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Artificial Intelligence in Drug Discovery and Design: A Comprehensive Review of Current Applications, Challenges, and Future Directions

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Abstract

Objectives: This study seeks to critically examine how artificial intelligence (AI) is used in drug discovery and drug design and in particular it intends to examine how AI is used in the identification of a target, optimization of leads, de novo design and prediction of pharmacokinetic and toxicological properties.

Evidence acquisition: The major scientific databases, such as PubMed, Scopus, and Google Scholar were searched systematically and extensively to retrieve evidence. The peer-reviewed articles devoted to the usability of machine learning, deep learning, and generative artificial intelligence in pharmaceutical research were thoroughly reviewed and synthesized to offer a current overview of the latest advances, issues, and perspectives.

Results: AI technologies exert a tremendous influence on the sphere of drug discovery making possible the biological and chemical investigation of a big data. The strategies enhance the precision of forecasting, reduce the time it takes to develop the medicine and reduce the cost. It has been primarily used in drug-target interactions prediction, virtual screening, de novo molecular design and customized medicine. Such models as deep learning architectures, graph neural networks and generative models are further advanced to enhance molecular design and optimization. Although these benefits exist, other issues, such as the quality of data, model interpretability, legal concerns and integrating AI predictions into the experimentation process, are present.

Conclusion: Artificial intelligence has been a paradigm shift in the pharmaceutical research that has introduced new methods to offer medicines development more efficiently and quicker. As it continuously evolves, it ought to lead to the discovery of improved and safer medicines. Data quality, explainable AI models, and data integration between computational prediction and experimental validation could be some topics of future research.

الذكاء الاصطناعي في اكتشاف وتصميم الأدوية: مراجعة شاملة للتطبيقات الحالية والتحديات والاتجاهات المستقبلية

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الخلاصة:
تهدف هذه الدراسة إلى تحليل تطبيق الذكاء الاصطناعي (AI) بشكل نقدي في اكتشاف وتصميم الأدوية مع التركيز بشكل خاص على تطبيقه في تحديد الهدف، وتحسين المركبات الرائدة، وتصميم الأدوية من الصفر، والتنبؤ بالخصائص الحركية الدوائية والسمية. أُجري بحثٌ منهجي وشامل في قواعد البيانات العلمية الرئيسة، بما في ذلك **PubMed** و **Scopus** و **Google Scholar** كما جرى تقييم وتحليل الدراسات المحكمة التي تناولت تطبيقات التعلم الآلي، والتعلم العميق، والذكاء الاصطناعي التوليدي في البحوث الصيدلانية بصورة شاملة، بهدف تقديم نظرة محدثة حول أحدث التطورات، والتحديات، والآفاق المستقبلية في هذا المجال.تُحدث تقنيات الذكاء الاصطناعي أثراً بالغاً في مجال اكتشاف الأدوية، إذ تُتيح التحليل البيولوجي والكيميائي للبيانات الضخمة. تُحسّن هذه الاستراتيجيات دقة التنبؤ، وتُقصّر دورة تطوير الأدوية، وتُخفّض التكاليف. تشمل استخداماتها الرئيسية التنبؤ بتفاعل الدواء مع هدفه، والفحص الافتراضي، والتصميم الجزيئي من الصفر، والطب الشخصي. ويجري تطوير نماذج مثل بنى التعلم العميق، والشبكات العصبية البيانية، والنماذج التوليدية لتحسين التصميم الجزيئي وتحسينه. على الرغم من هذه المزايا، توجد تحديات أخرى، منها قيود جودة البيانات، وقابلية تفسير النماذج، والمسائل القانونية، ودمج تنبؤات الذكاء الاصطناعي في الإجراءات التجريبية.يُمثل الذكاء الاصطناعي نقلة نوعية في أبحاث الصيدلة، إذ أتاح تقنيات جديدة لتطوير الأدوية بشكل أسرع وأكثر فعالية. ومع استمرار تطويره، يُتوقع أن يُسفر عن اكتشاف أدوية أفضل وأكثر أمانًا. ويمكن أن تشمل بعض مواضيع البحث المستقبلي جودة البيانات، ونماذج الذكاء الاصطناعي القابلة للتفسير، وتكامل البيانات بين التنبؤ الحاسوبي والتحقق التجريبي.

