J. Pharm. Res. 2023;22(3):103–112

Print ISSN: 0973-7200
Online ISSN: 2454-8405

Journal of Pharmaceutical Research

Review Article

Revolutionizing Drug Design with Artificial Intelligence: A Comprehensive Review of Techniques, Applications, and Case Studies

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ARTICLE INFO

Article history:
Received 11.09.2023
Accepted 09.10.2023
Published 30-12-2023

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https://doi.org/10.18579/jopcr/v22.3.23.54

ABSTRACT

Introduction: Artificial intelligence (AI) has the potential to revolutionize drug design and discovery by significantly reducing the time and costs involved in developing new drugs. This literature review aims to explore the use of AI in drug design, focusing on virtual screening, de novo drug design, and prediction of ADME properties. **Objective:** The objective of this review is to provide an overview of the AI techniques used in drug design and their applications in virtual screening, de novo drug design, and prediction of ADME properties. The review also aims to summarize the advantages and limitations of these approaches and present case studies and examples showcasing their use in drug design. **Methodology:** A comprehensive search of academic databases was conducted, and 11 relevant articles were selected for inclusion in this review. The selected articles were analyzed to identify the AI techniques used in drug design, their applications, advantages, and limitations. Case studies and examples were also examined to demonstrate the efficacy of AI in drug design. **Results:** AI techniques such as machine learning, deep learning, and reinforcement learning have been successfully used in virtual screening, de novo drug design, and prediction of ADME properties. Virtual screening involves the use of AI algorithms to identify promising compounds for further testing, while de novo drug design involves the generation of novel compounds using AI techniques. Prediction of ADME properties involves the use of AI to predict the absorption, distribution, metabolism, and excretion of drug candidates. The case studies and examples presented in this review demonstrate the potential of AI to accelerate drug design and discovery. **Conclusion:** AI has the potential to revolutionize drug design and discovery by significantly reducing the time and costs involved in developing new drugs. Virtual screening, de novo drug design, and prediction of ADME properties are among the most promising applications of AI in drug design. However, further research is needed to fully explore the potential of AI in drug design and overcome some of the limitations of current approaches.

Keywords: Artificial Intelligence; Drug Design; Virtual Screening; De Novo Drug Design; ADME Prediction

INTRODUCTION

Background on AI and drug design

Drug design is an important component of drug discovery since it involves the identification of molecules that potentially work as a therapeutic agent for a certain ailment. Traditional drug design procedures have been time-consuming and costly, requiring the synthesis and testing of enormous chemical libraries in order to identify active molecules. However, the introduction of artificial intelligence (AI) has transformed the drug discovery process, making it more efficient, cost-effective, and accurate.

Artificial intelligence (AI) is a subject of computer science that focuses on developing algorithms that enable machines to learn from data and do tasks that would ordinarily require human intelligence, such as image recognition, speech recognition, and natural language processing. The use of AI in drug research has improved drug safety and efficacy prediction, led to the discovery of new therapeutic targets, and resulted in the development of novel drug candidates.

Importance of AI in drug design

The use of AI in drug design has several advantages over traditional drug discovery methods. For starters, it minimizes the time and expense associated with medication discovery. To identify prospective medication candidates, AI systems may scan enormous amounts of data from numerous sources, such as chemical databases, electronic health records, and scientific literature. This eliminates the need for extensive and costly experimentation and optimization of chemical compounds.

Secondly, AI can accelerate the identification of drug targets. Identifying a medication's biological targets is a vital stage in drug research. To find potential targets for a given condition, AI systems can evaluate biological data such as genomes, proteomics, and metabolomics. As a result, more effective medications targeting specific biological pathways and molecules may be developed.

Thirdly, AI can improve the accuracy of predicting the safety and efficacy of drug candidates. Traditional drug development methods rely on expensive and time-consuming human trials and animal experiments.

With a high degree of accuracy, AI algorithms can forecast the pharmacokinetic and pharmacodynamic characteristics of drug candidates, including absorption, distribution, metabolism, excretion, and toxicity. This minimizes the need for lengthy preclinical testing while also speeding up the discovery of safe and effective medications.

