



Use of Artificial Intelligence in Drug Discovery and Development

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ABSTRACT:

The current era of artificial intelligence and machine learning is a important. It has drastically lowered the load on human beings and improved lifestyle. This article articulate the importance of artificial intelligence and machine learning accurately and precisely. This study of work backed to artificial intelligence and machine learning to provide drug discovery and development process. This can lead to remove the need for clinical trials. This study helps extensively to researchers to study molecules without creating any trials. This study paper shows that importance of artificial intelligence and machine learning in drug discovery and development process as well as its future prospects.

Keywords: Artificial intelligence, machine learning, deep learning, drug discovery

Introduction:

The significant development in the drug discovery process has changed practice medicine in extensively to treat the various kinds of diseases. One of the reason behind the medicinal advancement has the medicinal developments and testing of the drugs. New molecules are mostly searched by the universities and research center and new medicine is developed by the large scale laboratories and industries because of the requirements in the very expensive chemicals and toxicological and pharmacological screening in testing. Due to this the whole process are transferred to pharmaceutical industry known as Pharma which are purely intended for the development of the new drug entities.

Development of new drug has very lengthy procedure and not very affordable process since preclinical, pharmacodynamic, pharmacological, toxicological studies takes on an average 4 years to completed. Further potential drug goes through the drug screening procedure. A various biological assays are carried for the determination of activity and selectivity of the drug. As traditionally type and number of test depends upon pharmacological drug for example anti-infective drugs should be tested on infective organisms thoroughly, etc. the molecule is generally studied for understanding of specificity of the drug. Further testing are conducted in animal testing and human disease. This are the very time taking procedure and very expensive methods for drug discovery hence in this regards artificial intelligence and machine learning plays an important role in drug discovery and development process. And its future applications.

The impact of Artificial intelligence on the drug discovery process and potential cost savings :

Designing of novel compound with specific properties and activities is the one of important application in drug discovery . There is modification and identification process of existing compounds followed in traditional method.this traditional process is slow and labor intensive. For example study of algorithms .development of alpha fold which is a software of learning of biology throughly .

Successful case studies of AI driven drug discovery process:

The ability of AI to identify novel compounds with high potential for cancer treatment has recently been reported by Gupta, R. et al. These researchers trained DL algorithm on treating for cancer causing agents. As an output, novel compounds with high potential for cancer treatment were obtained, demonstrating the ability of AI to identify novel compounds.

The role of engagement between AI research scientist and pharmaceutical scientist:

For the development of novel and high-quality treatments for a range of diseases, collaboration between AI researchers and pharmaceutical scientists is essential. By combining their knowledge and expertise, they can improve efficient computing device learning algorithms and models aimed at predicting the efficacy of potential drug candidates and accelerating the drug improvement process.

The drug DSP-1181 invented by using artificial intelligence are goes for clinical trials:

Exscientia, which developed DSP-1181 in collaboration with Japan's Sumitomo Dainippon Pharma, noted that it had taken less than 12 months from the start of preclinical testing to the end, as opposing 4 long years traditionally by using methods the AI can create amazing results.

Benefits using Artificial Intelligence in drug discovery and development process:

The AI can predict drug properties as known as physicochemical properties of the new drug entities. This AI and ML are beneficial for both financial and ethical perspective. Use of AI and ML in drug discovery and development increase efficiency, accuracy as well as productivity. Artificial intelligence can predict the toxicity levels in found drug molecule. It can predict the Anti-Microbial properties in new drug molecule entity.

Drawback for using AI and ML in drug discovery and development process :

The major drawback is a Data integration.

Challenges pertaining to the AI in drug discovery process:

The first challenge arising is a occupational and skillset immobility in employee in industry.

Low level understanding on the methodology of algorithms in this process.

There is potential bias in algorithm which can create unequal access to medical treatment and unfair treatment of certain groups of people hence artificial intelligence and machine learning must be used in responsible and ethical manner.

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