الكلمات المفتاحية: الذكاء الاصطناعي، تصميم الأدوية من الصفر، الفحص الافتراضي، البحوث الصيدلانية.

INTRODUCTION

Artificial intelligence (AI) is a paradigm shift in pharmaceutical research, radically changing the traditional method of drug discovery and design. Over the last ten years, the blistering development of technology and the growing abilities of biomedical sciences allowed researchers to leave the traditional trial and error approach and adopt data-based and predictive modeling approaches [(1)]. In comparison to the traditional drug development cycle that depends mostly on experimental screening and extensive testing of the laboratory, AI can process enormous amounts of biological, chemical, and clinical data more quickly and efficiently. These data consist of genomic, proteomic, metabolomic and pharmacological data that are occasionally too elaborate to be examined using conventional statistical techniques in isolation The restrictions of the traditional pharmaceutical development further highlight the importance of AI in drug discovery [(2)].

The traditional pipeline is typically marked by long development cycles, high financial expenditures and low success rates, with numerous therapeutic candidates failing in either the preclinical or clinical phase because of toxicity, lack of efficacy, or unfavorable pharmacokinetic properties [(3)]. These constraints have created a strong need to develop new ways to improve productivity and reduce attrition rates. The objective of this paper is to critically assess the role of AI in the current drug discovery and design. It deals with certain significant applications such as discovery of targets, optimization of lead compounds, virtual screening, de novo drug design and prediction of pharmacokinetics and toxicological consequences [(4)].

These applications are crucial elements in the drug development process and AI has been found to be very promising to improve decision making and reduce experimental workload. Furthermore, this study highlights the major AI methods used in pharmaceutical research, such as machine learning (ML), deep learning (DL), graph neural networks (GNNs), transformer-based networks, and generative models [(5)].

The new computational approaches have made it possible to better model complex biological systems, anticipate drug-target interactions and screen molecular attributes such as binding affinity, toxicity and stability. In addition, the paper describes the opportunities of AI, such as acceleration of drug development cycle, decrease in cost of research, enhanced target validation and lead optimization plans. The role of AI in the growth of personalized medicine is also crucial to combine multi-omics and patient-specific clinical data and to adopt more customized and effective treatment techniques [(6)]. In the meantime, the paper discusses critically the key obstacles that hinder the widespread use of AI in drug discovery. These include data quality and availability, difficulty to interpret a model, regulatory and ethical issues, and the complexity of integrating AI based predictions with experimental techniques [(7)].

Evidence Acquisition

An extensive and systematic evaluation of literature was performed to evaluate the current state of the art

of artificial intelligence in drug discovery and drug design. The relevant studies were searched in the main scientific databases (PubMed, Scopus, web of science and Google Scholar). The search technique combined terms such as artificial intelligence, machine learning, deep learning, drug discovery, drug design, virtual screening, ADMET prediction, drug-target interaction and generative AI [8].

The inclusion criteria were limited to articles published in the years 2020-2025 to guarantee the material supplied is up-to-date and relevant. Good quality review articles as well as original pieces of research were taken into account. Articles were chosen based on the probability of supplying information about the application of AI in pharmaceutical research, such as, target discovery, molecular modeling, drug screening, lead optimization, and clinical prediction [9].

Comparative approach was given through literature on conventional drug discovery methodologies. Such studies proved the disadvantages of the out-of-date practices such as lengthy development process, expensive and high turnover. Such an analogy was needed to show the advantages of AI-based solutions compared to traditional ones [10]. The gathered literature was divided into a number of topic categories, such as:

- Conventionally limited drug discovery.
- Machine learning applications.
- Deep learning frameworks.
- De Novo Drug Design and generative AI.
- ADMET forecast.
- Repurposing drugs.
- Limits and challenges of AI.
- Ethical and regulatory issues.
- Prospects for the future.

