

Special Issue

Experimental and Theoretical Approaches to Protein-Targeting Drug Discovery: 3rd Edition

Message from the Guest Editors

Protein-driven biological processes are of fundamental importance in biomedicine because they are related to pathologies of enormous social relevance, including cancer, neurodegenerative disorders, and viral diseases, such as COVID-19 and other infectious conditions. 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. This Special Issue is open to the submission of both original articles and reviews that describe research and ideas on the themes outlined here for protein-based molecular strategies.

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Message from the Editorial Board

Biomolecules is a multidisciplinary open-access journal that reports on all aspects of research related to biogenic substances, from small molecules to complex polymers. We invite manuscripts of high scientific quality that pertain to the diverse aspects relevant to organic molecules, irrespective of the biological question or methodology. We aim for a competent, fair peer review and rapid publication. Please look at some of the exciting work that has been published in *Biomolecules* so far. We would be delighted to welcome you as one of our authors.

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