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Machine Learning Methods for Medicinal Chemistry

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Message from the Guest Editor

The concept of artificial intelligence (AI) is increasingly being used in predictive modeling and optimization of medical chemistry processes in drug discovery. One of the main goals of AI is to create machine learning (ML) platforms that enable gradual improvement in model performance. This Special Issue aims to introduce examples showing how current ML methods are used in various areas of the drug discovery process. The focus will be placed on some achievements using newer machine learning methods in designing tools capable of generating and assessing synthetic structures, as well as ligand binding and ADMET models.

Perspective topics include (but are not limited to):

- Recent advances in AI/ML algorithms;
- Applications of ML in structure generation;
- Prediction of target protein in drug design;
- Homology modeling/prediction of protein folding;
- Machine learning approaches to predicting protein–ligand interactions;
- In silico toxicity and ADMET modeling to optimize molecular properties;
- ML in drug metabolite and metabolic site prediction;
- ML-based biomarker discovery;
- Use of ML in synthesis planning.

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Message from the Editor-in-Chief

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