Purpose of the literature review

The purpose of this literature review is to provide an overview of the current state of AI in drug design. It will examine the different AI techniques used in drug discovery, such as machine learning, deep learning, and reinforcement learning, and their applications in virtual screening, de novo drug design, and prediction of ADME (absorption, distribution, metabolism, and excretion) properties.

The assessment will also emphasize the benefits and drawbacks of employing AI in drug discovery, as well as the field's obstacles and future possibilities. By examining the current research, this literature review aims to provide insights into how AI can improve the drug discovery process and lead to the development of more effective and safe drugs.

The Use of AI in Drug Design

Overview of AI techniques used in drug design (Table 1)

The integration of AI in drug discovery has led to the development of several techniques that aid in the identification of potential drug candidates. The following are the most commonly used AI techniques in drug design:

Machine learning

Machine learning is a type of AI that enables computers to learn patterns and make predictions based on data without being explicitly programmed. By examining enormous amounts of data from numerous sources, including chemical libraries, biological assays, and clinical trials, machine learning algorithms can forecast the biological activity of drug candidates.

Machine learning algorithms can also analyze the structure-activity relationship (SAR) of compounds to identify chemical features that contribute to their biological activity. Several studies have proven that machine learning algorithms may accurately discover innovative medication candidates[1–4].

Deep learning

Deep learning is a subset of machine learning that involves the use of artificial neural networks with multiple layers to learn representations of data. Deep learning algorithms in drug development can examine huge and complicated data sets, such as protein-ligand interactions, and predict the biological activity of drug candidates. Deep learning algorithms can also generate new compounds with desired properties, such as potency and selectivity, using generative models. Several studies have demonstrated the efficacy of deep learning algorithms in drug discovery[5–8] .

Reinforcement learning

Reinforcement learning is a type of machine learning that involves training an agent to take actions in an environment to maximize a reward. In drug discovery, reinforcement learning algorithms can optimize the chemical structure of a compound to achieve a specific biological activity while minimizing the risk of toxicity. Reinforcement learning algorithms can also optimize the dosage and frequency of administration of drugs to maximize their therapeutic effects. Several studies have shown the potential of reinforcement learning in drug discovery[9–12] .

Table 1: Examples of AI techniques used in drugdesign

AI technique	Description
Machine learning	Algorithms that use statistical methods to learn patterns in data
Deep learning	Neural network-based algorithms capable of learning from large datasets
Reinforcement learning	A type of machine learning that learns through trial-and-error interactions with the environment

Applications of AI in drug design (Table 2)

Virtual screening

Virtual screening is a computational method that involves screening large chemical libraries to identify potential drug candidates that bind to a specific target. AI algorithms, such as machine learning and deep learning, can be used to analyze the structure and properties of compounds and predict their affinity to a target. Virtual screening has the potential to drastically reduce the time and expense associated with identifying prospective medication candidates. Several studies have shown that virtual screening using AI algorithms can identify novel drug candidates with high accuracy[3,8,11].

De novo drug design

De novo drug design is a computational method that involves generating new compounds with desired properties, such as potency and selectivity, using generative models[2,5]. Deep learning and reinforcement learning AI algorithms can be used to develop new substances with specified chemical properties and predict their biological action[6,7]. De novo drug design can lead to the development of novel drug candidates that are not present in chemical libraries. Several studies have shown the potential of AI algorithms in de novo drug design[8,11].

Prediction of ADME properties

The absorption, distribution, metabolism, and excretion of medications in the body are referred to as ADME characteristics. Predicting ADME features accurately is critical for the creation of safe and effective medicines. Machine learning and deep learning AI systems can be used to predict ADME features of drugs with great accuracy. Several research have shown that AI systems are effective at predicting ADME qualities[3].

In conclusion, AI has revolutionized the drug discovery process by enabling the identification of potential drug candidates in a more efficient, cost-effective, and accurate manner. The use of AI techniques, such as machine learning, deep learning, and reinforcement learning, has led to significant advancements in virtual screening, de novo drug design, and prediction of ADME properties.

