



Molecular Dynamics Modeling and Simulation

Guest Editors:

Dr. Outi Salo-Ahen

Pharmaceutical Sciences and
Structural Bioinformatics
Laboratory, Faculty of Science
and Engineering, Abo Akademi
University, Biocity, Tykistökatu
6A, FI 20520 Turku, Finland

Dr. Parthiban Marimuthu

Structural Bioinformatics
Laboratory, Biochemistry, Faculty
of Science and Engineering, Abo
Akademi University, Biocity,
Tykistökatu 6A, FI 20520 Turku,
Finland

Deadline for manuscript
submissions:

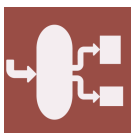
closed (30 November 2023)

Message from the Guest Editors

Molecular dynamics (MD) modeling is a powerful approach that can be used to simulate molecular motions and interactions over a period of time. In recent years, state-of-the-art computational platforms and advanced MD methods have made it possible to provide plausible explanations for various biological events, as well as predicting drug binding kinetics or material properties, thus reducing the need for tedious and expensive experimental procedures.

The aim of this Special Issue is to present a contemporary overview of the application of MD simulations in material and life sciences, especially in the context of drug discovery and development. Original research papers and short communications, as well as review articles that address the theoretical and methodological aspects of MD simulations, are all welcome. The submission of articles covering the topics listed below are particularly encouraged.





an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Giancarlo Cravotto

Department of Drug Science and
Technology, University of Turin,
Via P. Giuria 9, 10125 Turin, Italy

Message from the Editor-in-Chief

Processes (ISSN 2227-9717) provides an advanced forum for process/system-related research in chemistry, biology, material, energy, environment, food, pharmaceutical, manufacturing and allied engineering fields. The journal publishes regular research papers, communications, letters, short notes and reviews. Our aim is to encourage researchers to publish their experimental, theoretical and computational results in as much detail as necessary. There is no restriction on paper length or number of figures and tables.

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), Ei Compendex, Inspec, AGRIS, and other databases.

Journal Rank: JCR - Q2 (*Engineering, Chemical*) / CiteScore - Q2 (*Chemical Engineering (miscellaneous)*)

Contact Us

Processes Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

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

mdpi.com/journal/processes
processes@mdpi.com
[X@Processes_MDPI](https://twitter.com/Processes_MDPI)