



Role of Molecular Dynamics Simulations and Related Methods in Drug Discovery

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Message from the Guest Editor

Molecular dynamics simulations together with some related methods such as binding free energy calculation, Markov state model, etc., have been widely applied in the field of drug discovery due to their special advantages in uncovering the dynamics conformational features of protein and studying the thermodynamics and dissociation kinetics of protein–ligand interactions.

This Special Issue focuses on the various applications of molecular dynamics simulation and related computing methods in the drug discovery process, including virtual screening, binding free energy calculation, protein–ligand interaction, residence time, dissociation paths, and other related research articles. Studies providing such information are also welcome, which will help to elucidate the rationale for molecular modification and new drug development.





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Message from the Editor-in-Chief

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