Special Issue

The Application of Machine Learning to Molecular Dynamics Simulations

Message from the Guest Editor

Molecular dynamics allows for detailed study of the atomistic behavior of biomolecules, such as protein–ligand and protein–protein interactions and has played an important role in the field of drug discovery and development. Machine learning, through models like deep learning, accelerates the process, enabling faster predictions of key properties such as binding affinity, toxicity, and mechanisms of action. By combining machine learning algorithms with molecular dynamics simulations, we can achieve faster and more accurate simulations, leading to a deeper understanding of the properties and behavior of molecular systems. This Special Issue focuses on recent advances in machine learning to improve force fields, sampling, and property prediction in molecular dynamics simulations. The application of this approach can be primarily targeted at drug discovery, but can be extended to other aspects of protein structure and dynamics related to drug discovery. Innovative methods are also welcome to enhance the drug discovery process, the evaluation of mechanisms of action, and the study of atomistic details in biomolecular interactions.

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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