Unleashing the potential of AI in drug discovery: Opportunities and Limitation

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Abstract:
The Indian pharmaceutical industry is embracing the use of artificial intelligence (AI) in drug discovery, with a focus on neglected diseases, collaboration with international partners, and investment in research and development. AI is being utilized to identify new drug targets, optimize drug combinations, and develop personalized medicine. The Indian government is supporting the use of AI in drug discovery through the National Programme on Artificial Intelligence and the creation of the Centre of Excellence in Artificial Intelligence and Healthcare in collaboration with the Indian Institutes of Technology.However, there are also challenges associated with the use of AI in drug discovery in India. One of the main challenges is the need for high-quality data, which can be difficult to obtain in certain parts of the country. Additionally, there is a shortage of experts in AI, which can hinder the development and implementation of AI-based drug discovery platforms.Despite these challenges, there is significant potential for AI to revolutionize drug discovery in India, particularly for neglected diseases and personalized medicine. Indian pharmaceutical companies are collaborating with international partners to develop AI-based drug discovery platforms. Additionally, there is a growing number of startups focused on AI-based drug discovery, such as Bugworks Research and InMedPro. The Indian government has also launched initiatives to promote drug discovery for neglected diseases, such as the Open Source Drug Discovery project.The use of AI in drug discovery is transforming the pharmaceutical industry in India, with the potential to accelerate drug development, improve efficacy and safety, and develop personalized medicine. While there are challenges to overcome, the benefits of AI in drug discovery in India are clear. As this technologycontinues to advance, it is likely to revolutionize the way new drugs are developed and brought to market, improving the lives of millions of patients around the world.

KeyWords: Artificial Intelligence, Drug Discovery, Machine Learning, Algorithm

Introduction

Artificial intelligence (AI) is revolutionizing many areas of life, and drug discovery is no exception. Drug discovery is a complex and costly process that involves identifying potential drug candidates, optimizing them for efficacy and safety, and then testing them in clinical trials. AI has the potential to accelerate this process and make it more efficient by automating some of the most time-consuming and error-prone tasks.AI techniques such as machine learning (ML), natural language processing (NLP), and deep learning (DL) can be applied to vast amounts of data to identify new drug targets, predict the efficacy and safety of drug candidates, and even design new molecules from scratch. By leveraging these techniques, researchers can analyze data from a wide range of sources, including clinical trial data, scientific literature, and electronic health records, to generate insights and discover new treatments.One of the key benefits of AI in drug discovery is its ability to accelerate the drug discovery process. Traditional drug discovery methods can take many years and cost billions of dollars, but AI can help researchers identify promising drug candidates in a fraction of the time and at a fraction of the cost. Additionally, AI can help researchers identify drug candidates for rare or neglected diseases, where traditional drug discovery methods may be less effective.

AI can also help to optimize drug development by predicting the safety and efficacy of drug candidates in clinical trials. By analyzing data from previous clinical trials, researchers can identify biomarkers that are predictive of response to treatment, which can help to identify patients who are most likely to benefit from a particular drug. This can help to reduce the number of patients needed for clinical trials and increase the chances of success.

AI is a powerful tool for drug discovery that has the potential to revolutionize the way new drugs are developed and brought to market. However, there are also challenges associated with AI in drug discovery, including the need for large amounts of high-quality data, the need for rigorous validation of AI models, and the ethical considerations associated with the use of AI in healthcare. Nonetheless, the potential benefits of AI in drug discovery are significant and this technology is likely to play an increasingly important role in the future of drug discovery and development.[1]

Background:

