



Artificial Intelligence and Computer Aided Drug Design

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Message from the Guest Editor

Dear Colleagues,

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





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Message from the Editor-in-Chief

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