

**REVIEW ON: ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY  
AND DEVELOPMENT**

**\*<sup>1</sup>Achal Mandale, <sup>2</sup>Dr. Karishma Nikose, <sup>3</sup>Kirti Pandav, <sup>4</sup>Samiksha Thaware, <sup>5</sup>Siddesh Lande, <sup>6</sup>Sanjiwani Pawar**

**\*<sup>1,3,4,5,6</sup>Student in J.I.P.R, Kalamb,**

**<sup>2</sup>Associate Professor in J.I.P.R, Kalamb, PHD in Pharmaceutical Science,  
J.I.P.R, Kalamb, Dist. Yavatmal, Maharashtra (445001).**

Article Received on 09 Nov. 2025,  
Article Revised on 29 Nov. 2025,  
Article Published on 01 Dec. 2025,

<https://doi.org/10.5281/zenodo.17790055>

**\*Corresponding Author**

**Achal Mandale**

Student in J.I.P.R, Kalamb, Dist.  
Yavatmal, Maharashtra (445001).



**How to cite this Article:** \*<sup>1</sup>Achal Mandale, <sup>2</sup>Dr. Karishma Nikose, <sup>3</sup>Kirti Pandav, <sup>4</sup>Samiksha Thaware, <sup>5</sup>Siddesh Lande, <sup>6</sup>Sanjiwani Pawar. (2025) REVIEW ON: ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT. "World Journal of Pharmaceutical Research, 14(23), 1150-1167.

This work is licensed under Creative Commons Attribution 4.0 International license.

**ABSTRACT**

Artificial Intelligence (AI) focuses in producing intelligent modelling, which helps in imagining knowledge, cracking problems and decision making. Recently, AI plays an important role in various fields of pharmacy like drug discovery, drug development process, pharmaceutical manufacturing, quality control and quality assurance etc. In drug discovery, AI accelerates the identification of potential drug candidates by analysing vast datasets, predicting molecular interactions, and optimizing lead compounds. During the drug development process, AI aids in clinical trial design, patient stratification, and predicting drug safety and efficacy, significantly reducing time and cost. In pharmaceutical manufacturing, AI enables process optimization, predictive maintenance, and quality control, ensuring consistent and high-quality production. AI also plays a pivotal role in detection technologies, facilitating early disease diagnosis, biomarker identification, and

monitoring therapeutic responses. Furthermore, AI addresses current pharmaceutical challenges, including complex regulatory requirements, high attrition rates, and the need for personalized medicine. While the advantages of AI include faster timelines, cost savings, improved accuracy, and data-driven decision-making, disadvantages such as data quality issues, ethical concerns, over-reliance on algorithms, and regulatory hurdles must be carefully

managed. Overall, AI is poised to revolutionize the pharmaceutical landscape, offering transformative potential while requiring thoughtful implementation.

**KEYWORDS:** Artificial intelligence, AI and drug discovery, drug development, pharmaceutical manufacturing and Advantages and disadvantage of AI technology.

## INTRODUCTION

Artificial Intelligence (AI) is defined by the American Society of Health-System Pharmacists (ASHP) as “the theory and development of computer systems to perform tasks normally requiring human intelligence, such as visual perception, language processing, learning, and problem solving.”<sup>1</sup> In health-care, AI encompasses several subfields including machine learning (ML) which uses data and algorithms to mimic human learning, neural networks which are inspired by the human brain to process complex data, natural language processing (NLP) which allows computers to understand and generate human language, and generative AI which creates new content such as text, images, or models. These technologies serve as the foundation for large language models (LLMs) that power many clinical and educational applications in healthcare today. Among these, the most widely used and recognized form is generative AI tools such as ChatGPT which are being increasingly integrated into healthcare education and clinical support.<sup>[1]</sup>

Artificial Intelligence (AI) is a stream of science related to intelligent machine learning, mainly intelligent computer programs, which provides results in the similar way to human attention process. This process generally comprises obtaining data, developing efficient systems for the uses of obtained data, illustrating definite or approximate conclusions and self-corrections/adjustments. AI technology becomes a very fundamental part of industry for the useful applications in many technical and research fields.<sup>[2]</sup>

