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Impact of Artificial Intelligence in Drug Discovery and Development

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Abstract: *The field of drug discovery and development has been revolutionized by the integration of artificial intelligence (AI) technologies. AI has significantly impacted various stages of the drug development process, including target identification, lead optimization, pharmacokinetics, and toxicity prediction. This review paper provides an overview of the impact of AI in drug discovery and development, highlighting the advancements, challenges, and future prospects. It discusses the application of machine learning, deep learning, and other AI techniques in accelerating the drug discovery process, improving the efficiency of clinical trials, and reducing the overall cost of drug development. Additionally, this review examines the ethical and regulatory considerations associated with the use of AI in drug development. Overall, this paper emphasizes the transformative potential of AI in revolutionizing the pharmaceutical industry and improving patient outcomes.*

Keywords: Artificial intelligence, Computer assisted drug discovery, Machine learning, Toxicity Prediction, Clinical Trials, Ethical Considerations, Regulatory Frameworks

I. INTRODUCTION

Every aspect of life is constantly subject to change, and one of the main aims of humans is to control these changes for our benefit; this is especially true in the field of medicine and pharmaceuticals. These disciplines focus on the creation or discovery of chemical compounds and mixtures and their use to ease physical and psychological suffering. For many decades, the manufacturing of drug products has been controlled by a regulatory framework that safeguards the quality of final products by testing of raw materials, in-process materials, end-product characteristics, batch-based operations and fixed process conditions[1-3]. From the past two decades, the development of efficient and advanced systems for the targeted delivery of therapeutic agents with maximum efficiency and minimum risks has imposed a great challenge among chemical and biological scientists[4]. Further, the cost of development and time consumption in developing novel therapeutic agents was another setback in the drug design and development process[5]. To minimize these challenges and hurdles, researchers around the globe moved toward computational approaches such as virtual screening (VS) and molecular docking, which are also known as traditional approaches. However, these techniques also impose challenges such as inaccuracy and inefficiency[6]. Thus, there is a surge in the implementation of novel techniques, which are self-sufficient to eliminate the challenges encountered in traditional computational approaches. Artificial intelligence (AI), including deep learning (DL) and machine learning (ML) algorithms, has emerged as a possible solution, which can overcome problems and hurdles in the drug design and discovery process[7]. The use of artificial intelligence (AI) is increasing, and is likely to change how clinical examination and training is carried out. Doctors can participate in the development of this technology for use in the medical and pharmaceutical industries; this will ensure that the potential of AI to significantly improve medical care is fulfilled[8].

AI is currently used in the pharmaceutical industry in four main ways. The first is in the assessment of the severity of disease and the prediction of whether treatment will be successful for an individual patient, even prior to its administration. Secondly, it is used to prevent or solve complications during treatment. Its third main use is as an assistive technology to during treatment procedures or operations on patients. Lastly, it is used to determine the reasons behind the use of particular instruments or chemicals during treatment, and to develop or extrapolate new uses for instruments or chemicals to improve safety and efficacy. AI also has a more general role in the management and analysis of big data[9]. Moreover, implementing AI tools, including machine learning and data analytical approaches, is

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revolutionizing drug and pharmaceutical enterprises to identify and initiate a new therapeutic in contemporary times[10]. Artificial intelligence (AI) and machine learning (ML) have flourished in the past decade, driven by revolutionary advances in computational technology. This has led to transformative improvements in the ability to collect and process large volumes of data. Meanwhile, the cost of bringing new drugs to market and to patients has become prohibitively expensive. In the remainder of this paper, we use "R&D" to generally describe the research, science, and processes associated with drug development, starting with drug discovery to clinical development and conduct, and finally the life-cycle management stage. Developing a new drug is a long and expensive process with a low success rate as evidenced by the following estimates: average R&D investment is $1.3 billion per drug[11]; median development time for each drug ranges from 5.9 to 7.2 years for non-oncology and 13.1 years for oncology; and proportion of all drug-development programs that eventually lead to approval is 13.8%[12].

Machine Learning in Drug Discovery and Development

The use of machine learning is increasing in various avenues of the pharmaceutical industry, including drug discovery, enabling improvements in the industry as a whole. The achievements of machine learning are demonstrated by the expanding number of companies in which ML is key to their business structure. They stated that machine learning techniques has also been investigated by large pharmaceutical companies for use in drug research and development[13]. The extent of the capability of machine learning and its usefulness in the field of drug discovery; it is thus imperative that it must be incorporated in future advances in the field of drug discovery. The goal is to use high-throughput screening technologies to reduce the asset and work seriousness of medication disclosure. Machine learning may eventually minimize, if not eliminate, the necessity for live animal testing[14]. These studies demonstrate that machine learning is an extremely useful tool in drug discovery.

