Special Issue

Drug Discovery and Molecular Docking

Message from the Guest Editor

The process of drug development is complex, expensive, and time-consuming. In this scenario, computer-based methodologies for drug design have been demonstrated to have the predictive power useful to speed up the discovery of novel drug candidates. Among the several methodologies of computational chemistry for identification of biologically active molecules, molecular docking is being used increasingly in the pharmaceutical industry. Molecular docking evaluates ligand–target interactions and tries to reproduce native binding modes, thus accelerating estimations of binding affinity and ligand optimization techniques. The process of drug discovery mainly focuses on protein–ligand and, more recently, protein–protein docking. Indeed, many challenges still remain to be addressed such as protein flexibility, role of water molecules, and entropic effects. The goal of this Special Issue is, therefore, to solicit and publish the latest advances in molecular docking and to inform researchers in related fields of its potential.

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Deadline for manuscript submissions

closed (30 June 2020)

Molecules

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Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

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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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