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Molecular Dynamics Modeling and Simulation

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Message from the Guest Editors

Molecular dynamics (MD) modeling is a powerful approach that can be used to simulate molecular motions and interactions over a period of time. In recent years, state-of-the-art computational platforms and advanced MD methods have made it possible to provide plausible explanations for various biological events, as well as predicting drug binding kinetics or material properties, thus reducing the need for tedious and expensive experimental procedures.

The aim of this Special Issue is to present a contemporary overview of the application of MD simulations in material and life sciences, especially in the context of drug discovery and development. Original research papers and short communications, as well as review articles that address the theoretical and methodological aspects of MD simulations, are all welcome. The submission of articles covering the topics listed below are particularly encouraged.

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Message from the Editor-in-Chief

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