Chapter 62
Role of Artificial Intelligence and Machine Learning in Drug Discovery and Drug Repurposing

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ABSTRACT

Drug designing and repurposing is the most important field in the pharmaceutical industries and biomedical sciences. Because the challenges caused by drug such as low retention time, sensitivity can affect the efficacy of developmental process. As AI or ML has proven to be a potential activity in the health and biomedical sciences and from previous research it has found that AI can learn new data and transform it into the useful knowledge. So, in field of pharmacology, the aim is to design more efficient and novel vaccines using this method which is also cost effective. The underlying fact is to predict the molecular mechanism and structure for increased likelihood of developing new drugs. Clinical, electronic, and high-resolution imaging datasets can be used as inputs to aid the drug development niche. Moreover, the use of comprehensive target activity has been performed for repurposing a drug molecule by extending target profiles of drugs which also include off targets with therapeutic potential providing a new indication.

INTRODUCTION

Over the last few years, an immense progress has made in the fields of artificial intelligence, machine learning and bioinformatics and more research is needed for understand the data in biological science and related problems. Bioinformatics is a subdivision of science that involves the analysis of biological

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data using mathematical principles, statistical tools and certain algorithms in addition to computational approaches (Ezziane, 2006). Artificial intelligence is the ability to solve various problems related to human intelligence and in turn the simulation of these intelligence processes using computer systems or software. It involves machine learning that allows one to perform all of these tasks based on its training (Narayanan et al., 2002). Basic or structural bioinformatics tools use artificial intelligence and machine intelligence for the design of drugs and repurposing various novel compounds against many diseases such as cancer, neural inflammation and others using the silica approach by applying certain tools with principles of artificial intelligence and machine learning. Bioinformatics has been used to analyze data and logical conclusions. The huge amount of data obtained from whole genome sequencing projects and bioinformatics is used for the annotation of biological data in meaningful ways (Nicolas, 2020). Similarly a large collection of problems has been solved by combining the knowledge and abilities of artificial intelligence with bioinformatics approaches for the prediction of genes, studies involving the study of protein interactions, computational systems for drug design, repurposing drugs for better efficiency, next generation sequencing and development of other software. Therefore, both artificial intelligence and machine learning have useful applications in the field of bioinformatics. The proficiency of artificial intelligence can be changed by varying input data. Artificial learning is further classified into generalized and applied branches. Both of them are totally different where applied is involved in the use of machines and algorithms while applied to stimulate the data into expressions similar to the thoughts of humans automatically (Bülow, 2021). Current machine learning has overcome some of the barriers and has predicted a huge amount of data, increased computational power and the revival of neural networks. These algorithms can be trained for exploit further data and thus don't require human labor or programmers for data prediction (Mitra, 2005).

If safety testing has been performed then it will display compatibility of dosage with the new indications. Drug repurposing has been discovered by chance on the basis of random testing and exploration. For example in the market, sildenafil citrate was discovered as a hypertensive drug and then repurposed with Pfizer resulting in the formation of a new drug molecule Viagara for the treatment of erectile dysfunction proved by clinical studies directly from its formulation which in turn provided massive sales in addition to additional health benefits. From the last few years, several computational approaches have been proposed for the repurposing of drug molecules (Kumar et al., 2018). Popular information for this purpose has been acquired from in silico drug repurposing such as electronic records, gene based information, genetic expression response based profiles, mapping of the targeted complex molecules and phenotype- based profile assessment. Drug repurposing hubs and repurpose hub were recently surveyed. There is also some literature on drug design, discovery and optimization of lead during development, leading to the development of a totally novel molecule (Mellit & Kalogirou, 2008).

However, the aim of this review is to use artificial intelligence and machine learning programs that use publicly available data and information. The main point of emphasis is the comprehensive target based activity of the drugs for the discovery of drug molecules and repurposing where existing drug molecules have some target effects over recently identified target effects for the purpose of new indications (Chen et al., 2008). Hence it provides evidence for the further development of drug molecules and their commercialization. This is particularly true for the drugs that are not specific to any target but have the activity for a number of targets showing broad spectrum activity. For example in some cases cancer off target candidates are available which in addition to having anticancer activity also have potential for the production of new drugs. Here the point to consider is that repurposing us not only to cancer