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A SYSTEMATIC REVIEW ON ROLE AND IMPACT OF ARTIFICIAL INTELLIGENCE IN DRUG DESIGN

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Abstract

Drug discovery is a time-consuming, costly, and complex process with high attrition rates at multiple stages. Artificial intelligence (AI) has emerged as a transformative tool in modern drug design, offering the ability to analyze large chemical, biological, and clinical datasets, predict molecular interactions, and optimize compounds in silico. This review systematically examines the role, applications, tools, and impact of AI in drug discovery, focusing on machine learning, deep learning, natural language processing, and reinforcement learning. Key applications include target identification and validation, lead compound discovery, de novo drug design, drug repurposing, ADMET prediction, and clinical trial optimization. AI has demonstrated significant potential in reducing time and cost, improving predictive accuracy, and accelerating the development of novel therapeutics. The review also highlights AI-driven software platforms, challenges such as data quality and model interpretability, and emerging trends including integration with omics, personalized medicine, explainable AI, and fully automated drug design. Overall, AI is reshaping pharmaceutical research, offering unprecedented opportunities to enhance efficiency, innovation, and precision in drug development.

Keywords: Artificial Intelligence; Drug Discovery; Machine Learning; Deep Learning; Drug Design; Drug Repurposing; ADMET Prediction; Personalized Medicine.

1. Introduction

Target identification, lead compound discovery, preclinical testing, and clinical trials are typically included in the complicated, costly, and time-consuming process of drug discovery. A single drug's development can cost over $1 billion, require more than ten years, and have substantial attrition rates at every stage (Hessler & Baringhaus, 2018; Wang et al., 2018). Conventional methods frequently depend on labour-intensive experimentation, high-throughput screening, and trial-and-error techniques, which restrict productivity and creativity. Artificial intelligence (AI) has been a game-changing technology in drug design in recent years. It can analyse large datasets, anticipate chemical interactions, and optimise compounds in silico, all of which speed up the drug development process. (Li et al., 2025; Vamathevan et al., 2019).

From target identification and lead optimisation to drug repurposing and clinical trial design, artificial intelligence (AI) technologies, such as machine learning, deep learning, natural language processing, and reinforcement learning, have shown considerable promise in various phases of drug discovery (Huang et al., 2022; Singh et al., 2023). AI speeds up and lowers the cost of medication development by combining chemical, biological, and clinical data. It also improves prediction accuracy and facilitates the identification of new treatments. The purpose of this systematic review is to examine the function, uses, resources, and effects of AI in drug discovery, emphasising present achievements, constraints, and new developments influencing pharmaceutical research going forward.

AI's importance in drug discovery has been reinforced by recent developments in algorithm development, big data availability, and processing capacity. Multi-modal datasets, including chemical libraries, high-throughput screening findings, omics data, and real-world clinical information, can now be integrated by AI models to produce previously unachievable actionable insights (Huang et al., 2022; Vamathevan et al., 2019). Additionally, researchers may effectively explore large chemical spaces, find new therapeutic candidates, and optimise pharmacokinetic and safety profiles before entering expensive experimental phases thanks to AI-driven techniques including de novo drug creation, drug repurposing, and ADMET prediction. As a result, AI not only improves the efficiency and cost-effectiveness of drug development but also enhances innovation, paving the way for personalized medicine and next-generation therapeutics.

2. Overview of Artificial Intelligence in Drug Design

2.1 Definition and Scope of AI

Artificial intelligence (AI) makes it possible for robots to carry out activities like learning from data, identifying patterns, and making predictions that need human-like intellect. AI, such as machine learning, deep learning, and neural network models, is used in drug design to predict molecular features and interactions by analysing huge chemical and biological datasets (Hessler & Baringhaus, 2018; Li et al., 2025). Target identification, virtual screening, and ADMET prediction are only a few of the drug discovery pipeline's uses. It enables the automation of difficult operations and the analysis of high-dimensional data. Compared to conventional methods, this improves candidate selection, saves time and money, and increases accuracy (Hessler & Baringhaus, 2018; Wang et al., 2018; Li et al., 2025).

