APPLICATION OF ARTIFICIAL INTELLIGENCE IN CLINICAL TRIALS AND DRUG DEVELOPMENT

Addepalli Lakshmi Abhishek [1], Rachna Varma[2], Shweta Anand[3]
Department of Veterinary Pharmacology and Toxicology, COVAS, SVPUAT, Meerut (U.P)-250110
Corresponding author email: *abhishekaddepalli14@gmail.com*
DOI: https://doi.org/10.5281/zenodo.19997060

Abstract

The rise of Artificial Intelligence (AI) has triggered a revolution in the pharmaceutical industry, with the aim of tackling longstanding issues such as high drug development costs, long timelines, and low success rates in drug discovery and clinical trials. Traditional methods of drug development are resource-intensive and often inefficient, creating a strong demand for data-driven and automated solutions. In this review, the authors examine AI applications in drug discovery and clinical trial optimization, highlighting their role in enhancing efficiency, accuracy, and decision-making. Technologies like machine learning and deep learning are becoming increasingly valuable for identifying new drug targets, predicting molecular interactions, and optimizing synthesis pathways. In clinical studies, AI assists with patient recruitment, trial design and testing, real-time monitoring, and predictive analytics of treatment outcomes. Integrating large datasets—including genomics, electronic health records, and imaging data—also supports personalized medicine and improves patient stratification. Key findings suggest that AI can significantly shorten drug development timelines, cut operational costs, and increase the precision of clinical procedures. However, challenges such as data quality, algorithmic bias, legislation and regulation, and difficulties with data sharing still limit widespread adoption. Future efforts will likely focus on enhancing data integration, transparency, and regulatory frameworks to fully realize AI's potential in pharmaceutical research and healthcare innovation.

Keywords: Artificial Intelligence, Drug Discovery, Clinical Trials, Machine Learning, Personalized Medicine, Pharmaceutical Innovation

1. Introduction

1.1 Background of AI in Healthcare

Artificial Intelligence involves creating computational systems that mimic human intelligence and perform learning, reasoning, and decision-making. A branch called Machine Learning (ML) allows systems to learn from data and enhance their performance without explicit programming (Aung *et al*., 2021; Askin *et al*., 2023). The healthcare industry has experienced rapid change due to increased computing power, greater access to large biomedical datasets, and advances in algorithms like neural networks and deep learning. Over the last decade, AI has become more essential in biomedical sciences, supporting applications such as medical imaging, diagnostics, genomics, and predictive analytics. The combination of AI with multi-omics data and electronic health records has significantly advanced the understanding of diseases and clinical decision-making (Malamateniou *et al*., 2021; Liu et al., 2023).

1.2 AI should be used in Drug Development.

The traditional drug development process is slow and costly, taking an average of 10-15 years and costing billions of dollars from discovery to regulatory approval (Terranova *et*

al., 2024). Additionally, few drug candidates reach clinical trials, and many fail in the final stages due to lack of effectiveness or safety concerns (Bender & Cortes-Ciriano, 2021). These challenges emphasize the need for new methods to boost efficiency and lower failure rates. AI provides a promising solution by enabling faster data analysis, more accurate predictions of drug behavior, and better trial design, thereby speeding up the development process (Chopra *et al*., 2022).

1.3 Objectives of the Review

The focus of this paper is to thoroughly analyze how artificial intelligence has been applied in drug development and clinical trials, with an emphasis on target identification, medication design, and patient recruitment. It also seeks to identify main challenges in AI implementation, such as data bias, regulatory obstacles, and model interpretability, while exploring AI's future possibilities in pharmaceutical research and personalized medicine (de Brito Pontes & Netto, 2025; Zhang *et al*., 2025).

