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A REVIEW ON ROLE OF ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL INDUSTRY AND DRUG DISCOVERY

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Abstract

The process of finding new drugs could be completely transformed by artificial intelligence (AI), which offers increased speed, accuracy, and efficiency. This systematic review examines how artificial intelligence (AI) is developing to address issues facing the pharmaceutical industry, with a particular emphasis on drug discovery, supply chain disruptions, clinical trials, and trial operations. Through the application of AI algorithms that examine vast amounts of biological data, such as proteomics and genomics, scientists are able to pinpoint targets linked to disease and forecast how those targets may interact with possible therapeutic candidates. The most popular artificial intelligence (AI) technologies are deep learning and neural networks; potential technologies for clinical trial design are Bayesian nonparametric models. This review highlights the advantages and disadvantages of the many AI-based techniques used in pharmaceutical technology. However, the pharmaceutical industry's ongoing exploration and investment in AI present exciting opportunities for improving patient care and drug development procedures.

Keywords: Artificial intelligence (AI), Machine learning, Deep learning, Drug discovery, Disease diagnosis, Artificial Neural Network

INTRODUCTION

A subfield of computer science called artificial intelligence (AI) gives machines the ability to analyse complicated data and operate more productively. Artificial intelligence (AI) is the conglomeration of different intelligent processes and behaviours created by computational models, algorithms, or rules that enable a machine to simulate human cognitive functions like learning, solving problems, and so forth [1]. Artificial intelligence (AI) is the system's capacity to comprehend, acquire knowledge from outside sources of data, and generate precise and intended outcomes [2, 3]. It has been determined that artificial intelligence (AI) has a transformative impact on drug development [4]. For many A regulatory framework that protects the quality of finished products through testing of raw materials, in-process materials, end-product characteristics, batch-based operations, and fixed process conditions has governed the manufacturing of drug products for many years [5]. Our pharmaceutical industries are now involved in automation as well, allowing them to increase their production rates and make enormous profits in the pharmaceutical industry. The majority of them have used automated equipment and software in their businesses to produce pharmaceuticals more quickly; in other words, automation is becoming more and more commonplace throughout the world thanks to artificial intelligence [2]. Novel pharmaceutical innovations emphasize enhanced stability and high potency to meet unmet needs for disease treatment, ranging from small molecule drugs to biologics [6]. There are currently four main applications of AI in the pharmaceutical sector. The first involves determining the extent of the illness and forecasting a patient's likelihood of responding well to a particular treatment, even before it is started. Second, it's employed to avoid or address treatment-related complications. Utilizing it as an assistive technology for patients undergoing operations or treatment is its third primary use. Finally, it helps to develop or extrapolate

new uses for instruments or chemicals to improve safety and efficacy, as well as to ascertain the rationale behind the use of specific instruments or chemicals during treatment [5]. AI-based quantitative structure–activity relationship (QSRL) technologies, machine learning (ML), deep learning, virtual screening (VS), support vector machines (SVMs), deep virtual screening, deep neural networks (DNNs), recurrent neural networks (RNNs), and other algorithms are used in drug discovery for both drug screening and drug design [1]. In pharmaceutical product development, various AI models have been explored to enhance different aspects of the process as shown in **Fig.1** [7].