2.2 Types of AI Technologies Used in Drug Discovery

2.2.1 Machine Learning (ML)

Algorithms may learn from data and make predictions without explicit programming thanks to machine learning (ML), a fundamental AI technology. ML has been widely used in drug development for target identification, virtual screening, and quantitative structure–activity relationship (QSAR) modelling (Dara et al., 2021). Researchers can prioritise promising discoveries for additional experimental validation by using machine learning (ML) models to predict the activity, selectivity, and toxicity of drugs by analysing massive chemical and biological datasets. Support vector machines (SVMs), random forests, and gradient boosting models are examples of techniques that have been shown to be successful in increasing the speed and accuracy of candidate selection, which lowers the expense and duration of the early phases of drug development (Singh et al., 2023).

2.2.2 Deep Learning (DL)

A specialised branch of machine learning called deep learning (DL) models complex, high-dimensional data using multi-layered neural networks. DL is very useful in drug design for de novo molecular design, ADMET characteristics, and drug–target interaction prediction (Singh et al., 2023; Lac et al., 2024). Molecular graphs, sequences, and structural data can be processed by convolutional neural networks (CNNs) and recurrent neural networks (RNNs)

to produce precise biological activity predictions. DL models can identify new compounds and improve lead optimisation accuracy by revealing hidden patterns in chemical space that are challenging for conventional ML techniques to find (Lac et al., 2024).

2.2.3 Natural Language Processing (NLP)

The AI technique known as natural language processing (NLP), which was first created to comprehend human language, has been modified for use in drug discovery to extract information from unstructured text, including scholarly papers, patents, and clinical trial data (Bhat & Ahmed, 2025). NLP methods can automatically find connections between genes, proteins, and illnesses, offering information for target prioritisation and therapeutic repurposing. To find previously undiscovered molecular targets or therapeutic processes, for example, NLP-driven models may process millions of abstracts, greatly enhancing the data available for computational drug design (Singh et al., 2023).

2.2.4 Reinforcement Learning (RL)

According to Popova, Isayev, and Tropsha (2018), reinforcement learning (RL) is an AI paradigm where an agent learns to make the best choices by interacting with its surroundings and getting feedback in the form of incentives. RL and generative models have been used in drug discovery to explore chemical space and optimise molecule structures for desirable features including pharmacokinetics, potency, and selectivity. RL algorithms can independently suggest new compounds by setting reward functions based on chemical and biological criteria, which speeds up the creation of molecules with improved medicinal potential (Rashid & Ahmed, 2025).

Table 1: Key AI Technologies and Their Applications in Drug Discovery

AI Technology	Description	Applications in Drug Discovery
Machine Learning (ML)	Algorithms that learn patterns from structured data	Target identification, QSAR modeling, ADMET prediction
Deep Learning (DL)	Neural networks with multiple layers for complex pattern recognition	De novo drug design, molecular property prediction, protein-ligand binding prediction

Natural Language Processing (NLP)	Extraction and analysis of information from scientific literature	Literature mining for drug repurposing, target discovery
Reinforcement Learning (RL)	AI learns optimal strategies through trial-and-error	De novo drug design, molecule optimization
Explainable AI (XAI)	Techniques to interpret black-box AI models	Understanding molecular predictions, regulatory compliance

2.3 Comparison of AI-Based vs Traditional Drug Design

In order to find and optimise lead compounds, traditional drug discovery is a time-consuming and resource-intensive process that usually entails high-throughput screening, iterative chemical synthesis, and extensive in vitro and in vivo testing (Hessler & Baringhaus, 2018). With high attrition rates during preclinical and clinical stages, this traditional technique frequently takes 10–15 years and costs more than $1 billion each successful drug (Wang et al., 2018). AI-based drug design, on the other hand, uses computational models to predict molecular interactions, analyse large chemical and biological datasets, and optimise candidate compounds in silico, all of which speed up decision-making and lessen the workload associated with experiments (Li et al., 2025; Singh et al., 2023). AI systems, for instance, can anticipate ADMET qualities, find interesting therapeutic targets, virtually screen millions of compounds, and even create new molecular structures, all of which greatly reduce the time needed for drug development and increase the likelihood of success. AI enhances conventional techniques by increasing productivity, accuracy, and creativity, making the drug development process more economical and data-driven even if it cannot completely replace experimental validation (Hessler & Baringhaus, 2018; Li et al., 2025).