2. Fundamentals of AI in Drug Development

2.1 Machine Learning Techniques

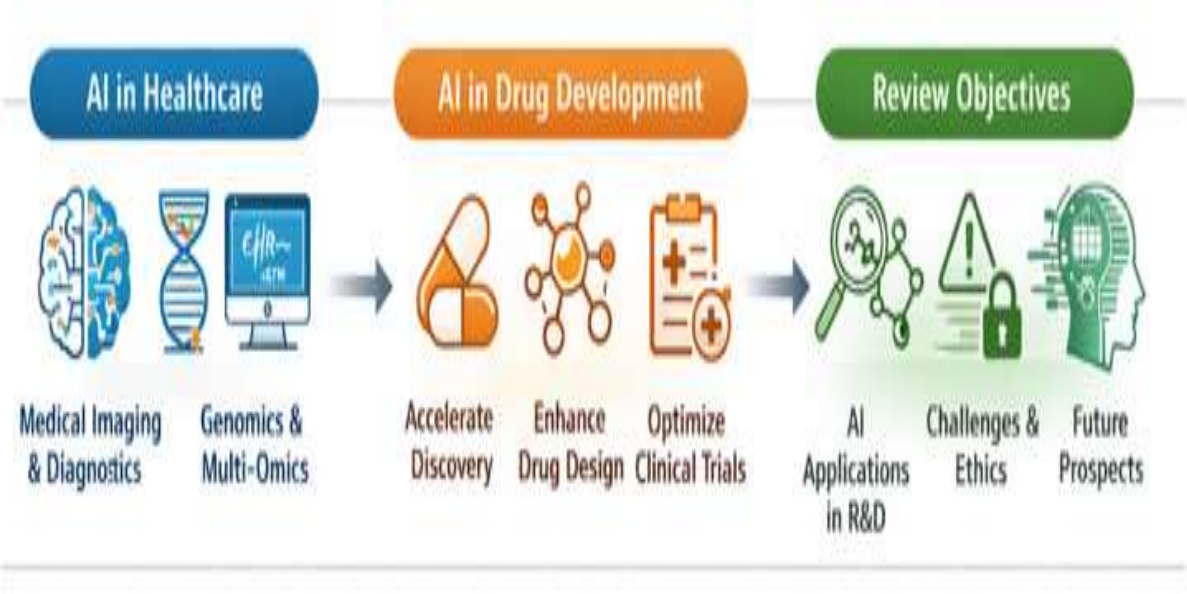
Machine learning (ML) is central for AI applications in drug development, as it enables prediction and pattern recognition from complex biomedical data. Support Vector Machines (SVMs) and Random Forests (RFs) are common algorithms used for classification and regression in prediction and quantitative structure-activity relationship (QSAR) modeling (drug-target and drug-drug interactions). Clustering and dimensionality reduction approaches exemplify unsupervised methods of learning employed to uncover latent patterns in high-dimensional data, like gene expression profiles. Deep learning approaches, particularly Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs), have significantly improved the analysis of complex data types such as medical images, molecular structures, and sequential biological data, thereby boosting the accuracy of drug discovery and clinical prediction methods (Le *et al*., 2024).

2.2 Data Sources

The development of AI-driven drugs relies on various extensive datasets. Genomic and proteomic data offer insights into disease causes and treatments targets by analyzing gene expression and protein interactions. Electronic Health Records (EHRs) provide real-world data on patients, including medical histories, treatment outcomes, and other demographic information, which are essential for patient stratification and for optimizing clinical trials (Araki *et al*., 2023). Radiology and pathological images are also imaging datasets used by AI models to identify disease patterns and predict treatment responses. When combined with heterogeneous data types, the strength and predictability of AI systems are enhanced in pharmaceutical research (Liu *et al*., 2023).

