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Review Article

Artificial Intelligence in Drug Discovery: A New Era of Pharmaceutical Innovation

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Drug discovery is a complex, time-consuming, and costly process that traditionally requires over a decade and billions of dollars to bring a single new molecule to market. In recent years, Artificial Intelligence (AI) has emerged as a transformative tool capable of accelerating and optimizing each stage of drug discovery—from target identification to clinical trials. By integrating techniques such as Machine Learning (ML), Deep Learning (DL), Natural Language Processing (NLP), and Neural Networks (NNs), AI can analyze vast biomedical datasets, identify hidden patterns, and predict drug-target interactions with remarkable accuracy. This technological shift not only reduces research costs but also improves success rates in drug development. This review aims to comprehensively discuss the role of AI in modern pharmaceutical research, highlighting its applications, case studies, challenges, and future prospects. Moreover, the article emphasizes how AI-driven models are reshaping the landscape of personalized medicine and drug repurposing, thereby ushering in a new era of pharmaceutical innovation.

Keywords: Artificial Intelligence, Drug Discovery, Machine Learning, Deep Learning, Neural Networks, Pharmaceutical Innovation.

INTRODUCTION

Drug discovery is among the most time-consuming and expensive processes in the pharmaceutical industry. The conventional drug development approach typically includes several sequential stages such as target identification, molecule discovery, lead optimization, preclinical testing, and clinical trials, which together may span 10–15 years and exhibit a success rate below 10% [1,2]. Artificial Intelligence (AI), defined as the simulation of human intelligence in machines capable of learning, reasoning, and decision-making, has recently transformed various scientific disciplines, including healthcare and pharmaceutical research [3,4]. Over the past few years, AI has had a remarkable influence on the pharmaceutical industry by minimizing manual effort, reducing research time, and improving decision accuracy [5,6]. In traditional drug discovery, molecular modeling and high-throughput screening rely heavily on trial-and-error experimentation, which is both costly and labor-intensive [7,8]. In contrast, AI-driven models—particularly those employing machine learning (ML) and deep learning (DL) algorithms—can analyze chemical structures, biological targets, and prior experimental or clinical data to rapidly identify the most promising drug candidates [9–11]. A notable example is DeepMind's AlphaFold, which has demonstrated the ability to predict protein structures with atomic-level precision, greatly enhancing target-based drug design [12]. Furthermore, leading pharmaceutical companies such as Pfizer, Novartis, and GlaxoSmithKline (GSK) have established AI-focused collaborations with technology firms to strengthen their research and development (R&D) processes [13,14]. Similarly, Indian companies such as Sun Pharma have also started integrating AI in quality control, process optimization, and data-driven manufacturing [15]. Overall, the use of Artificial Intelligence in pharmaceutical sciences holds enormous potential to shorten drug development timelines, reduce financial risk, and enhance therapeutic efficacy [16–18]. This review aims to provide a comprehensive overview of

how AI technologies are being utilized throughout the stages of drug discovery, discuss the current challenges in their implementation, and highlight future perspectives that could redefine pharmaceutical innovation and application [19,20].

2. Traditional Drug Discovery Process

Drug discovery is a long and step-by-step process that goes through several important phases before a new medicine becomes available in the market. The main stages include target identification, lead discovery, lead optimization, preclinical studies, and clinical trials [13]. In traditional research, scientists first choose a biological target—often a protein or enzyme linked to a particular disease. After that, thousands of chemical compounds are tested in the lab to find those that can best interact with the target [14]. This screening method, known as high-throughput screening (HTS), is costly and time-consuming, and it usually has a low success rate [15]. After finding potential lead molecules, medicinal chemists modify their structures to make them more active, selective, and safer for use. This stage is called lead optimization. However, even after this, many drug candidates fail in the preclinical or clinical testing stages because of poor pharmacokinetics, side effects, or lack of therapeutic action [16]. Studies have shown that only one out of about 10,000 tested compounds finally becomes an approved drug, and the complete process can take 10–15 years with an average cost of more than 2 billion USD [17]. These difficulties have created a strong need for more efficient and faster methods—and this is where Artificial Intelligence (AI) plays a major role [18]. AI can help reduce time and cost by quickly analyzing large amounts of data, finding patterns that humans might miss, and even predicting experimental outcomes before testing [19]. Instead of replacing traditional techniques, AI works alongside them, making every stage of the research process more efficient and accurate [20].