Table 2: Comparison of Traditional vs AI-Based Drug Design Approaches

Parameter	Traditional Drug Design	AI-Based Drug Design	Impact/Advantage
Time required	10–15 years	2–5 years for early-stage discovery	Accelerated pipeline, faster lead identification

Cost	>$1 billion per approved drug	Reduced due to in silico screening	Significant cost savings
Data handling	Manual, small datasets	Large-scale multi-modal data (omics, clinical, chemical)	More comprehensive insights
Predictive accuracy	Moderate, often trial-and-error	High, with ML/DL models predicting activity, toxicity, ADMET	Reduced attrition and higher success rates
Novelty	Limited by human intuition	Generative AI can propose novel molecules	Expands chemical space and innovation potential
Optimization	Iterative lab-based experiments	Computational optimization of ADMET, binding, toxicity	Efficient compound refinement

3. Applications of AI in Drug Discovery and Design

3.1 Target Identification and Validation

Target identification and validation, which involve identifying biomolecules—such as proteins, enzymes, or genes—that are connected to disease processes, are fundamental stages in the drug discovery process. Conventional methods rely on time-consuming, labour-intensive experimental assays and literature mining, which frequently produce insufficient results. By combining omics datasets (genomics, transcriptomics, and proteomics) to more accurately anticipate disease-associated targets, AI has revolutionised this approach (Huang et al., 2022). While deep learning algorithms can model intricate protein-protein interactions to evaluate druggability, machine learning models can examine correlations across several datasets to find previously undiscovered targets.

AI also helps with target validation, which enables researchers to rank the most promising targets for therapeutic benefit. By simulating downstream signalling and the network effects of target modulation, predictive models can lower the failure rates of experiments. AI speeds up the identification of actionable targets and helps with early-stage prioritisation by fusing high-dimensional data with pattern recognition, which eventually reduces time and expense in drug development pipelines (Vamathevan et al., 2019).

3.2 Lead Compound Discovery

In lead compound discovery, chemical entities are screened against verified targets to identify compounds with potential biological action. Through QSAR modelling, virtual screening, and structure-based predictions, AI improves this process (Dara et al., 2021). High-throughput prioritisation of potential compounds from millions of possibilities is made possible by machine learning algorithms' ability to evaluate chemical descriptors and forecast binding affinities. By suggesting novel compounds with anticipated bioactivity profiles, generative models significantly broaden chemical space and lessen the need for trial-and-error experimentation.

Beyond preliminary screening, AI helps in scaffold selection and activity prediction, finding compounds with the best pharmacodynamic and physicochemical characteristics (Chen et al., 2020). By increasing hit rates and reducing time spent on ineffective synthetic pathways, these techniques increase the efficiency of the early stages of drug development. The smooth transition from computational prediction to experimental validation is made possible by integration with laboratory automation.

3.3 De Novo Drug Design

Developing completely novel molecular entities that are optimised for the intended therapeutic effects is known as de novo drug design. In order to create compounds with high target specificity and advantageous ADMET profiles, artificial intelligence (AI), in particular deep generative models and reinforcement learning, makes it possible to explore large chemical spaces (Popova, Isayev, & Tropsha, 2018). AI can suggest new compounds not found in current chemical libraries by iteratively improving candidate structures based on reward functions (such as binding affinity or synthesis feasibility).

