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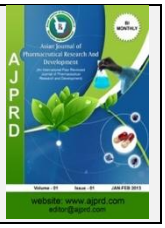

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Review Article

Artificial Intelligence Drug Discovery and Development

Subedar Ikra A., Bhandare Sangita N

Pravara Rural Education Society's College of Pharmacy (for Women), Chincholi, Nashik ,422102,Maharashtra, India

A B S T R A C T

The integration of Artificial Intelligence (AI) into drug discovery and development has revolutionized the pharmaceutical landscape by enabling faster, cost-effective, and data-driven innovations. Traditional drug discovery methods are time-consuming and expensive, often requiring over a decade and billions of dollars to bring a new drug to market. AI technologies such as Machine Learning (ML), Deep Learning (DL), and Natural Language Processing (NLP) significantly enhance each stage of the drug discovery pipeline—from target identification and virtual screening to lead optimization, toxicity prediction, and clinical trial design. By analyzing complex biological, chemical, and clinical datasets, AI facilitates the discovery of novel therapeutic targets, predicts molecular interactions, and improves drug safety and efficacy. Moreover, generative AI models accelerate de novo drug design, while AI-driven analytics enable personalized medicine and drug repurposing. Despite challenges such as data bias, interpretability, and regulatory constraints, AI's transformative potential continues to reshape pharmaceutical research, offering a faster, more efficient, and precise approach to developing next-generation therapeutics.

KEYWORDS: Artificial Intelligence (AI), Drug Discovery, Machine Learning (ML), Deep Learning (DL).

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*Address for Correspondence:

Subedar Ikra A, Pravara Rural Education Society's College of Pharmacy (for Women), Chincholi , Nashik ,422102,Maharashtra, India

INTRODUCTION

Drug discovery and development is still one of the most difficult and expensive processes in contemporary biomedical research. With a success rate of less than 10%, it takes 10 to 15 years and more than $2 billion USD on average to bring a single novel medicinal molecule to market (1). Traditional drug discovery relies mostly on empirical screening, repetitive experimental optimization, and serendipitous finds, all of which can result in inefficiency, high attrition rates, and increased development costs. One revolutionary approach to overcoming these obstacles is the incorporation of artificial intelligence (AI) into pharmaceutical research practices. AI helps scientists find and improve medication candidates more effectively by allowing robots to learn from data, spot intricate patterns, and make predictions (2). AI is capable of processing and analysing large chemical, genomic, and clinical datasets using sophisticated computer algorithms, which enables quicker and more precise identification of therapeutic targets, molecular interaction prediction, and evaluation of drug safety and efficacy (3). Artificial intelligence (AI)-powered tools like machine learning (ML), deep learning (DL), and natural language processing (NLP) have demonstrated great promise in a variety of drug discovery stages, from virtual screening and target identification to lead optimization, toxicity prediction, and drug repurposing (4). These models capture non-linear interactions and provide highly accurate predictions of pharmacological activity, outperforming conventional quantitative structure–activity relationship (QSAR) approaches (5). AI systems also speed up data curation and hypothesis creation by improving knowledge extraction from biomedical literature using NLP technologies. This feature is especially helpful for drug repurposing, which involves computationally screening current medications for novel indications (6). One example of AI's promise is the creation of DSP-1181, a chemical that was designed by AI to treat obsessive-compulsive disorder (OCD); the compound moved from design to human clinical trials in just one year, which is significantly faster than with conventional techniques (7).

By improving endpoint prediction, patient selection, and trial design, AI has also completely transformed clinical trial administration. By simulating patient responses, predictive analytics can assist researchers in determining the right dosage and reducing side effects (8). Moreover, interpretability offered by explainable AI (XAI) techniques enables scientists to comprehend the logic underlying computational predictions, boosting trust in AI-driven judgments (5). The synergy between AI and omics technologies—including genomics, proteomics, and metabolomics—fosters the development of precision and personalized medicine, tailoring treatments to individual patients based on genetic and molecular profiles (9). AI's integration into de novo drug design enables the generation of novel molecular structures with optimized pharmacokinetic and pharmacodynamic properties while reducing experimental workload (10). The development of precision and personalized medicine is facilitated by the collaboration of AI and omics technologies, such as proteomics, metabolomics, and genomics, which enable the customization of medicines for specific patients based on their genetic and molecular profiles (9). By integrating AI into de novo drug design, new molecular structures with improved pharmacokinetic and pharmacodynamic features can be created while the amount of experimental work is reduced (10). In summary, from target discovery to clinical validation, artificial intelligence is transforming the whole pharmaceutical pipeline. AI has potential for a paradigm shift toward quicker, more economical, and data-driven medication discovery and development by fusing computational power with biological knowledge. This will ultimately change the face of global healthcare in the future (7,9,10,11).

