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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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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