



Experimental and Theoretical Approaches to Protein-Targeting Drug Discovery II

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Message from the Guest Editors

Dear Colleagues,

Following a very successful first run, we are pleased to announce the launch of a second edition of the Special Issue “Experimental and Theoretical Approaches to Protein-Targeting Drug Discovery”.

Protein-driven biological processes are of fundamental importance in biomedicine because they are related to pathologies of enormous social relevance, including cancer, neurodegeneration, and viral diseases, such as the recent COVID-19 pandemic. In this Special Issue, we wish to focus on the novel experimental and theoretical approaches for drug discovery, design, and development, with particular attention being paid to the mechanisms of drug interference with protein-driven biological pathways. Contributions on nucleic acid–protein interaction, aptamers, peptide aggregation, nucleopeptide chemistry, and antimicrobial polyamino acids are also welcome as they could improve our overall knowledge of the amino-acid-based biochemistry at the interface between drug design and therapy. Other themes of interest are inherent to computational chemistry, in particular, to molecular docking and molecular dynamics, applied to protein and peptide science.





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