Overview of the Discovery Process

Drug discovery is a complex and exacting procedure that turns a scientific theory into a medicinal substance. It includes multiple pivotal phases, each with unique obstacles and approaches. By providing creative answers to conventional bottlenecks, the incorporation of Artificial Intelligence (AI) is having a growing impact on these phases (12,13).

Exploration and Progress

- Identifying and validating the target: The first stage is to determine which biological molecules—like proteins or genes—are essential to a disease. These targets have been verified to guarantee that modifying them can result in positive therapeutic effects. Machine learning algorithms and other AI approaches are currently used to analyse large biological datasets and anticipate possible targets (13,14).
- Hit Identification: To find "hits"—molecules that interact with the verified target—high-throughput screening (HTS) of compound libraries is carried out. The screening method is streamlined by AI models that help forecast a compound's binding affinity (13,15).
- Lead Optimization: Chemical changes are made to promising hits to improve its pharmacokinetic, potency, and selectivity. By forecasting molecular interactions and behaviour, AI-driven simulations can optimize these characteristics (12,13).

Preclinical Research

- In vitro and in vivo testing: To evaluate the safety and effectiveness of lead compounds, they are evaluated in lab and animal models. AI systems may lessen the need for animal testing by using preclinical data to forecast human reactions (12,16).
- Toxicology Studies: Prior to human testing, thorough investigations are carried out to detect any possible hazardous consequences. Artificial intelligence (AI) systems use chemical structure analysis to forecast toxicity, which helps detect negative effects early (13).
- Formulation Development: Researchers create the drug's formulation by choosing the best delivery system and dosage type. By forecasting the best delivery methods based on molecular characteristics, AI helps with medication formulation (15).

Clinical Research

- Phase I: Assesses the drug's pharmacokinetics, dose range, and safety in a small sample of healthy volunteers. In order to forecast the best dosage schedules and detect possible adverse effects, AI models examine early-phase data (16).
- Phase II: Performed on a wider patient population to evaluate the medication's effectiveness and adverse effects. By helping to identify subgroups that would benefit the most from the treatment, AI helps with patient stratification (13).
- Phase III: Involves extensive testing to verify the drug's efficacy, track side effects, and contrast it with conventional therapies. AI increases trial efficiency by analysing clinical trial data to find trends and forecast results (13,17).

Regulatory Review and Approval

- New Drug Application (NDA): The sponsor of the medication provides regulatory bodies with an NDA that includes thorough clinical trial data. Artificial intelligence (AI) models help with data analysis, problem detection, and regulatory compliance (13,15).
- Review Process: The FDA and other regulatory bodies examine the information to decide if the medication is safe and effective for general use. AI facilitates this procedure by identifying possible issues and automating data analysis (16).
- Approval: The medicine can be marketed if the advantages outweigh the hazards. AI keeps an eye on post-market data in order to identify any long-term negative consequences (13).

Post-Market Safety Monitoring

- Phase IV Trials: Following approval, the medication is observed for both uncommon and long-term side effects in the general population. To detect adverse events and

evaluate the drug's long-term safety profile, artificial intelligence models examine real-world data (13,16).

- Continuous Monitoring: Patients and healthcare professionals record side effects, which helps with the continuous evaluation of the medication's safety profile. To identify new safety concerns, AI systems compile and examine these reports (13).

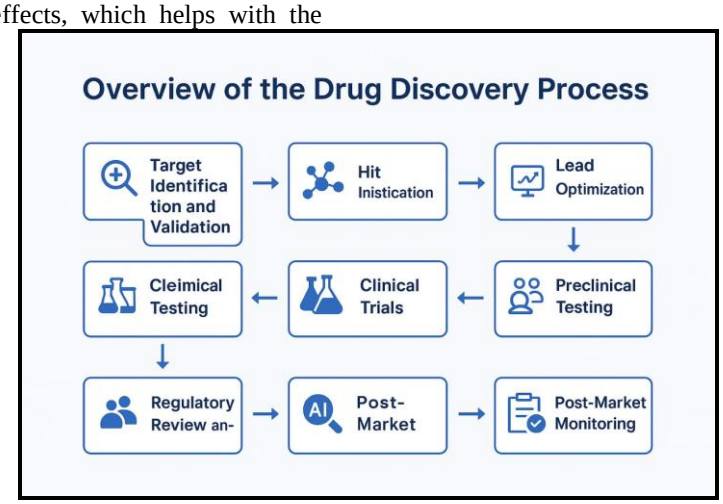

Figure 1: Overview of the Drug Discovery Process

Role of Artificial Intelligence In Drug Discovery and Development

Through the automation of information extraction from vast, diverse data sets and the creation of prediction models that lower trial costs and duration, artificial intelligence (AI) is revolutionizing drug discovery and early development (18). The entire pipeline uses AI techniques, from traditional machine learning (ML) to contemporary deep learning (DL) and generative modelstarget identification, hit/lead discovery, de-novo molecule design, ADMET and toxicity prediction, drug repurposing, biomarker discovery, and clinical-trial optimization (19). By combining clinical, biological, and chemical data, these techniques enhance multi-parameter optimization, expedite candidate selection, and aid in decision-making (20).

