

Special Issue

In Silico Activity Profiling of Natural Products

Message from the Guest Editors

In this Special Issue of *Molecules*, we invite the scientific community to submit original research contributions, short communications or review articles that report on the most recent achievements in the development and application of in silico approaches with a special focus on the investigation of natural products. Our aim is to allow the colleagues that work in this field to present their most advanced and reliable findings as well as prospective results. The studies can address pharmacokinetic and pharmacodynamic aspects of the bioactive compound making use of a broad arsenal of in silico approaches such as ligand- and structure-based methods, molecular dynamics simulations, as well as their combination. The incorporation of experimental means of verification of theoretical studies in submitted manuscripts will be considered as a plus.

Guest Editors

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Deadline for manuscript submissions

closed (15 May 2022)



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About the Journal

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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