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Artificial Intelligence Applications in Drug Discovery and Research

Seyma MINTAS [1], Canan SEVİMLİ-GUR [2,*]

Abstract

Existing drug treatments may be inadequate for all the prevalent and emerging diseases that people face every day. Therefore, the discovery and development of new drugs is an inevitable necessity to protect human health and treat diseases. Discovering a new drug involves many steps, such as selecting the drug with therapeutic effect from a large number of active compounds, determining the ADMET properties of the drug, and conducting clinical studies to determine its toxicity and side effect profile. It is a costly and time-consuming process. According to the California Biomedical Research Association, it takes an average of 12 years and $359 million to get a drug from the lab to the patient. With the increase in digitalization in the field of health, as in every field, scientists have resorted to artificial intelligence (AI) to solve the problem of cost and time. Pharmaceutical manufacturing companies have made major investments and developed numerous AI-based algorithms to be used in different stages of drug discovery. With the use of these algorithms in drug discovery and research, the money and time spent has decreased and efficiency has increased. This mini-review discusses AI applications in drug discovery and research.

Keywords: Medicine, drug research, artificial intelligence, ADMET, algorithm, Big Data.

1. Introduction

Although there is no universally accepted definition of the concept of artificial intelligence (AI) to date, it it is broadly described as the simulation of human intelligence by computers. It refers to software and systems that enable computers to perform actions that require human intelligence. It is a multidisciplinary field [1].

The data-intensive environment referred to as 'Big Data' necessitates the acquisition, integration, and analysis of vast datasets to address complex medical and scientific challenges. It is essential to utilize AI techniques to uncover meaningful hidden patterns. Machine learning (ML) and deep learning (DL) are the two most commonly used subfields/domains of AI in drug discovery. ML and DL algorithms are applied to Big Data to extract meaningful and actionable insights from complex and heterogeneous datasets. [2, 3].

Scanning Big Data in the pharmaceutical field with AI techniques has significantly shortened the drug discovery and development process. With the shortening of the process, drug discovery has become more economical.

AI algorithms leverage existing data to enhance analysis and evaluation, use from the identification of a drug candidate to the manufacturing process in the industry. Therefore, before the synthesis and experimental evaluation of the drug molecule, AI-driven analysis has an important place in evaluating the effectiveness and efficiency of drug candidates against the desired disease.

Commonly employed DL methods in drug discovery and development can be listed as convolutional neural network, recurrent neural network, restricted boltzmann machine, autoencoders, artificial neural networks, fuzzy expert system approach [1, 4].

2. Application of Artificial Intelligence Techniques to Drug Development Steps

After successfully undergoing preclinical testing, a drug candidate proceeds to clinical trials, which are conducted in three phases: Phase 1 focuses on drug safety evaluation in a small group of healthy volunteers; Phase 2 examines drug efficacy and safety in a small group of patients with the target disease; and Phase 3 involves large-scale efficacy and safety studies in diverse patient populations. Successful completion of clinical trials is mandatory for FDA evaluation and subsequent market approval. Failures at any of these three stages render the drug development process inefficient, reduces the value of the investment, and increases the cost. The two main reasons behind the high failure rates are incorrect patient selection and inefficient monitoring during trials. He integration of AI applications into drug discovery has significantly enhanced clinical trial success rates by mitigating issues such as improper patient selection and suboptimal monitoring.

*Corresponding author

Seyma MINTAS; Izmir Katip Celebi University, Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, Türkiye; e-mail: seymamintas11@icloud.com; 0009-0000-0340-8552

Canan SEVİMLİ-GUR*; Izmir Katip Celebi University, Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, Türkiye; e-mail: canan.sevimli.gur@ikcu.edu.tr 0000-0002-2210-5925

AI models also analyze relevant parameters such as toxicity, side effects, etc., thus increasing the success rate and thus reducing the cost of clinical trials. In drug discovery and development, AI can generally be used in steps such as cell classification and sorting, calculation of the properties of small molecules, organic compound synthesis of computational tools, design of novel compounds, development of experiments and prediction of the three-dimensional structure of target molecules.