The concept of using computers to simulate intelligent behaviour and critical thinking was first described by Alan Turing in 1950. In the book *Computers and Intelligence*, Turing described a simple test, which later became known as the “Turing test,” to determine whether computers were capable of human intelligence. Six years later, John McCarthy described the term artificial intelligence (AI) as “the science and engineering of making intelligent machines.”<sup>[3]</sup>

AI is a technology-based system involving various advanced tools and networks that can mimic human intelligence. At the same time, it does not threaten to replace human physical presence completely. AI utilizes systems and software that can interpret and learn from the input data to make independent decisions for accomplishing specific objectives. Its applications are continuously being extended in the pharmaceutical field.<sup>[4]</sup>

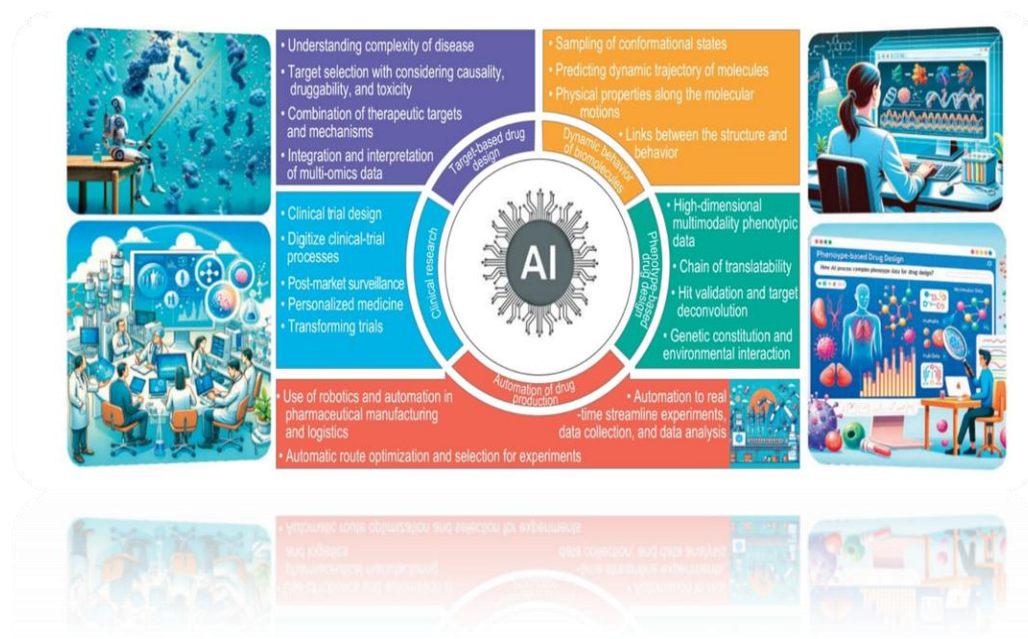
There is a strong emphasis on quality, accuracy, and conformity with regulations in the pharmaceutical production sector. The pressure on pharmaceutical producers to improve operational efficiency, reduce downtime, and guarantee product quality is rising as the global demand for pharmaceutical products rises.<sup>[5]</sup> The continuous evolution of AI, fuelled by advancements in machine learning and data science, has facilitated the development of innovative solutions to complex challenges in the pharmaceutical sector.<sup>[6]</sup>

AI, it is typically used as a general term to encompass all methods that the pharmaceutical industry is implementing, such as machine learning (including deep learning), natural language processing, and computer or machine vision. All these innovations, despite being labelled AI, reflect differing analytical approaches. AI depicts machines or systems that have the ability to perform independent decision making and can be described as “an entity (or collective set of cooperative entities), able to receive inputs from the environment, interpret and learn from such inputs, and exhibit related and flexible behaviours and actions that help the entity achieve a particular goal or objective over a period of time.”<sup>[7]</sup>

