

Special Issue

Role of Molecular Dynamics Simulations and Related Methods in Drug Discovery

Message from the Guest Editor

Molecular dynamics simulations together with some related methods such as binding free energy calculation, Markov state model, etc., have been widely applied in the field of drug discovery due to their special advantages in uncovering the dynamics conformational features of protein and studying the thermodynamics and dissociation kinetics of protein–ligand interactions. This Special Issue focuses on the various applications of molecular dynamics simulation and related computing methods in the drug discovery process, including virtual screening, binding free energy calculation, protein–ligand interaction, residence time, dissociation paths, and other related research articles. Studies providing such information are also welcome, which will help to elucidate the rationale for molecular modification and new drug development.

Guest Editor

Prof. Dr. Huanxiang Liu
Faculty of Applied Science, Macao Polytechnic University, Macao
999078, China

Deadline for manuscript submissions

closed (30 April 2025)



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 5.6
CiteScore 10.0
Indexed in PubMed



mdpi.com/si/161730

*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 5.6
CiteScore 10.0
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)* 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, CAPus / SciFinder, and other databases.

Journal Rank:

JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore
- Q1 (Inorganic Chemistry)