2.1. Artificial intelligence applications in literature screening

Nowadays, literature review has become one of the cornerstones of academic and scientific research. However, increasing information density makes it difficult for researchers to carry out this process more efficiently and effectively. In this context, AI technologies optimize literature review processes and provide significant advantages to researchers.

Literature review was a time-consuming process that was usually carried out manually in the past. In traditional searches, researchers could scan a limited number of databases and had difficulty summarizing or analyzing the results. However, the support of AI with technologies such as natural language processing (NLP), ML, and data mining has created a revolutionary transformation in this field.

AI-based systems can scan millions of articles, reports, and data sets in seconds and provide researchers with comprehensive and customized results. These systems are not only used for scanning the literature, but also for tasks such as summarizing, thematic analysis, and trend identification. AI stands out with the following application areas in literature review:

a. Intelligent Search Engines and Databases: Platforms such as Google Scholar, PubMed and Semantic Scholar offer the most appropriate results for users' search terms with AI-based algorithms. These systems have the ability to analyze users' past search behavior and provide suggestions.

b. Automatic Summarization: AI systems can analyze long articles, summarize them and quickly present the main idea of the article to the researcher. For example, important sections of articles can be identified and summarized in plain language using NLP techniques.

c. Thematic and Textual Analysis: ML can classify large numbers of studies under certain themes or concepts. This allows researchers to easily organize related literature and identify critical trends.

d. Citation and Relationship Analysis: AI systems can determine which studies are more influential and gaps in the literature by examining citation relationships between studies. For example, it is possible to determine the main studies and subfields in a field with methods such as "Citation Network Analysis".

e. Systematic Review and Meta-Analysis: AI-powered tools allow systematic reviews and meta-analyses to be conducted more quickly and objectively. These tools greatly simplify the processes of filtering data, assessing quality, and summarizing results.

AI technologies will be increasingly used in literature review processes and will increase the quality of research. In particular, explainable AI and DL techniques will make systems in this field more user-friendly and reliable. In addition, it will be possible to provide researchers with a more personalized experience by developing AI solutions specific to different disciplines.

In the literature review, AI applications provide great contributions to scientific progress by accelerating academic research. The development of innovative and ethical systems that are suitable for the needs of researchers will ensure that these technologies are used more widely and effectively [13, 14].

2.2. Use of artificial intelligence in the preclinical stage

Preclinical studies are a critical phase in which safety and efficacy data are evaluated, forming the basis of drug development and biomedical research. This process is usually costly, time-consuming, and data-intensive. However, in recent years, the use of AI technologies in this field offers great potential to accelerate processes and increase accuracy.

At the preclinical stage, AI is used in areas such as analyzing various types of biomedical data, evaluating drug candidates, and optimizing experiments. The main applications of AI include methods such as ML, DL, and NLP. These technologies offer effective solutions for both in vitro and in vivo studies. The subsequent sections provide a detailed examination of the principal applications of AI in the preclinical stage, including its pivotal contributions to drug candidate identification, experimental design optimization, and other critical processes.

a. Identification and Optimization of Drug Candidates: AI can predict new drug candidates that are suitable for biological targets by analyzing large molecular data sets. For example, it is used in ligand-based screening to predict the biological activity of chemical compounds. Additionally, target identification is facilitated through molecular dynamics simulations and bioinformatics analyses, which enable the identification of potential target

proteins and pathways. Moreover, structure-activity relationship (SAR) analysis, powered by machine learning algorithms, accelerates drug optimization by predicting relationships between chemical structure and biological activity.

b. Toxicity and Safety Assessment: AI is developing alternative models to reduce toxicity testing in laboratory animals. For instance, in silico toxicity prediction leverages AI to predict safety profiles by correlating chemical properties with biological effects. Additionally, the combination of AI with organ-on-a-chip technology, which integrates microfluidic systems, enables more accurate modeling of the toxic responses of human organs.

