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Molecular Docking in Drug Discovery

Guest Editor:

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Deadline for manuscript submissions:
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Message from the Guest Editor

Dear Colleagues,

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.

Dr. Micholas Dean Smith
Guest Editor

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Message from the Editor-in-Chief

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