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Artificial Intelligence Driven Drug Discovery: Computational Strategies, Translational Challenges, and Future Directions

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ABSTRACT

Artificial intelligence (AI) is transforming drug discovery by enabling data-driven prediction, optimization, and design across the pharmaceutical development pipeline. Advanced machine learning (ML) and deep learning (DL) architectures, including graph neural networks, reinforcement learning frameworks, and generative models, facilitate target identification, virtual screening, de novo molecular design, and prediction of pharmacokinetic and toxicity profiles with enhanced speed and scalability. By integrating multi-omics datasets, cheminformatics, and high-throughput screening outputs, AI platforms can uncover complex structure-activity relationships that are often inaccessible through conventional computational methods. Despite these advances, the translational reliability of AI models remains constrained by data heterogeneity, limited high-quality annotated datasets, algorithmic bias, and challenges in model interpretability. Ethical considerations, reproducibility, and regulatory acceptance further influence clinical applicability. Strategies such as data augmentation, transfer learning, explainable AI (XAI), and hybrid modeling approaches that combine in silico predictions with experimental validation are emerging to address these limitations. This review critically evaluates the computational frameworks underpinning AI-assisted drug discovery, examines current methodological bottlenecks, and outlines integrative strategies to enhance predictive robustness and translational impact. The convergence of AI with systems biology, high-performance computing, and automated laboratory platforms is poised to accelerate therapeutic innovation while reducing attrition rates and development costs.

Keywords: *Computational pharmacology, Graph neural networks, Multi-omics integration, Explainable artificial intelligence, In silico drug design*

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