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Structural and Computational-Driven Molecule Design in Drug Discovery

Guest Editors:

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Deadline for manuscript submissions:
closed (26 February 2024)

Message from the Guest Editors

Drug development is a complicated, high-risk, expensive, and lengthy process along with several stages such as target identification, lead discovery and lead optimization. In this process, the congruence between computational and experimental outcomes is a mainstay for the exploration of novel compounds. Besides, in the drug development process, many drug candidates could not pass the trials successfully due to the inadequate ADMET properties. Therefore, in silico ADMET analysis is attractive and a cost-saving strategy for a large number of compounds prior to applying expensive and time-consuming in vitro and in vivo ADMET estimation.

This Special Issue aims to provide deep mechanistic insights into strategies in structural dynamics studies and computational methods. It is our great pleasure to invite you to submit original research articles and reviews in a Special Issue on “Structural and Computational-Driven Molecule Design in Drug Discovery”. Research areas may include (but are not limited to) the following: Structural dynamics studies Computer-aided drug design Molecular dynamics simulations Molecular docking Virtual screening QSAR In silico ADMET.

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Message from the Editor-in-Chief

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We hope to handle your contribution to *Pharmaceuticals* soon.

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