Additionally, this method facilitates multi-objective optimisation by concurrently balancing pharmacokinetic characteristics, potency, and selectivity. By combining reinforcement learning with predictive ADMET models, AI reduces late-stage failures and enhances innovation potential in drug discovery (Rashid & Ahmed, 2025). De novo design has been applied successfully to develop lead candidates for oncology, infectious diseases, and neurological disorders.

3.4 Drug Repurposing

Drug repurposing offers a quicker and less expensive path to clinical use by identifying new therapeutic uses for already-approved medications. By combining biological, chemical, and clinical data to identify new drug-disease connections, AI speeds up this process (Zhou et al., 2021). Alternative targets can be predicted and pertinent information can be extracted from literature using machine learning, graph-based models, and natural language processing. Notably, AI was able to prioritise candidates, lower costs, and accelerate time-to-market during the COVID-19 pandemic by identifying antivirals with potential efficacy against SARS-CoV-2 (Zhou et al., 2021).

3.5 ADMET Prediction (Absorption, Distribution, Metabolism, Excretion, Toxicity)

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3.6 Optimization of Drug Candidates

Lead compounds must be optimised to increase their potency, selectivity, and safety after they have been found. AI makes this possible by simulating molecular changes to improve therapeutic qualities through predictive models of structure–activity connections (Lac et al., 2024). Reinforcement learning techniques reduce experimental trial-and-error cycles by iteratively proposing chemical alterations guided by predetermined objectives.

Additionally, AI helps forecast toxicity and off-target effects, ensuring that candidate compounds are safer before moving on to preclinical or clinical trials. AI greatly reduces lead optimisation durations and increases the likelihood of clinical success by combining multi-objective optimisation with predictive modelling (Singh et al., 2023).

3.7 Clinical Trial Design and Prediction

By predicting trial outcomes, optimising inclusion criteria, and identifying patient subgroups likely to respond to therapy, AI aids in the design of clinical trials (Beam & Kohane, 2018). By analysing actual patient data, machine learning models may foresee adverse events, simulate trial outcomes, and direct dosage methods, all of which increase trial efficiency.

Additionally, AI makes adaptive trial design possible, which maximises statistical power and patient safety by dynamically modifying procedures depending on ongoing trial data (Miotto et al., 2018). By increasing trial design accuracy, this shortens trial duration, lowers expenses, and increases the possibility of regulatory clearance.

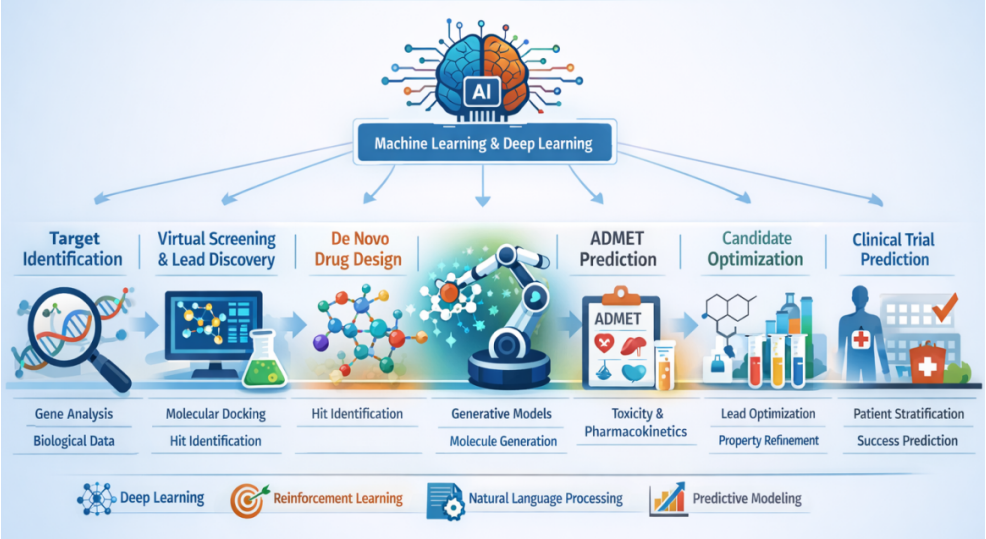

Figure 1: Workflow of AI-Driven Drug Discovery

4. Tools, Algorithms, and Platforms in AI-Driven Drug Design

4.1 Commonly Used Machine Learning Models

AI-driven drug design makes extensive use of machine learning (ML) models to forecast molecular characteristics, bioactivity, and toxicity. Random Forest (RF) provides resilience for ADMET prediction and QSAR modelling by constructing several decision trees and