2.3 AI Architecture in Pharma

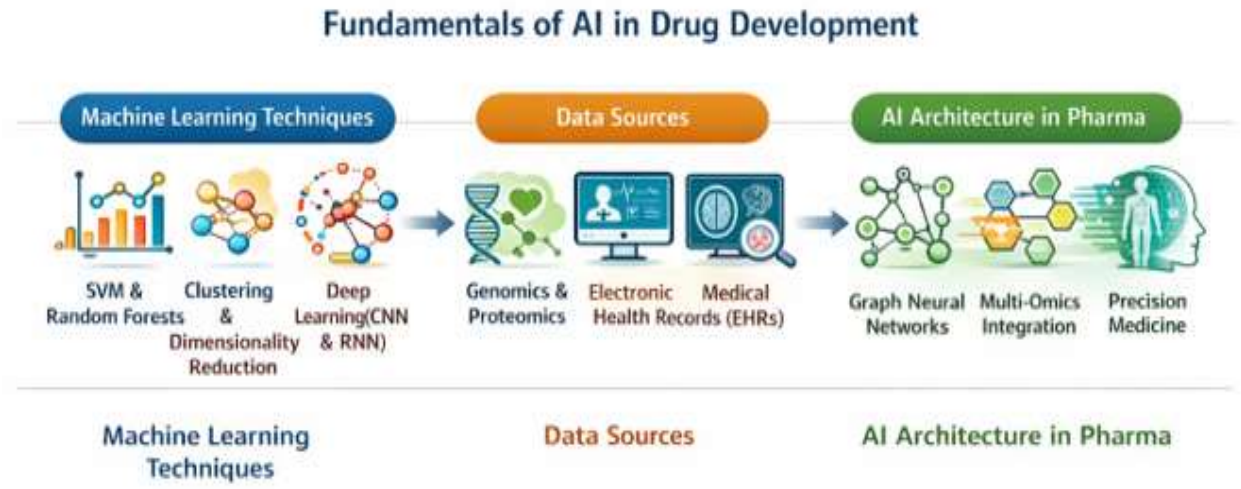
Complex biological systems, in which molecules, proteins, and genes interact, have advanced AI architectures, specifically graph-based learning models. Graph neural networks (GNNs) are more effective at modeling interactions and drug-target relationships than traditional models (Beis *et al*., 2023). Moreover, multi-omics integration combines genomics, transcriptomics, proteomics, and metabolomics to provide a complete view of disease pathways and treatment. This patient-centered strategy will improve precision medicine by enabling more effective forecasts of therapeutic effects and tailored treatment plans (Baltrusaitis *et al*., 2019; Chen et al., 2023).



3. AI in Drug Discovery and Development

3.1 Target Identification and Validation

For the analysis of large-scale genomic and proteomic data has enabled AI to greatly improve target identification and validation, as it can reveal associations between disease and pathways and the related genes important to the disease. Biomarker discovery is performed by machine learning algorithms that identify patterns, mutation expression matches, mutation profiles, and matching protein interactions, so making it possible to identify novel therapeutic targets (Beis *et al*., 2023; Le *et al*., 2024). Genomic data analysis processes can be enhanced by AI-based solutions to select targets with greater clinical relevance and easier targeting.



3.2 Lead Compound Identification

Lead Compound Identification entails determining the lead compound used to produce the lead-based product (e.g., lead-free gasoline).Virtual screening is one of the AI methods that has transformed conventional drug discovery, particularly in lead compound detection. The prediction of the biological activity of compounds and their affinity with target proteins is performed with the help of Quantitative Structure-Activity Relationship (QSAR) models and molecular docking simulations (Chopra *et al*., 2022). Moreover, government by AI of small-molecule libraries, such as deep generative models, enables the search for new compounds based on pharmacological characteristics, thereby eliminating the requirement to screen many compounds in experiments (Cosentino & Hormozdiari, 2023).

3.3 Synthesis Planning & Automation

The vision of automation is to design synthesis and engineering tools to enhance the design of nanoproducts and improve their quality. <|human|>Synthesis Planning and Automation 5.3 Synthesis planning and automation the vision of synthesis planning and automation is to develop synthesis tools and engineering tools to design better nanoproducts and to improve their quality.

AI also plays a very important role in synthesis planning through retrosynthetic analysis, where complex molecules are broken down into simpler precursors. Reaction predictor models help identify potential reactions and determine the optimal ones. When combined with automated laboratory systems, such as robotic systems and high-throughput screening technologies, AI enables precise and reproducible experimental execution. This automation is crucial for reducing human error, speeding up the synthesis process, and improving the overall efficiency of drug development (Connor *et al*., 2022; He *et al*., 2019).