1. Target discovery & validation: AI identifies disease-relevant targets and ranks those with greater therapeutic potential by analysing multi-omics, literature, and high-throughput data (21). Maps of disease-gene-pathway interactions and new intervention strategies are proposed by network-based machine learning and representation learning. Compared to manual curation, this improves throughput and finds targets that are not immediately apparent (19).
   2. Virtual screening and hit discovery: Compared to traditional docking alone, machine learning and deep learning models (such as graph neural networks) can quickly score vast compound libraries for anticipated binding or activity, enabling significantly bigger virtual screens (20). These methods enhance the experimental hit pool and lessen the strain of experimental screening (22).
2. Generative design and de-novo chemistry: GANs, transformer-based models, and variational autoencoders are examples of generative models that generate new chemical structures that are optimized for a variety of characteristics, including potency, solubility, and synthetic accessibility (23). Generative AI suggests candidates who balance intricate property trade off, speeding up lead optimization cycles (24).
3. ADMET, safety, and toxicity prediction: By anticipating pharmacokinetics and toxicity endpoints in advance, machine learning models help to minimize late-stage failures (20). Early lead de-risking and triage are facilitated by predictive ADMET models; however, domain applicability and external validation are still crucial (25).
4. Phenotypic discovery and drug repurposing: AI examines clinical records, transcriptomics, and phenotypic screens to suggest current medications for novel indications, cutting down on time by utilizing established safety profiles (19). Often, network and embedding techniques are employed to repurpose assumptions (21).
5. Biomarkers, clinical trials, and patient stratification: AI assists in the identification of predictive biomarkers from imaging and omics data, facilitating improved patient stratification and cost-effective, power-efficient adaptive trial designs Additionally, by anticipating eligibility and likely respondents, machine learning optimizes recruitment and site selection (18,22).
6. Implementation, regulatory, and reproducibility considerations: AI has many obstacles to overcome, including limitations in label data for certain endpoints, bias in data, model interpretability, reproducibility, and regulatory acceptance, despite its great potential (22). Collaboration with regulators, open reporting, and prospective validation are necessary for a safe transition to clinical usage (23).

AI Techniques and Algorithms Used

By producing new compounds, automating data processing, and forecasting molecular characteristics, artificial intelligence (AI) has completely changed the drug discovery and development process. Conventional drug discovery is expensive, time-consuming, and frequently fails, requiring more than ten years. AI solves these problems by using algorithms that can identify intricate chemical and biological patterns in large datasets, greatly increasing accuracy and efficiency (7).

Machine Learning Techniques

AI-driven drug development is built on machine learning (ML) techniques. Biological activity, drug-target interactions, and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiles are frequently predicted using supervised algorithms like Random Forest (RF), Support Vector Machines (SVM), and Gradient Boosting (XGBoost) (2). These algorithms categorize substances as active or inert against particular targets by analysing molecular fingerprints and chemical descriptors (such as ECFP and MACCS). Pattern recognition, compound grouping, and the discovery of new scaffolds are aided by unsupervised learning methods such as principle component analysis (PCA) and k-means clustering (5). Effective model training with less label data is another benefit of semi-supervised learning, which is typical in pharmaceutical datasets (26).

Deep Learning Models

1. Deep Learning (DL) has proven to be incredibly effective in tasks involving medication formulation and prediction. Using 2D or 3D pictures of chemical structures, Convolutional Neural Networks (CNNs) are used for structure-based virtual screening and ligand-binding affinity prediction (27). SMILES strings (Simplified chemical Input Line Entry System) are examples of sequential data that Recurrent Neural Networks (RNNs) and Transformers evaluate to predict chemical characteristics and produce novel drug-like compounds (28).
2. Graph Neural Networks (GNNs) are among the most potent deep learning designs in this field. In order to facilitate direct learning from molecular structures without the need for manual feature extraction, they encode molecular graphs in which atoms serve as nodes and bonds as edges (29).

