Special Issue

Artificial Intelligence and Computer Aided Drug Design

Message from the Guest Editor

Artificial Intelligence (AI) is gaining more and more importance in the pharmaceutical sector, deeply transforming the drug discovery process. In drug discovery, AI helps in predicting the efficacy and safety of molecules and gives researchers a much broader chemical pallet for the selection of the best molecules for drug testing and delivery. With the huge amount of clinical and pharmaceutical data available to date, AI algorithms find suitable drugs, which can be repurposed for an alternative use in medicine. Moreover, with the help of AI, it becomes easier to run clinical tests, diagnose diseases and provide the most effective treatment for a particular disease. In this Special Issue, we would like to discuss new approaches based on AI in the drug discovery process and in the repositioning of old molecules, together with their impact on the pharmaceutical pipeline. The goal is to provide an overview of the sectors where AI might play a crucial role in the pharmaceutical world in the next years.

- Computer aided drug design
- Machine learning, deep learning
- Big data
- Virtual screening
- Drug discovery and repurposing
- Drug-target interaction

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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