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Integrating AI-Driven Virtual Screening with High-Throughput Experimental Validation in Drug Development

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ABSTRACT

High costs, long timelines, and high rates of failure are the typical characteristics of the traditional drug development process, particularly in the early phases of compound identification and validation. The integration of high-throughput experimental validation with virtual screening using artificial intelligence has emerged as a game changer in modern drug development. In contrast to traditional computer-based approaches, AI-based virtual screening employs machine learning and deep learning algorithms to rapidly and correctly prioritize lead compounds, model drug-target interactions, and evaluate large chemical libraries. The chemical search space is significantly narrowed down by these virtual approaches, enabling focused experimental efforts. Nevertheless, biological efficacy and safety cannot be ensured by computer predictions; experimental confirmation is necessary. The candidates selected by AI can be validated rapidly and in parallel by using high-throughput experimental validation platforms, which include automated biochemical and cell-based assays that provide sound biological data on efficacy, selectivity, toxicity, and primary pharmacokinetic properties. High-throughput validation and AI-assisted screening complement each other to enhance lead identification, reduce false-positive rates, and accelerate lead optimization with reduced resource consumption. Furthermore, the combined strategy facilitates the exchange of feedback between AI models and experimental data, leading to a continuous enhancement of prediction accuracy. This paper examines the basic methodologies, recent technological advances, and practical applications of integrating high-throughput experimental validation with AI-based virtual screening in drug discovery. The future outlook on developing reliable, scalable, and efficient AI-assisted drug discovery platforms is also discussed, along with key considerations such as data quality, interpretability, and experimental scalability.

Keywords: *Artificial intelligence; Virtual screening; High-throughput screening; Drug discovery; Machine learning.*

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