Special Issue

Molecular Big Data, Computing, and Atomic-Level Simulation for Drug Discovery and Biology

Message from the Guest Editor

Current development of machine learning algorithms and data technology make drug discovery and biology gain new challenges and opportunities to solve a scientific big problem. In particular, diverse unstructured data (e.g., real world data) as well as public databases are considerable to improve the applicability domain and predictive power in molecular simulations. In the same way we can find a shortcut to reach the summit of a mountain through searching uncertain different paths, a scientific big problem can be solved through investigating different methodologies of diverse research area (at a glance, unrelated). This issue covers recent diverse and novel approaches of atomic-level simulations using algorithms and data technologies. In this issue, unconventional or unexpected methods are recommended to suggest innovative prediction of atomic level molecular mechanics or biological activity. However, the prediction can also be conducted by current major methods (e.g., molecular dynamics simulations, docking simulations, QSAR, pharmacophore modeling) using well-encoded unique data.

Guest Editor

Prof. Mi-hyun Kim
Gachon University, Incheon, Korea

Deadline for manuscript submissions

closed (31 March 2021)

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)