

AI-Enabled Virtual Screening and Drug Repurposing in Pharmacy

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ABSTRACT

The world is transforming using Artificial Intelligence. Pharmaceutical companies are currently using traditional medicine discovery, which is a lengthy and costly process, and most discovered drugs could not obtain relevant regulatory approval for patient use due to their unsuitability. A Virtual Screening (VS) approach is a new method to improve the research and development lifecycle. The VS process reduces the initial level of research required to discover potential drug components for a disease. Deep Learning (DL) algorithms play a vital role with VS. DL can understand the patterns within an existing dataset. The drug discovery process applies algorithms to understand the pattern of different chemical compounds with diseases. On the other hand, Drug Repurposing is the process of finding new therapeutic applications for drugs that are already on the market, providing a quicker, inexpensive alternative to conventional drug development. The approach takes advantage of existing knowledge about a drug's pharmacokinetics, pharmacodynamics, safety, and manufacturing processes, dramatically reducing development times. AI approaches, including machine learning, enhance the identification of suitable biological targets, predict drug-disease associations, and facilitate the analysis of complex biological data and literature. Case studies demonstrate the effectiveness of AI in rapidly repurposing drugs, such as remdesivir during the COVID-19 pandemic. However, challenges remain, including data bias, model interpretability, and ethical considerations. Overall, AI-enabled virtual screening and drug repurposing represent a promising and cost-effective strategy in pharmaceutical research. With continued methodological improvements and proper validations, these technologies have the potential to accelerate drug development and support more targeted therapeutic interventions.

Keywords: Artificial Intelligence, Virtual Screening, Drug Repurposing, Deep Learning, COVID-19 pandemic



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