Generative Models for De Novo Drug Design

New approaches to creating compounds with desired pharmacological characteristics have been made possible by generative algorithms. To create new chemical structures that are optimized for potency, selectivity, and drug-likeness, variational autoencoders (VAEs), generative adversarial networks (GANs), and reinforcement learning (RL) techniques are being used more and more (30). Effective optimization is made possible by RL-based models, which iteratively alter molecules according to "reward" functions determined by target affinity or ADMET scores (31).

AI in ADMET Prediction and Toxicity Modeling

Costly late-stage failures can be avoided by forecasting ADMET qualities early in the development process. ML and DL models use big datasets like Tox21 and ChEMBL to predict pharmacokinetic parameters (32). Researchers can better comprehend why particular chemicals are expected to be harmful by using Explainable AI (XAI) techniques, which improve interpretability, while ensemble learning methods that combine many models improve prediction accuracy (33).

Integration and Future Prospects

In closed-loop discovery systems, AI suggests compounds, automated labs synthesis and test them, and the data from these processes retrains the models (11). AI approaches are also being combined with robots and automation. Multi-modal models that integrate clinical data, proteomics, and genomes are the focus of future research in order to accomplish precision-based and customized drug discovery (9).

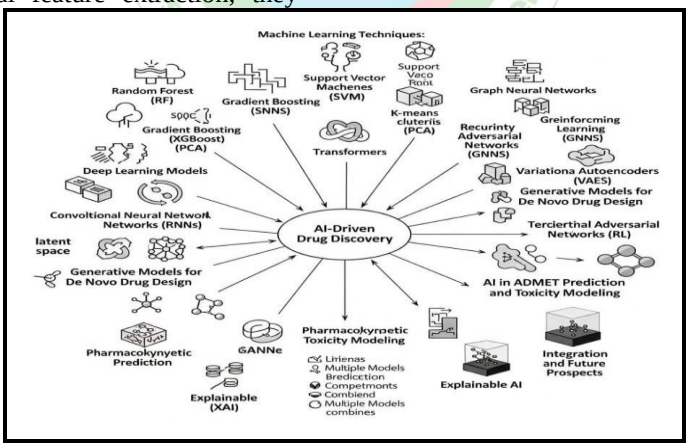

Figure 2: AI Drivenin Drug Discovery

Application of AI in Drug Discovery

It usually takes more than ten years and billions of dollars to bring a new drug to market due to the lengthy, resource-intensive, and complex process of drug discovery and development. As large-scale biological, chemical, and clinical data becomes more readily available, artificial intelligence (AI) has become a potent instrument to speed up and improve this process. Through the drug development pipeline, researchers may analyze complicated datasets, anticipate chemical interactions, create novel compounds, and make data-driven decisions thanks to artificial intelligence (AI) tools like machine learning (ML), deep learning (DL), and natural language processing (NLP). Pharmaceutical research can increase accuracy, creativity, and safety in drug development while cutting down on time, expense, and failure rates by incorporating AI (2,34).

All phases of drug development are affected by AI applications, including hit screening, de novo drug design, lead optimization, ADMET prediction, preclinical and clinical trial design, and target identification, which involves identifying putative genes and proteins linked to disease. By forecasting outcomes that were previously impossible or

difficult to predict using conventional approaches, AI not only speeds up each step but also improves decision-making (2,3,27).

1. Target Identification

- Identifying genes and proteins linked to disease is accomplished by AI and machine learning algorithms that examine extensive biological datasets, such as proteomics, metabolomics, and genomics.
- Understanding intricate biological networks and forecasting target-disease correlations are made easier by deep learning algorithms.
- Information from biomedical literature is extracted using natural language processing (NLP) systems such as IBM Watson and BioBERT to identify new medicinal targets. This increases the accuracy of drug target selection and speeds up the discovery of pertinent biomarkers (2,27,34).

2. Hit Identification / Virtual Screening

- By examining chemical structures and binding affinities, AI-powered virtual screening makes it possible to quickly forecast ligand-receptor interactions.
- By more accurately recognizing hits, deep neural networks and convolutional models perform better than conventional molecular docking.
- In comparison to traditional experimental screening, platforms such as Atom Net and Deep Dock use 3D CNN models to predict binding sites and affinities of millions of compounds in silico, which drastically cuts down on time and expense (3,35,36).

3. De Novo Drug Design

- AI-based generative models, such as Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs), create new drug-like compounds with certain physicochemical characteristics.
- These models are able to produce molecules that are optimized for target affinity, bioavailability, and solubility even prior to synthesis.
- Reinforcement learning systems continuously improve performance against predetermined goals, further optimizing produced molecules (31,37,38).