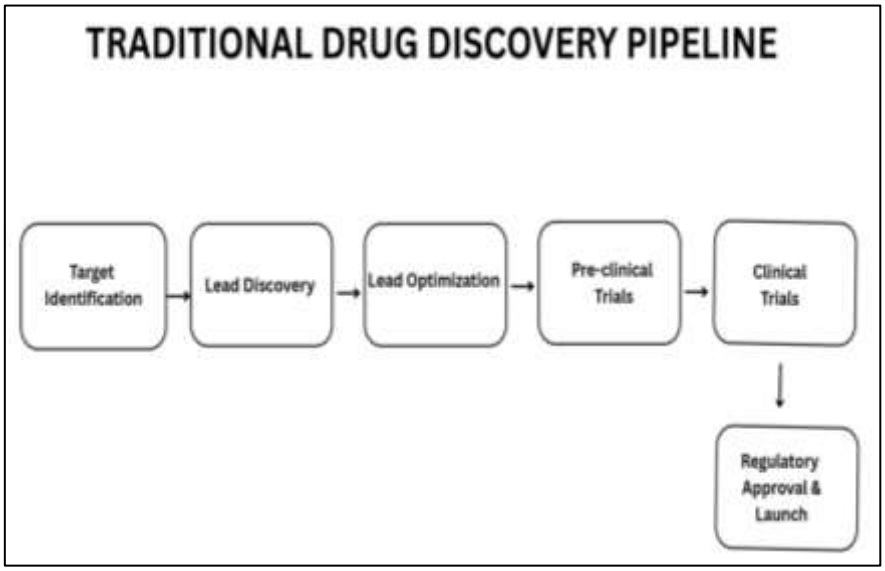

Figure 1: - Traditional Drug Discovery Pipeline

3. Overview of Artificial Intelligence in Drug Discovery

Artificial intelligence (AI) is the use of computer systems that, without explicit programming for every task, are able to learn from data, identify patterns, and make predictions. AI is used in drug research to evaluate chemical libraries, forecast molecular activity, create novel compounds, and enhance drug characteristics [21].

Definition and Concept of AI

The origins of Artificial Intelligence (AI) trace back to the 1950s, when John McCarthy first described it as “the science and engineering of creating intelligent machines” [15]. In the modern era, AI represents an integration of mathematics, statistics, and computer science, used to design algorithms capable of learning and adapting from data. Within the field of drug discovery, AI technologies are capable of evaluating millions of chemical structures and biological

interactions with far greater speed and precision than traditional human analysis [16]. The fundamental objective of AI is not to replace researchers, but rather to enhance scientific decision-making by delivering accurate and data-driven insights that complement human expertise [17].

Machine Learning (ML)

Machine Learning (ML), a vital subset of Artificial Intelligence, enables systems to learn automatically from large and complex datasets to make informed predictions or decisions. Within the field of drug discovery, ML models are widely used to forecast drug–target interactions, assess ADMET properties (Absorption, Distribution, Metabolism, Excretion, and Toxicity), and estimate the bioactivity of new chemical compounds [22]. ML acts as the core framework of AI applications in pharmaceutical research. These algorithms analyze vast chemical, biological, and pharmacological datasets to uncover hidden correlations that are often difficult for humans to identify. By learning from previously available data, ML models can predict the activity, safety, or toxicity of novel drug candidates with remarkable accuracy [5,7]. Several well-established ML approaches—such as Support Vector Machines (SVMs), Random Forests (RF), and k-Nearest Neighbor (kNN) algorithms—play crucial roles in virtual screening, lead optimization, and ADMET prediction [8,12]. For instance, Random Forest algorithms are capable of predicting the binding affinity of small molecules with protein targets, allowing researchers to identify potential drug candidates more efficiently [9].

