Special Issue

Exploring Protein-Ligand Interaction: Key Insights for Drug Discovery

Message from the Guest Editors

The extensive research into protein aggregation processes may offer significant insight into the key mechanisms of cellular malfunction caused by aggregation, opening new pathways for drug development. The interactions between natural and synthetic ligands/drugs, and organic/inorganic nanoparticles with proteins may lead to: (i) alteration of the biological and pharmacological activities of ligands/drugs, their delivery to cells and tissues, and their potential antioxidant capacity; (ii) partial modifications of protein physiological functions, with loss of their native structure and even inactivation. This Special Issue is devoted to new contributions into protein–ligand interactions studied under physiological and/or pathological conditions using both experimental and theoretical approaches. Experimental and computational techniques may be taken into consideration. Such studies are essential for understanding biological control mechanisms and provide an experimental and theoretical basis for the discovery, design and development of new drugs and novel therapeutic strategies.

- protein
- ligand
- molecular docking
- molecular dynamics simulation

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Message from the Editor-in-Chief

Biomedicines (ISSN 2227-9059) is an open access journal devoted to all aspects of research on human health and disease, the discovery and characterization of new therapeutic targets, therapeutic strategies, and research of naturally driven biomedicines, pharmaceuticals, and biopharmaceutical products. Topics include pathogenesis mechanisms of diseases, translational medical research, biomaterial in biomedical research, natural bioactive molecules, biologics, vaccines, gene therapies, cell-based therapies, targeted specific antibodies, recombinant therapeutic proteins, nanobiotechnology driven products, targeted therapy, bioimaging, biosensors, biomarkers, and biosimilars. The journal is open for publication of studies conducted at the basic science and preclinical research levels. We invite you to consider submitting your work to Biomedicines, be it original research, review articles, or developing Special Issues of current key topics.

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