

Special Issue

Artificial Intelligence and Machine Learning in Drug Development

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.

Guest Editor

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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.

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