Special attention was given to the studies which tested machine learning models to predict drug-target interactions, molecular properties, and biological activity. The works are critical because they demonstrate that AI can result in a reduction in the number of experiments and can improve the efficiency of drug discovery in the initial phases [11]. The research of deep learning was also examined because it is capable of processing high-dimensional data, which is complex. They are convolutional neural networks, recurrent neural networks, and transformer-based models, that have found extensive applications in predicting protein structure and molecular representation, and analyzing biological sequences [12]. The inclusion of generative AI studies was due to its being a significant breakthrough in the field of drug design. Variational autoencoders, generative adversarial networks, and diffusion models are models that can generate new molecular structures with specific pharmacological properties [13]. Literature on ADMET prediction was also examined and pharmacokinetics and toxicity are still key elements that define drug development success. Models based on AI have the capability of forecasting these properties at early stages of the development process and thus lower the chances of failure at the late stage [14]. Moreover, literature on the multi-omics integration was examined to learn how AI can be used to integrate genomic, proteomic, and clinical data to discover new therapeutic targets and help in personalized medicine practices [15].

RESULTS

Artificial intelligence (AI) has transformed drug discovery by introducing data-driven approaches that improve the efficiency, accuracy, and scalability of the conventional drug development process. Unlike traditional strategies that rely heavily on experimental screening and iterative trial-and-error optimization, AI enables the analysis of large-scale biological and chemical datasets to identify promising drug candidates, optimize molecular properties, and support decision-making throughout the discovery pipeline. As illustrated in Figure 1, AI is increasingly integrated across multiple stages of drug discovery, where it accelerates candidate identification, supports molecular optimization, and improves research productivity while reducing the time and cost associated with pharmaceutical development [16].

AI Applications in Advanced Drug Formulation and Physical Pharmacy

The application of artificial intelligence (AI) in medicine has become one of the most promising enabling technologies in developing more advanced pharmaceutical formulations, as it enables the rational design and optimization of drug delivery systems. The algorithms of machine learning (ML) can be applied efficiently to complex formulation datasets to predict the critical quality attributes (CQAs), such as the particle size, drug loading, encapsulation efficiency, dissolution behavior, and stability of the formulations. As a result, predictive models based on AI minimize the workload of an experiment, speed up the formulation development process, and enhance the optimization of pharmaceutical products in general [17,18].

Artificial intelligence has become a revolutionary technology in the logical design of nanomedicines, such as lipid nanoparticles, liposomes, polymeric nanoparticles, nano micelles, noisome, and nanosuspensions. Complex formulation and

manufacturing data can be combined using machine learning and deep learning algorithms to predict critical quality attributes (CQAs), such as particle size, polydispersity index, zeta potential, encapsulation efficiency, drug loading, release behavior, and formulation stability. These predictive functions decrease the use of empirical trial-and-error experimentation, speed up formulation optimization, and enhance formulation reproducibility. Moreover, AI aids the Quality-by-Design (QbD) paradigm to determine important material features (CMAs) and important process parameters (CPPs), enables effective formulation design, process optimization, and scalable pharmaceutical production Taken together, these developments propel the effective translation of nano-pharmaceutical formulations between laboratory studies and clinical and industrial practice [19,20].

Moreover, AI-enabled predictive models demonstrate notable potential to optimize formulations of poorly water-soluble drugs to predict solubility improvements, dissolution behavior, drug release kinetics, and oral bioavailability and then subject them to experimental validation. These models can minimize the need to use empirical trial-and-error methods to formulate a drug, optimize its formulation, and increase the chances of a successful product development, which explains why AI is becoming an increasingly important part of pharmaceutical formulation and physical pharmacy [21,22].