4. Optimizing Leads

- AI helps medicinal chemists forecast structure–activity relationships (SAR), which improves the stability, safety, and efficacy of lead compounds.
- ML models anticipate how slight changes in chemical structure affect biological performance by analyzing molecular descriptors. Moreover, AI-guided optimization techniques predict possible toxicity and off-target effects, lowering the chance of failure in preclinical phases (2,32).

5. ADMET Prediction

- AI forecasts a molecule's pharmacokinetic and safety profile by predicting its absorption, distribution, metabolism, excretion, and toxicity features.
- In order to assess cytotoxicity, hepatotoxicity, and metabolic stability, tools such as DeepTox and ADMET Predictor employ neural networks.
- Drug safety and efficacy are ensured and expensive late-stage failures are avoided using early AI-based ADMET analysis (3,39).

6. Studies, Preclinical and Clinical

- AI helps with preclinical toxicity evaluations, dose estimations, and the selection of suitable animal models.
- AI helps clinical researchers recruit, stratify, and monitor patients in real time using wearable data and electronic health records.
- Machine learning increases trial efficiency and success rate by predicting patient reactions and designing adaptive clinical trials (34, 40).

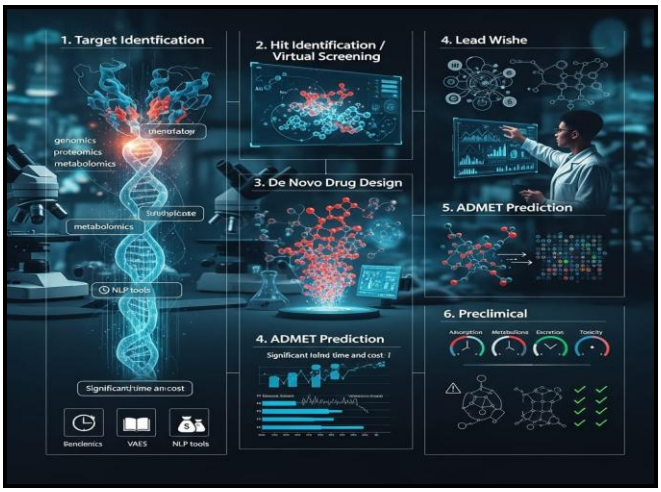

Figure 3: Application of AI in Drug Discovery

Real-World case studies of Ai In drug discovery and Development

1. Bayer + AWS: Reaction Optimization with Generative AI

Bayer and Amazon Web Services (AWS) worked together in 2024 to apply generative AI to forecast the circumstances of chemical reactions. The AI platform reduces experimental planning from weeks to hours and improves repeatability by recommending the best solvents, catalysts, and temperatures based on past reaction data and machine learning. This illustrates how AI speeds up early-stage drug development and practical laboratory chemistry (41).

2. Atomwise: Multi-Target Screening Large Scale

In 2024, 318 verified drug candidates from various therapeutic domains were assessed by Atom Net, a deep learning platform that is atom-wise. By identifying new chemical scaffolds for 235 targets, the AI-driven method drastically cut down on time and expenses as compared to conventional high-throughput screening. This example demonstrates the scalability of AI for drug discovery pipelines with several targets (42).

3. Exscientia + Recursion Pharmaceuticals: Integration of AI-Powered Drug Design

For $688 million, Recursion Pharmaceuticals purchased Exscientia in 2024, combining its high-throughput phenomics technology with Exscientia generative AI molecular design. In terms of industrial-scale AI integration in drug development, this combination expedites preclinical candidate selection while maximizing computational forecasts and experimental validation (43).

4. Predictive Pharmacology AI by Iambic Therapeutics

In order to forecast the pharmacokinetics, toxicity, and general medication performance of early-stage medicines, Iambic Therapeutics created the Enchant AI model in late 2024. The technology speeds up drug optimization and lowers preclinical attrition, with an accuracy of ~0.74 compared to ~0.58 for earlier models (44).

5. AI-Powered Antibiotic Research at the University of Pennsylvania

In 2024, scientists discovered new drugs by using AI to mine about a million chemicals from microbiome datasets. 79% of projected compounds exhibited antibacterial efficacy, according to experimental validation, demonstrating AI's capacity to quickly investigate chemical spaces and combat antibiotic resistance (45).

6. Deep Mind's Alphafold for Predicting Protein Structure

Highly accurate 3D protein structure predictions are still possible using DeepMind's AlphaFold (2024–2025 upgrades), which makes it easier to find druggable areas for biologics and small compounds. These days, pharmaceutical companies use AlphaFold to speed up target validation and structure-based drug design (46).