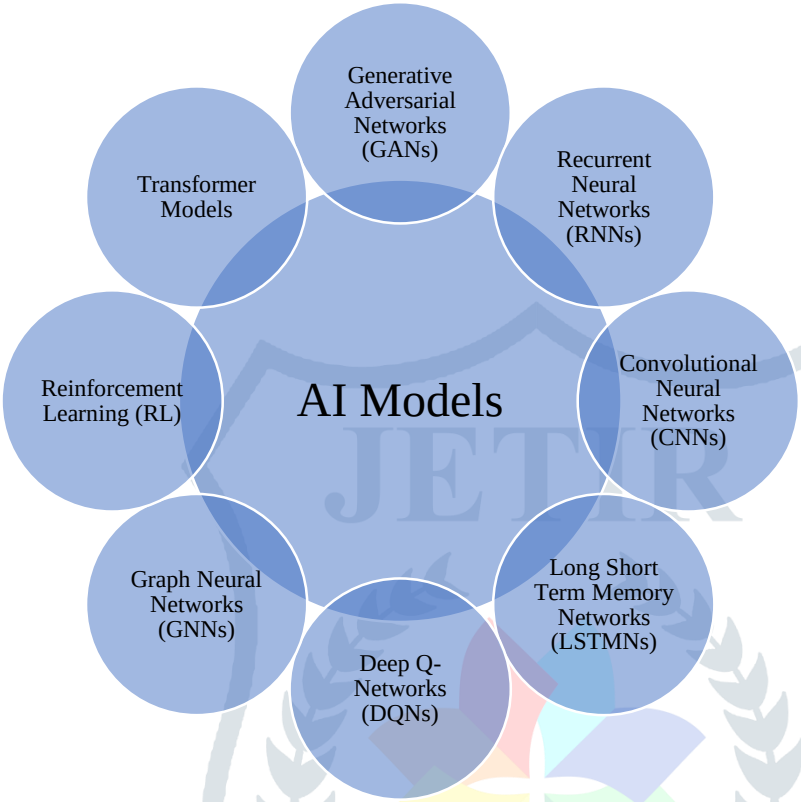

Figure 1. Commonly used AI models in the pharmaceutical industry

Machine Learning

Algorithms that can be created to assess and forecast based on novel and intricate features are referred to as machine learning [4]. ML transmits information through electronic impulses in an exact manner similar to that of human brain neurons. Their intricate algorithms, which are essentially mathematical models, learn from and forecast future data by utilizing underlying algorithms found in the provided data and information. It can generate precise answers and resolve a variety of intricate mathematical issues in the data [2, 9]. Machine learning is being used in many different aspects of healthcare. Identifying and diagnosing diseases, creating customized therapies, finding and producing drugs, conducting clinical trials, radiology and radiotherapy, smart electronic health records, and anticipating epidemic outbreaks are a few of these fields [4,8]. The drug development industry finds AI/ML techniques attractive because of their automated nature, predictive capabilities, and anticipated increase in efficiency. Over the past 15 to 20 years, ML techniques have been applied with increasing sophistication in drug discovery. Because of the COVID-19 pandemic's increased reliance on digital technology for patient data collection, the use of AI/ML in clinical trials may accelerate even further [10].

Deep Learning

Artificial neural networks, or deep learning (DL), are a kind of machine learning (ML) that is loosely modelled after the architecture of the human brain [9]. An input, several hidden, and an output compartment are features of DL neural networks. It is capable of learning even the most complicated modules with sufficient data provided by various neurons and input sets, and it can produce extremely accurate results. In addition to other cutting-edge techniques like initialization schemes and neural activation functions, the most often used processing methods are gradient-based optimization techniques and the backed-propagation algorithm.

Recurrent neural networks (RNN), conventional neural networks (CNN), and graph neural networks (GNN) are the three types of processing techniques [2].

Artificial Neural Network

There is another term for ANNs: the "Digitalized Human Brain." The brain compartment is made up of three main compartments: the input compartment, the hidden compartment, and the output compartment. Neural networks, or brain neurons, establish connections between these three compartments. 11–12 The hidden compartment, which is where data analysis is done, is connected to the input compartment, where we feed our input data. That means that in response to input data, it will either forward the data toward the output compartment or back-propagate (deny the input data). It lessens the intricacy of the statistical modeling utilized in drug discovery studies involving pharmacokinetics, pharmacodynamics, QSAR modeling, and HTVS. Its exceptional interpreting power aids in the discovery of new drugs by interpreting both linear and non-linear computational parameters.