Artificial intelligence (AI) has the potential to revolutionize the drug discovery process by enabling the identification of new drug targets, optimization of drug candidates, and prediction of drug safety and efficacy. While AI-based drug discovery has gained significant momentum in recent years, its roots can be traced back to the 1950s when the first AI models were developed.In the 1960s and 1970s, researchers began using machine learning algorithms to develop predictive models for drug toxicity and efficacy. However, the use of AI in drug discovery remained limited due to the lack of computing power and the difficulty of obtaining large datasets of biological and chemical information.In the 1980s and 1990s, advances in computing power and the emergence of high-throughput screening techniques enabled researchers to generate large datasets of biological and chemical information. This, in turn, led to renewed interest in the use of AI in drug discovery. One of the earliest examples of AI-based drug discovery was the development of the DENDRAL system in the 1960s. DENDRAL was a computer program that used machine learning algorithms to predict the structure of organic molecules based on mass spectroscopy data. The system was able to predict the structures of several molecules with a high degree of accuracy, demonstrating the potential of AI in drug discovery.In the 1990s, researchers began using neural networks to predict the toxicity and efficacy of drugs. Neural networks are machine learning algorithms that are modeled after the structure of the human brain. They are capable of learning from large datasets of biological and chemical information and making predictions based on that information. In 1992, researchers at IBM developed a neural network-based system called SIMS that could predict the toxicity of compounds based on their chemical structure. SIMS was able to predict the toxicity of several compounds with a high degree of accuracy, demonstrating the potential of AI in drug discovery. In the late 1990s and early 2000s, the emergence of high-throughput screening techniques enabled researchers to generate large datasets of biological and chemical information. This, in turn, led to renewed interest in the use of AI in drug discovery. In 2000, researchers at Pfizer developed a neural network-based system called the Virtual Ligand Screening (VLS) system. VLS was designed to predict the binding affinity of compounds to a particular protein target. The system was able to identify several compounds with high binding affinities, demonstrating the potential of AI in drug discovery. In 2003, the pharmaceutical company GlaxoSmithKline (GSK) established a collaboration with the University of California, San Francisco (UCSF) to develop AI-based drug discovery platforms. The collaboration resulted in the development of the GSK-UCSF Center for Excellence in Chemical Methodologies and Library Development, which focused on the development of new methods for compound library synthesis and screening. In 2006, the pharmaceutical company AstraZeneca established a collaboration with the Karolinska Institute in Sweden to develop AI-based drug discovery platforms. The collaboration resulted in the development of the AstraZeneca-Karolinska Institutet Integrated Cardio Metabolic Centre (AIMC), which focused on the development of new treatments for cardiovascular and metabolic diseases. In 2012, the startup company Berg Health was founded with the goal of developing AI-based drug discovery platforms. Berg Health developed a system called the Interrogative Biology platform, which used machine learning algorithms to analyze large datasets of biological information and identify new drug targets. The system was used to identify several potential drug targets for diseases such as cancer and Alzheimer's disease.

In 2015, the pharmaceutical company Pfizer established a collaboration with IBM to develop AI-based drug discovery platforms. The collaboration resulted in the development of the Pfizer-IBM Watson Immuno- Oncology Discovery.[2]

- **How AI is being used in drug discovery:**

A] **Identifying Drug Targets**:

AI can be used to identify new drug targets by analyzing large amounts of biological data. For example, researchers can use ML algorithms to identify genes that are differentially expressed in diseased versus healthy tissues. These genes can then be prioritized as potential drug targets. NLP can also be used to analyze scientific literature to identify potential drug targets.

B] **Designing New Molecules**:

AI can be used to design new drug molecules by predicting the properties of small molecules and generating new molecules that are likely to have the desired properties. For example, researchers can use DL algorithms to generate new molecules with specific properties such as potency, selectivity, and pharmacokinetics. These molecules can then be synthesized and tested for efficacy.

C] **Predicting Efficacy and Safety:**

AI can be used to predict the efficacy and safety of drug candidates by analyzing large amounts of data from preclinical and clinical trials. For example, ML algorithms can be used to predict the toxicity of drug candidates based on their chemical properties. DL algorithms can also be used to predict the response to treatment based on genetic or other biomarker data.

D] **Repurposing Existing Drugs:** AI can be used to identify new uses for existing drugs by analyzing large amounts of data from clinical trials, electronic health records, and scientific literature. For example, researchers can use ML algorithms to identify drugs that have potential for repurposing based on their chemical structure or mechanism of action.

E] **Optimizing Clinical Trials:**

AI can be used to optimize clinical trials by identifying patient populations that are most likely to respond to a particular drug. For example, ML algorithms can be used to identify biomarkers that are predictive of response to treatment, which can help to identify patients who are most likely to benefit from a particular drug. This can help to reduce the number of patients needed for clinical trials and increase the chances of success.

- **Indian scenario for the use of AI in drug discovery:**

Growth of AI in the Indian Pharma Industry: The Indian pharmaceutical industry is rapidly adopting AI in drug discovery, with many companies investing in this technology. The Indian government is also promoting the use of AI in drug discovery through initiatives such as the National Programme on Artificial Intelligence.

