Special Issue

Advances in Computer-Aided Drug Design Strategies

Message from the Guest Editor

Computer-aided drug design has become a cornerstone of current scientific research and is of phenomenal importance in pharmacy, revolutionising the way we approach the understanding of biological phenomena and drug discovery as well as development. From virtual screening to molecular dynamics simulations of increasingly large and complex systems, and from structure-based to ligand-based approaches, computer-aided tools are streamlining processes that were once costly, laborious, and time-consuming. Recent developments in artificial intelligence and machine learning offer a new level of predictive accuracy, enabling researchers to model complex biological systems, predict drug interactions, and optimise pharmacokinetic properties with remarkable precision. These strategies not only improve efficacy, but also reduce the financial costs and potential ethical issues associated with large-scale in vivo and in vitro studies.

This Special Issue aims to bring together original research, analyses, and case studies that demonstrate how cutting-edge computational techniques are being used to address the pressing challenges of drug discovery.

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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