Applications of Artificial Intelligence in drug Discovery [6-7,14-15]

Drug discovery and research have been transformed by AI in many ways. Several of the key contributions made by AI in this field includes the following:

- Identifying the Target
- Virtual Screening
- The Structure-Activity Relationship (SAR)
- Drug Repurposing
- Enhancement of Potential Medicines
- De Novo Drug Design
- Anticipation of Toxic Effects

Identifying the Target

AI systems are able to identify possible therapeutic targets by analysing a variety of data types, including clinical, proteomic, and genetic data. Through the identification of disease-associated targets and molecular pathways, artificial intelligence (AI) assists in the development of medications that can regulate biological processes.

Virtual Screening

Artificial Intelligence facilitates the effective screening of extensive chemical libraries to find promising drug candidates with a high probability of binding to a particular target. Artificial Intelligence (AI) helps researchers save time and resources by prioritizing and selecting compounds for experimental testing by simulating chemical interactions and predicting binding affinities.

The Structure-Activity Relationship (SAR)

The relationship between the molecular structure and biological function of a chemical compound can be represented by artificial intelligence models. This enables scientists to create compounds with desired properties, like high potency, selectivity, and advantageous pharmacokinetic profiles, in order to optimize drug candidates.

Drug Repurposing

The relationship between a chemical compound's molecular structure and biological function can be represented by artificial intelligence models. By creating compounds with desired properties like high potency, selectivity, and advantageous pharmacokinetic profiles, researchers can use this to optimize drug candidates.

Enhancement of Potential Medicines

AI algorithms have the potential to analyze and improve various aspects of medication candidates, including pharmacokinetics, safety, and efficacy. By doing this, researchers can increase the effectiveness of pharmaceuticals while lowering the possibility of unfavorable outcomes.

De Novo Drug Design

Reinforcement learning and generative models are two tools that AI algorithms can use to suggest new chemical structures that resemble drugs. AI broadens the chemical space and supports the creation of novel therapeutic candidates by drawing on knowledge from chemical libraries and experimental data.

Anticipation of Toxic Effects

AI systems can forecast drug toxicity by examining a compound's properties and chemical structure. AI systems have the potential to predict which drugs will be dangerous by analysing the molecular formulas and properties of substances. Machine learning algorithms that have been trained on toxicology databases are able to recognize potentially dangerous structural features or predict negative effects. By doing so, researchers can reduce the possibility of unfavourable reactions in clinical trials and prioritize safer chemicals.

Using AI models and tools has led to significant advancements in the field of drug discovery. Some of the popular AI model tools used for drug discovery as shown in **Fig.2**.

