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From Molecules to Medicines: The Role of Artificial Intelligence in Accelerating Drug Discovery

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Abstract: *The integration of artificial intelligence (AI) into drug discovery is revolutionizing traditional pharmaceutical research by accelerating and optimizing the development of new therapeutics. Leveraging machine learning (ML) and deep learning (DL) techniques, researchers can now process and analyze vast molecular datasets to identify, design, and refine bioactive compounds with greater efficiency and precision.*

This review highlights the transformative impact of AI across key stages of the drug discovery pipeline, including target identification, virtual screening, lead optimization, and pharmacokinetic/ pharmacodynamic (PK/PD) modeling. AI enables high-throughput prediction of molecular interactions, facilitates the discovery of novel drug candidates, and enhances decision-making by providing accurate predictive models. Furthermore, AI supports the development of personalized medicines by integrating genomic, clinical, and real-world data to tailor treatments to individual patients.

Applications such as molecular docking, QSAR modeling, and deep neural networks allow for rapid identification of promising compounds and help mitigate late-stage failures by predicting efficacy and toxicity early in the process. Virtual screening powered by AI significantly reduces the need for costly and time-consuming experimental assays, while lead optimization benefits from AI's ability to predict molecular modifications that enhance drug-likeness and safety.

Despite its promise, AI in drug discovery faces challenges including data heterogeneity, model interpretability, and regulatory uncertainty. Ensuring the reliability, transparency, and ethical use of AI models remains a priority for future research.

This review provides a comprehensive overview of current AI applications in drug discovery, the benefits realized thus far, and the challenges that must be addressed to fully harness its potential.

Keywords: Artificial intelligence (AI), Drug Discovery, Machine learning, Virtual Screening, Natural Language Processing (NLP), Target Identification, Lead Optimization, Personalized medicine.

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