Artificial Intelligence (AI) has recently been developed into a sizzling topic in the area of medical care industry. The biopharmaceutical industries are making efforts to approach AI to enhance drug discovery process, reduce research and development expenses, diminish failure rates in clinical trials and ultimately generate superior medicines. The accessibility of immense statistics in life sciences and a speedy development in machine learning algorithms led to an evolution of AI-based start-up companies focused on drug discovery over the recent years. Numerous remarkable AI- biopharmaceutical alliance were declared in 2016-2017 that include Pfizer and IBM Watson, Sanofi Genzyme and Recursion Pharmaceuticals, AstraZeneca, Abbvie, Merck, Novartis, GSK and Exscientia, etc.<sup>[8]</sup>

The advent of the third wave of artificial intelligence (AI) heralds a new era in drug discovery. AI-powered techniques can be characteristic of identifying features that are difficult for humans to interpret from big and high-dimensional data in biomedical research.

That's why there is so much enthusiasm for AI in drug discovery, not only in academia but also in industry. Booming AI tools are revolutionizing nearly every stage of the drug discovery process, indicating the substantial potential to transform the speed and economics of the industry. Our previous review provided a comprehensive overview of developments in this area. Due to space limitations, we focus here only on the frontiers of the five technologies or phases of drug development mentioned below (Fig 1)



**Figure 1: Example modules and their challenges in AI enhanced drug development pipeline. Cartoon figures were drawn with the assistance of DALL.**<sup>[9]</sup>

AI can be broadly classified based on the technology's capabilities and scope upon application. 'Narrow' or 'Weak' AI refers to the development of technology designed to perform repetitive and well-defined tasks or functions. A frequently used technique within this category and the healthcare realm is "machine learning". In recent years, it has been applied to areas such as disease outbreak forecasting and stratification of treatment strategies within development of personalised medicine. Through the collation of baseline data on patient- and disease-specific characteristics, application of machine learning to these repetitive and often predictive-modelled tasks have demonstrated significant reductions in therapeutic and diagnostic errors often encountered in human medical practice.<sup>[10]</sup>

While there are many definitions of AI, it has often been described as "the theory and development of computer systems to perform tasks that normally would require human cognition, such as perception, language understanding, reasoning, learning, planning, and

problem-solving.”<sup>2</sup> Machine learning is a key part of many AI tools, and the United States Food and Drug Administration defines machine learning as “an artificial intelligence technique that can be used to design and train software algorithms to learn from and act on data. New technologies are emerging at a rapid pace, forcing health care providers to consider adopting these technologies to optimize patient care. While the application of AI is expanding rapidly in health care, there are also many applications within the field of health care education. Multiple surveys demonstrate that health profession students have a basic understanding of AI principles, are aware of AI technologies they are using, are familiar with AI topics discussed in the medical community, and perceive AI positively.”<sup>[11]</sup>

### **AI in Drug Discovery**

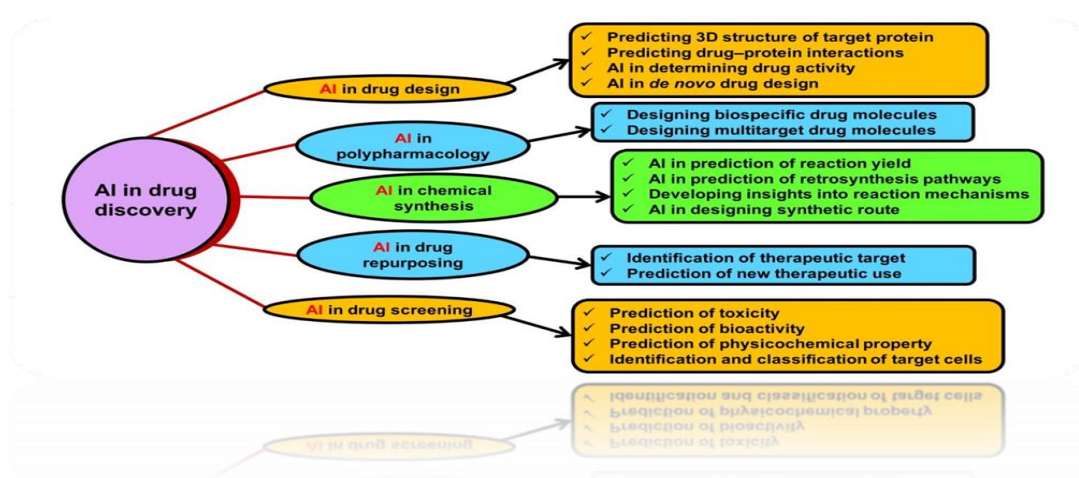
Developing drugs is perhaps one of the most expensive and riskiest processes in the world, costing over \$2 billion for a typical drug. About 90% of potential drugs fail to attain FDA approval. The early stage of developing drugs primarily comprises the discovery and preclinical trials that often involve animal testing where drug candidates are proposed to address certain biological targets that cause a disease. Once a drug candidate-target pair is found and verified during the preclinical trial phase, the drug enters the later clinical trials stage. If the drug succeeds in these trials, the last stage involves the FDA deciding whether to grant final approval.

