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Recent Developments on Protein–Ligand Interactions: From Structure, Function to Applications 2.0

Guest Editor:

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closed (15 March 2024)

Message from the Guest Editor

Dear Colleagues,

Protein–ligand interactions play a fundamental role in most major biological functions, but also in drug discovery. With the increasing structural information of proteins and protein–ligand complexes, molecular modeling, 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. For instance, one main application is to identify tractable chemical start-points that non-covalently modulate the activity of a biological molecule. This new information brings questions that affect chemistry, biology, and even pose specific computer problems. Papers related to any aspect of protein–ligand analysis and/or prediction using computational approaches, as well as new developments dedicated to these tasks, will be considered for this Special Issue.

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Message from the Editor-in-Chief

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