One of the most beneficial advances of artificial intelligence is machine learning (ML)-based drug-target interaction prediction. Complex data can be fed into ML algorithms to obtain molecular structure-related biological activity correlations.

According to a summary provided in Table 1, various AI methods are involved in different phases of the drug discovery process, with their use providing unique advantages [23].

Besides its predictive properties, machine learning in drug discovery adheres to a clearly defined and systematic workflow that involves a number of interdependent steps, such as data collection, preprocessing, feature extraction, model development, training, validation, and performance evaluation [24].

The foundation of this process is high quality data collection, which depends on the quality and diversity of biological and chemical data sources since the quality of machine learning models largely depends on the quality of the input data [25]. The stage of preprocessing entails cleaning of raw data, normalization of data and transforming data into a standard form and to reduce noise that would cause models to perform poorly [26]. The extraction and encoding of characteristics also make it possible to convert complex molecular structures and biological data into valuable numerical data that are easily handled by machine learning algorithms [27].

These pictures play a significant role in the analysis of the latent trends in terms of drugs-target interactions and molecular properties [28]. Then it trains models on huge amounts of data, to learn how to correlate inputs with desirable outputs. Lastly, validation processes are done to check the generalizability of the model and prevent overfitting [29]. Accuracy, precision, recall and area under the curve (AUC) are among the performance evaluation criteria of predictive capabilities [30]. Also, hyperparameter optimization and iterative optimization is usually employed to increase the stability and reliability of the model [31]. Such a methodology is crucial to comprehending and maximizing AI-assisted drug development and discusses a means of translating computational predictions into valuable experimental results [32]. Figure 2 shows the entire machine learning process of drug development.

The AI in drug discovery has been enhanced using deep learning (DL) approaches. The neural networks such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs) and models that use transformers are particularly useful with high-dimensional and heterogeneous data. The models are able to take molecular structures, protein sequences and biomedical information and to create accurate predictions of binding affinity, biological activity and drug response [33].

Graph neural networks (GNNs) have emerged as powerful deep learning models for molecular representation in drug discovery. GNNs unlike traditional methods that use descriptors to describe molecules model molecules as graphs with atoms as nodes and chemical bonds as edges, and directly learn structural and relational information. This graphical model enhances the modeling of physicochemical, biological, and pharmacological characteristics, and molecular interactions with biological targets. In accordance with Figure 3, GNNs can be used to identify and optimize promising drug candidates based on integrating both molecular and biological data, enhancing the accuracy and efficiency of AI-based drug discovery [30,34].

Transformer-based models are likewise of tremendous interest these years. They are very efficient in dealing with sequential data, and have been extensively utilized for protein structure prediction, chemical language modeling, and drug-

target interaction studies. This has made them more accurate in their forecasts and scaled in drug discovery process [35].

Variational autoencoders (VAEs), generative adversarial networks (GANs) and diffusion models are examples of generative deep learning models that have transformed de novo molecular design by allowing the creation of new molecular structures with specified physicochemical and biological characteristics. These models efficiently explore the chemical space, optimize molecular characteristics, and accelerate the identification of promising drug candidates for further development [36].

Generative AI can be used to provide De Novo Drug design, in which new molecules are designed computer-aided and then synthesized in the lab. This greatly speeds up the process of drug discovery at an early stage and gives a chance to optimize compounds to achieve better efficacy, safety, and pharmacokinetic characteristics [37]. Generative models have also been combined with reinforcement learning (RL) to optimize molecules even more. Under this approach, AI systems continuously optimize molecular structures in terms of desired objectives, such as the optimization of biological activity or minimization of toxicity. This self-directed learning enhances the lead optimization efficiency and chances of discovering drug candidates with success [38].

