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The Role of Molecular Docking in the Design of Targeted Therapeutic Entities and Nanomaterials

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Deadline for manuscript submissions:
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Message from the Guest Editors

Molecular docking has become a useful computational technique for aiding in drug design by providing insights on interactions and dynamics of molecules and nanomaterials within biological systems. The docking of therapeutic entities and/or nanomaterials enables the prediction of preferred orientations and binding capacities of the developed therapeutics and nanostructures with the target site, thus, providing the capability to predict and achieve superior pharmacological activities. Given the wide variety of pharmacological targets and biomedical applications of nanoconstructs, this research area has received considerable interest.

Accordingly, authors are invited to submit high-quality research articles regarding topics such as, but not limited to, molecular docking studies for designing novel compounds and/or nanomaterials for various biomedical applications. Review submissions highlighting the latest advances in the study of the design and biological interactions of novel active entities (i.e., active molecules and nanomaterials) with pharmacological targets are also encouraged.

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