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Computational Methods in Drug Design

Guest Editor:

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closed (31 July 2022)

Message from the Guest Editor

Molecular modeling and computational chemistry have become essential in the medicinal chemistry field today. In silico strategies represent powerful weapons commonly applied to accelerate drug discovery, design, and optimization campaigns, as well as to improve the knowledge and understanding of the biological processes implied in the mechanism of action of known drugs.

On these basis, this Special Issue is focused on the development of valuable and innovative computer-aided drug design approaches, as well as on successful applications of in silico techniques and strategies in all aspects and stages of the drug design process. Scientists are thus invited to submit original research articles and reviews dealing with all kinds of molecular modeling studies applied to drug design, such as virtual screening studies, computer-aided hit-to-lead and lead optimization campaigns, molecular modeling studies focused on drug–target interactions and dynamics, development and application of target-fishing approaches, generation of innovative computational tools and models for the prediction of pharmacodynamics, and pharmacokinetic ligand properties.

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Message from the Editor-in-Chief

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