7. Takeda + Nabla Bio: AI-Powered Antibody Development

Nabla Bio and Takeda collaborated in 2025 to use AI in the discovery of antibody and protein therapeutics. Nabla's Joint Atomic Model (JAM) platform speeds up development and lowers R&D expenses by quickly producing candidate biologics for difficult targets. This collaboration demonstrates AI's growing significance in the discovery of biologics (47).

AI-Developed Pharmaceuticals Entering Clinical Trials: Isomorphic Labs

DeepMind technology is being used by Alphabet's Isomorphic Labs to create new medications; AI-designed candidates are currently getting close to human trials. Drug discovery timelines are accelerated and effective molecular design is made possible by the platform's prediction of protein-ligand interactions (48).

Evaxion Biotech: AI-Driven Vaccine Development

Evaxion Biotech employs AI to optimize antigen candidates and anticipate immunogenic epitopes in order to create vaccines. The technology sped up the development of immunotherapies for cancer and infectious diseases in 2024, cutting design times from months to a few weeks. Faster clinical candidate identification and customized vaccination tactics are made possible by AI-driven epitope prediction (49).

Beneficial AI: Repurposing Drugs and Developing New Therapies

Benevolent AI finds drug-disease correlations by using machine learning and knowledge graphs. More quickly than with conventional techniques, the platform predicted possible candidates that entered preclinical validation in 2024 by repurposing existing drugs for uncommon and neurological disorders. This proves that AI is useful for finding new targets and repurposing drugs in a systematic manner (50).

Healx: AI for the Treatment of Rare Diseases

Healx uses data mining and artificial intelligence to repurpose licensed medications for rare disorders. The business found potential candidates in 2025 to treat Niemann-Pick disease type C, and within two years, they advanced to clinical testing. Knowledge graphs, machine learning, and natural language processing are all used in this platform to effectively find new therapeutic opportunities (51).

Phenomic AI with Multi-Omics from Recursion Pharmaceuticals

Identifying possible treatments for a variety of illness indications was made possible by Recursion's 2025 expansion of their AI platform, which combined high-throughput cellular imaging with multi-omics data. AI's capacity to integrate various biological datasets for expedited candidate selection was demonstrated by the platform's effective prioritization of more than 200 drugs for preclinical validation (52).

De Novo Molecule Design in Insilico Medicine

Deep learning and generative AI were utilized in Insilico Medicine to create small medicines for idiopathic pulmonary fibrosis. Their product, ISM001-055, entered Phase 1 clinical trials in 30 months instead of the customary 4–6 years by combining target identification, molecule generation, and in-silico screening. This example demonstrates how AI can significantly shorten the time needed for early-stage drug development (35).

CHALLENGES AND LIMITATIONS OF AI INDRUG DISCOVERY

Drug development is being revolutionized by artificial intelligence (AI), which speeds up virtual screening, target identification, de novo drug creation, and clinical trial optimization. Although AI has great potential, there are a number of obstacles and restrictions that limit its use, applicability, and dependability in pharmaceutical research (2,53,54).

1. Accessibility and Quality of Data

To produce precise predictions, AI models need substantial, carefully selected, high-quality datasets. In drug discovery, pertinent datasets that primarily cover well-studied targets or compounds are frequently infrequent, dispersed, or inconsistent. Heterogeneity is added by variations in reporting standards, laboratory settings, and experimental procedures, which could lower model accuracy (2). Additionally, low-quality data might reinforce preexisting biases, leading to inaccurate expectations for new drug targets or underrepresented groups (40).

2. Openness and Interpretability

A lot of AI algorithms, especially deep learning models, function as "black boxes," making predictions without providing context. This opacity diminishes trust and regulatory acceptance by making it hard for researchers to comprehend why a molecule is categorized as dangerous or active (55). Model outputs must be evaluated and confirmed scientifically, which requires transparent and explainable AI (XAI) techniques (54).

3. Including Experimental Validation

While AI can produce predictions for possible medication candidates, these findings need to be validated by clinical trials, in vitro, or in vivo experiments. It is difficult to translate in silico predictions into biological systems because of intricate chemical interactions, unexpected pharmacokinetics, and off-target effects (3). This drawback emphasizes that AI is a technology that complements laboratory investigations rather than taking their place.

4. Training Data Bias

If specific chemical classes, illnesses, or patient populations are overrepresented in training datasets, AI models may be biased. These biases have the potential to distort model predictions, hence restricting their applicability to underrepresented populations or goals (7). For example, pharmacological responses in different ethnic groups may not be reliably predicted by models that were mostly trained on datasets from the Western population.

5. Ethical and Regulatory Difficulties

Data privacy, intellectual property, patient permission, and accountability for AI-driven judgments are just a few of the ethical and regulatory issues that arise when AI is used in medication development. Developers face uncertainty while regulatory bodies such as the FDA and EMA continue to establish frameworks for AI applications (16,53). Transparency in automated decision-making and fair access to medications produced by AI are ethical issues.

