Special Issue

Machine Learning in Drug Discovery

Message from the Guest Editor

Time consumption, high cost, and great risk, significant attrition rates, among other factors, are hallmarks of drug discovery. Nevertheless, drug discovery has moved into a new paradigm with the introduction of machine learning technologies. Especially, the innovation and sophistication of machine learning algorithms as well as the development of high-throughput computing machines have further expedited the revolution. In fact, machine learning has been extensively applied to tasks including but not limited to homology modeling; hit identification; lead optimization; drug repurposing, de novo drug design; drug absorption, distribution, metabolism, excretion, and toxicity (ADME/Tox) assessments; and drug formulation development. The objective of this Special Issue is attempting to comprehensively cover all aspects associated with the applications and innovation of machine learning in drug discovery. In addition, it aims to explore the advantages and limitations of every machine learning algorithm and/or scheme. Finally, the future directions of machine learning and their applications will be addressed.

Guest Editor

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