Special Issue

Molecular Docking in Drug Discovery

Message from the Guest Editor

The accurate in silico prediction of small molecule-receptor complex geometries, i.e., molecular docking, offers great promise in driving the rational development of novel small-molecule therapeutics. Despite successes over the past 20 years in aiding drug development, persistent open questions as to how to improve both the accuracy of ligand-binding pose and affinity predictions, while also increasing computational efficiency, remain. It is important to note, that although these open questions remain, recent methodological developments are now providing pathways towards overcoming previously “undruggable” targets. In this Special Issue, we seek to highlight methodological reviews, novel molecular docking approaches, and new performance benchmarks, to guide future methodological development. Innovative applications of current docking methods are also of interest, particularly docking campaigns against traditionally “undruggable” targets.

Guest Editor

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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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