

Special Issue

New Insights in Artificial Intelligence for Drug Design and Target Discovery

Message from the Guest Editor

In recent years, emerging multimodal large language models, including text-based and biological data-driven foundational models, have become powerful tools for analyzing biomedical text and extracting valuable information on proteins, nucleic acids, and chemical compounds. These models facilitate the identification of novel drug candidates and accelerate biomolecule target discovery. Deep generative models represent another frontier in drug design, enabling the creation of novel chemical entities with desired properties. Furthermore, integrating multi-omics data with AI methods is crucial for understanding drug responses, identifying biomarkers, and discovering potential drug combinations.

We invite researchers to contribute original research articles and review papers that explore the promising applications of AI in the fields of biology and medicine. This Special Issue aims at providing novel insights into the evolving research paradigms of drug design and target discovery by integrating diverse AI methodologies, computational biology techniques, and bioinformatics.

Guest Editor

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