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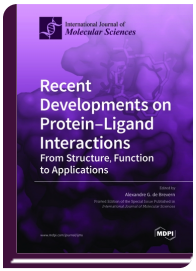
Recent Developments on Protein–Ligand Interactions



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Protein–ligand interactions play a fundamental role in most major biological functions. The number and diversity of small molecules that interact with proteins, whether naturally or not, can quickly become overwhelming. They are as essential as amino acids, nucleic acids or membrane lipids, enabling a large number of essential functions. One need only think of carbohydrates or even just ATP to be certain. They are also essential in drug discovery. With the increasing structural information of proteins and protein–ligand complexes, molecular modelling, molecular dynamics, and chemoinformatics approaches are often required for the efficient analysis of a large number of such complexes and to provide insights. Similarly, numerous computational approaches have been developed to characterize and use the knowledge of such interactions, which can lead to drug candidates. "Recent Developments on Protein–Ligand Interactions: From Structure, Function to Applications" was dedicated to the different aspect of protein–ligand analysis and/or prediction using computational approaches, as well as new developments dedicated to these tasks. It will interest both specialists and non-specialists, as the presented studies cover a very large spectra in terms of methodologies and applications. It underlined the variety of scientific area linked to these questions, i.e., chemistry, biology, physics, informatics, bioinformatics, structural bioinformatics and chemoinformatics.

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