6. High Costs of Computation and Resources

The process of creating AI models is computationally demanding and calls for cloud computing, GPUs, and domain knowledge. Entry hurdles for smaller institutions may arise from a lack of financing and infrastructure (54). Concerns about sustainability in pharmaceutical research are also raised by the significant energy consumption of training huge models.

7. Cross-System Generalization in Biology

AI models frequently have trouble extrapolating from the particular dataset they were trained on. Models that perform well on training data but badly on unknown chemicals or targets are said to be overfit (53). Because chemical and biological systems are so varied and intricate, this is especially important in the drug discovery process.

8. Implications for Ethics and Society

The automation of drug discovery procedures presents moral questions about reproducibility, human oversight, and fair access to healthcare. If AI forecasts are misused or relied upon excessively without professional oversight, unexpected outcomes may ensue (40). For medication research to remain accountable and ethically sound, human oversight is necessary.

9. Problems with Reproducibility and Benchmarking

In AI-driven drug discovery, reproducibility is difficult because of proprietary datasets, model parameter non-disclosure, and uneven methodology. Comparing models and assessing their dependability is challenging in the absence of conventional benchmarking (2,55).

10. Data Privacy and Security Concerns

AI in drug discovery often relies on patient or clinical trial data, which must comply with data privacy laws such as GDPR. Breaches or misuse can have legal and ethical implications, and restricted data sharing can limit model performance (16).

11. Limited Domain Expertise

AI Teams AI specialists may lack deep biological or pharmacological knowledge, while domain experts may not understand AI methodologies. This gap can

lead to misinterpretation of model outputs or suboptimal model development. Interdisciplinary collaboration is essential to ensure AI models are both technically robust and biologically meaningful (56).

12. Trust and Public Perception

Widespread use of AI in drug development is contingent upon public, regulatory, and researcher trust. Acceptance may be hampered by worries about "black-box" AI, unethical use, or an excessive dependence on computer predictions. Building trust in AI-assisted drug discovery requires open datasets, validation studies, and transparent communication (57).

13. Data Representation and Imbalance

The fairness and generalizability of machine learning applications can be seriously jeopardized by the very unbalanced distributions found in real-world pharmaceutical datasets. For example, biased or underperforming AI models may result from having a large number of instances of successful designs compared to those with issues (58).

14. Model Over fitting and Assessment Criteria

AI models are frequently created to perform exceptionally well on past benchmarks that are unlikely to predict their future performance. Because of this, only a small number of these models are ever reported to offer potential benefits, such finding novel and powerful drug leads for a therapeutic target (59).

15. Combining Data from Multiple Omics

Due to variations in data kinds, sizes, and noise levels, integrating heterogeneous omics data (genomics, proteomics, and metabolomics) into AI models can be difficult. Predictive accuracy may be decreased if these datasets are not appropriately integrated (60).

FUTURE PERSPECTIVE

Drug development and discovery are rapidly changing due to artificial intelligence (AI). AI has the ability to speed up the development of new treatments, improve clinical trial design, and advance personalized medicine as computational techniques advance. In the future, the efficiency, accuracy, and moral delivery of novel medications could be completely transformed by combining AI with generative models, multi-omics data, and actual patient data (60,61,62).

Through increased productivity, accuracy, and creativity, artificial intelligence (AI) is transforming the drug discovery and development process. Looking ahead, a number of new developments suggest how artificial intelligence will influence pharmaceutical research in the years to come (19,62,64,65).