A] **Collaboration with International Partners:** Indian pharmaceutical companies are collaborating with international partners to develop AI-based drug discovery platforms. For example, in 2020, Sun Pharma partnered with HitGen to develop small molecule leads using AI and DNA-encoded library technology.

B] **Focus on Neglected Diseases:** AI is being used in India to identify new drug targets and drug candidates for neglected diseases such as tuberculosis and malaria. The government has also launched initiatives to promote drug discovery for neglected diseases, such as the Council of Scientific and Industrial Research's Open Source Drug Discovery project.

C] **Startups in AI-Based Drug Discovery:** India has a growing number of startups that are focused on AI- based drug discovery. For example, Bugworks Research is developing AI-powered antibiotics for drug- resistant infections, while InMedPro is using AI to identify novel drug candidates for cancer.

D] **Investment in Research and Development:** The Indian government has allocated significant funding for research and development in AI-based drug discovery. For example, in 2020, the government announced the creation of the Centre of Excellence in Artificial Intelligence and Healthcare in collaboration with the IITs.

E] **Challenges:** There are also challenges associated with the use of AI in drug discovery in India, such as the need for

high-quality data and expertise in AI. However, there is significant
potential for AI to transform drug discovery in India, particularly for neglected diseases and personalized medicine.[3]

- **Global Scenario:**

The use of artificial intelligence (AI) in drug discovery is rapidly gaining momentum in the global pharmaceutical industry. AI technologies such as machine learning, natural language processing, and predictive analytics are being used to improve the efficiency of drug development, reduce the cost of research and development, and bring personalized medicine to patients.

One of the main ways that AI is being used in drug discovery is to identify new drug targets. Traditional drug discovery involves a trial-and-error approach, which can be time-consuming and expensive. Using machine learning algorithms, AI can analyze large datasets of biological information, such as genetic data or protein structures, to identify potential targets for new drugs. This can significantly reduce the time and cost of drug discovery by providing researchers with a more focused set of targets to investigate.

AI is also being used to optimize drug candidates. By analyzing large datasets of chemical and biological information, AI can predict which drug candidates are most likely to be effective, as well as which ones are likely to have undesirable side effects. This can help researchers to prioritize which candidates to pursue, reducing the number of drug candidates that fail in clinical trials.

Another area where AI is making a significant impact is in predicting the safety and efficacy of drugs. By analyzing large datasets of clinical trial data, AI can identify patterns in how drugs interact with different patient populations. This can help researchers to identify which patients are most likely to benefit from a particular drug, as well as which patients are most likely to experience adverse side effects.[4]

- **Future aspect:**

The future of AI in drug discovery is incredibly promising, and it is likely to have a significant impact on the development of new treatments for a wide range of diseases. Here are some more details on the potential future applications of AI in drug discovery:

A] **Personalized Medicine:**

One of the most promising areas of application for AI in drug discovery is personalized medicine. AI algorithms can analyze large amounts of data on a patient's genetics, medical history, and lifestyle factors to predict how they will respond to specific drugs. This information can be used to develop personalized treatment plans that are tailored to the individual patient.

B] **Drug Repurposing:**

AI can help identify existing drugs that can be repurposed for new indications, reducing the time and cost of developing new drugs. By analyzing large datasets of biological and chemical information, AI algorithms can identify potential drug candidates for diseases that are not the original intended use of the drug.

C] **Drug Safety:**

AI can help predict the safety of drugs by analyzing large datasets of biological and chemical information, reducing the risk of adverse drug reactions. This can save pharmaceutical companies significant amounts of time and money by reducing the need for costly clinical trials.

D] **Drug Optimization:**

AI can help optimize drug candidates by predicting their safety and efficacy, reducing the need for costly and time-consuming clinical trials. By analyzing large datasets of biological and chemical information, AI algorithms can predict how a drug will behave in the human body and identify potential safety concerns before clinical trials begin.

E] **Precision Drug Synthesis:**

AI can help optimize the synthesis of drugs by predicting the most efficient and cost-effective routes of synthesis. This can help pharmaceutical companies save time and money by reducing the need for trial and error in drug synthesis.

