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Artificial Intelligence for Drug Discovery-Resources, Application and Challenges

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Abstract: *Artificial intelligence (AI) has infused various sectors, including the drug discovery, where it has been utilized to efficiently identify new chemical moieties with desirable properties. Conventional wet laboratory testing, validations, and synthetic procedures are costly and time-consuming for drug discovery. The future in artificial intelligence (AI) techniques has revolutionized their applications to medicinal chemistry and drug discovery. Altogether with accessible data resources, AI techniques are changing the approach of drug discovery. In previous ten years, a series of AI-based models have been developed for various steps of drug discovery. Meanwhile, the algorithms used to modify AI-based models for drug discovery is argued. Subsequently, the applications of AI techniques in pharmaceutical analysis including predicting drug toxicity, drug bioactivity, and drug physicochemical property is discussed. Furthermore, AI-based models for de novo drug design, drug-target structure prediction, drug-target interaction, and binding affinity prediction is discussed. Moreover, it is also highlighted the modern applications of AI in drug activity prediction and nano-medicine design. Finally, the challenges and future perspectives on the applications of AI to drug discovery are discussed here*

Keywords: artificial intelligence; drug discovery; medicinal chemistry

I. INTRODUCTION

Medicinal chemistryand drug discoveryis a process through which new medications against diseases are synthesized. It involves the use of a wide variety of technologies and expertise. In general, discovering and developing a drug costs billions of rupees and time period of ten to twelve years on an average[1].The lessefficacy and high-cost of conventional methods have become the hurdles of drug discovery. Therefore, developing new methods to deal with such a time-consuming and expensive task is necessary.[2]

Artificial intelligence is a field within technology, focuses on developing methods that empower devices to perform tasks typically associated with human sense, such as thinking and learning. AI is having a revolutionary impact on various fields of our lives and spreading across numerous industry sectors, with the pharmaceutical fieldtoo[3]. The value of AI is immense as it serves as a technology that can significantly reduce the extensive time and financial investments required for the discovery of a new drug. When used properly, an AI technology helpsanalyzelarge amounts of data, such as structure, functional group, and chemical information, to identify potential drug molecules and predict drug efficacy or toxicity[4]. By evaluating complex datasets and identifying hidden patterns, machine learning (ML) or deep learning (DL) algorithms can find novel targets associated with multitasking data and help find for novel chemical molecules with potent biological activities. They have not only expedited the identification of potential drug candidates but have also proven invaluable in the process of drug repurposing.[5]In the realm of medicinal chemistry, AI has shown promising results in the discovery of new chemical scaffolds with therapeutic potential. It has the capacity to scrutinize vast chemical spaces and extract meaningful patterns, thereby significantly reducing the time required for identifying potential drug candidates.[6] ML/DL algorithms can be trained to predict the biological activities, pharmacokinetic properties, and also toxicity profiles of molecules[7]. Now a days DL methods can generate novel molecular structures that match desired therapeutic profiles[8-9]. Molecular docking, the method that predicts the interaction between a small molecule and a protein has traditionally been a computationally intensive task. Now a day, AI is being utilized to predict the likelihood of molecular binding, its strength, and the most energetically favourable position, thereby automating this critical process. In addition, it can be utilized to optimize the chemical structures of drug molecule for

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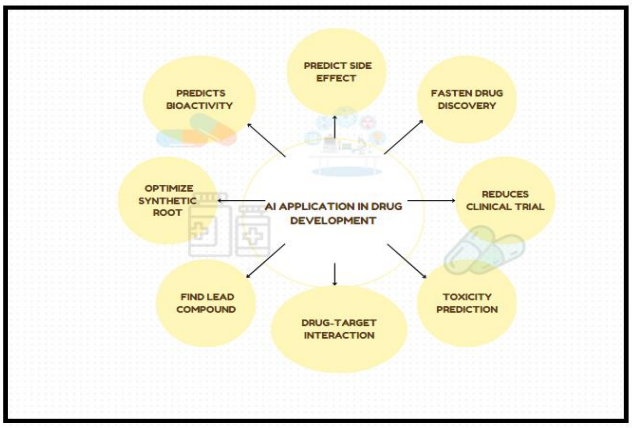
enhanced efficacy and reduced toxicity. While the promise of AI in medicinal chemistry is profound, the integration of AI into drug discovery pipelines presents on-going challenges[10]. Issues related to the quality and availability of data, interpretability of AI models, and regulatory considerations persist. However, as we head to the on-going digital transformation, it becomes increasingly evident that AI-based approaches hold immense ability to revolutionize drug discovery and reform the field of medicinal chemistry. The main purpose of this article is not only to outline the breakthroughs AI has facilitated but also to critically evaluate where it falls short or poses new challenges.



AI in Drug Discovery

AI has transformed medicinal chemistry by providing novel tools and approaches for drug discovery, such as deep generative models for molecular design, as well as the extrapolation of drug–target interactions or drug toxicity.[11]

AI plays a significant role in medicinal chemistry by accelerating drug discovery and development. It can:

Drug Design: AI algorithms help design novel compounds with desired properties, reducing the time and cost of drug development.

Predictive Analytics: AI models can predict a molecule's pharmacokinetics, toxicity, and bioavailability.

Drug Repurposing: AI identifies existing drugs that can be repurposed for new medical uses.Biomarker Discovery: AI assists in identifying relevant biomarkers for disease diagnosis and prognosis.

Virtual Screening: AI-based virtual screening techniques quickly analyze large chemical databases to find potential drug candidates.

Optimization: AI optimizes chemical synthesis processes to make drug production more efficient.Personalized Medicine: AI tailors treatments based on a patient's genetic and molecular profile.AI is revolutionizing medicinal chemistry, making drug discovery more efficient and effective.

