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Computational Methods in Drug Design and Discovery

Guest Editor:

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Deadline for manuscript submissions:
closed (31 December 2022)

Message from the Guest Editor

Dear Colleagues,

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.

Prof. Dr. Pedro Silva
Guest Editor

Keywords:

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

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th 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 multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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