Deep Learning (DL)

Deep Learning (DL) is an advanced branch of Machine Learning (ML) that makes use of artificial neural networks to process complex and non-linear data patterns. DL models—particularly Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs)—have achieved remarkable accuracy in predicting biological activities and molecular structures [24]. A well-known breakthrough in this area is AlphaFold, created by DeepMind, which can accurately predict 3D structures of proteins using deep learning techniques. This innovation has completely changed the field of structural biology and has made it much easier for researchers to discover and design new drug targets [1]. Essentially, Deep Learning can be viewed as a specialized form of ML that employs multiple layers of neural networks to automatically extract meaningful features from large datasets. In the area of drug discovery, DL models such as CNNs and RNNs are used for structure–activity relationship (SAR) modeling, molecular property prediction, and even de novo molecule generation [13,14]. For example, CNNs can study molecules in both 2D and 3D representations to predict their biological effects, whereas RNNs learn from known chemical structures to create new, drug-like molecules with desired characteristics [15,16].

Natural Language Processing (NLP)

Natural Language Processing (NLP) enables artificial intelligence systems to read, understand, and interpret scientific text, including research papers, patents, and clinical reports. Using NLP, AI can automatically extract meaningful data from thousands of published studies in a fraction of the time it would take human researchers [25]. Through AI-driven literature mining, NLP can uncover new relationships between diseases and genes and even propose potential therapeutic targets or treatment strategies, thereby assisting scientists in drug discovery and clinical research.

Reinforcement Learning (RL)

Reinforcement Learning (RL) is another powerful branch of AI where the system learns through trial and error, guided by feedback in the form of rewards or penalties. In drug discovery, RL techniques are used to generate new molecules that possess specific biological or chemical properties [26]. For instance, generative AI models trained with reinforcement learning can design novel compounds that are more active, stable, and less toxic than existing drugs, helping researcher's discover improved therapeutic candidates more efficiently.

AI Platforms in the Pharmaceutical Industry

Several AI-driven platforms have already demonstrated practical success in the pharmaceutical sector. AtomNet, for example, uses deep

convolutional neural networks to predict the binding interactions between small molecules and protein targets [4]. Similarly, Insilico Medicine applies generative AI algorithms for de novo drug design and has successfully identified multiple drug candidates that have progressed into clinical trial phases [5]. Another important initiative, DeepChem, provides open-source tools that support the building and evaluation of machine learning models in chemistry and biology, making AI technology more accessible to researchers worldwide [27]. Together, these platforms show that AI is no longer limited to theory — it has become a practical and essential tool in modern drug discovery and development.

Generative Models (GANs and VAEs)

Among the most sophisticated AI architectures in use today are Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs). These models can create entirely new chemical structures that possess desirable pharmacological and physicochemical properties [18].A GAN consists of two interconnected networks — a generator, which produces new molecular designs, and a discriminator, which evaluates them for authenticity. Through this continuous competition, GANs learn to generate highly realistic and optimized molecular structures. Both GANs and VAEs have shown promise in de novo drug design, lead optimization, and exploration of novel chemical space, thereby accelerating the discovery of innovative therapeutics [19,20].

Graph Neural Networks (GNNs)

Molecular structures are often represented as graphs, where atoms act as nodes and bonds serve as edges. Graph Neural Networks (GNNs) are particularly effective for analyzing such data, as they can learn and interpret the complex relationships between atoms and molecular substructures [21]. These models are widely used for predicting binding affinity, estimating toxicity, and modeling drug–target interactions [22]. Unlike traditional AI models, GNNs can capture the true three-dimensional connectivity of molecules, resulting in more precise and reliable predictions [23].

4. AI Algorithms Used in Drug Discovery

Artificial Intelligence (AI) utilizes several computational models designed to mimic human learning and decision-making. In the field of drug discovery, these algorithms analyze massive amounts of biological and chemical data to identify promising drug candidates more quickly and accurately than conventional techniques. Commonly used AI algorithms include Support Vector Machines (SVMs), Random Forests (RF), Neural Networks (NNs), Deep Learning models, and Graph Neural Networks (GNNs).

Support Vector Machines (SVMs)

Support Vector Machines (SVMs) are supervised machine learning algorithms primarily used for classification and regression tasks. In drug discovery, they help predict the biological activity of chemical compounds and identify potential lead molecules from vast compound libraries. SVMs work by distinguishing active and inactive compounds using molecular descriptors such as molecular weight, lipophilicity, and hydrogen bond donors.

Example: SVM-based models have been effectively utilized in virtual screening to discover HIV protease and kinase enzyme inhibitors [1].

