Special Issue

Molecular Computational Research in Pharmacological Structure–Efficacy

Message from the Guest Editors

This Special Issue collates research on molecular computational approaches to elucidate the intricate relationships between chemical structure and pharmacological efficacy. Recent advancements in quantum mechanics, molecular docking, molecular dynamics simulations, and free energy calculations have considerably improved the rational design and optimization of drug candidates. These methodologies offer in-depth insights into molecular recognition, binding affinity, and mechanistic pathways, leading to a greater understanding of drug–target interactions at the atomic level. We invite the submission of original research and review articles that utilize computational tools to predict bioactivity, investigate structure–activity relationships (SAR), or model enzymatic and receptor-mediated processes. Studies that bridge experimental and theoretical perspectives are particularly encouraged, especially those focusing on novel therapeutic targets and innovative computational strategies. This initiative aims to promote the development of more effective and selective pharmacological agents through data-driven and mechanism-based design.

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