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Computer-Aided Molecular Modeling and Simulation in Drug Design

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Message from the Guest Editors

Computer-aided molecular modeling and simulation has become an essential tool in drug design, allowing researchers to study and understand molecular interactions between a drug candidate and its target. This field combines principles from computational chemistry, bioinformatics, and biophysics to simulate and visualize the behavior of molecules at the atomic level. Many computational methods are also used to predict the toxicity and pharmacokinetic properties of drug candidates. For example, QSAR models can be used to predict the activity of a drug candidate based on its chemical structure, while ADME models can predict how the drug candidate will behave in a person's body. Overall, computer-aided molecular modeling and simulation techniques are important tools in modern drug design, allowing researchers to identify potential drug candidates more efficiently and accurately than traditional experimental methods can. In this Special Issue, we aim to draw together research from experts in the field that highlight traditional and new computational methods and strategies to discover and design new drugs for clinical treatments.

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Message from the Editor-in-Chief

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