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Latest Advances in Computational Chemistry and Molecular Docking for Biological Macromolecules

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Message from the Guest Editors

In recent decades, the application of computational chemistry in biochemical and biomolecular sciences has progressively grown with significant developments in methodology, software, and computer hardware. Computational chemistry methods range from molecular mechanics (MM) and molecular dynamics (MD) calculations based on approximate classical potentials to ab initio approaches based on quantum chemistry. Molecular docking is a simplified form of MM and MD calculations used to search for the most energetically and geometrically suitable complex between two or more molecules, e.g., ligands and proteins. Therefore, it plays an important and irreplaceable role in rational drug design. This Special Issue is dedicated to presenting the results of recent developments in the methods and application of computational chemistry techniques for studying the structure, dynamics, and function of biological macromolecules. Of particular interest are computational methods aimed at understanding the formation of intermolecular complexes and providing an efficient tool for the discovery of novel protein-targeted drugs.

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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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