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Computational Chemical Biology 2021

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Deadline for manuscript submissions:
closed (31 March 2022)

Message from the Guest Editors

Molecular modeling tools are extremely helpful in predicting properties and supplying important explanations that allow a complex comprehension of biological systems. The use of simulation techniques leads to an easier discovery of interactions and interaction types between molecular systems. For example, computational chemistry techniques significantly improve the prediction of active sites and finding of groups of geometric and electronic properties for optimal interaction with specific biological targets and an adequate biological response.

We invite authors to submit original research that contributes to the development of new methodologies for the improvement of prediction of properties, theoretical features to understand biological systems, and the exploration of biological functions.

Potential topics include but are not limited to:

- Computational structure–activity relationship;
- Development of calculations of reactivity properties of ligands and targets;
- Development of methodologies to improve the properties prediction in biological systems;
- The role of simulation in biological systems properties prediction;
- Molecular docking;
- Molecular dynamics.

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Editor-in-Chief

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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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