F] **Drug Design:**

AI can help design new drugs by predicting how they will interact with biological targets in the body. By using machine learning algorithms to analyze large datasets of biological and chemical information, AI can help identify

promising drug candidates that are more likely to be effective.

G] **Drug Delivery:**

AI can help optimize drug delivery methods by predicting how drugs will be absorbed and distributed throughout the body. By using machine learning algorithms to analyze large datasets of biological and chemical information, AI can help identify the most effective drug delivery methods for specific drugs.[5]

- **Advantages of AI in Drug Discovery:**

Artificial intelligence (AI) has transformed drug discovery by boosting the effectiveness and accuracy of the process. Here are some of the benefits of artificial intelligence in drug discovery:

A. **Speeding up drug discovery:** AI algorithms can quickly analyze large amounts of data from various sources, including scientific literature, clinical trials, and genomic data, to identify potential drug targets and predict the effectiveness of a drug candidate. This significantly speeds up the drug discovery process, reducing the time and cost required to bring a drug to market.

B. **Identifying new drug targets:** AI can help identify new drug targets that were previously unknown or unexplored. Machine learning algorithms can analyze large datasets to identify patterns and relationships between different molecules, proteins, and genes, leading to the identification of new targets for drug development.

C. **Improving drug efficacy and safety:** AI can help predict the efficacy and safety of a drug candidate before it is tested in clinical trials. Machine learning algorithms can analyze the chemical structure of a drug candidate and predict its pharmacokinetics, toxicity, and potential side effects, enabling researchers to optimize the drug design and minimize the risk of adverse effects.

D. **Personalized medicine**: AI can help develop personalized medicine by analyzing individual patient data, including genetic and molecular profiles, to predict the most effective treatment for a particular patient. This approach can lead to more effective and targeted treatments with fewer side effects.

E. **Repurposing existing drugs**: AI can help identify new uses for existing drugs that were originally developed for a different condition. By analyzing the molecular structure and properties of existing drugs, AI algorithms can identify potential new uses for these drugs, speeding up the drug development process and reducing costs.[6]

Disadvantages of AI in Drug Discovery:

While AI has many benefits in drug discovery, there are some potential drawbacks to consider which are as follows:

a. **Limited data availability:** AI relies heavily on large datasets for training and validation, but in some cases, there may be limited or incomplete data available, which can impact the accuracy and reliability of AI models.

b. **Lack of transparency:** Some AI models can be complex and difficult to interpret, which can make it challenging for researchers and regulators to understand how the model arrived at a particular result or prediction.

c. **Biased data:** AI models can be influenced by biased data, leading to inaccurate or biased predictions. This is particularly important to consider when using AI in personalized medicine, where demographic and genetic factors may impact the accuracy of the model.

d. **Ethical considerations:** The use of AI in drug discovery raises ethical concerns around the ownership of data, privacy, and the potential for bias or discrimination.

e. **Cost and infrastructure:** The use of AI requires specialized hardware and software, as well as skilled personnel, which can be expensive and require significant investment in infrastructure.

f. **Limitations of AI models**: AI models can only make predictions based on the data that they have been trained on. This means that there may be limitations to the types of questions that AI can answer, and it may not be suitable for all aspects of drug discovery.[7]

- **Comparision of artificial intellience in drug discovery all over the globe:**

Artificial intelligence (AI) has become an increasingly popular tool for drug discovery in recent years. It can help accelerate the drug discovery process by identifying potential drug targets, predicting the activity of new compounds, and optimizing the design of clinical trials. Here is a comparison of how AI is being used in drug discovery all over the globe:

A] **North America:**

North America is a hub for AI-based drug discovery. Many startups and established companies are working on developing AI-powered drug discovery platforms. The United States has the largest number of AI-based drug discovery companies, followed by Canada. In North America, many AI-based drug discovery companies are located in Silicon Valley and the Boston area. These companies are using machine learning algorithms and other AI technologies to analyze large amounts of data and identify potential drug targets. Some companies, such as Atomwise and Insilico Medicine, are using AI to design new molecules that can be used as drugs. Others, such as Recursion Pharmaceuticals, are using AI to screen existing drugs for new therapeutic uses.

