

## Special Issue

# Molecular Dynamics Simulations of Metal-Binding Proteins and Nucleic Acids

### Message from the Guest Editor

More than one-third of all known proteins encoded need at least one metal ion to perform their biological function. Various metal-containing cofactors require dedicated biosynthetic enzymes for their assembly. Metal ions are also crucial to tune and stabilize the three-dimensional (3D) structure of nucleic acids, and to promote intermolecular interactions. To understand how the aforementioned processes work, it is necessary to investigate the 3D structure and mobility of the involved macromolecules at the atomic level. Molecular dynamics (MD) simulations complement experimental information and generate new hypotheses on the molecular and cellular functions of metal ions. Among the specific challenges posed by the MD of metal-binding macromolecular systems, a particularly relevant one is the parametrization of the metal site. This is obviously crucial to achieve an accurate interpretation of the data.

### Guest Editor

Prof. Dr. Antonio Rosato

Department of Chemistry and Center for Magnetic Resonance,  
University of Florence, 50019 Sesto Fiorentino, Italy

### Deadline for manuscript submissions

closed (30 April 2023)



## International Journal of Molecular Sciences

an Open Access Journal  
by MDPI

Impact Factor 4.9  
CiteScore 9.0  
Indexed in PubMed



[mdpi.com/si/125631](https://mdpi.com/si/125631)

*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)