Random Forest (RF)

Random Forest (RF) is an ensemble-based machine learning algorithm that builds multiple decision trees and combines their outputs to achieve higher prediction accuracy. In drug discovery, RF is extensively applied for ADMET prediction (Absorption, Distribution, Metabolism, Excretion, and Toxicity), target identification, and compound classification.

Key Advantages:

- Efficiently processes large and complex datasets
- Minimizes overfitting by averaging results from multiple trees
- Ranks feature importance, helping identify key molecular properties

Example: RF models have been effectively utilized to predict blood–brain barrier permeability and evaluate toxicity profiles of new chemical entities [2].

Artificial Neural Networks (ANNs)

Artificial Neural Networks (ANNs) are computational models inspired by the neural structure of the human brain, where interconnected "neurons" work in multiple layers to process information. These networks learn complex data patterns and are capable of predicting molecular interactions and disease associations with high accuracy

Applications:

- Prediction of ligand–receptor binding affinity
- Structure–Activity Relationship (SAR) modeling
- Detection of off-target interactions

Example: ANN-based models have been successfully applied to identify multi-target ligands for neurological diseases such as Alzheimer's [3].

Deep Learning (DL)

Deep Learning, a specialized branch of machine learning, employs multi-layered neural networks to understand complex and non-linear patterns in biomedical datasets. It has proven highly effective in image-based drug discovery, de novo molecular design, and protein–ligand docking studies.

Prominent Models:

Convolutional Neural Networks (CNNs): Used to analyze and interpret 3D molecular or structural images.

Recurrent Neural Networks (RNNs): Designed to process sequential biological information, such as amino acid or protein sequences.

Example: CNN-based deep learning frameworks have been successfully applied in cell image screening to predict compound activity and effects automatically, eliminating the need for manual data labeling [4].

Graph Neural Networks (GNNs)

In the field of chemistry, molecular structures are best represented as graphs, where atoms act as nodes and bonds serve as edges. Graph Neural Networks (GNNs) are capable of learning directly from these graph-based representations, making them exceptionally useful for predicting molecular properties and designing new drug candidates.

Example: Advanced GNN models such as GraphDTA and Chemprop have emerged as leading computational tools for accurately predicting drug–target binding affinities [5].

Reinforcement Learning (RL)

Reinforcement Learning (RL) allows algorithms to make step-by-step decisions by learning from rewards and penalties. In the field of drug discovery, RL models are used to generate and refine new molecular structures by optimizing multiple properties such as potency, solubility, and toxicity at the same time.

Example: Companies like DeepMind and Insilico Medicine have successfully applied RL-based models to design a novel fibrosis drug in just 46 days, demonstrating its remarkable efficiency in accelerating drug development [6].