AI has also transformed virtual screening, such as the deep learning-based docking platform GNINA combines convolutional neural networks with traditional molecular docking to enhance ligand–protein binding pose detection and binding affinity rescoring, and thus reduce false-positive hits and enhance the identification of active compounds during virtual screening .This AI- aided solution improves accuracy and efficiency of early-stage drug discovery by supporting the speedy screening of large libraries of chemicals and prioritizing most promising candidate molecules to be experimentally validated [39]. AI can be used to identify and validate targets as well. Multi-omics data (genomics, proteomics, and transcriptomics) can be used to identify genes, pathways, and biomarkers related to disease through AI models. It helps in identifying new therapeutic targets and enhances the precision of drug development programs [40].

Artificial Intelligence (AI) is also critical in personalized medicine. With the incorporation of patient-specific data, such as genetic and clinical data, AI models have the potential to forecast personal treatment responses and help to create individualized treatment plans [41].

Moreover, artificial intelligence made a tremendous advance in predicting pharmacokinetic and toxicological properties. AI-based ADMET prediction tools enable the early identification of compounds with unfavorable absorption, distribution, metabolism, excretion, and toxicity profiles, thereby facilitating compound prioritization, reducing late-stage attrition, and improving the overall efficiency and success rate of drug discovery and development [42]. Drug repurposing is another major application of AI applications. AI can find new therapeutic uses for known chemicals through computer study of current medications and biological processes. This saves on development time and cost, as repurposed medications are generally proven to be safe [43]. In general, the use of AI in drug discovery has resulted in greater efficiency, lower costs, better predicted accuracy, and faster development times However, the efficiency of these methods is related to the quality of data, dependability of the model and the ability to integrate them with the experimental validation processes [44].

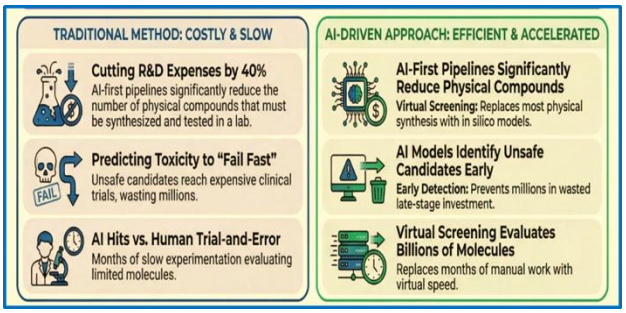

Figure (1): Comparison between traditional and AI-driven drug discovery in terms of time, cost, and success rate.

Table (1): Applications of Artificial Intelligence Techniques in Drug Discovery and Their Advantages.

Technique	Application in Drug Discovery	Advantage
Machine Learning	Prediction of drug-target interactions	Scalable and fast
Deep Learning	Molecular property prediction	High accuracy
Generative Models (GANs, VAEs)	De novo drug design	Novel molecule generation
Reinforcement Learning	Lead optimization	Adaptive improvement
Graph Neural Networks	Molecular structure modeling	Captures complex relationships
Transformer Models	Protein structure & sequence analysis	Handles large-scale data

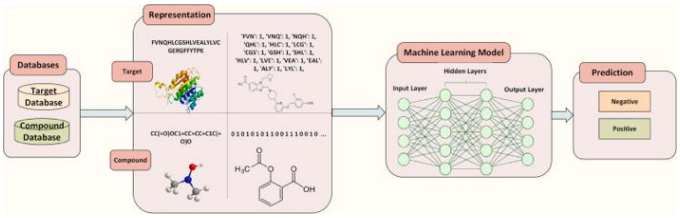

Figure (2): Schematic representation of the machine learning pipeline in drug development. Key processes such as data collection, preprocessing, feature engineering, model training, validation and prediction of molecular interactions and drug characteristics.