B] **Europe:**

Europe is also home to a number of AI-based drug discovery companies. Countries such as the UK, Germany, and France are leading the way in this field. The European Union has also launched the European Health Data and Evidence Network (EHDEN), which aims to use AI and machine learning to analyze healthcare data. Europe has a long history of pharmaceutical research and development, and AI is becoming an increasingly important tool in this field. Many European companies are using AI to analyze large amounts of data from electronic health records, clinical trials, and other sources to identify potential drug targets and develop new drugs.

C] **Asia:**

In Asia, China is leading the way in AI-based drug discovery. The Chinese government has invested heavily in AI research, and many startups have emerged in recent years. Japan and South Korea are also investing in AI-based drug discovery, with several companies working on developing AI-powered platforms. China is one of the fastest- growing markets for AI-based drug discovery. The Chinese government has invested heavily in AI research and has launched several initiatives to support AI-based drug discovery, such as the National Major Science and Technology Projects for "Significant New Drugs Development" and "Precision Medicine".

D] **Australia:**

Australia has a growing biotech sector, with several companies using AI in drug discovery. The Australian government has also launched the Biomedical Translation Fund, which provides funding to companies working on developing new medical technologies, including AI-based drug discovery. Australia has a growing biotech sector, with several companies using AI in drug discovery. Companies such as Cyclica and EMBL Australia are using AI to analyze large datasets and identify potential drug targets. The Australian government has also launched the Biomedical Translation Fund, which provides funding to companies working on developing new medical technologies, including AI-based drug discovery.[8]

- **General Statistical data all over the globe about AI in drug discovery:**

AI in drug discovery is a relatively new field, and statistical data on its global use is not yet widely available. However, here are a few data points that provide some insight into the current state of AI in drug discovery:

A] **Funding:**

Investment in AI-based drug discovery has been increasing rapidly in recent years. According to a report by CB Insights, global funding for AI-based drug discovery companies reached a record high of $2.3 billion in 2020, up from $1.3 billion in 2019.

B] **Patent filings:**

There has been a significant increase in the number of patent filings related to AI in drug discovery. According to a study by Clarivate, the number of patent applications in this field increased by 34% between 2017 and 2019, with the United States, China, and Japan accounting for the majority of filings.

C] **Clinical trials:**

AI-based drug discovery companies are beginning to move their products into clinical trials. According to a report by GlobalData, there were 104 clinical trials involving AI-based drug discovery products in 2020, up from 59 in 2019. D]

Applications:

AI is being used in drug discovery to identify new drug targets, design new molecules, optimize drug development processes, and improve clinical trial design. According to a survey by the Pistoia Alliance, 95% of respondents believe that AI will be critical to the future of drug discovery.[9]

- **Distinction between national and international programmes related to AI in drug discovery:**

National and international programs related to AI in drug discovery have distinct differences in their scope, funding, and organizational structure. Here are a few key distinctions between national and international programs:

A] **Scope:**

National programs tend to focus on the specific needs and challenges of a particular country's pharmaceutical industry and healthcare system. For example, a national program in the United States may prioritize the development of AI tools to improve the efficiency and cost-effectiveness of drug development processes, while a program in India may focus on developing affordable and accessible AI-based diagnostic tools for diseases that are prevalent in that region. In contrast, international programs tend to have a broader, global scope, and may focus on addressing common challenges faced by the pharmaceutical industry and healthcare systems worldwide.

B] **Funding:**

National programs are typically funded by government agencies or private industry within a particular country. For example, the US National Institutes of Health (NIH) has established programs such as the Accelerating Medicines Partnership (AMP) to support the development of AI tools for drug discovery. In contrast, international programs may be funded by multiple governments or organizations, and may involve collaboration between industry, academia, and government agencies from different countries.

C] **Organizational structure:**

National programs are typically organized within a single country, and may involve collaboration between different universities, research institutes, and industry partners within that country. In contrast, international programs may involve multiple organizations and institutions from different countries, and may be coordinated by international organizations such as the World Health Organization or the International Union of Pure and Applied Chemistry.

National and international programs related to AI in drug discovery have different goals, funding sources, and organizational structures, but both play an important role in advancing this field and improving the development of new medicines for patients.

- **Components of Artificial intelligence in drug discovery:**

The field of artificial intelligence (AI) in drug discovery involves a variety of different components and techniques, each of which plays a critical role in the development of new medicines. Here are a few key components of an AI-based drug discovery department:

A] **Data management:**

The use of AI in drug discovery requires large amounts of data, including information about biological systems, chemical compounds, and clinical trial results. Effective data management is essential for ensuring that this data is accurate, standardized, and accessible to researchers.