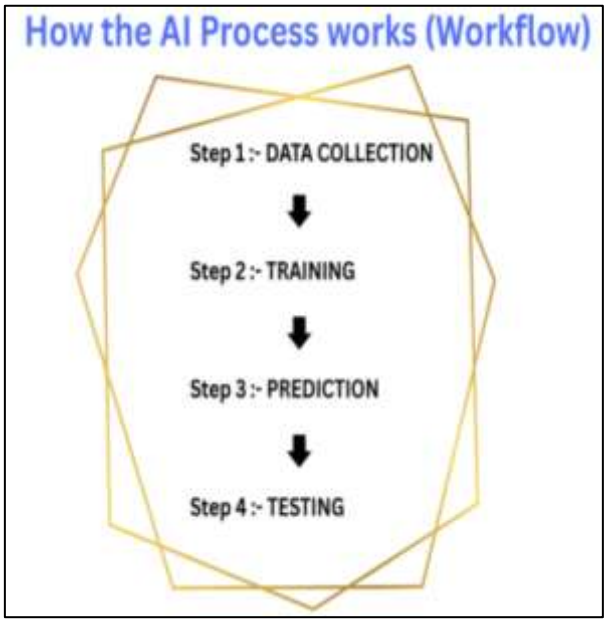

Figure 2: - AI Algorithm Workflow in Drug Discovery

5. Applications of AI in Drug Discovery

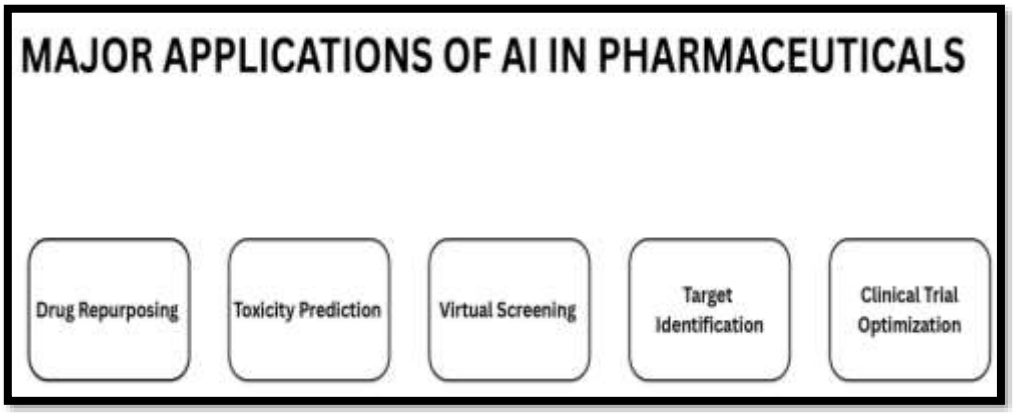

Figure 3: - Applications of AI in Drug Discovery

Artificial Intelligence (AI) has become an integral part of nearly every stage of modern drug discovery. Its greatest strengths lie in speed, precision, and data-handling capability, allowing researchers to analyze massive biological and chemical datasets that would otherwise take years to process manually. The following section highlights the key applications of AI in pharmaceutical research and development.

Target Identification

The initial stage of drug discovery focuses on identifying a biological target, typically a protein or enzyme associated with a disease. Artificial Intelligence (AI) assists researchers by analyzing genomic, proteomic, and clinical datasets to determine which targets are most responsive to therapeutic intervention [28]. Machine Learning algorithms can uncover hidden relationships between genes and diseases, while Deep Learning models help in analyzing protein 3D structures to locate possible binding regions.

Examples:

1. AlphaFold predicts protein folding patterns, helping scientists identify potential druggable targets [1].

2. AI-based systems like Deep Target and BenevolentAI analyze extensive biomedical databases to propose novel targets for complex conditions such as cancer and Alzheimer's disease [31].

Lead Discovery

After selecting a biological target, the next goal is to find potential compounds (leads) that can bind effectively to it. Traditional high-throughput screening methods are costly and time-consuming, but AI significantly accelerates this process.

Virtual screening: AI models predict which chemical compounds are most likely to interact with the target structure [29].

Generative models: Deep learning algorithms design new molecules with specific desired biological properties [26].

Example: The AtomNet platform employs convolutional neural networks (CNNs) to predict molecular interactions accurately and identify promising leads [4].

Lead Optimization

Once potential leads are discovered, they must be optimized to enhance efficacy, selectivity, and safety. AI systems can forecast how chemical modifications influence bioactivity and ADMET properties (Absorption, Distribution, Metabolism, Excretion, and Toxicity) [30]. Moreover, Reinforcement Learning (RL) algorithms can recommend structural changes to achieve optimal molecular properties [26].

Drug Repurposing

AI also enables the rediscovery of new applications for existing drugs, saving both cost and development time. Machine learning models analyze drug databases and disease pathways to identify additional therapeutic uses [31].

Example: During the COVID-19 pandemic, AI-based screening rapidly identified antiviral candidates from existing drugs within weeks — a task that would traditionally take months [11].

Toxicity Prediction

Ensuring safety is a crucial step in drug development. AI-powered systems predict toxic or adverse effects even before laboratory testing. By studying chemical structures and biological data, ML and DL models can detect compounds with potential safety concerns [32]. This early prediction reduces the likelihood of failures during preclinical and clinical testing stages.

Clinical Trial Optimization

AI also transforms clinical trial management by enhancing both speed and accuracy:

Patient stratification: AI selects the most appropriate candidates for trials using real-world clinical and genomic data.

Outcome prediction: Predictive algorithms estimate drug efficacy and possible side effects in diverse populations [33].

NLP integration: Natural Language Processing (NLP) scans patient records and clinical data to match eligibility criteria efficiently.