c. Cell Culture and Experiment Optimization: AI-based algorithms analyze processes such as cell proliferation, differentiation, and gene expression in in vitro experiments. For example, deep learning methods are employed in cell imaging to classify, count, and analyze cell phenotypes. Furthermore, AI optimizes experimental parameters in experimental design, leading to significant savings in both time and cost.

d. Studies on Animal Models: AI enables more efficient analysis of data from animal models. For instance, AI algorithms are used in behavioral analysis to evaluate neurological disorders or the effects of drugs by monitoring animal behavior. Additionally, AI facilitates the analysis of physiological data collected from sensors, allowing for continuous monitoring of biomarkers such as heart rate and respiration.

e. Biomarker Development: AI plays an important role in the discovery of new biomarkers for disease diagnosis and treatment targets. Validation of biomarkers can be done more quickly and accurately by analyzing genomic, proteomic and metabolomic data.

The role of AI in preclinical studies is expanding. Explainable AI, in particular, will enable these technologies to gain wider acceptance by providing transparency in regulatory processes. In addition, the integrated use of AI with large data sets obtained from biobanks will enable more sensitive and effective drug development processes.

In preclinical studies, AI offers faster, more cost-effective, and more ethically sustainable solutions than traditional methods. However, in order for these technologies to realize their full potential, challenges such as data quality, algorithm reliability, and regulation must be overcome. AI will continue to play an important role in scientific progress as a critical tool shaping the future of biomedical research [15,16].

2.3 Use of artificial intelligence peptide synthesis and small molecule design

Advancements in artificial intelligence have significantly transformed peptide synthesis and small molecule design, two fundamental areas in modern drug development. These innovations are particularly evident in the work of Yan et al. (2020), who developed a Convolutional Neural Networks (CNN)-based platform for the identification of antimicrobial peptides (AMPs) [5].

Peptide synthesis and small molecule design are fundamental to modern drug development processes. However, these processes often involve time-consuming, costly, and complex computational steps. AI is accelerating research processes and increasing accuracy by offering innovative approaches to the design of peptides and optimization of small molecules.

Peptides are short amino acid sequences that play a key role in natural biological processes. Especially in the design and production of therapeutic peptides, AI offers significant advantages with the following applications:

a. AI in Peptide Design: AI is used in the design of peptides with desired biological properties. For instance, it enables sequence prediction by identifying amino acid sequences that exhibit targeted biological effects, with deep learning algorithms often used to predict peptides with high binding affinity. Additionally, AI facilitates the optimization of artificial peptides through molecular dynamics simulations and algorithms that suggest modifications to improve the stability and solubility of peptides.

b. Optimization of Peptide-Synthesis Pathways: AI can enhance efficiency by optimizing sequencing and synthesis protocols. For example, in Solid Phase Peptide Synthesis (SPPS), AI is used to optimize reaction conditions, increasing efficiency and reducing byproduct formation. Additionally, AI-supported models facilitate reagent prediction by selecting appropriate reagents for chemical reactions and optimizing synthesis conditions.

c. Development of Therapeutic Peptides: In the development of therapeutic peptides, AI plays a crucial role by predicting binding affinity to biological targets, analyzing immunogenicity, and optimizing pharmacokinetic properties. Similarly, in the design of small molecules, AI significantly contributes to drug discovery processes by facilitating the creation of molecular structures that interact effectively with biological targets. AI scans the vast chemical space and identifies molecules with high biological activity. For example, Generative Adversarial Networks (GANs) are used to generate new chemical structures, scanning millions of potential small molecules to produce candidates suitable for biological targets. Additionally, AI models predict structure-activity relationships (SAR), guiding the design process by revealing connections between molecular structures and biological activity. AI also optimizes chemical synthesis processes by predicting the outcomes of reactions. Tools such as retrosynthesis analysis automatically determine synthesizable pathways for complex molecules, with

examples including platforms like ASKCOS and Synthia. Furthermore, AI aids in reagent selection by predicting the most suitable reagents for chemical reactions, streamlining synthesis pathways and improving efficiency. In preclinical studies, AI predicts the pharmacokinetic and toxicological profiles of molecules through ADMET (Absorption, Distribution, Metabolism, Elimination, and Toxicity) analysis. This helps guide safer molecule design and reduces the risk of adverse effects. Additionally, machine learning models predict toxic side effects, enabling the creation of chemical structures with improved safety profiles.