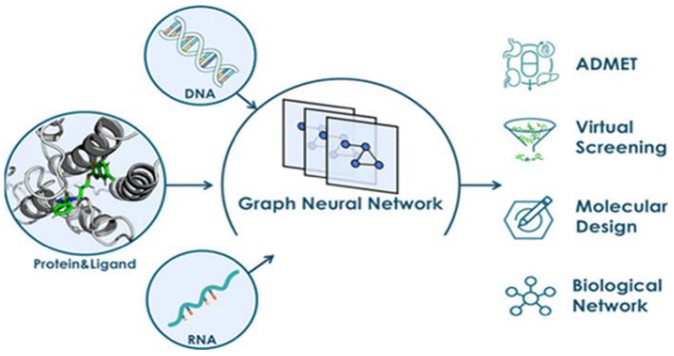

Figure (3): Schematic illustration of drug development using graph neural networks (GNNs): The encoding of the drug molecules as graphs (where the atoms are the nodes and the bonds are the edges) yields more faith to the process of modeling the molecular interactions, physicochemical properties, and drug-target interactions.

Real-World Case Studies of AI in Drug Discovery

Case Study 1: INS018_055 (Insilico Medicine)

A representative example of AI-driven drug discovery is INS018_055, a first-in-class small-molecule inhibitor developed for idiopathic pulmonary fibrosis (IPF). Using a generative AI platform, computational models were applied to identify a novel therapeutic target, generate chemically feasible molecules, and optimize lead compounds with favorable pharmacological characteristics. This combined workflow allowed the process to proceed to preclinical candidate nomination in about 18 months, significantly speeding up the traditional discovery process. After the successful preclinical testing and good Phase I safety result, INS018_055 entered Phase II clinical testing, which constitutes one of the best real-world evidence of the translational potential of AI in contemporary drug discovery [45,46].

Case Study 2: DSP-1181 (Ex Scientia)

The other example which has been well documented is DSP-1181, a drug candidate that was being developed by Exscientia in partnership with Sumitomo Pharma to cure obsessive-compulsive disorder (OCD). To achieve this, computational models based on AI were used to accelerate the discovery of hits, molecular optimization, and lead selection, thus allowing the discovery of a clinical candidate within a much shorter time than traditional drug discovery approaches. DSP-1181 later became the first AI-designed small molecule to enter Phase I clinical trials and the practicality of AI in enhancing the speed and efficiency of pharmaceutical research and development [2,3].

DISCUSSION

As the results of this review show, artificial intelligence (AI) has fundamentally changed the current drug discovery process, allowing to make decisions based on data at every step of the pharmaceutical development process. AI has penetrated many drug development phases such as target discovery, virtual screening, lead optimization and pre-clinical prediction of pharmacokinetic and toxicological characteristics. This combination has made the process of candidate selection much more efficient, but has also greatly lowered the time and expense of traditional drug discovery methodologies, which makes AI an efficient technology in supporting decisions in pharmaceutical research [1].

In addition to initial drug discovery, AI has shown significant potential in pharmaceutical formulation, allowing it to predict all-important quality characteristics, such as particle size, encapsulation efficiency, dissolution behavior, and formulation stability, and optimize the formulation beforehand. Such predictive abilities aid rational design of sophisticated drug delivery systems and reduce the experimental burden and hasten the formulation development, thus, enhancing the efficiency of pharmaceutical product development [22].

The other significant result pointed out in this review is the role of AI in structure based drug design. Hybrid artificial intelligence and molecular docking and structure-based virtual screening has enhanced prediction of protein-ligand interactions and identification and prioritization of promising lead compounds. AI-based solutions are able to enhance the efficiency and accuracy of docking processes but computational predictions are viewed as supplementary to experimental investigations and must be validated by molecular dynamics simulations and biological validation prior to clinical translation [47].

The recent developments in generative AI have also increased the range of computational drug discovery to include de novo molecular design and multi-objective optimization of candidate molecules.

Though such strategies can dramatically speed up molecular innovation, successful clinical translation remains contingent upon close collaboration with medicinal chemistry, experimental validation, and multidisciplinary pharmaceutical research, with AI being used to complement and not substitute the traditional pharmaceutical research processes [48]. In addition to its proven utility in drug discovery, AI is becoming more and more useful in precision medicine, combining genomic, transcriptomic, proteomic, imaging and clinical data. Such multimodal strategy allows more effective stratification of patients and aids in making individual therapeutic decisions The clinical utility of these models, however, is subject to the availability of a variety of standardized datasets and strong external validation to ensure consistent performance with heterogeneous populations of patients [49].