Table 2: Applications of AI in drug design

Application	Description
Virtual screening	Use of computational methods to identify compounds with potential to bind to a target
De novo drug design	Design of new compounds from scratch using computational methods
Prediction of ADME properties	Prediction of Absorption, Distribution, Metabolism, and Excretion properties of a compound

Virtual Screening [Figure 1]

Definition and Importance of Virtual Screening in Drug Discovery

Virtual screening is an in silico drug discovery approach that uses computational algorithms to predict the potential of small molecules to bind to a target protein of interest. This approach has become an essential part of drug discovery and is widely used in the primitive stages of drug development. It allows for the rapid screening of large chemical libraries to identify compounds with the desired biological activity, reducing the time and cost involved in traditional screening methods as mentioned by Lavecchia in 2015[12]. Virtual screening can also provide valuable insights into the binding modes of small molecules with target proteins, aiding in the development of more effective drug candidates[12–15].

AI Approaches for Virtual Screening

AI has been widely applied to virtual screening, particularly in the development of predictive models for drug-target interactions. The three main AI approaches for virtual screening are structure-based, ligand-based, and hybrid virtual screening[16].

- Structure-based virtual screening

Structure-based virtual screening (SBVS) involves the use of a target protein's three-dimensional structure to identify potential drug candidates that can interact with it. This approach typically involves molecular docking, where small molecules are docked into the binding site of the target protein to predict their binding affinity and binding modes . AI techniques such as machine learning and deep learning have been used to improve the accuracy and efficiency of molecular docking as mentioned by Ashtawy and Mahapatra in 2019[17].

- Ligand-based virtual screening

Ligand-based virtual screening (LBVS) uses the chemical and physical properties of known ligands to identify potential drug candidates that have similar properties. This approach involves the construction of a predictive model based on a training set of ligands with known activity against the target protein as mentioned by Yang et al.(2022) and Nag et al.(2022). Machine learning algorithms such as support vector machines (SVMs) and random forests have been applied to LBVS to improve the accuracy of the predictive models[14,16].

- Hybrid virtual screening

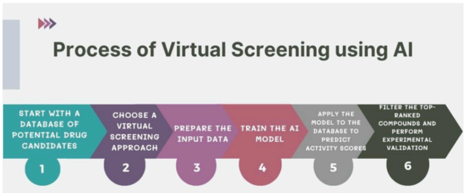

Fig. 1: Flowchart for the process of virtual screening using AI

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Advantages and Limitations of Virtual Screening [Table 3]

Virtual screening offers several advantages over traditional screening methods, including its ability to screen large chemical libraries in a short time frame, and the cost-effectiveness of the approach as mentioned by Lavecchia in 2015. Virtual screening can also provide valuable insights into the binding modes of small molecules with target proteins, aiding in the development of more effective drug candidates [12].

However, there are also some limitations associated with virtual screening. For example, virtual screening is only as good as the quality of the target protein's structure used in the screening process as mentioned by Shen et al. Yang et al. claim that the calibre of the training data utilized to develop the prediction models used in virtual screening also influences their accuracy. As a result, it's critical to make sure the training data used to build the prediction models is of high quality and representative of the target protein-ligand interactions [13,14].

Table 3: Advantages and limitations of virtual screening

Advantages	Limitations
Can screen large compound libraries efficiently	Accuracy of virtual screening depends on the quality of the model
Cost-effective compared to experimental screening	Limited ability to predict binding affinity
Can identify novel scaffolds	Limited ability to predict selectivity

De Novo drug design (Figure 2)

Definition and importance of de novo drug design

De novo drug design is the process of creating novel medications from the ground up, with no prior knowledge of their chemical structures or qualities. This method of drug discovery is gaining popularity since it enables for the development of medications that are customized to specific targets and have optimum features. When contrasted with traditional drug discovery methodologies, de novo drug design has the perceived advantage of altering the drug development process because it can save significant amounts of time and resources.

AI approaches for de novo drug design

- Generative models

Generative models, such as variational autoencoders (VAEs) and generative adversarial networks (GANs), have been used for de novo drug design. VAEs are neural networks that can learn the underlying patterns in a dataset and generate new data that follows those patterns. GANs are a kind of generative model that are made up of two neural networks: 1) a generator that generates new data and 2) a discriminator that differentiates between real and fake data.