3.4 ADMET Prediction

Absorption, Distribution, Metabolism, Excretion, and Toxicity prediction models regarding drug candidates are commonly developed using AI-driven approaches. Random forest and deep learning models are machine learning models that use chemical descriptors and bio-data to predict toxicity and pharmacokinetic behavior during the early stages of the development process (Goller *et al*., 2020; Cosentino & Hormozdiari, 2023). This minimizes failures in the late stages and improves the safety profile of candidate drugs.

3.5 Drug Repurposing

Although AI has the potential to find novel therapeutic uses for already-approved medications, it has emerged as a potent tool for drug repurposing. By analyzing clinical data, drug-disease molecular interactions, and disease networks, AI models can reveal hidden connections between medications and illnesses, facilitating the creation of efficient treatments more quickly. (Zhang *et al*., 2025; de Brito Pontes & Netto, 2025). This techniques is especially useful in urgent health situations because it requires less development time, costs less, and faces fewer regulatory hurdles compared with standard drug discovery methods.

AI in Drug Discovery and Development

Section	Key Concepts	AI Applications
Target Identification & Validation	Genomic & proteomic analysis, biomarker discovery	ML identifies disease pathways, gene targets
Lead Compound Identification	QSAR, molecular docking, compound screening	AI predicts drug activity & generates novel molecules
Synthesis Planning & Automation	Retrosynthesis, reaction prediction, robotics	AI plans synthesis & automates lab processes
ADMET Prediction	Absorption, Distribution, Metabolism, Excretion, Toxicity	Artificial intelligence predicts pharmacokinetics & toxicity early

Drug Repurposing	Drug-disease interaction analysis	AI identifies new uses for existing drugs

4. AI in Clinical Trials

4.1 Clinical Trial Phases Overview

Drug safety and effectiveness are assessed through four phases in clinical trials. Phase I emphasizes safety and dosing in a small group of healthy volunteers, while Phase II evaluates effectiveness and side effects in a larger group of patients. Phase III aims to demonstrate the drug's effectiveness and compare it to existing treatments in large-scale studies. Phase IV involves post-marketing surveillance, focusing on long-term safety and outcomes in a broad patient population (International Journal of Surgery, 2023; Liu *et al*., 2023). AI is increasingly utilized at each stage to improve efficiency and decision-making.

4.2 Patient Recruitment & Selection

The process of recruiting and selecting patients will be used for enrolling participants in the clinical trial, a key factor. AI matching systems employ machine learning algorithms and natural language processing to analyze electronic health records and identify more candidates. NLP helps extract useful clinical data from unstructured information, improving the speed and accuracy of recruitment (Araki *et al*., 2023; de Brito Pontes & Netto, 2025).

4.3 Trial Design Optimization

AI can be utilized in adaptive trial design, where interim data analysis can be adjusted in real time to enhance trial efficiency and lower costs. It can be utilised to optimize dosage by simulating pharmacokinetics and pharmacodynamics, ensuring the therapeutic dose is optimal (Terranova *et al*., 2024).

4.4 Predictive Analytics

Machine learning and deep learning models enable predictive analytics for survival and treatment response. These models use historical and real-time data to predict patient outcomes, improving decision-making and increasing trial success rates (Saady *et al*., 2025; Wong *et al*., 2021).

4.5 Monitoring and Safety

With AI, it is possible to continuously monitor clinical trials, as adverse events can be detected promptly and risks can be predicted. Even advanced algorithms can identify early safety signals, reduce patient risk, and improve the integrity of the trial (Ranchon *et al*., 2023).

4.6 Data Analysis and Management.

AI can provide more effective data management of the large, complex datasets generated during trials. With automated reporting systems, data analysis and regulatory documentation can be simpler, more accurate, and less manual (Gosselin *et al*., 2021).

