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Drug Discovery and Molecular Docking

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Message from the Guest Editor

Dear Colleagues,

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.

Dr. Maria Cristina De Rosa
Guest Editor

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Message from the Editor-in-Chief

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