

Special Issue

Advances in Drug Design and Drug Discovery

Message from the Guest Editor

Drug design and discovery is a dynamic field that has witnessed rapid progress due to the integration of computational sciences, structural biology, and biotechnology. Artificial intelligence (AI) and machine learning now allow prediction of drug-target interactions and optimization of chemical structures, accelerating early development stages. Structure-based drug design, powered by cryo-electron microscopy and crystallography, provides precise insights into molecular interactions, enabling the creation of highly selective drugs. Omics technologies—including genomics, proteomics, and metabolomics—are driving the identification of disease-associated pathways and biomarkers for personalized therapies. Beyond small molecules, biologics, and advanced modalities such as monoclonal antibodies, RNA-based therapeutics, and gene-editing approaches are expanding treatment possibilities. Collectively, these advances are transforming drug discovery into a more precise, efficient, and patient-centered process. While challenges remain, the innovations of the past decade mark a significant step forward in the development of safe and effective therapeutics.

Guest Editor

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