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Modulating Target Protein Function through the Binding of Small Molecules

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Message from the Guest Editor

Dear Colleagues,

This Special Issue aims to highlight the concept that small molecule binding can modulate target protein function in a variety of ways. Such 'binders' can affect protein activity through competitive, noncompetitive or uncompetitive binding. Particularly, ligand binding can influence not only protein structure but also protein dynamics. The latter expands the scope of a binder-based approach to translate small molecules to medicines, through the stabilization of pharmacologically desired conformational states of target proteins or by shifting the populations of different conformational states. We encourage contributions on the computational study of ligand binding altering the structure and dynamics of proteins, leading to: (1) inhibiting a function, (2) enhancing a function and (3) conferring a novel function of the proteins.

In this Special Issue, research areas may include (but not limited to) the following: small molecule binding changes target protein structure, stability, and conformational dynamics, shifts protein conformational distributions, or alters interaction with its effector(s) or tendency to be chemically modified by cellular enzymes.

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