Special Issue

New Insights in Artificial Intelligence for Drug Design and Target Discovery

Message from the Guest Editor

In recent years, emerging multimodal large language models, including text-based and biological data-driven foundational models, have become powerful tools for analyzing biomedical text and extracting valuable information on proteins, nucleic acids, and chemical compounds. These models facilitate the identification of novel drug candidates and accelerate biomolecule target discovery. Deep generative models represent another frontier in drug design, enabling the creation of novel chemical entities with desired properties. Furthermore, integrating multi-omics data with AI methods is crucial for understanding drug responses, identifying biomarkers, and discovering potential drug combinations.

We invite researchers to contribute original research articles and review papers that explore the promising applications of AI in the fields of biology and medicine. This Special Issue aims at providing novel insights into the evolving research paradigms of drug design and target discovery by integrating diverse AI methodologies, computational biology techniques, and bioinformatics.

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Deadline for manuscript submissions

20 November 2025

International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/224920

International Journal of Molecular Sciences
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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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