B] **Machine learning algorithms:**

Machine learning is a type of AI that involves the use of algorithms to automatically learn patterns and insights from large datasets. In drug discovery, machine learning algorithms can be used to identify new drug targets, predict the activity of potential drug compounds, and optimize drug development processes.

Natural language processing (NLP): NLP is a type of AI that involves the use of algorithms to analyze and interpret human language. In drug discovery, NLP can be used to extract useful information from scientific literature, such as the results of clinical trials or the structure of chemical compounds.

C] **High-performance computing (HPC):**

The use of AI in drug discovery requires significant computational resources, including large-scale data storage, powerful processors, and specialized hardware such as graphics processing units (GPUs). HPC is essential for running

complex AI algorithms and analyzing large datasets.

D] **Collaboration tools:**

Collaboration is key to the success of an AI-based drug discovery department, and requires effective communication and collaboration tools. This may include virtual collaboration platforms, project management tools, and data sharing platforms.

An AI-based drug discovery department requires a range of different components and techniques, all working together to improve the efficiency and effectiveness of drug discovery processes.

- **Limitations of AI in drug discovery:**

While AI has great potential in drug discovery, there are several limitations and challenges that need to be addressed before its widespread adoption. Here are some of the major limitations of AI in drug discovery:

A] **Data quality and quantity:**

AI algorithms require large quantities of high-quality data to accurately learn patterns and make predictions. However, many datasets used in drug discovery may be incomplete, biased, or of poor quality, leading to inaccurate predictions and reduced effectiveness of AI-based approaches.

B] **Overfitting:**

AI algorithms can also suffer from overfitting, which occurs when the algorithm becomes too specialized to the training data and is unable to generalize to new data. Overfitting can be particularly problematic in drug discovery, where small datasets and complex biological systems can make it difficult to generalize from one dataset to another.

Interpretability:

Many AI algorithms, particularly deep learning algorithms, are considered "black boxes" because it can be difficult to understand how they arrive at their predictions. This lack of interpretability can make it difficult to identify potential biases in the algorithm or to determine how to improve its performance

C] **Lack of domain expertise:**

AI algorithms require significant domain expertise to develop and apply effectively. However, many drug discovery projects involve complex biological systems and chemical compounds, requiring expertise from multiple fields such as biology, chemistry, and pharmacology.

D] **Regulatory hurdles:**

The use of AI in drug discovery may also face regulatory hurdles, particularly in relation to the validation and approval of AI-based models for use in drug development.

E] **Cost:**

The use of AI in drug discovery requires significant investment in hardware, software, and expertise. For smaller companies or research institutions with limited resources, the cost of implementing AI-based approaches can be prohibitive.[10]

Conclusion:

Artificial intelligence (AI) has the potential to revolutionize drug discovery and development. In recent years, AI technologies have been increasingly applied in drug discovery research, particularly in the early stages of the process. One of the main benefits of using AI in drug discovery is that it can help scientists quickly analyze large amounts of data, such as genomic and proteomic data, to identify potential drug targets and drug candidates. AI can also be used to predict the efficacy and toxicity of candidate drugs, which can help reduce the number of failed drug trials and speed up the drug development process.

Another advantage of using AI in drug discovery is that it can help identify new uses for existing drugs. By analyzing large amounts of data from clinical trials and other sources, AI can identify potential uses for drugs that have already been approved by regulatory agencies.

AI can also help optimize clinical trials by identifying patient subgroups that are most likely to respond to a

particular drug, which can help reduce the cost and time required for clinical trials.

However, there are also some challenges associated with using AI in drug discovery. One of the main challenges is the quality and reliability of the data used to train AI models. Inaccurate or biased data can lead to incorrect predictions, which can have serious consequences in drug development.

Another challenge is the lack of transparency and interpretability of AI models. In some cases, it may be difficult to understand how an AI model arrived at a particular prediction, which can make it difficult to validate the model's results.

In conclusion, AI has the potential to transform drug discovery and development by enabling faster and more efficient identification of drug targets and drug candidates. However, there are also challenges associated with using AI in drug discovery that need to be addressed in

order to fully realize its potential. With continued research and development, AI is likely to play an increasingly important role in drug discovery and development in the years to come.

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