AI is supported by numerous advanced tools and technologies that facilitate peptide synthesis and small molecule design. For example, AlphaFold, a deep learning-based tool, has revolutionized protein structure prediction and protein-peptide interaction analysis, providing unprecedented accuracy in understanding molecular dynamics. Schrödinger Maestro offers robust capabilities for small molecule pharmacophore modeling and molecular docking, enabling precise predictions in drug design workflows. Similarly, open-source platforms like DeepChem assist in chemical modeling and design, while ChemProp leverages machine learning for molecular property prediction, further enhancing the efficiency and precision of these processes.

As algorithms and big data technologies continue to evolve, the role of AI in peptide synthesis and small molecule design will expand even further. Explainable AI and hybrid modeling approaches are expected to provide more reliable and practical solutions, ensuring the broader applicability of AI-driven methods in drug discovery. Additionally, the integration of AI algorithms with high-performance computing (HPC) systems is anticipated to significantly enhance the speed and accuracy of molecular simulations, enabling faster and more effective drug development.

Despite its transformative potential, realizing the full benefits of AI in peptide synthesis and small molecule design requires addressing several challenges. Issues such as data quality, algorithm reliability, and regulatory compliance must be carefully managed to ensure the safe and effective deployment of these technologies in drug discovery and development [17, 18].

2.4. Use of AI to define drug dosage and drug delivery efficiency

Optimization of drug dosage and delivery systems is of critical importance in modern medicine and pharmacology. In order to provide effective and safe treatment, drugs must be administered in the correct dosage and delivered to biological targets with high efficiency. In these processes, AI offers significant innovations with data analytics, predictive modeling and optimization algorithms.

Drug dosage varies according to the physical and biological characteristics of the individual. While traditional dosage determination methods are usually based on clinical trials and data from the general population, AI can make more precise and personalized dosage calculations with individual patient data.

AI plays a crucial role in personalized dosage optimization by analyzing individual patient characteristics such as genetic profile, age, weight, gender, and comorbidities. Traditional methods often fail to capture these individual differences, but AI provides a solution through advanced modeling techniques. Pharmacokinetic and pharmacodynamic (PK/PD) models powered by AI can precisely simulate the absorption, distribution, metabolism, and excretion of drugs, enabling tailored dosage recommendations. Furthermore, AI leverages pharmacogenetic data to assess the impact of genetic variations on drug metabolism and provides personalized dosage recommendations based on genetic factors, enhancing treatment accuracy and safety.

In addition to personalized optimization, AI supports dynamic dosage management by utilizing real-time patient monitoring. AI-powered closed-loop systems can dynamically adjust dosages in response to biological feedback, ensuring optimal therapeutic outcomes while minimizing toxicity risks. These systems also help in therapeutic index optimization by balancing the potential toxic effects of drugs with their therapeutic benefits. Moreover, ML algorithms analyze historical clinical data to predict side effect profiles and identify safe dose ranges, further enhancing patient safety and improving treatment precision.

AI is also revolutionizing drug delivery systems by ensuring that drugs are delivered to their targets at the right dose to maximize therapeutic effect. In targeted drug delivery systems, AI algorithms optimize the binding efficiency of nanoparticles to biological targets, enhancing the precision of nanotechnology-based delivery methods. Additionally, ML-based ligand-selection models identify the most suitable ligands for surface modifications of drug delivery systems, further improving their targeting capabilities.

AI also contributes to the development of controlled release systems, which are designed to provide sustained and controlled drug release over time. It models drug release profiles to maintain therapeutic levels effectively and uses DL algorithms to evaluate the biocompatibility and biodegradability of materials employed in these systems. This ensures both safety and efficiency in drug delivery. Furthermore, AI simulates and analyzes how drugs distribute within the body, predicting their concentrations in specific tissues. Pharmacological modeling

tools predict drug delivery times and concentrations at target sites, while molecular dynamics simulations analyze drug behavior in both intracellular and extracellular environments, enhancing delivery efficiency.