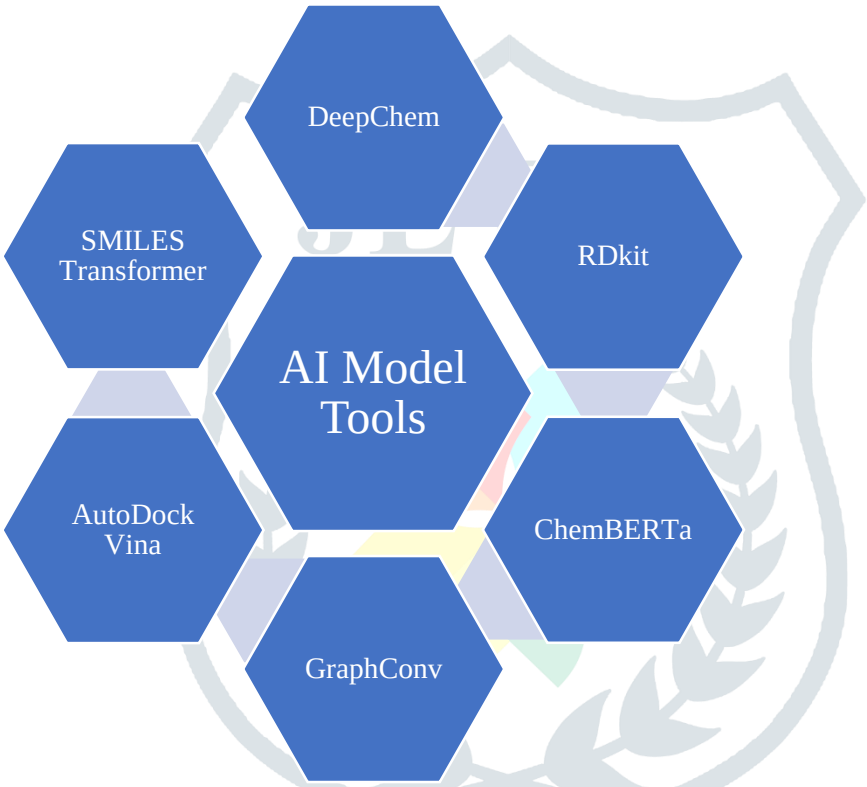

Figure 2. Popular AI model tools used for drug discovery

Challenges and Limitations of Using AI in Drug Discovery [16]

There are several challenges and limitations of using AI in drug discovery that must be considered are as follows [5, 17-22]:

- Ineffective integration of data. This issue arises from the diversity that exists among datasets, which may include candidate, processed, raw, or metadata data.
- A significant amount of data is needed for training AI-based methods.
- Immobility of occupation and skill set: A large number of individuals employed in the pharmaceutical sector today lack the training or credentials required to manage AI systems.
- The accuracy and dependability of the results can frequently be impacted by the small quantity of data that is available, the poor quality of the data, or inconsistent data.
- Moral implications
- Ensuring the just and moral application of AI in the creation of novel therapeutic substances.

Several strategies and approaches can be used to overcome the obstacles faced by AI in the context of chemical medicine [23-26].

Use of data augmentation: In order to augment already-existing datasets, synthetic data must be generated. As a result, the amount and variety of data that can be used to train machine learning algorithms may rise, increasing the precision and dependability of the outcomes.

Use of explainable AI (XAI) methods: We seek to offer clear, understandable justifications for the predictions generated by machine learning algorithms. This can help allay worries about fairness and bias in AI-based methods and provide us a better grasp of the underlying assumptions and mechanisms that underlie the predictions.

Limitations [27-28]

• Traditional experimental procedures and the knowledge and experience of human researchers cannot be replaced by current AI-based methodologies.
• AI can only make predictions based on the data that is currently available; human researchers must then evaluate and explain the findings.

Future Scope

In the pharmaceutical sector, artificial intelligence primarily has the ability to lower costs and boost productivity [39]. Writing business apps has benefited from machine learning approaches, which can handle complicated analyses with large, heterogeneous, and high-dimensional information collections without the need for human input. Coordination of many massive data repositories may be best achieved by combining human expertise and experience with machine learning, especially deep learning. Many facets of drug development and discovery should be made possible by AI innovation, which is predicted to standardize computer-supported medication plan strategies. Improvements in medication due to better analysis of vast and complicated datasets should follow from the coordinated development of mechanization and innovations coming from merging technologies [5, 29–30].

Conclusion

With the development of cutting-edge technologies like artificial intelligence and machine learning, the idea of computers is expanding continuously. AI and ML have enormous potential to develop cutting-edge technology, automate tasks, and digitize society. The pharmaceutical industry's ability to successfully use AI and machine learning into drug development, screening, and repurposing is influenced by a number of factors. AI-based models can mimic medication distribution and clearance in the body, predict pharmacokinetic parameters, and optimize drug dosage and administration methods.

This comprehensive analysis of the literature demonstrated how artificial intelligence (AI) and machine learning can increase the effectiveness and precision of medication development. As this article discusses, the majority of the pharmaceutical industry are currently moving toward robots and machines to create fully automated systems. All things considered, the use of AI technologies has enormous potential to expedite medication development, enhance patient outcomes, and completely transform the pharmaceutical sector.

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