aggregating findings (Dara et al., 2021). Support Vector Machines (SVMs), which are especially useful for smaller datasets with fewer samples, classify molecules by identifying the best hyperplanes in descriptor space (Chen et al., 2020).

By capturing intricate nonlinear correlations in chemical and biological data, artificial neural networks (ANNs) make it possible to predict pharmacokinetics, solubility, and binding affinities (Singh et al., 2023). When combined, RF, SVM, and ANNs offer a flexible toolkit for early-stage drug development that combines prediction accuracy, scalability, and interpretability to speed up candidate selection.

4.2 Deep Learning Architectures

Convolutional Neural Networks (CNN)

One kind of deep learning model that is especially well-suited for examining spatial or grid-like data, including chemical structures depicted as graphs or three-dimensional grids, is the convolutional neural network (CNN) (Lac et al., 2024). CNNs outperform conventional machine learning models in capturing intricate nonlinear interactions in drug design by extracting hierarchical characteristics from chemical structures to predict binding affinity, biological activity, and pharmacokinetic aspects.

CNNs have been used in protein-ligand interaction prediction, virtual screening, and de novo drug discovery to enable automated feature extraction and lessen reliance on manually created descriptors (Chen et al., 2020; Lac et al., 2024). CNNs improve prediction accuracy and speed up early-stage drug development processes by directly learning structural patterns from molecular representations.

Recurrent Neural Networks (RNN)

Deep learning models called Recurrent Neural Networks (RNNs) are perfect for analysing molecular sequences like SMILES strings or protein sequences because they can analyse sequential data by retaining recollection of prior inputs (Lac et al., 2024). By capturing the connections between sequence segments that conventional models could miss, RNNs can predict molecular characteristics, bioactivity, and chemical reaction outcomes in drug discovery.

RNNs have been used in de novo drug design, peptide and protein modelling, and reaction outcome prediction, enabling the automated synthesis of novel compounds with desired characteristics (Chen et al., 2020). In addition to existing deep learning architectures like CNNs and GNNs, RNNs enhance forecast accuracy and facilitate the exploration of novel chemical space by identifying sequential patterns in chemical or biological data.

Graph Neural Networks (GNN)

For molecular representations where atoms are nodes and bonds are edges, Graph Neural Networks (GNNs), deep learning models created especially to work with graph-structured data, are perfect (Lac et al., 2024). GNNs are able to accurately predict chemical characteristics, bioactivity, and interactions between substances and targets by capturing the topological and relational information of molecules.

By directly learning from molecular graphs without the need for manually created descriptors, GNNs outperform typical ML models in drug discovery applications such as virtual screening, drug–target interaction modelling, and molecular property prediction (Chen et al., 2020). GNNs improve the identification of promising drug candidates and enable de novo molecule creation by efficiently modelling intricate structural interactions.

4.3 AI-Based Software Platforms and Databases

With readily available tools for molecular design, virtual screening, and predictive modelling, AI-based software platforms and databases are becoming crucial to contemporary drug discovery. A deep learning platform called AtomNet uses 3D structural data to predict protein–ligand binding, allowing for high-throughput virtual screening of millions of molecules (Wallach et al., 2015). DeepChem is an open-source framework that combines deep learning and machine learning techniques for generative molecule design, ADMET modelling, and molecular property prediction (Ramsundar et al., 2019). Chemprop provides precise activity and toxicity predictions without the need for manual feature engineering by using graph neural networks to predict molecular attributes directly from chemical structures (Yang et al., 2019).