In drug design, generative models can be trained on a dataset of known molecules to learn their structural features and generate new molecules with similar properties. For example, the REINVENT system developed by Olivecrona et al. (2020) uses a VAE to generate novel drug-like molecules with desired properties [15].

- Reinforcement learning

Another AI approach used in de novo drug design is reinforcement learning. Reinforcement learning teaches an agent to make decisions depending on incentives from the environment. The environment can be depicted through molecular structures in drug design, and benefits can be based on the projected attributes of the molecules.

For example, Blaschke et al.'s (2021) Reinvent 2.0 system employs reinforcement learning to build unique molecules with desirable features. The system predicts the properties of molecules using a deep neural network and optimizes the attributes of created molecules using a reinforcement learning technique [6].

- Hybrid approaches

Hybrid approaches that combine multiple AI techniques have also been used for de novo drug design. For example, the Deep Reinforcement and Generative Network (DRAGON) system developed by Lo et al. (2018) combines reinforcement learning and generative models to generate novel molecules with desired properties [15], [18].

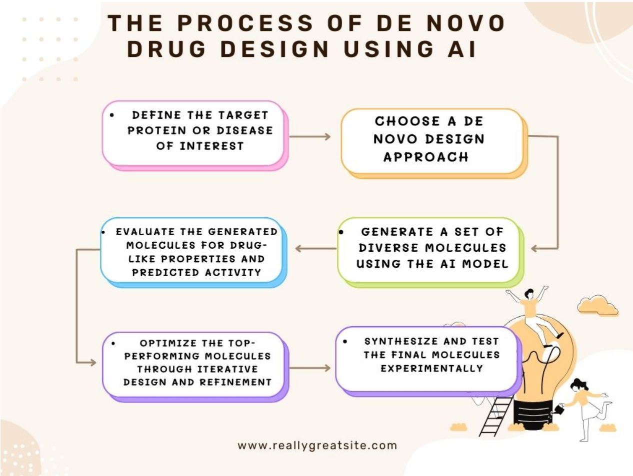

Fig. 2: Flowchart for the process of de novo drug design using AI

Advantages and limitations of de novo drug design

De novo drug design has several advantages over traditional methods of drug discovery. It enables the development of medications customized to specific targets and can lead to the discovery of novel chemical scaffolds that would not have been discovered using existing methods. Furthermore, as compared to standard drug discovery procedures, de novo drug creation can save large amounts of time and resources.

However, de novo drug design also has limitations. The generated molecules may not have optimal pharmacological properties or may have undesirable side effects. In addition, the generated molecules may be difficult or expensive to synthesize, and their efficacy and safety need to be validated through rigorous testing.

Overall, de novo drug design has the promise to transform the drug discovery process, but more study is required to fully assess its efficacy and limitations. Future predictions indicate that AI innovations like generative models and reinforcement learning will have a big impact on drug development. These technologies have shown promising outcomes in de novo drug creation.

Prediction of ADME Properties (Figure 3)

- Definition and importance of ADME properties in drug discovery

ADME properties (absorption, distribution, metabolism, and excretion) are key factors in determining the pharmacokinetic behaviour of drugs, and thus their efficacy and safety. Therefore, the prediction of ADME properties is an essential step in drug discovery and development. Traditional experimental methods for evaluating ADME properties are time-consuming and costly, which makes computational methods an attractive alternative. AI-based methods have shown promise in predicting ADME properties, which can accelerate drug discovery and reduce the cost of development.

AI approaches for predicting ADME properties

- Quantitative Structure-Activity Relationship (QSAR) modelling

QSAR modelling is a popular approach for predicting ADME properties using AI. QSAR models use statistical methods to correlate the structural features of compounds with their ADME properties. These models can predict a variety of ADME features including as solubility, permeability, and clearance[19] .

- Deep learning

Deep learning has also shown promise in predicting ADME properties. Deep learning models can learn complex relationships between chemical structures and ADME properties, making them potentially more accurate than traditional QSAR models. A variety of ADME parameters, including solubility, permeability, and toxicity, have been predicted using deep learning models.