Example: IBM Watson Health applied AI tools to forecast trial success rates and optimize study design, reducing the overall time-to-market for oncology drugs [12].

De Novo Drug Design

De novo drug design involves creating entirely new molecular entities from scratch, bypassing the need for physical compound synthesis during the early discovery phase. AI models use molecular fingerprints and SMILES strings to design novel compounds with desired pharmacological properties. Graph-based algorithms further enable property-driven molecule generation.

Example: A collaboration between AstraZeneca and NVIDIA successfully employed generative AI to develop new antibiotic candidates targeting drug-resistant bacteria [9].

ADMET Prediction

Testing a compound's ADMET characteristics is one of the costliest stages in pharmaceutical R&D. AI models help predict these profiles early in the discovery process, significantly reducing the risk of failure in later trials. Commonly used models include Support Vector Machines (SVMs) and Random Forests (RFs). AI-based tools such as DeepTox and ADMETlab 2.0 deliver accurate toxicity and pharmacokinetic predictions, enhancing drug safety assessments.

Example: The DeepTox model outperformed conventional QSAR techniques by predicting compound toxicity across multiple benchmark datasets [10].

SUMMARY

AI has revolutionized the process of drug discovery, making it faster, more accurate, and less expensive. Platforms such as AlphaFold, AtomNet, and Insilico Medicine illustrate how AI can rapidly convert data-driven concepts into viable drug candidates [1,4,5]. The subsequent part of the discussion will focus on the challenges and limitations of AI, alongside its future prospects within pharmaceutical research.

6. Challenges and Future Prospects of Artificial Intelligence in Drug

Discovery

Although artificial intelligence (AI) has revolutionized various stages of drug discovery, several challenges persist that must be addressed to achieve its full potential in pharmaceutical research and development.

Data Quality and Availability

The efficiency of AI models largely depends on the quality and comprehensiveness of the datasets used for training. Incomplete, biased, or noisy data can result in unreliable or misleading predictions [34]. Moreover, several publicly available databases lack consistent or sufficient information, particularly concerning rare diseases or uncommon chemical compounds. Privacy regulations associated with clinical and patient data further restrict access, thereby slowing the development and validation of AI algorithms [35].

Model Interpretability

A significant limitation of AI, particularly deep learning-based systems, is their lack of transparency. These models often function as "black boxes," making it difficult for researchers to interpret the rationale behind specific predictions. This opacity hampers scientific validation and reduces confidence among clinicians, pharmaceutical scientists, and regulatory bodies [36]. Ensuring interpretability and explainability in AI models is therefore essential for their ethical and effective deployment in drug discovery.

Regulatory Challenges

The integration of AI into the pharmaceutical domain presents complex regulatory challenges. Current frameworks and guidelines for validating AI models in drug development are still evolving [37]. While agencies such as the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMA) are developing regulatory pathways, the approval of AI-generated drug candidates remains intricate and time-consuming. Establishing standardized evaluation procedures will be vital for the safe and efficient adoption of AI technologies in this field.

Ethical Concerns

Ethical considerations are central to the responsible use of AI in healthcare and drug research. Potential biases within datasets can lead to unequal or inappropriate therapeutic recommendations [38]. Furthermore, overreliance on AI-driven decisions without adequate human supervision may compromise patient safety. Therefore, maintaining transparency, accountability, and human oversight is essential in AI-assisted drug development.

Computational Limitations

Despite the advanced capabilities of AI, its successful implementation requires significant computational infrastructure. Training deep learning models demands high-performance graphics processing units

(GPUs) and extensive memory, resources that may not be accessible in all research laboratories. Consequently, smaller institutions may find it difficult to reproduce or validate large-scale AI studies, limiting broader adoption of these technologies [39].

FUTURE PERSPECTIVES

In spite of the challenges mentioned above, the future of AI in drug discovery appears highly promising. Several emerging trends highlight its transformative potential:

1. Multimodal AI Systems: Integrating chemical, genomic, and clinical data can enable more accurate predictions and drug-target interactions [40].
2. Generative AI Models: These can design novel molecular structures with desired pharmacological properties more efficiently than traditional computational methods [26].
3. Integration with Robotics: The combination of AI and automated laboratory systems can facilitate high-throughput experimentation with minimal human intervention.
4. Personalized Medicine: AI can contribute to the design of drugs tailored to individual genetic profiles, enhancing therapeutic efficacy and minimizing adverse effects [41].
5. Global Collaboration: Cloud-based AI platforms promote international data sharing and collaborative research, accelerating innovation in drug discovery.

