

Artificial Intelligence In Drug Discovery And Development: A Comprehensive Review

A Detailed Review of Applications, Advancements, Challenges, and Future Prospects of AI in Pharmaceutical Research

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Abstract: Artificial Intelligence (AI) has emerged as a transformative force in pharmaceutical research, reshaping every stage of the drug discovery and development pipeline. Traditional drug discovery is slow, costly, and characterized by high failure rates, typically requiring 10–15 years and billions of dollars to successfully bring a single drug to market. The rapid growth of biological data, advancements in computational power, and the development of sophisticated machine learning (ML) and deep learning (DL) algorithms have positioned AI as a powerful solution to address these challenges. AI-driven platforms can efficiently analyze complex datasets, identify novel drug targets, predict molecular interactions, optimize lead compounds, and evaluate pharmacokinetic and toxicity profiles with greater accuracy and speed than conventional methods. Additionally, AI enhances virtual screening, accelerates *de novo* drug design, and supports drug repurposing by uncovering hidden patterns in biomedical data. In drug development, AI plays a crucial role in optimizing formulation design, predicting drug performance, and improving clinical trial efficiencies through patient stratification, real-time monitoring, and adaptive trial designs. Regulatory sciences are also gradually integrating AI to streamline decision-making and improve pharmacovigilance systems. Several real-world successes—including AI-designed molecules entering clinical trials, the use of AI in COVID-19 vaccine development, and breakthroughs such as AlphaFold in protein structure prediction—demonstrate the transformative potential of AI in modern drug discovery.

Despite these advancements, challenges such as data quality issues, model interpretability, integration barriers, and ethical considerations remain significant. Nevertheless, AI continues to evolve rapidly and is expected to play an increasingly central role in future pharmaceutical innovation. This review provides a comprehensive overview of AI applications, methodologies, successes, limitations, and emerging trends in drug discovery and development.

Keywords: Artificial Intelligence, Machine Learning, Deep Learning, Drug Discovery, Drug Development, Virtual Screening, *De novo* Drug Design