5. Integration of AI with Personalized Medicine

Artificial Intelligence (AI) plays a crucial role in advancing personalized medicine through a data-driven approach that focuses on each patient's unique traits. Patient stratification, where machine learning models categorize clinical, genomic, and demographic data into subgroups with similar disease patterns or treatment responses, is also an important application. This stratification improves clinical trial design and enhances overall treatment outcomes by ensuring patients receive the most suitable interventions (Liu *et al*., 2023; Araki *et al*., 2023). Precision therapeutics is further improved by AI, which predicts individual patients' responses to specific medications based on their genetic makeup, lifestyle factors, and medical history. AI models can identify disease biomarkers and enhance treatment plans by integrating multi-omics data, including genomics, proteomics, and metabolomics, thereby reducing adverse effects and increasing effectiveness (Le *et al*., 2024; Beis *et al*., 2023).

AI in Clinical Trials

Section	Key Aspects	AI Applications

Clinical Trial Phases (I–IV)	Safety, efficacy, comparison, post-marketing	AI supports decision-making across all phases
Patient Recruitment & Selection	EHR analysis, eligibility criteria	ML & NLP identify suitable participants
Trial Design Optimization	Adaptive trials, dose optimization	AI adjusts trials in real-time, simulates PK/PD
Predictive Analytics	Survival prediction, treatment response	ML/DL models predict outcomes and success rates
Monitoring & Safety	Adverse event detection, risk assessment	AI enables real-time monitoring and early alerts
Data Management & Analysis	Big data handling, reporting	Automated systems improve accuracy & efficiency

This method is changing healthcare into a targeted and efficient system. Additionally, by integrating wearable and mobile health solutions with remote monitoring systems, digital health has enabled the usage of AI in personalized medicine. These technologies provide real-time patient data that AI analyzes to deliver ongoing health updates, identify early signs of disease, and recommend adaptive treatments. AI combined with digital health platforms can boost patient engagement and adherence and support the shift toward proactive and preventive healthcare (Ranchon *et al*., 2023; Chen *et al*., 2023).

6. Regulatory and Ethical Considerations

6.1 Regulatory Frameworks

The rise of Artificial Intelligence in drug development and clinical trials has prompted regulatory agencies to develop frameworks that ensure safety, productivity and transparency. The U.S. Food and Drug Administration (FDA) has released guidelines on AI/ML-based systems that focus on a lifecycle approach, including continuous monitoring, validation, and algorithm updates (U.S. Food and Drug Administration, 2023). These frameworks are based on risk, with regulatory oversight adjusted to the potential harm AI systems might pose to patient safety and clinical outcomes. These practices aim to balance innovation with compliance, expecting AI-powered tools to be high quality and capable of adapting to changing data inputs and model performance (Liu *et al*., 2023; Askin *et al*., 2023).

6.2 Ethical Issues

The adoption of AI in healthcare is also crucial for ethics, including confidentiality, bias, and transparency. Using large-scale patient data, like electronic health records with other genomic information, raises concerns about privacy and secure data handling. It is vital to follow data protection laws to keep patient trust (Jeyaraman *et al*., 2023). Additionally, bias in datasets remains a major problem, as under-representation of certain groups can lead to unfair results and limit the usefulness of AI models (Bender & Cortes-Ciriano, 2021). These biases can be reduced by using diverse, high-quality data. Moreover, making complex AI models understandable is a challenge that lead to the creation of Explainable AI (XAI), providing clear and understandable explanations for model predictions. For AI in healthcare to gain clinical acceptance, regulatory approval, and ethical use, increasing transparency is essential (Kleinberg, 2018; Aung *et al*., 2021).

7. Challenges and Limitations

Although the technology for drug development and clinical trials is still making significant progress through artificial intelligence (AI), various obstacles still limit its widespread application. Data quality and availability pose major challenges because of these models need large, well-labeled datasets for training. However, biomedical data is often incomplete, scarce, or unavailable due to privacy restrictions and high acquisition costs, especially for rare diseases (Bender & Cortes-Ciriano, 2021; Liu *et al*., 2023). Additionally,