Overall, AI should not be viewed as a replacement for human expertise but rather as a transformative tool that enhances decision-making, reduces development costs, and expedites the discovery of novel therapeutics [42].

CONCLUSION

Artificial intelligence (AI) has revolutionized modern pharmaceutical research by making drug development processes faster, more efficient, and cost-effective. AI-driven technologies have helped overcome long-standing challenges in areas such as target identification, molecular design, clinical trial optimization, and drug repurposing. Advanced algorithms—including deep learning, graph neural networks, and reinforcement learning—enable researchers to analyze vast chemical spaces, predict complex biological interactions, and design innovative drugs with improved safety and efficacy. However, despite its growing impact, the full-scale adoption of AI in drug discovery faces barriers related to data reliability, model transparency, regulatory acceptance, and ethical concerns. Addressing these issues will require global collaboration, improved data infrastructures, and stronger partnerships between computational scientists and pharmaceutical professionals. In the future, the integration of AI with breakthrough technologies such as quantum computing, cloud-based simulations, and multi-omics analysis will further advance pharmaceutical innovation. AI is evolving from a supportive tool into a foundational element of next-generation drug discovery and precision medicine. With sustained research efforts and ethical application, artificial intelligence holds the potential to redefine healthcare by delivering safer, more effective, and affordable therapies to patients around the world.

REFERENCES

1. Jumper J, Evans R, Pritzel A, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021; 596:583-589.
2. Tunyasuvunakool K, Adler J, Wu Z, et al. Highly accurate protein structure prediction for the human proteome. Nature. 2021; 596:590-596.
3. Kovalevskiy O, et al. AlphaFold two years on: Validation and impact. Proc Natl Acad Sci U S A. 2024;121: e2305678121.
4. Wallach I, Dzamba M, Heifets A. AtomNet: A deep convolutional neural network for bioactivity prediction in structure-based drug discovery. J Chem Inf Model. 2015; 55:1953-1962.
5. Zhavoronkov A, et al. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nat Biotechnol. 2019; 37:1038-1040.
6. Kola I, Landis J. Can the pharmaceutical industry reduce attrition rates? Nat Rev Drug Discov. 2004; 3:711-715.
7. Vamathevan J, Clark D, Czodrowski P, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019; 18:463-477.
8. Parvathaneni M, et al. Application of artificial intelligence and machine learning in drug

