International Journal of
Molecular Sciences

IMPACT FACTOR 5.6 | Indexed in: PubMed | CITESCORE 7.8

an Open Access Journal by MDPI

Molecular Dynamics Simulations of Metal-Binding Proteins and Nucleic Acids

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)

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.

International Journal of
Molecular Sciences

IMPACT FACTOR 5.6 | Indexed in: PubMed | CITESCORE 7.8

an Open Access Journal by MDPI

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

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.

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 & Molecular Biology*) / CiteScore - Q1 (*Inorganic Chemistry*)

Contact Us

International Journal of Molecular Sciences Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/ijms
ijms@mdpi.com
𝕏@IJMS_MDPI