

Comparative Analysis of AI-Driven Drug Discovery and Drug Repurposing

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Abstract: Artificial intelligence (AI) is essentially remodelling pharmaceutical research and development, which calls for a comparative analysis of its use in de novo drug discovery (DNDD) and drug repurposing (DRP). This review of the literature compares the strategic and methodological divergence of these two avenues. DNDD uses generative AI to canvass immense chemical space to produce high-risk, high-reward new entities but takes 10–17 years and more than \$2 billion. In contrast, DRP utilizes predictive AI and network-based approaches (e.g., Graph Neural Networks, multi-omics integration) to predict novel therapeutic applications for known, safety-tested compounds. DRP provides shortened timelines (3–12 years), significantly lower costs, and triple the success rate. Success in DNDD is dependent on fidelity of generative models and synthesizability, whereas DRP depends upon the ability to perform scalable, explainable multi-omics data integration. Ultimately, the two plans are complementary, with DRP offering clinical speed and DNDD guaranteeing long-term pipeline invention.

Keywords: Artificial Intelligence (AI), Drug Discovery, Drug Repurposing, Generative AI, Predictive Modeling, Multi-omics, Graph Neural Networks, Precision Medicine