These platforms greatly lower the computational barrier for researchers, enabling the incorporation of sophisticated AI models into drug development processes without requiring a high level of programming knowledge. They speed up the entire drug development process

by merging cutting-edge algorithms with high-quality chemical databases to enable quick lead identification, molecular optimisation, and drug repurposing (Ramsundar et al., 2019; Yang et al., 2019). Additionally, these platforms facilitate scalability and reproducibility, increasing the efficiency and accessibility of AI-driven medication design in both academic and commercial contexts.

5. Impact of AI on Drug Design

5.1 Reduction in Time and Cost of Drug Discovery

By enabling in silico screening, predictive modelling, and automated lead optimisation, AI has greatly improved the drug development process by lowering reliance on drawn-out experimental processes. According to Hessler and Baringhaus (2018), traditional drug development frequently requires ten to fifteen years and more than a billion dollars for each authorised medication. Businesses can save a significant amount of time and money by using AI technologies to quickly choose potential candidates, cut down on experimental iterations, and expedite preclinical research (Li et al., 2025).

For instance, while traditional high-throughput screening may take months or years, AI-driven platforms may digitally screen millions of compounds in a matter of days. In addition to reducing late-stage attrition, computational optimisation of ADMET characteristics and binding affinities early in the pipeline also lowers development costs (Singh et al., 2023). These efficiencies make drug discovery more agile and economically sustainable, particularly for rare diseases or urgent therapeutic needs.

5.2 Improvement in Accuracy and Predictive Power

By identifying intricate patterns in chemical, biological, and clinical datasets, AI improves the precision and predictive capacity of drug discovery. When predicting bioactivity, toxicity, and pharmacokinetics, machine learning and deep learning models perform better than conventional QSAR and statistical methods (Zhang et al., 2020; Lac et al., 2024). More accurate predictions of drug-target interactions and off-target effects are made possible by the ability of graph neural networks, convolutional neural networks, and other architectures to capture chemical structural relationships and sequence dependencies.

In order to produce comprehensive forecasts, AI can also use multi-modal datasets, such as omics, structural biology, and clinical trial data. This improves total drug development

success rates by lowering the probability of failure during preclinical and clinical stages. AI transforms predictive drug creation by enabling researchers to concentrate on candidates with the best chance of success by fusing speed and accuracy (Huang et al., 2022).

5.3 Success Stories and Case Studies

AI has already produced some noteworthy drug discovery success stories. For example, DeepMind's AlphaFold significantly improved protein structure prediction, speeding up target-based drug design (Jumper et al., 2021), while AtomNet discovered new inhibitors for protein targets that were experimentally confirmed (Wallach et al., 2015). During the COVID-19 pandemic, AI also made it easier to quickly repurpose medications by finding already-existing substances that might have antiviral properties (Zhou et al., 2021).

AI has been used by pharmaceutical corporations in oncology, infectious diseases, and uncommon genetic abnormalities, leading to improved drug candidates and quicker lead identification. According to case studies, artificial intelligence (AI) not only saves money and time but also fosters creativity by making it possible to find chemicals that would have been difficult to detect with traditional techniques (Li et al., 2025; Singh et al., 2023). These achievements demonstrate AI's revolutionary potential in contemporary medication design.

5.4 Limitations and Challenges

AI in drug design has a number of drawbacks despite its revolutionary potential. Because AI models need big, diversified, and well-annotated datasets to generate accurate predictions, data quality and availability continue to be major challenges. The incompleteness, bias, and inconsistency of many public chemical and biological datasets might impair model performance and restrict generalisability across various pharmacological targets or disease domains (Huang et al., 2022; Walters & Murcko, 2020).

The interpretability of AI models is another difficulty. CNNs, RNNs, and GNNs are examples of deep learning architectures that frequently function as "black boxes," making it challenging for academics and regulatory bodies to comprehend how predictions are made. In high-stakes decision-making, this lack of openness might impede confidence, model validation, and adoption (Rudin, 2019). Widespread adoption is further hampered by ethical and legal issues such patient data privacy, intellectual property, and accountability for AI-

driven judgements. For the safe, dependable, and responsible application of AI in drug discovery, adherence to ethical standards and legal frameworks is crucial (Topol, 2019).