The integration of AI with various advanced technologies has significantly improved drug dosage and delivery systems. DL algorithms are extensively used in PK/PD analyses and toxicity predictions, while Bayesian optimization is employed to refine controlled release systems and analyze clinical data. Reinforcement learning has proven effective in optimizing dynamic dosage management and drug delivery system performance. Additionally, retrosynthesis analysis supported by AI determines ideal chemical pathways for drug synthesis and carrier system design, streamlining drug development processes and enhancing efficiency. The use of AI in drug dosage and delivery systems has the potential to provide more effective, faster and more economical treatment methods in the future. In particular, explainable AI models will increase the trust in AI in clinical decision-making processes. In addition, smart drug delivery systems integrated with biosensors will maximize treatment effectiveness with real-time monitoring and dosage adjustments.

AI is a powerful tool that supports personalized medicine and precision treatment approaches in defining drug dosage and delivery efficiency. The speed, accuracy and cost advantages offered by AI will reshape drug development and application processes. However, data management, regulation and ethical issues need to be addressed in order for these technologies to be implemented effectively and safely [19, 20, 21].

2.5. Use of artificial intelligence in predicting bioactive agents and monitoring drug release

Development of bioactive agents and monitoring of drug release processes are key to pharmaceutical research and clinical applications. Conducting these processes using traditional methods can be time-consuming and costly. AI offers powerful tools for predicting bioactive molecules, optimizing drug release mechanisms, and real-time monitoring by analyzing large datasets.

Bioactive agents are molecules that provide therapeutic effects by exhibiting specific interactions in biological systems. AI plays an important role in identifying these molecules and predicting their properties.

AI plays a transformative role in discovering new molecules by predicting bioactive agents through the analysis of large molecular databases. DL algorithms are particularly effective in identifying potential new molecules by learning the relationships between chemical structures and biological activity. Additionally, AI-powered quantum chemistry simulations assist in the selection of effective molecules by predicting their energy profiles and interaction potentials at the molecular level, enabling more accurate predictions in early-stage drug discovery.

Predicting the ADMET properties of bioactive molecules is another critical application of AI in drug development. ML models analyze the physicochemical properties of molecules to predict their ADMET profiles with high accuracy. Furthermore, feature-selection algorithms identify promising candidates by evaluating the effects of molecular structures on toxicity and bioavailability, streamlining the drug development pipeline.

AI also contributes significantly to modeling ligand-target interactions, simulating the interactions of bioactive agents with biological targets to predict mechanisms of action. Docking simulations powered by AI identify molecules with strong interactions by analyzing their molecular binding energies, while tools such as AlphaFold predict protein structures and ligand binding sites, facilitating target-oriented molecule discovery.

In drug delivery systems, AI provides innovative approaches for the design, optimization, and monitoring of controlled release mechanisms. AI-based simulations and data analytics optimize drug release profiles by improving timing and dosage control, ensuring that therapeutic levels are maintained consistently. DL algorithms play a key role in material design by evaluating the biodegradability and biocompatibility properties of drug carrier materials, further enhancing the efficiency of release systems.

AI also enables real-time monitoring of drug release processes by analyzing sensor data. For example, biosensor integration allows for immediate assessment of treatment efficacy by measuring the amount of drug released and biomarker levels in the patient. Closed-loop control systems, powered by AI, dynamically adjust release mechanisms based on real-time data, optimizing the release process to ensure maximum therapeutic benefit.

Furthermore, AI enhances the simulation and visualization of drug distribution within the body. Pharmacokinetic modeling tools optimize release strategies by predicting how drugs are distributed across tissues and how they access their targets. Molecular dynamics analyses add another layer of insight by simulating the intracellular and extracellular release dynamics of drugs, providing a deeper understanding of their behavior in biological systems.

