Special Issue

Computational Methods for Drug Discovery and Design

Message from the Guest Editor

In recent decades, drug design processes have been often assisted by computational methods. Such methods have been crucial to sustain the current development of medicinal chemistry research. These computational methods belonging to the fields of pharmaceutical modeling, molecular modeling and simulation, cheminformatics, bioinformatics, computational chemistry, and biochemistry. These methods encompass tools that contribute to the finding of novel drugs or the processing of available information for creating useful knowledge about the interactions between bioactive ligands and their biological targets.

In this Special Issue, we are seeking original articles, short communications, or review articles focusing on the use of computational methods for drug design processes. Papers employing the computational methods available for in silico drug design, such as docking, molecular dynamics, QSAR, pharmacophore modeling, virtual screening, free energy calculations, density functional theory applications, and QM/MM, are welcome. Papers combining both experimental and computational studies are also desired.

Guest Editor

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Deadline for manuscript submissions

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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