discovery and development. J Drug Deliv Ther. 2023;13(1):151-158.
9. Laddha C, Shelke A, Vaidya Y, et al. A review on artificial intelligence in drug discovery & pharmaceutical industry. Asian J Pharm Res Dev. 2023;11(3):45-51.
10. Hasselgren C, Oprea TI. The role of AI in drug discovery. ChemBioChem. 2024;25: e202300567.
11. Beck BR, et al. Predicting commercially available antiviral drugs that may act on SARS-CoV-2 through a drug-target interaction deep learning model. Comput Struct Biotechnol J. 2020; 18:784-790.
12. Wadighare UA, Deshmukh SP. A review on artificial intelligence and machine learning used in pharmaceutical research. GSC Biol Pharm Sci. 2024;26(1):191–198.
13. Scannell JW, Blanckley A, Boldon H, Warrington B. Diagnosing the decline in pharmaceutical R&D efficiency. Nat Rev Drug Discov. 2012; 11:191-200.
14. Parvathaneni M, et al. Application of artificial intelligence and machine learning in drug discovery and development. J Drug Deliv Ther. 2023;13(1):151-158.
15. Kola I, Landis J. Can the pharmaceutical industry reduce attrition rates? Nat Rev Drug Discov. 2004;3:711-715.
16. Dhudum R, Ganeshpurkar A, Pawar A. Revolutionizing drug discovery: A comprehensive review of AI applications. Drugs and Drug Candidates. 2024;3(1):148-171.
17. Parvathaneni M, et al. Application of artificial intelligence and machine learning in drug discovery and development. J Drug Deliv Ther. 2023;13(1):151-158.
18. Serrano DR, et al. Artificial intelligence applications in drug discovery and development review. Open Access J Pharm Res. 2024; 5:22-38.
19. Vamathevan J, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019; 18:463-477.
20. Dhudum R, et al. Revolutionizing drug discovery: A comprehensive review of AI applications. Drugs and Drug Candidates. 2024;3(1):148-171.
21. Parvathaneni M, et al. Application of artificial intelligence and machine learning in drug discovery and development. J Drug Deliv Ther. 2023;13(1):151-158.
22. Yao R, et al. Knowledge mapping of Graph Neural Networks for drug discovery. Front Pharmacol. 2024; 15:1234567.
23. Zhang O, Lin H, Zhang H, et al. Graph neural networks in modern AI-aided drug discovery. J Chem Inf Model. 2024; 64:789-802.
24. Jumper J, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021; 596:583-589.
25. Dhudum R, et al. Revolutionizing drug discovery: A comprehensive review of AI applications. Drugs and Drug Candidates. 2024;3(1):148-171.
26. Zhong Z, Barkova A, Mottin D. Knowledge-augmented graph machine learning for drug discovery: A survey. arXiv preprint. 2023; arXiv:2302.08261.
27. DeepChem. Open-source toolkit for deep-learning in chemistry and biology [Internet]. 2023 [cited 2025 Dec 21]. Available from: https://deepchem.io
28. Nag S, Baidya ATK, Mandal A. Deep learning tools for advancing drug discovery and development. 3 Biotech. 2022; 12:110.
29. Wallach I, Dzamba M, Heifets A. AtomNet: A deep convolutional neural network for bioactivity prediction. J Chem Inf Model. 2015; 55:1953-1962.
30. Parvathaneni M, et al. Application of artificial intelligence and machine learning in drug discovery and development. J Drug Deliv Ther. 2023;13(1):151-158.
31. Beck BR, et al. Predicting commercially available antiviral drugs for SARS-CoV-2 using deep learning. Comput Struct Biotechnol J. 2020; 18:784-790.
32. Wadighare UA, Deshmukh SP. A review on artificial intelligence and machine learning used in pharmaceutical research. GSC Biol Pharm Sci. 2024;26(1):191–198.
33. Ocana A, et al. Integrating artificial intelligence in drug discovery and early development. Biomark Res. 2025; 13:7.
34. Serrano DR, et al. AI applications review. Open Access J Pharm Res. 2024; 5:22-38.
35. Vamathevan J, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019; 18:463-477.

36. Zhang O, Lin H, Zhang H, et al. Deep lead optimization: Leveraging generative AI for structural modification. arXiv preprint. 2024; arXiv:2404.19230.
37. FDA. Artificial intelligence and machine learning in drug development guidance [Internet]. 2023. Available from: https://www.fda.gov/media/155618/download
38. Naik N, Hameed BMZ, Shetty DK, et al. Legal and Ethical Consideration in Artificial Intelligence in Healthcare: Who Takes Responsibility? Front Surg. 2022; 9:266.
39. Karimian G, Petelos E, Evers SMAA. The ethical issues of the application of artificial intelligence in healthcare: A systematic scoping review. AI Ethics. 2022; 2:539-551.
40. Veeresh Kumar R, Saxena C, Mukul K, Brijay H. The role of artificial intelligence in modern drug discovery and development. Asian J Pharm Res Dev. 2025;13(2):79-81.
41. Dhudum R, Ganeshpurkar A, Pawar A. Revolutionizing drug discovery: A comprehensive review of AI applications. Drugs and Drug Candidates. 2024;3(1):148-171.
42. Mouchlis VD, Afantitis A, Serra A, et al. Advances in de Novo drug design: from conventional to machine learning methods. Int J Mol Sci. 2021; 22:1676.
43. Tovar A, Eckert H, Bajorath J. Comparison of 2D fingerprint methods for multiple-template similarity searching on compound activity classes of increasing structural diversity. ChemMedChem. 2007; 2:208-217.
44. Carracedo-Reboredo P, Linares-Blanco J, Rodriguez-Fernandez N, et al. A review on machine learning approaches and trends in drug discovery. Comput Struct Biotechnol J. 2021; 19:4538-4558.

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