- Hybrid approaches

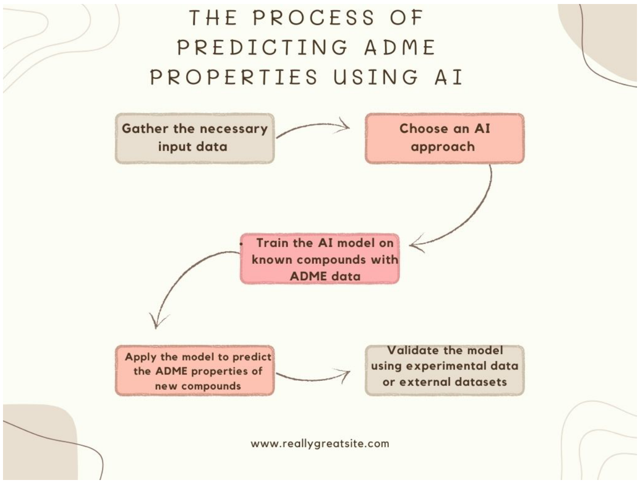

Fig. 3: Flowchart for the process of predicting ADME properties using AI

Advantages and limitations of predicting ADME properties using AI [Figure 4]

The use of AI for predicting ADME properties has an upper hand over traditional experimental methods, including speed, cost-effectiveness, and the ability to analyze large amounts of data. Additionally, AI-based methods can predict ADME properties at an early stage of drug development, which can help to prioritize compounds for further testing and reduce the number of compounds that fail in later stages of development.

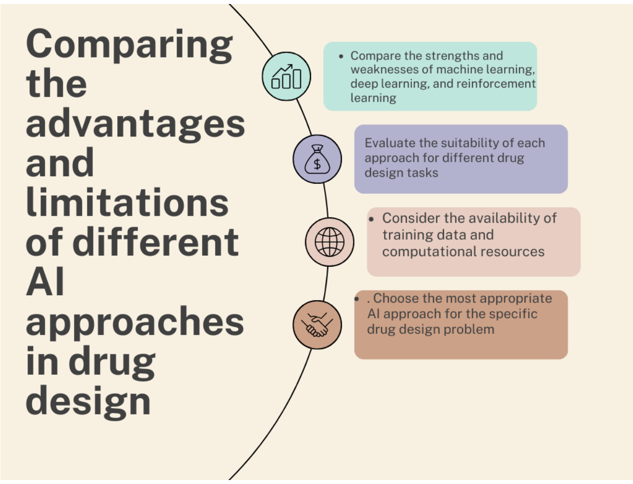

Fig. 4: Flow chart for Advantages and limitations of predicting ADME properties using AI

Case Studies and Examples

Overview of case studies and examples showcasing the use of AI in drug design

Several case studies have demonstrated the potential of AI in expediting the drug discovery process. In this section, we will discuss some examples of the use of AI in virtual screening, de novo drug design, and prediction of ADME properties.

Virtual screening case studies

Identification of inhibitors for SARS-CoV-2

The COVID-19 pandemic has led to a pressing need for effective treatments for the disease caused by the SARS-CoV-2 virus. Virtual screening using AI has been used to identify potential inhibitors of the virus. For example, Janiesch et al. (2020) used a deep learning approach to screen a library of over 1 billion compounds and identified 6 compounds that showed promising activity against the virus[20].

Discovery of novel PDE2 inhibitors

Phosphodiesterase 2 (PDE2) is a promising therapeutic target for several neurological disorders. In a study by Jiménez-Rosés et al. (2021), a combination of molecular docking and machine learning was used to identify novel PDE2 inhibitors. The study identified several compounds with high binding affinity to PDE2, demonstrating the potential of AI in accelerating drug discovery for neurological disorders[21].

De novo drug design case studies

Reinforcement learning for de novo design of drug-like molecules

Reinforcement learning has been used to design new molecules with desirable properties. In a study by Zhavoronkov et al. (2019), a reinforcement learning algorithm was trained to generate novel molecules with specific properties, such as high potency and low toxicity. The algorithm was able to generate novel compounds that showed promising activity against several drug targets[22].

Generative models for de novo design of novel kinase inhibitors

Generative models have also been used to design new molecules. In a study by Xiong et al. (2023), a generative model was trained to generate new kinase inhibitors. The study demonstrated that the generative model was able to generate novel compounds with high potency and selectivity against several kinases[23].

