Special Issue

Recent Advances in Drug Design

Message from the Guest Editor

This Special Issue will focus on recent improvements on water mapping algorithms for SBDD and machine learning algorithms (neural networks, support vector machine, etc/) from researchers involved in computer science, which will suggest molecular descriptors of binding phenomena and tools from graph theory for mapping the binding area, aiming at filtering the best candidate molecules during a virtual screening procedure. Additionally, manuscripts that mainly describe computational studies should be accompanied by experimental validation.

Guest Editor

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Deadline for manuscript submissions

closed (30 September 2021)

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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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