data integration is complicated by the lack of standardization in data formats, presentation, collection methods, and reporting systems across institutions, which affects model quality (Shanbhogue *et al*., 2021). Bias and generalizability are other key challenges, as applying AI models to diverse populations can produce inaccurate or unfair results because of limited or unrepresentative training datasets. The underrepresentation of certain ethnic and demographic groups in clinical and genomic data worsens this issue (Jeyaram *et al*., 2023). Furthermore, an unpredictable regulatory system is a major obstacle since the current guidelines for AI/ML-based systems are still evolving, making it difficult to ensure compliance and acceptance across different jurisdictions (U.S. Food and Drug Administration, 2023). Lastly, the gap between computational predictions and clinical outcomes, despite some promising results, is the lack of success of drugs developed with AI that have surpassed Phase II clinical trials. That is why BSI is emphasized as a means of facilitating the translational success of AI in pharmaceutical research through improved validation schemes, robust datasets, and cross-disciplinary collaboration (Askin *et al*., 2023; Terranova *et al*., 2024).

8. Future Perspectives

The future of AI (Artificial Intelligence) in drug development and clinical trials is filled with transformational changes with the incorporation of emerging technologies. The convergence of AI and quantum computing is a promising direction, as it can address complex molecular simulations and optimization problems at unprecedented speeds, accelerate drug discovery, and increase predictive power (Cova *et al*., 2022; Li *et al*., 2024).

The other innovation that is emerging is the utilisation of digital twins in clinical trials where virtual patients are developed through real-time biological and clinical data. Such models enable disease progression and treatment response to be simulated, making it possible to design trials more efficiently and spare patients unnecessary risks, with trials tailored to them (Liu *et al*., 2023). There is also increasing significance of real-world evidence (RWE) due to electronic health data records, wearable devices, and patient registries. Analysis of RWE by artificial intelligence enhances the process of clinical decision-making, regulatory filing and post-marketing monitoring as it helps to understand the real performance of the drug in real-life conditions (Araki *et al*., 2023; Ranchon *et al*., 2023). Moreover, software based on generative AIs in drug design is reshaping the ability to design novel molecules with artificially selected medicinal actions by applying deep learning architectures to generate candidates with preferable pharmacological activities, thereby reducing the time and expense incurred during the initial stage of discovery (Cosentino & Hormozdiari, 2023). Lastly, fully automated drug discovery pipelines (which combine AI and robotics with high-throughput experimentation), will also be developed, which is likely to develop end-to-end autonomous systems to streamline the entire drug development lifecycle and to increase efficiency, reproducibility, and innovation (Connor *et al*., 2022; He *et al*., 2019).

9. Conclusion

Pharmaceutical research and development are rapidly evolving with the adoption of Artificial Intelligence (AI), which is data-driven and effective in improving efficiency, accuracy, and innovation throughout the drug discovery and clinical trial process. Since its introduction in target identification, molecule design, patient recruitment, and predictive analytics, AI has demonstrated the ability to save time in development and reduce operational costs, thereby increases success rates. The potential of AI to analyze large amounts of multi-dimensional data enables more informed decision-making and facilitates the transition to

personalized medicine, ultimately enhancing patient outcomes (Terranova *et al*., 2024; Liu *et al*., 2023). Besides, AI-based solutions have facilitated previously complicated procedures, including clinical trial design, safety assessment, and pharmacokinetic modeling, among others, thereby making drug development pipelines faster and more certain (Chopra *et al*., 2022; Ranchon *et al*., 2023). Nonetheless, with lot of issues persist, including data quality problems, algorithmic bias, transparency concerns, and regulatory changes. These issues need to be addressed to guarantee that AI technologies are implemented in healthcare in an ethical and responsible manner (Bender & Cortes-Ciriano, 2021; Askin *et al*., 2023). To sum up, although AI offers vast potential to transform pharmaceutical R&D, its use must be accompanied by continuous advances in data governance, regulatory transparency, and model inference to be effective. Joint work between scientists, players in the industry, and the regulators would be instrumental in realizing the full capability of AI and see its fair and sustainable utilization in the improvement of healthcare systems around the world.

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Cite this article:
Addepalli Lakshmi Abhishek, Rachna Varma, Shweta Anand. (2026). Application of artificial intelligence in clinical trials and drug development. Vet Farm Frontier, 03(04), 61–70. https://doi.org/10.5281/zenodo.19997060