



Research Advances on the Protein-Protein Interactions and Development of Therapeutics

Guest Editor:

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Message from the Guest Editor

Several diseases are the result of aberrant protein–protein interactions involving endogenous or pathogen-derived proteins. A blockade of such undesirable interactions has proven clinical benefits and has been identified as a prime target for the drug design. Due to the flat and wide interface, some protein targets are certainly inappropriate for the development of small drug molecules; in addition, production of monoclonal antibodies against such protein molecules is expensive and challenging due to the short half-life of antibodies.

In this Special Issue, we invite authors to submit their studies on protein–protein interaction and the development of therapeutics using various computational methods such as protein structure prediction, molecular docking, molecular modelling, molecular dynamics simulation, and free energy calculations. Research themes include treatments for cancer and neurological disorders, alternatives to overcome antibiotic resistance, and drugs to treat zoonotic infectious diseases.

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