

Special Issue

Artificial Intelligence Advancing Computer-Aided Drug Discovery

Message from the Guest Editor

Artificial Intelligence (AI) is transforming drug development by tackling complex challenges in biomedical research and significantly expediting the discovery process. To further streamline candidate selection and reduce downstream failures, AI is essential in the early-stage evaluation of pharmacokinetic and toxicological profiles, such as absorption, distribution, metabolism, excretion, and toxicity. Clinical development timeframes, research expenses, and the possibility of success are drastically reduced by using AI in large biological datasets and advanced predictive algorithms. This Special Issue, titled "Artificial Intelligence Advancing Computer-Aided Drug Discovery", highlights the recent progress of applying AI in computer-aided drug discovery. Submissions of original research and reviews on AI-assisted approaches, including target identification, compound screening, ADMET prediction, and multi-omics integration, are welcome. Studies on innovative algorithms, hybrid experimental–computational workflows, and AI-driven drug development are also encouraged.

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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