1. Accelerated Drug Development: By simplifying preclinical validation, lead optimization, and target selection, AI has the potential to significantly shorten drug development timelines. In order to find interesting chemicals, machine learning algorithms can quickly examine massive datasets, cutting down the time needed from years to months (61). This acceleration is especially important for pandemics and emerging diseases, where quick therapy development is necessary.
2. Integration of Multimodal Data: Future AI systems will incorporate multiple data types, including genomics, proteomics, metabolomics, electronic health records, and real-world evidence. This multimodal approach facilitates patient classification, increases prediction accuracy, and aids in the development of customized treatments based on each patient's unique genetic and environmental characteristics (60).
3. Generative AI Models: New chemical architectures, their interactions, and lead compound optimization are all being done with generative AI models. The development of novel drug candidates with enhanced efficacy and decreased toxicity is made easier by these models' ability to investigate enormous chemical regions that are hard for humans to assess by hand (66).
4. Improved Predictive Modeling: AI predictive models are getting better at predicting pharmacokinetics, off-target effects, and drug-target interactions. This lowers late-stage failures and related expenses by enabling researchers to rank compounds with a higher chance of success (5).
5. Regulatory Evolution: In order to assess and authorize AI-assisted drug discovery methods, regulatory bodies like the FDA and EMA are adjusting to AI technologies. This change in regulations will make it easier to safely and responsibly incorporate AI into standard drug development processes (67).
6. Collaborative Industry Partnerships: There is a growing number of partnerships among biotech companies, pharmaceutical corporations, and AI startups. Through collaborative endeavors, superior AI skills and domain expertise can be used to effectively share computational resources, enhance medication creation, and address complex diseases (68).
7. Cost and Resource Optimization: AI can maximize the use of resources by anticipating failed candidates in advance and concentrating on molecules that show promise. Drug discovery becomes more sustainable and scalable as a result of this efficiency, which lowers material and financial costs (62).
8. Equitable and Ethical Drug Development: As AI gets more and more integrated into drug discovery, ethical issues will become more important. Maintaining public trust and social responsibility requires ensuring objective datasets, protecting patient privacy, and facilitating fair access to AI-developed treatments (60).
9. Integration with Robots and Automation: By combining AI with robots and automated lab platforms, high-throughput testing, quick prediction validation, and scalable compound synthesis will be

possible, greatly speeding up experimental workflows (69).

10. AI for Neglected and uncommon Diseases: By spotting treatment possibilities for neglected and uncommon diseases, AI is in a unique position to fill gaps in the market. By quickly investigating possible therapeutic targets and repurposing current medications, it can shorten the time and expense of developing treatments for underserved disorders (70).

11. Personalized Medicine: By forecasting particular drug reactions using genetic, proteomic, and environmental data, AI can customize treatments for individual patients (57). Precision healthcare is supported, side effects are reduced, and efficacy is increased through personalized medicine.

12. Virtual Screening Optimization: AI speeds up big compound libraries' in silico screening, finding possible hits more quickly than with conventional techniques. In the early phases of drug discovery, this increases efficiency and aids in prioritizing compounds for experimental validation (71).

13. Drug Repurposing: AI can find novel therapeutic uses for medications that already exist, cutting down on development time and utilizing known safety profiles. When it comes to promptly addressing new health emergencies, this strategy is especially helpful (72).

14. Multi-Omics Integration: Researchers can find new biological targets and pathways for complicated diseases using AI-driven integration of heterogeneous omics information, which reduces the need for trial-and-error experimentation and supports mechanism-based drug design (73).

15. AI-powered Clinical Trial Optimization: By evaluating past data and forecasting trial results, AI can enhance clinical trial design, patient recruitment, and monitoring. This raises the likelihood that permits will be granted, lowers expenses, and promotes efficiency (74).

16. All things considered, advancements in ethics, laws, and collaboration are equally as important to the future of AI in drug research as technological advancements. By incorporating these perspectives, AI will be able to transform the pharmaceutical sector by enabling faster, more efficient, and more equitable drug development processes (5,60,61,62,66,67,68,70).

CONCLUSION

Artificial Intelligence is transforming the paradigm of drug discovery and development by enhancing efficiency, accuracy, and innovation across the pharmaceutical pipeline. Through data-driven modeling, AI enables early identification of promising drug candidates, reduces attrition rates, and accelerates clinical development. Its integration with multi-omics data, automation, and generative algorithms supports personalized and precision medicine, minimizing costs and development time. However, the successful adoption of AI requires addressing challenges related to data quality, model transparency, ethical concerns, and regulatory compliance. Collaborative efforts among researchers, industry leaders, and policymakers are crucial to ensuring responsible AI implementation. As advancements continue, AI holds the promise to revolutionize global healthcare by enabling faster, safer, and more equitable access to novel therapeutics.

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This work highlights the transformative role of Artificial Intelligence (AI) in revolutionizing modern drug discovery and development. The authors — Ms. IkraSubhedar and Mrs. Sangita Bhandare from Pravara Rural Education Society's College of Pharmacy (For Women), Chincholi Nashik — present a comprehensive perspective on how AI-driven methodologies, integrating

Machine Learning (ML), Deep Learning (DL), and Generative Modeling, are reshaping the pharmaceutical landscape through innovation, precision, and efficiency. This study emphasizes the application of AI algorithms in target identification, lead optimization, ADMET prediction, and clinical trial design, enabling faster and more cost-effective therapeutic development. Furthermore, it highlights the potential of AI in supporting personalized medicine and drug repurposing, ensuring safer and more effective treatments. This perspective envisions a technology-driven, data-centric approach that promises to accelerate pharmaceutical research and transform the future of global healthcare through intelligent and ethical innovation.

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