A variety of AI tools and algorithms support these advancements in bioactive agent discovery and drug delivery systems. Machine learning techniques, including regression and classification algorithms, are extensively used to analyze molecular properties and release profiles. Deep learning models are particularly effective in predicting the biological activity and ADMET profiles of molecular structures. Bayesian optimization is employed

to refine drug delivery system designs, while molecular simulation software such as GROMACS and AutoDock, combined with AI-powered pharmacokinetic tools, provide robust platforms for simulation and analysis. These technologies collectively enhance the precision, efficiency, and scalability of drug discovery and delivery processes.

The use of AI in the prediction of bioactive agents and drug release monitoring processes will enable the development of more effective and sensitive treatment methods in the future. Hybrid AI systems will be one of the cornerstones of personalized medicine by being integrated with sensor technologies and bioinformatics tools. In particular, explainable AI will improve clinical decision processes and increase the reliability of AI in the healthcare sector [22, 23, 24].

2.6. Use of artificial intelligence in identifying adverse drug reactions

Adverse drug reactions (ADRs) are a term used to describe unexpected and often harmful effects of medications. According to the World Health Organization, ADRs pose a significant burden to the global healthcare system and are estimated to account for 5-10% of hospitalizations. In this context, AI has emerged as a powerful tool for faster, more accurate, and proactive identification and management of ADRs.

AI plays a pivotal role in the identification and prevention of ADRs by utilizing advanced technologies such as big data analytics, ML, DL, and natural language NLP. These technologies enable the comprehensive analysis of vast and complex datasets, offering innovative solutions to enhance patient safety and improve pharmacovigilance systems.

Through data analysis and association identification, AI collects and examines extensive data from sources such as electronic health records, side effect reports, genetic profiles, and even social media. By analyzing these datasets, AI algorithms can uncover previously undetected drug-reaction relationships, providing critical insights into the causes and patterns of ADRs. This capability is particularly valuable for identifying subtle or rare reactions that might otherwise go unnoticed.

AI also contributes significantly to the prediction and risk assessment of ADRs. DL models, in particular, have shown exceptional capability in predicting ADRs for individual patients by analyzing genetic predispositions, environmental factors, and medical histories. These models support the development of personalized treatment plans by identifying potential risks associated with specific drugs before they are administered, thereby improving patient outcomes and minimizing harm.

In the area of ADR monitoring and reporting, AI-driven NLP systems automatically extract and report ADR information from clinical notes, scientific literature, and social media content. Platforms such as Google Health AI and IBM Watson exemplify the application of these technologies, enabling the efficient detection and communication of ADR-related information to healthcare professionals and regulatory authorities.

A range of AI tools supports these efforts, including ML models and algorithms like Support Vector Machines (SVM), Random Forests, and advanced techniques such as XGBoost, which offer high accuracy in ADR classification and prediction across large datasets. Similarly, NLP tools such as SpaCy and BERT are used to extract structured information from unstructured text, with systems like the FDA's Sentinel System leveraging these technologies for pharmacovigilance.

DL applications, including Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs), further enhance ADR detection by analyzing genetic data and clinical images. Transformer models, such as BERT and GPT, extend this capability by learning from vast datasets, enabling accurate predictions and insights into ADR mechanisms.

AI-powered pharmacovigilance platforms provide an additional layer of support for ADR identification and prevention. For example, VigiBase, the World Health Organization's global pharmacovigilance database, employs AI algorithms to analyze ADR reports from across the globe. Similarly, the FDA's Adverse Event Reporting System (FAERS) integrates AI to track and analyze ADR data efficiently, improving regulatory oversight and patient safety.

By leveraging these advanced technologies, AI significantly enhances the efficiency and accuracy of ADR identification, prediction, and prevention, contributing to safer drug development and more effective pharmacovigilance practices.

AI has the potential to revolutionize ADR identification and prevention. In the future, Prediction accuracy will increase with more data sets and advanced algorithms. ADRs can be monitored instantly with real-time data from IoT devices. Integration of regulatory processes with AI will accelerate drug safety assessments. AI has become an integral part of pharmacovigilance studies and plays a critical role in improving patient safety and treatment success [25, 26, 27].

