



## Protein–Ligand Interactions: Target Identification and Drug Discovery 2.0

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### Message from the Guest Editor

For many bioactive compounds, there is a lack of knowledge of the specific molecular targets involved, the effects of these substances on protein structure, and how they can modulate different cellular pathways and functions. This Special Issue focuses on recent studies aiming to investigate protein–ligand interactions with a special aim of elucidating the molecular modes of action of drugs as well as natural bioactive compounds. Studies highlighting information on target proteins and how interactions with a drug may affect a protein’s structure and biological activity will be welcome. Computational results accompanied by validation experiments are also sought after. This information will help to elucidate the molecular basis for many drugs’ activities and the development of new drugs.





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## Message from the Editor-in-Chief

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