Special Issue

Drug Discovery: New Concepts Based on Machine Learning

Message from the Guest Editors

The ML/AI-based methodology era enables and opens new avenues that can boost the growth of new methods and their increasing importance. The computational-aided drug design exposes the impacts on drug discovery (new targets, the targeting of small molecules, targeted protein–protein interactions, SAR generation using data-driven experimental databases and integrated platforms, drug delivery pathways, etc.). The Special Issue will cover the following topics: targeting small molecules;
protein–protein interactions;
protein dynamics;
docking studies;
logP and pKa computational methods;
solvation-free energy;
QSPR/QSAR studies;
fragment-based drug discovery (FBDD). We also welcome papers dedicated to computational and machine learning for drug discovery. The new ML approach for drug design and CADD was developed and designed for de novo drug design methods to generate a space for novel chemical compounds with desirable properties in a cost-efficient manner. We are happy to welcome papers dedicated to fragment-based drug discovery (FBDD) as a powerful tool to recognize and classify a new compound as the initial point for drug development.

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