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Advances in Computational Chemistry for Drug Design, Discovery and Screening

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Message from the Guest Editors

New advances in computational biology such as molecular modeling, molecular dynamics, virtual screening, and, more recently, artificial intelligence play more and more important roles. Many tedious and time-consuming steps can be replaced or facilitated by these technologies. This could lead to noticeable savings in the costs of modern drug discovery, in terms of both time and finance.

Contributions to this Special Issue may cover all advances related to computational drug discovery, including new target identification, virtual screening, drug design, lead optimization, properties prediction by artificial intelligence, binding energy calculation, WebGL based real-time simulation and data analysis, molecular dynamics simulation, and drug re-purposing.

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Message from the Editor-in-Chief

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