2.7. Prediction of protein folding and protein-protein interactions

Machine and statistical learning approaches such as K-nearest neighbor algorithm, Naive Bayesian algorithm, Support Vector Mechanism, Artificial Neural Networks and Random Forest are used to predict inhibition in PPIs.

2.8. Structure-based and ligand-based virtual screening

ML models such as PARASHIFT, HEX, USR and ShaPE algorithms have been developed for LBVS. Tools such as MTiOpenScreen, FlexX-Scan, CompScore, PlayMolecule BindScope, GeauxDock and ENRI have been developed for SBVS.

2.9. QSAR modeling and drug redesign

Various algorithms and tools such as VEGA platform, QSAR-Co, FL-QSAR, Meta-QSAR, Transformer-CNN, Cloud 3D-QSAR have been developed for QSAR modeling.

2.10. Prediction of mode of action and toxicity of compounds

Different web-based tools such as LimTox, pkCSM, admetSAR and Toxtree can be given as examples.

2.11. Identification of molecular pathways and polypharmacology

Text mining-oriented databases such as DisGeNET, STITCH, STRING are widely used to detect gene-disease relationships, drug-target relationships and molecular pathways, respectively.

2.12. Application of AI in de novo drug design

In de novo drug design, AI plays a critical role in designing molecules from scratch, optimizing their properties, and ensuring they possess targeted biological activity. Compared to traditional methods, the use of AI in this field offers faster and more cost-effective solutions, streamlining the drug discovery process.

AI algorithms are employed to explore the vast chemical space, enabling the creation of entirely new molecules tailored to specific needs. Among the most prominent methods, Generative Adversarial Networks (GANs) utilize a competitive framework between two neural networks to generate novel molecular structures. Similarly, Variational Autoencoders (VAEs) learn the patterns of chemical structures and use this knowledge to recreate and design new, similar molecules. Reinforcement Learning (RL) further enhances the process by improving the alignment of designed molecules with desired target properties.

These advanced AI techniques enable the generation of unique chemical structures that are optimized for specific biological targets, making de novo drug design a powerful and efficient approach to discovering innovative therapeutic solutions.

2.13. Example of neurodegenerative diseases in the use of AI

AI is playing an increasingly significant role in drug discovery, as demonstrated by numerous advancements and applications in the field. For example, Ponzoni et al. (2019) combined decision tree algorithms, quantitative association rules, and hierarchical clustering to identify potential risk genes associated with Alzheimer's disease through gene expression profiling of patient and control samples. They further utilized protein-protein interaction networks, autoencoders, and support vector machines (SVMs) to predict novel target genes associated with Parkinson's disease [6].

The pharmaceutical industry has heavily invested in AI-based applications to streamline drug discovery and development. Xie et al. (2018) developed a model capable of predicting drug-target interactions using transcriptome data from the L1000 database of the Integrated Network-Based Cellular Signatures Library, achieving an impressive accuracy of 98% [7, 8]. Deep learning (DL) methods have also been applied to identify nutraceuticals with anti-aging and anti-cancer properties that mimic the effects of FDA-approved drugs like metformin and rapamycin without causing adverse effects. By mapping the gene-level pathways of these compounds and analyzing over 800 potential alternatives from the LINCS dataset, DL classifiers predicted safer compounds for further development [8].

Prominent technology companies have also contributed to this revolution in drug discovery. Microsoft developed an AI-based system called "Hanover" to assist in identifying optimal cancer treatments by analyzing extensive medical datasets [9]. Similarly, IBM, in collaboration with Pfizer, introduced IBM Watson, a cloud-based platform designed to accelerate drug discovery by analyzing patient-specific data such as medical lab

reports and identifying potential relationships across datasets. The platform also enables personalized treatment plans by engaging patients in dynamic, data-driven interactions with doctors [9].

Koneksa Health has taken a unique approach with its AI-driven software, which integrates mobile and wearable devices to streamline clinical trials by analyzing biomarker data. Biomarkers, which are substances or data indicative of diseases and measurable in body fluids such as blood or urine, are collected and analyzed by this software, expediting the drug development process. The software allows for efficient data sharing with healthcare providers and pharmaceutical companies conducting clinical trials.

