Special Issue

Recent Advances in Structure-Based Inhibitor/Drug Design

Message from the Guest Editors

This Special Issue aims to report recent progress in the field of structure-based inhibitor and drug design, a pivotal approach that relies on the precise three-dimensional structures of therapeutic targets to rationally develop potent and selective compounds. By elucidating biomolecular interactions and the structures and functions of biomolecules through techniques such as X-ray crystallography, NMR, and molecular dynamics simulations, this strategy enables the rational design of molecules that selectively bind and modulate target functions. Additionally, the integration of bioinformatics, Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) is accelerating the prediction and optimization of drug candidates. This Special Issue will collect the latest research and review papers focused on these advances, providing valuable insights to promote future drug discovery and development. Submissions may include original research, comprehensive reviews, or perspectives.

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Deadline for manuscript submissions

31 March 2027

Biomolecules

an Open Access Journal by MDPI

Impact Factor 5.6
CiteScore 9.3
Indexed in PubMed

mdpi.com/si/253350

Biomolecules
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