Special Issue

Computational Pharmacology in Drug Discovery

Message from the Guest Editor

Computational pharmacology is an interdisciplinary field that uses computational techniques to study the behavior of drugs in the human body.

Computational pharmacology and AI are two powerful tools that have revolutionized the way drugs are discovered and developed. The combination of these two technologies has allowed researchers to develop powerful algorithms and computer models to simulate the effects of potential drugs on the human body. This has enabled them to rapidly identify potential drug candidates and develop them much more efficiently than ever before. In addition, AI has allowed for the development of more accurate and detailed models of how drugs interact with their targets, which can help scientists better understand the mechanisms of action of new drugs. AI can also be used to analyze large datasets of clinical data to identify potential biomarkers for drug efficacy and safety, allowing researchers to make informed decisions about which drugs should be developed.

Guest Editor

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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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