We focus on AI's effect on the early stage of drug discovery because the early stage is particularly crucial to the entire innovation process in that discovering more drug candidates initially will likely lead to more clinical trials and approvals. Furthermore, because an average drug can take more than 10 years to develop and because many advances in machine learning are too recent, it may be too early to capture AI's effect on later stages.”<sup>[12]</sup>

Artificial Intelligence has recently been developed into a sizzling topic in the area of medical care industry. The biopharmaceutical industries are making efforts to approach AI to enhance drug discovery process, reduce research and development expenses, diminish failure rates in clinical trials and ultimately generate superior medicines. The accessibility of immense statistics in life sciences and a speedy development in machine learning algorithms led to an evolution of AI-based start-up companies focused on drug discovery over the recent years. Numerous remarkable AI-biopharmaceutical alliance were declared in 2016-2017 that include Pfizer and IBM Watson, Sanofi Genzyme and Recursion Pharmaceuticals, AstraZeneca, Abbvie, Merck, Novartis, GSK and Exscientia, etc.”<sup>[8]</sup>

The vast chemical space, comprising >10<sup>60</sup> molecules, fosters the development of a large number of drug molecules. However, the lack of advanced technologies limits the drug development process, making it a time-consuming and expensive task, which can be addressed by using AI. AI can recognize hit and lead compounds, and provide a quicker validation of the drug target and optimization of the drug structure design. Different applications of AI in drug discovery are depicted in Figure no.2

Role of artificial intelligence (AI) in drug discovery. AI can be used effectively in different parts of drug discovery, including drug design, chemical synthesis, drug screening, polypharmacology, and drug repurposing.<sup>[4]</sup>



**Fig. No. 2: AI in drug discovery.**

Another key application of AI in drug discovery is the design of novel compounds with specific properties and activities. Traditional methods often rely on the identification and modification of existing compounds, which can be a slow and labour-intensive process. AI-based approaches, on the other hand, can enable the rapid and efficient design of novel compounds with desirable properties and activities. For example, a deep learning (DL) algorithm has recently been trained on a dataset of known drug compounds and their corresponding properties, to propose new therapeutic molecules with desirable characteristics such as solubility and activity, demonstrating the potential of these methods for the rapid and efficient design of new drug candidates.<sup>[13]</sup>

Cui and Zhu aimed to determine whether AI can predict the physicochemical properties (solubility, partition coefficient, dissociation constant) of different drugs, using a neural network called ResNet. The increased yield and reduced extraction time of polysaccharides

from different sources showed that this network was more accurate in predicting the solubility of the molecules when compared to other non-AI based models. This showed that AI can be integrated into the drug development procedure in order to improve its efficiency.<sup>[14]</sup>

The process of Drug Discovery affects the whole pharmaceutical sector including all the phases such as a preliminary phase of research from target Discovery and validation to the discerning of molecules. A variety of streams can be used to initiate the identification of small therapeutic molecules. New research can lead to awareness of different diseases with different routes of drug administration and can be developed to take part in pharmaceutical companies to run large-scale trials and other waste programs, in order to identify the targeted molecular compounds. This process is mostly performed at the beginning of lead Discovery, with the prospect of taking identified compounds in the right way through preclinical and clinical trials.<sup>[15]</sup>

