What Are the Applications of AI in Drug Repurposing?

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Abstract

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Introduction

Drug repurposing, the process of identifying new uses for existing drugs, has emerged as a promising strategy to accelerate the development of new therapies. Traditional drug discovery is a lengthy and expensive process, with a high failure rate. By repurposing existing drugs, which have already been tested for safety in humans, researchers can significantly reduce the time and cost of drug development. In recent years, artificial intelligence (AI) has revolutionized the field of drug repurposing, enabling scientists to analyze vast amounts of data and identify potential new drug-disease relationships with unprecedented speed and accuracy [1].

AI-Powered Drug Repurposing

AI algorithms can be applied to various stages of the drug repurposing pipeline, from target identification to clinical trial optimization. Here are some of the key applications of AI in drug repurposing:

Identifying New Drug-Disease Relationships

One of the primary applications of AI in drug repurposing is to identify novel connections between drugs and diseases. Machine learning models can be trained on large datasets of drug and disease information, including chemical structures, protein targets, gene expression data, and clinical trial results. By analyzing these complex datasets, AI algorithms can uncover hidden patterns and predict potential new indications for existing drugs. For example, AI models can identify drugs that have similar molecular or cellular effects to drugs that are already approved for a particular disease, suggesting that they

may also be effective for that disease [2].

Predicting Drug Efficacy and Toxicity

AI can also be used to predict the efficacy and toxicity of drugs for new indications. By analyzing data from preclinical and clinical studies, AI models can learn to predict how a drug will perform in a new disease context. This can help researchers to prioritize the most promising drug candidates for further investigation and to avoid wasting resources on drugs that are unlikely to be effective or safe. For instance, deep learning models have been used to predict the binding affinity of drugs to their targets, which is a key determinant of drug efficacy [1].

Optimizing Clinical Trials

AI can also be used to optimize the design and execution of clinical trials for repurposed drugs. By analyzing data from previous clinical trials, AI models can help researchers to identify the most appropriate patient populations for a particular drug, to determine the optimal dose and treatment schedule, and to predict the likelihood of success of a clinical trial. This can help to increase the efficiency and success rate of clinical trials, and to bring new therapies to patients more quickly [1].

Success Stories

Several drugs have been successfully repurposed with the help of AI. For example, an AI-powered platform was used to identify that baricitinib, a drug approved for rheumatoid arthritis, could be effective in treating COVID-19. This led to a clinical trial that showed that baricitinib could reduce mortality in hospitalized COVID-19 patients. Another example is the use of AI to identify that a drug originally developed for Alzheimer's disease could be effective in treating a rare genetic disease called NGLY1 deficiency.

The Future of AI in Drug Repurposing

The application of AI in drug repurposing is still in its early stages, but it has the potential to transform the field of drug discovery. As AI algorithms become more sophisticated and as more data becomes available, we can expect to see even more success stories of AI-powered drug repurposing in the years to come. By leveraging the power of AI, we can accelerate the development of new therapies for a wide range of diseases and improve the lives of patients around the world.

References

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