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Computational Methods in the Design of Anticancer Drugs

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Deadline for manuscript submissions:
closed (31 January 2024)

Message from the Guest Editors

Dear Colleagues,

In recent decades, computational methods have become an essential tool in the drug design process as they are able to reduce research costs and accelerate the development process. The application of computational methods in the design of anticancer drugs has proved to be very effective. Given the wide variety of very different tumor forms and the multiplicity of possible pharmacological targets, this research area is very fruitful.

This Special Issue on "Computational methods in the design of anticancer drugs" aims to collect the most recent discoveries in the field of anticancer drug design with the aid of computational methods, such as structure-based drug discovery and ligand-based drug discovery classical or de novo drug design (molecular docking, virtual screening, pharmacophore mapping, similarity searching, QSAR modeling), molecular dynamics and the development of machine learning methods. These are some types of computational approaches that we would like to highlight in this Special Issue.

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