Pharmaceutical companies are making substantial investments in AI to improve efficiency and reduce costs. GlaxoSmithKline, for instance, allocated $43 million to Exscientia, an AI-driven company based in Scotland, to expedite drug development while reducing costs by up to 75% [10]. AstraZeneca is collaborating with Berg to develop biomarkers and treatments for neurological diseases, further illustrating the industry's reliance on AI for innovation [10].

Historical contributions to AI in drug discovery also highlight its foundational importance. Corwin Hansch, known as the "father of computer-aided molecular design," pioneered the use of AI algorithms for predicting the physicochemical properties and biological activities of drug compounds. His work enabled the detailed prediction of chemical structures and their pharmacological properties, laying the groundwork for modern AI-based drug discovery methods [11].

SwissADME has also emerged as a significant resource in the field. This free, user-friendly web tool evaluates the pharmacokinetics and medicinal chemistry properties of small molecules, integrating robust computational methods to facilitate global accessibility and open scientific collaboration [12].

These advancements demonstrate the transformative potential of AI in drug discovery, offering faster, more cost-effective, and highly precise solutions for addressing complex medical challenges.

3. Conclusion and Discussion

Although AI seems to be creating and transforming the future of healthcare, it has yet to produce substantial efficacy in certain areas. The lack of any FDA-approved drugs developed solely using AI serves as a significant indicator of its current limitations. This situation is due to both the shortcomings of AI applications compared to humans and the disadvantages that the pharmaceutical industry itself provides to drug discovery.

A key distinction between AI and human intelligence lies in the latter's ability to empathize, a trait AI fundamentally lacks. The most important difference is the ability to empathize. So while various forms of AI have surpassed human performance, they lack higher-level background knowledge and are not as capable of forming relationships as the human brain. They can be trained to do a single task.

The pharmaceutical sector faces significant barriers to AI implementation, including limited open data sharing, inconsistent data formatting, and a disproportion between available ‘data’ and actionable ‘information’. However, overcoming these obstacles is most possible with the development of AI applications. Advancements in ML algorithms and the adoption of DL approaches have significantly enhanced the accuracy and precision of AI applications. However, overcoming these obstacles is most possible with the development of AI applications. The deepening of AI and its transformation into ML algorithms; later on, with the development of these algorithms and the widespread use of the DL approach, the accuracy and precision in AI applications have increased significantly. Considering all these developments, we can say that there is high hope for the elimination of the handicaps we mentioned.

Drug discovery is a complex and lengthy process that often spans many years and costs billions of dollars. However, artificial intelligence (AI) has the potential to transform and accelerate traditional methods. By offering significant innovations at various stages of drug discovery, from molecule design to clinical trials, AI is reshaping drug development processes.

One of the most notable impacts of AI is the shortening of drug development times. Traditional processes typically take 10-15 years, but with AI, this timeline is expected to be reduced by 30-50%. This acceleration will enable faster drug delivery to the market, allowing patients earlier access to treatments. Furthermore, AI is advancing personalized medicine by analyzing genetic variations to develop individual treatment plans. For instance, it can design patient-specific molecules for cancer immunotherapies.

AI also enables the design of challenging molecules by creating new compounds that can target biologically difficult targets, such as protein-protein interactions. This innovation allows researchers to address problems that are difficult to solve with traditional chemistry. Moreover, AI significantly reduces research and development costs, potentially cutting development expenses, which range from $2-3 billion, by 20-40%.

The success rate of clinical trials may also improve through more accurate predictions of toxicity, side effects, and efficacy profiles of clinical candidates. Additionally, AI's efficiency in drug discovery could increase access to affordable medicines in low-income areas, further broadening the reach of life-saving treatments.

Considering these developments, there is substantial hope for overcoming many of the existing challenges in drug discovery. While persistent obstacles remain, there is little doubt that AI will bring transformative changes to the field in the near future.

Declaration of Interest

The authors declare that there is no conflict of interest.

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