### **Drug Development Process**

Drug development is the process of bringing a new drug molecule into clinical practice; in its broadest definition, it includes all stages from the basic research of finding a suitable molecular target to large-scale Phase III clinical studies that support the commercial launch of the drug to post-market pharmacosurveillance and drug-repurposing studies. During the drug development process, chemical entities that have the potential to become therapeutic agents are identified and thoroughly tested, and the entire process is lengthy and costly.<sup>[16]</sup>

The first step in drug development is the identification of novel chemical compounds with biological activity. This biological activity can arise from the interaction of the compound with a specific enzyme or with an entire organism. The first compound that shows activity against a given biological target is called a 'hit'. Hits are often found during the screening of chemical libraries, computer simulation or screening of naturally isolated materials, such as plants, bacteria and fungi. The identification of a lead molecule is the second step in drug development. A lead is a chemical compound that shows promising potential that can lead to the development of a new drug as a treatment of disease.<sup>[17]</sup>

The developments in drug discovery have changed the practice of medicine tremendously that converting once fatal diseases into a kind of routine therapeutic exercises. One reason of this medicinal advancement has been an enhancement in the methods of developing and

testing new drugs. A new drug usually does not imitate an existing drug in chemical structure that necessitates the discovery of a new molecule. The new molecules are mostly found by the public sector as universities and research centres while the development of a new medicine, is usually done by industrial laboratories due to the requirement of very expensive chemicals, pharmacologic and toxicological screening and thorough testing. Due to these obstacles, therefore, the recent advancements are ascribed to the pharmaceutical industry as a pharma with its multibillion dollar corporation that is devoted to drug development and marketing. Development of a new drug is a very lengthy and highly expensive process since only, preclinical, pharmacokinetic, pharmacodynamic and toxicological studies include a multitude of *in silico*, *in vitro*, *in vivo* experimentations that traditionally last in average 4 years.<sup>[18]</sup>

artificial intelligence (AI) and machine learning (ML) technologies, which promise to quicken and improve the process. AI and ML models have shown the ability to analyse enormous datasets, discover insightful patterns, and generate predictions for identifying prospective drug candidates and targets. Lead optimization<sup>[3]</sup>, virtual screening, compound design, and medication repurposing are just a few of the domains where the use of AI and ML in drug development has already produced promising outcomes. These models have the potential to greatly overshoot the success rate of drug discovery and decrease the time and expense involved as they become more complex and potent. As AI and ML models become more complicated, a major issue in the area has emerged, which is the lack of transparency and interpretability.<sup>[19]</sup>

### **AI in Pharmaceutical Manufacturing**

The AI-driven process optimization in pharmaceutical manufacturing includes optimizing the formulation of tablets, capsules, and injections to reduce production time and costs; improving packaging processes for blister packs and vials to increase efficiency; and automating quality control inspections for detecting defects and ensuring product consistency. The pharmaceutical manufacturing industry is undergoing a transformation through the application of AI, which utilizes machine learning algorithms to analyse extensive datasets, optimize complex drug formulation processes, and enhance production efficiency. Machine learning algorithms can improve production scheduling by examining historical data and predicting periods of high demand, resulting in more effective resource allocation and increased productivity.<sup>[20]</sup>

Pharmaceutical production faces not just stringent quality controls but also the expectations of a dynamic market. The pharmaceutical industry is under continual pressure to boost output while decreasing prices and introducing new products more rapidly. To be competitive in this ever-changing market while maintaining the highest quality standards, new strategies are needed.<sup>[5]</sup>

The innovative “Chemputer” system facilitates digital mechanization in the synthesis and production of molecules, unifying many chemical signatures and executing by utilizing a scripting software code named “Chemical Assembly (CHASM)”. This has been utilized opportunely for the formation and production of diphenhydramine hydrochloride, rufinamide, and sildenafil, with the harvest and cleanness notably identical to hand-operated synthesis.