Although the current developments in AI-assisted drug discovery have made significant strides in this field, there are still a number of challenges that impede its use in pharmaceutical research,

most of them connected to data quality and model interpretability. Therefore, AI ought to be seen as a complement to the traditional method of drug discovery, but as an alternative solution because even computational predictions have to be carefully tested in the laboratory. The combination of explainable AI, quality biomedical data, generative AI, and automated experimental systems is predicted to drive future progress, as shown in Figure 4, to enhance the effectiveness, consistency, and translatability of AI-based drug discovery [50].

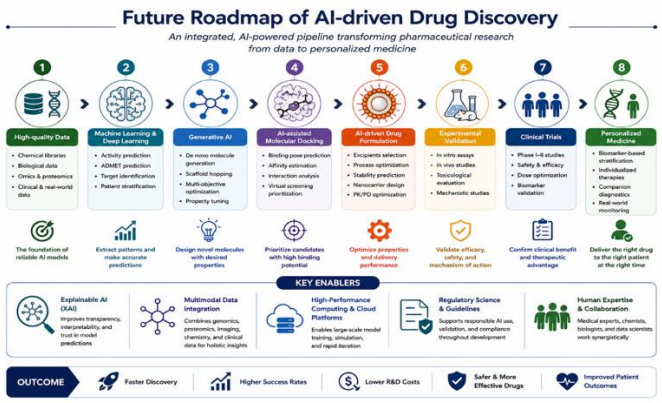

Figure (4): Future roadmap of AI-driven drug discovery. Proposed framework illustrating the integration of high-quality biomedical data, machine learning, generative AI, AI-assisted molecular docking, advanced pharmaceutical formulation, experimental validation, clinical translation, and precision medicine. Key enabling components, including explainable AI, multimodal data integration, regulatory science, and multidisciplinary collaboration, collectively facilitate the development of reliable, efficient, and clinically translatable AI-driven pharmaceutical research.

CONCLUSION

AI has served as a key enabling technology in current pharmaceutical research, enhancing various drug discovery steps, including target identification and molecular design, pharmaceutical formulation and early ADMET prediction. The AI based solutions, as has been talked about in this review, can be used to streamline research processes, cut down on the time taken to develop solutions and also assist in making more informed decisions throughout the drug development pipeline. Although these have been made, there are still various scientific and regulatory obstacles that pose a constraint to a wider application, especially regarding data quality, model interpretability, and experimental validation. Overcoming these shortcomings with standardized datasets, explainable AI, and multidisciplinary teamwork will be essential to guarantee the quality and clinical usability of AI-assisted drug discovery. On the whole, AI must be considered as a complementary technology, which enhances, but not substitutes traditional pharmaceutical research. The future developments will be based on the combination of computational intelligence with medicinal chemistry, automated experimentation, and biological validation to expedite the creation of safer, more effective, and tailored therapeutics.

FINDINGS

The results of this review indicate that the artificial intelligence (AI) is an emerging enabling technology throughout the pharmaceutical development pipeline. AI-based methods are used to enhance the target of interest, virtual screening, molecular design, pharmaceutical formulation, and the early prediction of pharmacokinetic and toxicological effects, increasing the efficiency of the research process and decreasing the development duration and expense. The increasing contributions of AI to multi-omics and clinical data integration in the pursuit of precision medicine and personalized treatment plans are also noted in the review. Nevertheless, effective deployment of AI in drug discovery still relies on the quality of datasets, interpretable models, and extensive experimental validation to have valid and clinically generalizable results.

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CONFLICT OF INTEREST

The author(s) declare no conflict of interest, financial or otherwise.

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