Special Issue

Computational Methods in Drug Design and Discovery

Message from the Guest Editor

When properly applied, computational chemistry methods can provide unmatched detail regarding chemical reactivity, mechanistic pathways, and the formation of supramolecular complexes today. This Special Issue aims at collecting outstanding contributions of cutting-edge computational methodologies to the broad field of medicinal chemistry. We welcome manuscripts describing original research on the computational development of novel drugs, the analysis of the molecular interaction between known drugs and their cellular targets, as well as the computationally assisted exploration of the chemical space for medicinal purposes (such as in silico screening, QSAR, etc.). We are especially interested in manuscripts describing the reaction mechanisms of covalent drugs, the computational improvement of current drugs toward higher selectivity/better pharmacokinetic parameters, and the detailed analysis of the interactions underlying the stability of novel protein/ligand complexes.

Keywords:

- computational screening
- reverse screening
- molecular dynamics
- reaction mechanisms
- covalent inhibitors

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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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