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Small Molecule Drug Discovery with Anti-microbial and Anti-cancer Properties

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Message from the Guest Editors

The journey of discovering effective treatments for infectious diseases and cancer has been a challenging and evolving process. Historically, drug discovery often relied on trial and error, resulting in lengthy and resource-intensive endeavors. However, the advent of computational methods has transformed this landscape, ushering in a new era of accelerated and targeted drug development. However, these traditional methods often yielded limited success due to the complex nature of diseases and the immense diversity of potential drug candidates. In the realm of modern drug design, computer-aided molecular modeling and simulation techniques stand as indispensable tools. They empower researchers to identify potential drug candidates with greater efficiency and precision than conventional experimental approaches. Topics of interest for this Special Issue may include, but are not limited to, natural product-derived antimicrobials and anticancer compounds, in silico screening of small molecules, molecular dynamics simulations in rational drug design, machine learning approaches for drug design, network pharmacology for drug discovery, and the structure-based design of PROTACs.

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Message from the Editor-in-Chief

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