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Protein–Ligand Interactions: Target Identification and Drug Discovery

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Message from the Guest Editor

This Special Issue focuses on recent studies aiming to investigate protein–ligand interactions with a special aim to elucidate the molecular mode of action and the target proteins of specific drugs as well as natural compounds. Certainly, the interaction with a drug may affect both protein conformation and biological activity, but, for many bioactive compounds, there is a lack of knowledge of their specific molecular targets, their effects on protein structure, and how they can modulate different cellular pathways and functions. Studies providing such information will be welcome; they will help to elucidate the molecular basis for many drug activities and the development of new drugs.



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Message from the Editor-in-Chief

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