International Journal of
*Molecular Sciences*

IMPACT FACTOR 4.9
Indexed in: PubMed
CITESCORE 8.1

an Open Access Journal by MDPI

# Role of Molecular Dynamics Simulations and Related Methods in Drug Discovery

Guest Editor:

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

Deadline for manuscript submissions:
**closed (30 June 2024)**

## 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.

International Journal of
*Molecular Sciences*

IMPACT FACTOR 4.9 | Indexed in: PubMed | CITESCORE 8.1

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 and 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