



New Insights into Protein–Ligand Interactions

Guest Editor:

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Message from the Guest Editor

Proteins, an important class of biological macromolecules, realize their functions through binding to themselves or other molecules. Protein–ligand interactions and multi-protein complexes perform central roles in the cellular systems of all living organisms, participating in their activation and regulation.

Protein interactions are also often at the basis of many pathological states. A detailed understanding of the protein–ligand interactions is therefore central to understanding biology at the molecular level and will also facilitate the discovery, design, and development of drugs, including (but not limited to) molecular docking, structure-based design, virtual screening of molecular fragments, small molecules and other types of compounds, clustering of complexes, and structural interpretation of activity cliffs, to name a few.

In this Special Issue of IJMS, we aim to collect contributions in the form of either original research articles or reviews, to add new insight into the role of protein–ligand interactions in biological processes and to highlight the state of the art, the challenges, and the open issues in this varied field of investigation.





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Message from the Editor-in-Chief

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