ADME prediction case studies (Figure 5)

Prediction of drug-induced liver injury using machine learning

Drug-induced liver injury (DILI) is a major cause of drug failure during development. Machine learning approaches have been used to predict the risk of DILI for new drug candidates. In a study by Yang et al. (2020), a machine learning algorithm was trained to predict the risk of DILI based on the chemical structure of the drug candidate. The algorithm was able to accurately predict the risk of DILI for several drugs, demonstrating the potential of AI in predicting ADME properties[14].

Predicting pharmacokinetics of drug candidates using deep learning

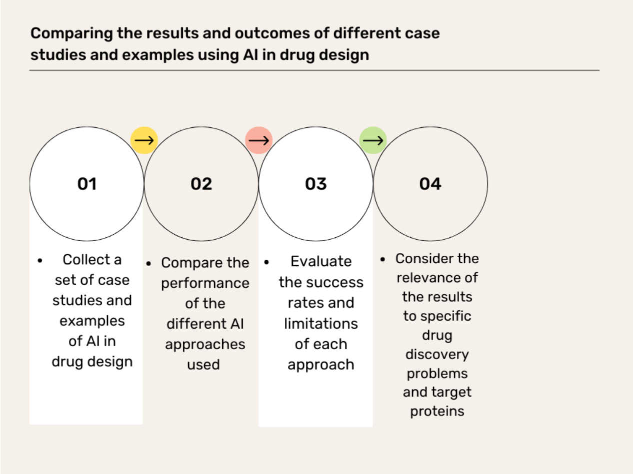

Fig. 5: Flow chart forcomparing outcome of different case studies and examples using AI

Overall, these case studies demonstrate the inherent potential of AI in accelerating drug discovery and development. Virtual screening, de novo drug design, and prediction of ADME properties are just a few examples of how AI can be applied in drug discovery. AI can not only save time and reduce costs, but also help identify new drug candidates with required properties.

Future Directions and Challenges

The use of AI in drug design has brought about numerous advantages, including speedier and more accurate identification of drug candidates, cost reduction, and increased efficiency. However, some difficulties must still be overcome before AI's full potential in drug creation can be realized.

Challenges

1. Limited availability of high-quality data: The availability of high-quality data is crucial for the success of AI

models in drug design. However, the data required for training such models is often limited and may be biased, leading to inaccurate predictions.
2. Interpretability and explainability: AI models used in drug design can be complex and difficult to interpret, leading to difficulties in understanding how they make predictions. This makes identifying any flaws or biases in the models difficult, and it makes evaluating their safety and effectiveness difficult for regulators.
3. Lack of diversity in chemical space: AI models used in drug design are often trained on a limited set of chemical structures, leading to a lack of diversity in chemical space. This can limit the applicability of the models to new chemical structures.
4. Ethical considerations: The use of AI in drug design raises ethical concerns, such as data privacy and bias in decision-making.

AI in drug design is a promising field that intends to use artificial intelligence approaches to speed the discovery and development of new medications. However, AI in drug creation confronts some issues including data privacy, bias, and openness.

Data privacy relates to the safeguarding of sensitive and personal information created or used by AI models. AI models, for example, may analyse genomic data or patient medical records to find new drug targets or candidates. However, this data may contain personally identifying information that bad actors might misuse or expose. AI in drug design should ensure that data is acquired, kept, and processed securely and ethically, and that data owners retain ownership over their data.

Bias refers to AI models' biased or erroneous depiction of specific groups or results. For example, AI models may learn from past or present data that reflects human biases or limits, such as discrepancies in drug trials or access based on race, gender, or location. This could result in AI models that favour or discriminate against specific demographics or outcomes, affecting medicine quality and safety. As a result, artificial intelligence in drug creation should ensure that the data is diverse, representative, and balanced, and that the AI models are fair, accountable, and explainable.

Transparency refers to the openness and clarity of AI models' procedures and outputs. AI models, for example, may employ complicated or black-box algorithms that are difficult for humans to comprehend or interpret. This may result in AI models that are obscure or untrustworthy, affecting stakeholders' trust and confidence. As a result, AI in drug creation should ensure that AI model approaches and outcomes are accessible, intelligible, and verifiable.

