

AI and Machine Learning in Modern Drug Design and Discovery

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Abstract: *The pharmaceutical industry is experiencing a paradigm shift driven by artificial intelligence (AI) and machine learning (ML). These technologies are accelerating drug discovery processes, improving target identification, optimizing molecular design, and predicting pharmacokinetic and toxicological properties with remarkable precision. Traditional drug discovery, characterized by high costs, extended timelines, and low success rates, is being transformed by computational intelligence. AI-based models can process massive datasets, identify hidden correlations, and simulate biological interactions that are otherwise challenging through conventional methods. This review explores the role of AI and ML in modern drug design, focusing on their applications in target identification, de novo drug design, lead optimization, and clinical trials. Furthermore, the review discusses the ethical and regulatory considerations in AI integration, future prospects, and the challenges that remain in achieving full automation and interpretability in pharmaceutical innovation.*

Keywords: Artificial Intelligence, Machine Learning, Drug Discovery, Deep Learning, QSAR, Molecular Docking, Pharmacoinformatics

