Special Issue

Protein-Ligand Interactions: Deciphering the Molecular Targets and the Mechanisms of Action of Drugs and Natural Compounds

Message from the Guest Editor

This Special Issue focuses on recent studies that aimed to investigate protein–ligand interactions, with a special aim to elucidate the molecular mode of action and the protein targets of drugs as well as natural compounds, and the cellular pathways involved. Indeed, protein–ligand interactions may affect both protein conformation and biological activity. However, for many bioactive compounds there is a lack of knowledge of their molecular targets, their effects on protein structure, and how they can modulate different cellular pathways and functions. Studies providing such information are welcomed and will help to elucidate the molecular basis for many drugs activity and the development of new drugs.

Guest Editor

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Message from the Editor-in-Chief

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