There are different methods to ensure the transparency of AI models, depending on the purpose and the audience of the transparency. Some of the common methods are:

- Openness: Openness entails making the AI models' research papers, code, and data available so that anybody may access, understand, and validate them. This has the potential to encourage collaboration and trust between the AI community and the general public. OpenAI, for example, is a group that makes its research papers and code available online[24,25] .

- Explainability: This refers to making AI models more intelligible by explaining how they make judgments or predictions. This can help consumers more effectively trust and employ AI models. IBM, for example, provides tools that facilitate model evaluation and provide insights into the model's logic[26,27] .

- Interpretability: This entails analysing the internal representations and behaviour of AI models to make them more intelligible. This can aid researchers in identifying and correcting potential biases and faults in AI models. DotData, for example, is a start-up that provides techniques for visualizing and evaluating AI model features and outputs[28] .

These are some of the methods to ensure the transparency of AI models, but there are also other methods such as robust testing, benchmarking, and evaluation. Transparency is not a one-time process, but a continuous and collaborative effort that involves different stakeholders and domains. Transparency is essential for building fair, reliable, and trustworthy AI systems.

Future directions (Figure 6)

Integration of multi-omics data holds the promise of revolutionizing and revitalizing drug design by amalgamating diverse datasets such as genomics, proteomics, and metabolomics. The synthesis of these intricate layers of information could substantially augment the precision and predictive prowess of AI models, leading to more effective drug development.

Explainable AI stands as a pivotal advancement in the AI landscape, particularly in the realm of drug design. With the advent of models that offer explanations for their decisions, the opacity surrounding AI's decision-making processes diminishes. This newfound transparency not only bolsters our comprehension of AI models but also facilitates the identification of potential pitfalls and biases, fostering greater trust and reliability.

The convergence of quantum computing and AI represents a transformative junction in drug design. The integration of quantum computing's immense computational capacity holds the potential to propel AI models to unprecedented heights. By enabling the prediction of molecular properties with remarkable precision and facilitating intricate simulations of chemical reactions, this amalgamation could usher in a new era of accurate drug development.

The imperative development of ethical frameworks emerges as a pressing need in the domain of AI-driven drug design. As these technologies become increasingly influential, ethical considerations come to the forefront.

Table 4: Methods to ensure transparency of AI models

Method	Description	Example
Openness	Making the research papers, code, and data of the AI models public	OpenAI publishes its research papers and code online
Explainability	Making the AI models more understandable by providing explanations of how they make decisions or predictions	IBM offers tools that simplify the process of model evaluation and provide insights into the model's logic
Interpretability	Making the AI models more understandable by analysing their internal representations and behaviour	dotData provides techniques for visualizing and interpreting the features and outputs of the AI models

Constructing robust ethical frameworks can effectively navigate concerns related to bias, fairness, and accountability, ensuring that the progress in drug design remains ethically sound and aligned with societal values.

AI has the potential to revolutionize drug design, but several challenges need to be addressed to fully realize this potential. Future research should focus on developing new AI models that can integrate multi-omics data and enhance the interpretability of AI models. Additionally, the development of ethical frameworks can help address the ethical concerns associated with the use of AI in drug design.

The potential impact of AI on the job market in drug discovery and a need for transparency and ethical considerations in the use of AI for drug design along with its' impact on drug pricing and accessibility are key considerations.

The use of AI in drug design is a rapidly growing field, and there have been significant advances in AI techniques for drug discovery. In particular, deep learning has emerged as a powerful tool for predicting molecular properties and drug-target interactions. Additionally, the potential of generative models and graph neural networks is being explored for de novo drug design.

Despite these advances, there are several challenges and limitations associated with the use of AI in drug design. One significant challenge is the need for large amounts of high-quality data to train AI models effectively. Another limitation is the lack of interpretability and transparency of AI models, which can make it difficult for researchers to understand how the model arrived at its predictions.

There are also ethical and societal implications to consider with the use of AI in drug design. For example, there is a concern that the use of AI may lead to job displacement in the drug discovery industry. Additionally, there is a need for transparency and ethical considerations in the use of AI for drug design, particularly with regards to issues of data privacy and bias. Finally, the impact of AI on drug pricing and accessibility is also an important consideration.

