Special Issue

Applied Deep Learning and Machine Learning in Drug Design and Discovery

Message from the Guest Editor

This Special Issue focuses on the application of deep learning and machine learning techniques in the field of drug design and discovery. It aims to explore the innovative ways in which these advanced computational approaches are being employed to accelerate drug development, optimize molecular structures, predict drug–target interactions, and enhance our understanding of complex biological systems. The articles featured in this issue will showcase cutting-edge research and developments at the intersection of artificial intelligence, chemistry, and biology, contributing to the advancement of pharmaceutical science and therapeutics. Keywords:

- drug design
- drug discovery
- artificial intelligence
- machine learning
- deep learning
- drug–target interactions
- drug–drug interactions

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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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