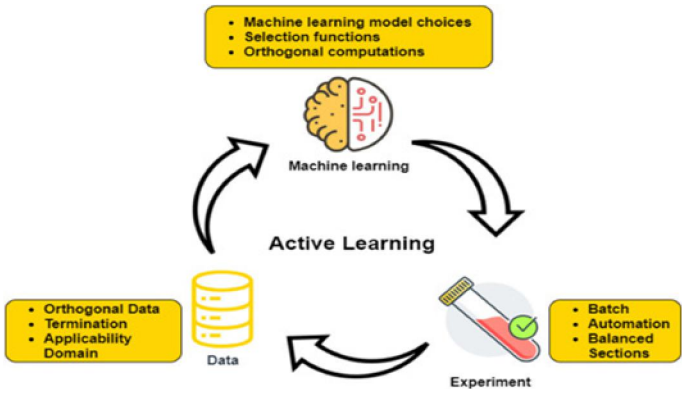

Fig.1 - Machine learning in Drug discovery and development

Application Point

Artificial intelligence and machine learning-aided drug discovery in central nervous system diseases -

To the numerous neurological disorders, the development of drugs in the central nervous system (CNS) disorders is a challenging area. With the rapid growth of biomedical data that enabled by advanced experimental technologies, AI and ML have emerged as an indispensable tool to draw meaningful insights and improve decision making in drug discovery. Due to the advancements in AI and ML algorithms, now the AI/ML-driven solutions have an unprecedented potential to accelerate the process of CNS drug discovery with better success rate[15].

Artificial intelligence in clinical trials

The main purpose of clinical trials is to address the safety and efficacy of a new drug candidate by measuring the predefined biomarkers. The utilisation of AI may reduce the cost, delays and failures in clinical trials. It helps in all the

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stages of clinical trials, from the design of study protocol to completion of the trial. The data required for the training of AI can be obtained from the real-world data such as electronic health records (EHR), insurance records, medical imaging, wearable's.

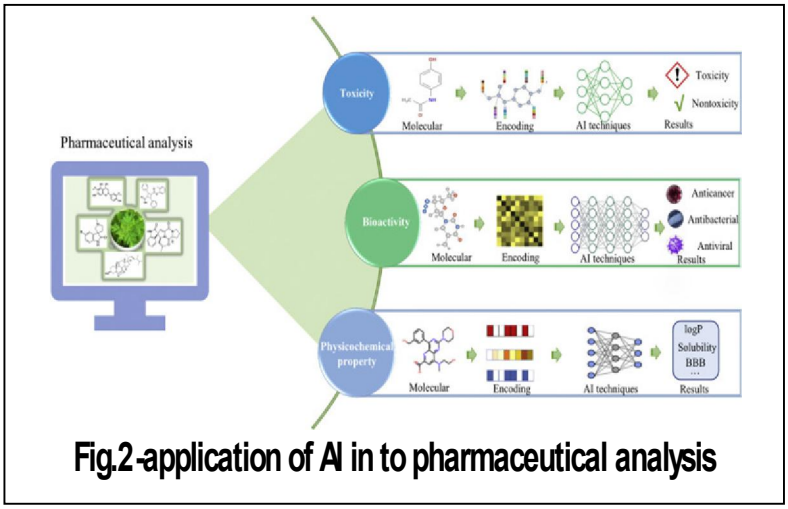

Fig.2-application of AI in to pharmaceutical analysis

Artificial intelligence in Pharmacovigilance-

Pharmacovigilance is defined as the science and activities related to detection, finding, assessment, understanding and prevention of adverse effects. Some of the tasks include the Drug-Drug Interactions (DDI) (is a condition when one drug influences the activity of another drug), DDIs extraction from biomedical literature and DDI classification. ML techniques like feature-based and kernel-based methods are used specifically for text mining and they are applied for biomedical literature.