As the field of AI in drug design emerges, it is critical to overcome these issues and constraints in order to ensure that AI is both effective and ethical. Collaboration between AI and drug discovery professionals will be important in addressing these issues and realizing AI's potential in drug creation.

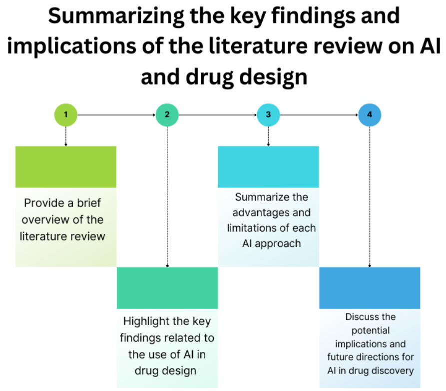

Fig. 6: Flow chart for summarizing literature review using AI for drug design

CONCLUSION

The use of AI in drug design has revolutionized the drug discovery process, with a significant impact on the speed, efficiency, and cost of drug development. This literature review has provided an overview of AI techniques used in drug design, applications of AI in drug design, and case studies showcasing the use of AI in drug design.

Virtual screening is a widely used application of AI in drug design. The AI approaches for virtual screening include structure-based, ligand-based, and hybrid virtual screening. The advantages of virtual screening are its high speed, low cost, and ability to identify potential lead compounds, but it has some limitations such as the accuracy of predicted binding affinity and the inability to consider conformational flexibility.

De novo drug design is another promising application of AI in drug design, which involves designing new molecules from scratch. The AI approaches for de novo drug design include generative models, reinforcement learning, and hybrid approaches. The advantages of de novo drug design are its ability to generate novel compounds and reduce the time and cost of drug development, but its limitations include the limited size of the generated molecule space and the challenge of balancing novelty and drug-likeness.

Prediction of ADME properties is an essential aspect of drug discovery, which can be facilitated by AI approaches such as QSAR modelling, deep learning, and hybrid approaches. The advantages of predicting ADME properties using AI are its ability to screen large compound libraries and identify compounds with favourable ADME profiles, but the limitations include the limited availability of high-quality data and the challenge of predicting complex interactions in vivo.

Overall, AI has the potential to significantly accelerate the drug discovery process, from identifying potential lead compounds to optimizing their ADME profiles. However, the successful integration of AI into drug discovery requires the collaboration of experts in AI, drug discovery, and experimental validation. The continued development and application of AI techniques in drug design are expected to lead to a more efficient and cost-effective drug development pipeline, benefiting both patients and pharmaceutical companies.

Here are the key takeaways from the review:

1. AI Revolutionizes Drug Design: Artificial Intelligence (AI) has emerged as a transformative tool in drug design, significantly accelerating the process..
2. Applications of AI: AI techniques, including machine learning, deep learning, and reinforcement learning, are applied in virtual screening, de novo drug design, and predicting ADME properties.
3. Virtual Screening: AI-powered virtual screening efficiently identifies potential drug candidates, offering a cost-effective and rapid alternative to experimental screening.
4. De Novo Drug Design: AI enables the creation of entirely new molecules from scratch, potentially leading to ground-breaking drug discoveries.
5. ADME Property Prediction: AI accurately predicts Absorption, Distribution, Metabolism, and Excretion properties, crucial for understanding a drug's behaviour in the body.
6. Case Studies Validate AI's Impact: Various case studies demonstrate AI's effectiveness, from identifying inhibitors for SARS-CoV-2 to designing novel kinase inhibitors.
7. Challenges Remain: While AI shows immense promise, challenges such as data availability, model interpretability, and ethical considerations must be addressed.
8. Future Directions: Integrating multi-omics data, developing explainable AI models, and potentially incorporating quantum computing are future directions to enhance AI's role in drug design.
9. Ethical Implications: Considerations about data privacy, bias, and job displacement in the drug discovery industry should be taken into account.

The review underscores that AI, when used judiciously, holds immense potential to revolutionize drug discovery, ultimately benefiting patients and the pharmaceutical industry.

Acknowledgement

The author acknowledges the contribution and support provided by the Department of Pharmacology, RUHS-College of Medical Sciences, Jaipur.

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