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Recent Approaches of Artificial Intelligence in Drug Discovery

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Abstract

Artificial intelligence (AI) and machine learning (ML) are bringing major changes to drug discovery by helping to overcome long-standing problems such as high costs, slow development, and low success rates. This review discusses recent progress (2019–2024) in the use of AI/ML throughout the drug discovery process—from identifying drug targets to clinical development. It highlights different techniques, including deep learning, graph neural networks, and transformers, and explains how they are applied in areas such as target identification, lead discovery, hit optimization, and safety testing. We compare the strengths and drawbacks of these approaches and outline key factors needed for success, including high-quality data, reliable model validation, and ethical practices. The review also points out current challenges, such as limited data access, poor model interpretability, and difficulties in translating findings into clinical use. Finally, we suggest future directions to fully realize the potential of AI in creating safer, more effective, and affordable medicines. The overall aim is to promote responsible and transparent integration of AI into pharmaceutical research.

Keywords: Artificial Intelligence , Machine Learning , Drug Discovery , Deep Learning, Graph neural networks , Target Identification.