Drug bioactivity prediction-

In reality, a large number of drugs derived from natural products are ineffective due to the lack of bioactivity. Hence, drug bioactivity assessment has become an active area in drug discovery. Although in vitro and in vivo experiments can mimic the functions of molecules in the human body, they are still time-consuming and expensive. Given their cost-effectiveness and time economy, AI techniques have been effectively applied to predicting drug bioactivities, such as anticancer, antiviral, and antibacterial activities.

Application of AI to pharmaceutical analysis

Pharmaceutical analysis involves the processes of identification, determination, quantification, and purification of pharmaceutical raw materials; it is an essential part of drug discovery. Qualitative and quantitative analyses are the two major types of experimental methods in pharmaceutical analysis. Although these techniques exhibit high accuracy, their cost for screening novel drug candidates from a huge amount of natural products is still expensive. Compared with experimental techniques, the costs required by computational methods are negligible. Hence, AI techniques have been used in pharmaceutical analysis to complement experimental techniques.

De novo drug design

The concept of de novo drug design (DNDD) based on AI with diverse techniques (e.g.: the autoencoders-AE, graph neural networks-GNNs, GAN, CNN, and the recurrent neural networks-RNNs) aims at generating novel compounds (previously unknown) with desired properties. Normally, the algorithms contained two steps: firstly, from the worthy databases (CHEMBL, ZINC, PubChem), the model automatically generated new molecules based on rules (SMILES, molecular graph); secondly, reinforcement learning methods speed up to explore the novel regions to design structures with promising activities[16].

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II. DISADVANTAGE/CHALLENGES

A well-known drawback of deep learning is its poor performance in medium-to-low data scenarios. Further insight might be provided into these scenarios by chemogenomic-based approaches alongside exploiting additional genomic or biological interactome data sources.[17]

Another commonly-claimed drawback of deep-learning approaches is their high computational cost. Deep learning typically entails longer training and evaluation times than many other machine-learning approaches without specialized hardware such as consumer-grade graphical processing or tensor-processing units[18].

A third but related difficulty is scepticism about machine learning and AI in the pharmaceutical industry owing to a lack of understanding on the methodology of algorithms, known as the "black box" phenomenon, and a lack of trust for the results generated. Those who are sceptical may be reluctant to use the data generated using AI and machine learning, wasting both time and money, and holding the industry back with regards to efficiency.[19]

Data limitations - The development of AI algorithms cannot be separated from the drive of data. High-quality and accurate data can sometimes enable simple models to outperform complex models. There are many excellent publicly accessible databases for data research, including TTD, ChEMBL, DrugBank, CMAP, and PRIDE, but the amount of data is insufficient to support more complex research. The construction of AI algorithms relies heavily on high-quality and sufficient data. The acquisition of high-quality data is a very important issue for sophisticated and complex biological systems, due to the limitations of current technology, and it is costly to process this data into standard data with high confidence. The method, time, and place of operation of each batch of data acquisition are different, making it more difficult to process the acquired data into uniform and valid data[20].

III. FUTURE PROSPECTS

The main potential of AI in the pharmaceutical industry is to reduce costs and increase efficiency[21]. Reports have shown that a few companies are engaging in silico synthetic planning into their whole course, accessing target molecules through the use of AI and ML; this has proven to be a beneficial technique in predictive chemistry and synthetic planning of small molecules. ML for Pharmaceutical Discovery and Synthesis (MLPDS) consortium, composed of MIT and 13 chemical and pharmaceutical companies, is developing and evaluating a data-driven synthesis planning program. The integration of predictive models into the medicinal chemistry synthesis workflow, the use of these models in MLPDS member companies, and the outlook for this field[22]

IV. CONCLUSION

The introduction of artificial intelligence has resulted in tremendous growth in the pharmaceutical sector's various key areas. It had revolutionized traditional approaches to drug discovery and development by using modernized computational approaches. Many pharmaceutical behemoths have begun to implement these sophisticated technologies to develop personalized medicine. This systematic literature review showed that AI and machine learning can improve the efficiency and accuracy of drug discovery and development. These technologies not only augment process efficiency, but also in some cases reduce or eliminate the need for clinical trials by conducting simulations in their place, and also allow researchers to study molecules more extensively without trials, reducing costs as well as ethical concerns. Integrating AI and machine learning is likely to revolutionise drug development in time, but there are still a number of barriers like cleaing of unstructured and heterogeneous dataset, occasional incompetency of the computing device etc. may impede this. Once these barriers are removed, advancements in AI and machine learning can be more widely implemented and improved, signaling the start of a new age for the pharmaceutical industry.

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