Clinical trial optimization: AI can analyze patient data from clinical trials to identify patient subgroups that may respond better to a particular drug or predict potential adverse events. This helps optimize the design and recruitment strategies for clinical trials.

AI in medicinal chemistry

It refers to the application of artificial intelligence (AI) techniques in the field of chemistry to aid in the discovery and development of new drugs. It involves the use of machine learning algorithms, data mining, and predictive modeling to analyze large datasets of chemical compounds and generate insights that can guide the design and optimization of drug molecules.

Some ways in which AI is utilized in medicinal chemistry include:

Compound generation: AI algorithms can generate new chemical compounds with desired properties by predicting their structures and properties based on existing data. This helps in the exploration of chemical space and the identification of novel drug candidates.

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Property prediction: AI can predict various properties of chemical compounds, such as solubility, stability, and bioactivity, based on their molecular structures. This enables researchers to prioritize and select compounds with the highest likelihood of success for further development.

Drug repurposing: AI algorithms can analyze large databases of existing drugs and their known targets to identify potential new therapeutic uses for approved drugs. This allows for the repurposing of existing drugs to treat different diseases, potentially saving time and costs compared to developing entirely new drugs.

Toxicity prediction: AI can predict the potential toxicity of chemical compounds based on their structural features and known toxicological data. This helps in identifying compounds with a lower risk of adverse effects and reducing the likelihood of drug failures during development.[13-15]

Optimization of drug properties: AI can assist in optimizing the properties of drug molecules, such as potency, selectivity, and pharmacokinetics. By analyzing large datasets of chemical and biological information, AI algorithms can suggest modifications to improve the desired properties of drug candidates.

The use of AI in medicinal chemistry has the potential to accelerate the drug discovery process by rapidly exploring vast chemical space and generating insights that can guide decision-making. It allows researchers to leverage computational power to analyze and interpret complex chemical data, leading to more efficient and effective drug discovery efforts. However, it is important to note that AI is a tool that complements human expertise and judgment in medicinal chemistry, and the final decision-making still relies on the knowledge and experience of researchers.

Authenticity in AI

AI is often seen as a key that can be changing the methods to produce the perfect output, often regardless of input. Whether the AI challenge is to design the perfect image of a cat from a model trained on images of cats, a car that is able to drive itself without making a single mistake, or a drug that can be designed to treat a disease safely and efficaciously. While AI is not the answer to every challenge, it is a useful tool that if used correctly can help to augment current understanding and drive new discoveries. Within medicinal chemistry and drug discovery, the best AI is not necessarily that can automatically design a new drug, but one or many different AIs, that allow better understanding and the design of new inputs, throughout the drug discovery process from target selection, hit identification, lead optimization to preclinical studies and clinical trials.[12]

Prediction of Drug–Target Interaction (DTI)

Drug pharmacophore and targeted receptor cells interaction precisely should give faster and efficient output in practice. Drugs control our body's physiological activities to exert therapeutic effects, which are achieved through the interaction between the drug and its target protein, known as drug–target interaction (DTI). Conventionally, the drug discovery approach has been based on the "one molecule–one target–one disease" paradigm, where the drug yields therapeutic effects by regulating its target. In this approach, it is necessary to test whether a particular protein could be a specific drug target for treatment. The importance of DTI research is increasingly recognized, especially regarding side effects, drug repositioning, quantitative structure activity relationand drug resistance. The power of AI is apparent in this target identification and virtual screening. The research carried out on the aspects of ML-based DTIs, namely, prediction of existing ligand binding sites, binding affinity, and binding poses, is eventually aimed at bringing us faster to more efficient drug discovery.[17]

Challenges

The AI techniques are not considered asresourceful tools for the discovery of drug due to the following challenges.

The key point is the availability of high-quality data that can be used to train AI technique-based models. While the amount of chemical and biological data is increasing, the issue of poor data quality delays the full use of these data.

Quantity of data is plays second vital role for the applications of AI techniques, the number of positive inputs is smaller than that of negative ones. The inputdifference problem will directly affect the predictions of the models.

Another typical issue of AI technique-based models for drug discovery is the lack of understanding and interpretability. A model's interpretability is the degree to which humans can understand the processes it uses to arrive at its result. In most cases, the proposed models fall short in interpreting their biological and pharmaceutical meanings. Hence, trusting the predictive results obtained by AI techniques is difficult for experimental scientists.

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These issues exclude their applications to drug discovery and development. Hence, developing open-source tools or packages, which will become precious sources in the near future, is necessary some resources are shown in table 1. It is believable that AI techniques will bring innovative changes for this area.

Table 1.-The resources for AI is majorly from following databases-

S.N.	Database	Link
1	ChEMBL	https://chembl.gitbook.io/chembl-interface-documentation/downloads
2	Drug bank	https://go.drugbank.com/data_packages
3	PubMed Central (PMC)	https://pubmed.ncbi.nlm.nih.gov/
4	National centre for biotechnology information	https://www.nibib.nih.gov/content/national-center-biotechnology-information-ncbi
5	National library of medicine	https://www.ncbi.nlm.nih.gov/pmc/

II. CONCLUSIONS AND FUTURE PERSPECTIVES

Over the past few years, we have perceived the wide applications of AI techniques to various steps of our day today lives and it has changed our lifestyle unexpectedly likewise it would also change the drug discovery and development in medical field in near future undisputedly. The bang of AI techniques has made important contributions to the acceleration of drug discovery. The application of Chat Generative Pre-Trained transformer is also an encouraging topic in medicinal chemistry and development. Subsequently, AI can provide methods to identify potential target molecules, design new drugs, and optimize the pharmacodynamics of drug candidates with reduced toxicity and side effects.

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