



Artificial Intelligence and Machine Learning in Drug Development

Guest Editor:

Dr. Irina Moreira

1. Life Sciences Department,
Coimbra University, Coimbra,
Portugal

2. CNC - Center for Neuroscience
and Cell Biology, University of
Coimbra, Coimbra, Portugal

irina.moreira@cnc.uc.pt

Deadline for manuscript
submissions:

30 April 2022

Message from the Guest Editor

Human biological complexity and genomic variability lead to different responses to therapeutic approaches at both the individual and population levels. Molecular profiling is now able to stratify diseases into their distinct molecular subtypes for matching with appropriate drugs, thus beginning to shape a translational systems medicine for better tailored predictive and pharmacotherapeutic guidance. This new research paradigm, powered by state-of-the-art artificial intelligence (AI)/machine learning (ML)-based prediction algorithms, presents great challenges and opportunities for researchers in the field.

This Special Issue welcomes original research, short communications, and review papers. Potential topics include, but are not limited to, the application of AI/ML to: target identification and characterization; protein networks/pathways prediction; mechanism of disease; drug–target complex formation and characterization; drug identification; drug repurposing; generation of novel drug candidates; drug efficacy metrics; and toxicology, biopharmaceutical properties prediction, etc. Wet-lab and clinical-data-based submissions with biomolecular experiments are welcomed.





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, CAPus / SciFinder, and many other databases.

Journal Rank: JCR - Q1 (*Biochemistry & Molecular Biology*) / CiteScore - Q1 (*Inorganic Chemistry*)

Contact Us

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

Tel: +41 61 683 77 34
Fax: +41 61 302 89 18
www.mdpi.com

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