6. Future Perspectives and Emerging Trends

6.1 Integration of AI with High-Throughput Screening and Omics

One significant development in drug discovery is the integration of AI with multi-omics data and high-throughput screening (HTS). To find disease pathways, therapeutic targets, and possible drug candidates, AI models may examine large datasets from genomes, transcriptomics, proteomics, and metabolomics (Huang et al., 2022). By combining these insights with HTS, bioactive chemicals can be identified more quickly and efficacy can be predicted in a variety of biological situations.

Network-based drug development, in which AI finds connections between genes, proteins, and small molecules throughout intricate disease networks, is further supported by this integration. By utilising patterns in omics datasets that are challenging for conventional techniques to identify, this technology improves the capacity to create multitarget medications or repurpose already-existing molecules.(Vamathevan et al., 2019).

6.2 AI in Personalized Medicine

AI is being used more and more in personalised medicine to customise treatments according to each patient's unique genetic, epigenetic, and clinical characteristics. Optimal dosing techniques, toxicity risks, and patient-specific therapeutic responses can all be predicted by machine learning algorithms (Topol, 2019). This precise method increases efficacy, decreases side effects, and makes it possible to choose medication candidates for clinical trials more logically.

AI models can assist stratified clinical trial designs and expedite the development of precision therapies by identifying subpopulations that are likely to respond to a medication by merging patient-level multi-omics data with real-world clinical datasets (Huang et al., 2022). Due to the considerable patient heterogeneity in cancer and uncommon genetic illnesses, this trend is especially significant.

6.3 Explainable AI (XAI) in Drug Discovery

Explainable AI (XAI) is becoming a vital tool for solving the deep learning black-box problem in drug creation. The goal of XAI approaches is to increase regulatory acceptance and trust by offering comprehensible insights into how AI models create predictions (Rudin, 2019). The molecular substructures or biological characteristics that contribute most to projected bioactivity, for instance, can be identified using attention mechanisms or feature importance studies.

XAI bridges the gap between computational predictions and experimental biology by facilitating decision-making, model validation, and hypothesis creation. XAI promotes cooperation between computational scientists and experimental researchers while enabling safer and more responsible AI-driven drug discovery through increased transparency (Jiménez-Luna et al., 2020).

6.4 Potential for Fully Automated Drug Design

By combining robotic synthesis platforms, generative AI, reinforcement learning, and predictive ADMET models, fully automated drug creation is becoming more and more possible (Rashid & Ahmed, 2025). These systems can create, optimise, and assess drug candidates on their own, reducing the need for human participation and speeding up the discovery process.

Completely automated pipelines promise to speed up chemical space research and the creation of new treatments by lowering time, expense, and experimental workload. Ongoing developments point to a future in which AI-driven drug design can function as a largely self-contained, end-to-end system, even though complete automation faces difficulties with data quality, model interpretability, and experimental validation (Popova, Isayev, & Tropsha, 2018).

7. Conclusion

Drug development has been completely transformed by artificial intelligence, which makes it possible to identify and optimise therapeutic candidates more quickly, effectively, and precisely. AI can drastically cut down on the time and expense of drug development by using sophisticated computer models to analyse complicated datasets, forecast molecular interactions, create new drugs, and optimise pharmacokinetic and safety profiles. Emerging concepts like integration with multi-omics, personalised medicine, explainable AI, and

completely automated drug creation offer exciting paths for future innovation, even though issues like data quality, model interpretability, and regulatory considerations still exist. All things considered, artificial intelligence (AI) is a revolutionary paradigm in pharmaceutical research, boosting innovation, productivity, and success rates while opening the door for the next wave of safe and efficient treatments.

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9. Conflict of Interest

The author(s) declare that there are no conflicts of interest regarding the publication of this review.

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