“Discrete Element Modelling (DEM)” is extensively employed in the pharmaceutical sector, such as in evaluating the partition of powders constituting a binary mixture, the fallout of altering blade speed and geometry, foretelling the probable route of the tablets for the encapsulation procedure, together with scrutiny of time expended by tablets in the spray section. ANNs, coupled with fuzzy paradigms, examined the interrelationship among machine settings as well as the issue of capping to pare tablet capping on the production line.<sup>[21]</sup>

The role of collaboration between AI researchers and pharmaceutical scientists is crucial in the development of innovative and effective treatments for various diseases. By combining their expertise and knowledge, they can create powerful algorithms and machine-learning models intended to predict the efficacy of potential drug candidates and speed up the drug discovery process. This collaboration can also help improve the accuracy and efficiency of clinical trials, as AI algorithms can be used to analyse the data collected during these trials to identify trends and the potential adverse effects of the drugs being tested. This can help pharmaceutical companies to make informed decisions about which drug candidates to pursue and can speed up the overall drug development process. Furthermore, collaboration between AI researchers and pharmaceutical scientists can also help to improve the accessibility and affordability of healthcare. By using AI algorithms to analyse data from large populations, they can be used to identify trends and patterns that can help predict the effectiveness of potential drug candidates for specific patient populations, which can help tailor treatments to the needs of individual patients. An illustrative example is the collaboration between the pharmaceutical company Merck and the AI company Numerate to

develop AI-based approaches for medicinal chemistry. Many new companies are currently arising around this area of research and their impact is expected to be significant in the short term. By working together, they can help to identify new targets for drug development and improve the effectiveness of existing treatments, ultimately benefiting patients and improving their quality of life.<sup>[13]</sup>

### **AI in quality control and quantity assurance**

Manufacturing of the desired product from the raw materials includes a balance of various parameters. Quality control tests on the products, as well as maintenance of batch-to-batch consistency, require manual interference. This might not be the best approach in each case, showcasing the need for AI implementation at this stage. The FDA amended the Current Good Manufacturing Practices (cGMP) by introducing a 'Quality by Design' approach to understand the critical operation and specific criteria that govern the final quality of the pharmaceutical product.<sup>[4]</sup>

Artificial Intelligence (AI) has a range of applications in pharmaceutical manufacturing that enhance quality control processes. These applications utilize AI's capabilities for data analysis, pattern recognition, and automation to ensure the production of safe and high-quality pharmaceutical products. Here are some specific applications to improve quality control and decision making in pharmaceutical manufacturing:

- **Visual Inspection and Defect Detection:** AI-powered computer vision systems analyze images of pharmaceutical products, packaging, and labels to identify defects, inconsistencies, and impurities. This automated visual inspection ensures that only products meeting stringent quality standards move forward in the production process. AI performs visual inspection and defect detection in pharmaceutical manufacturing through a combination of advanced technologies, including image recognition, machine learning, and computer vision.
- **Data Collection:** Images of pharmaceutical products, packaging, and labels are captured using cameras and sensors positioned at different points in the manufacturing process. These images serve as the input data for the AI system.
- **Data Preprocessing:** The collected images undergo preprocessing, which may include resizing, normalization, noise reduction, and enhancement. This ensures that the images are in a consistent format and quality, making them suitable for analysis.

- **Training Data Preparation:** A labelled dataset of images is created, where each image is annotated to indicate the presence or absence of defects. These annotations serve as the ground truth for training the AI model.
- **Model Training:** A machine learning model, often a convolutional neural network (CNN) due to its effectiveness in image analysis, is trained using the labelled dataset. The model learns to identify patterns and features associated with defects and non-defective products.
- **Defect Detection:** During real-time production, the AI model analyses images of products as they passthrough the inspection point. The model compares the extracted features from these images to the features it learned during training. If the features match those associated with defects, the model classifies the product as defective.
- **Continuous Learning and Improvement:** This process of continuous learning improves the model's accuracy and reduces false positives and negatives over time
- **Integration with Manufacturing Line:** The AI system is integrated into the manufacturing line, often in real-time, to ensure prompt defect detection and decision-making. Integration may involve synchronization with other production control systems and equipment.
- **Feedback Loop:** This feedback loop helps manufacturers identify root causes and take corrective actions to prevent similar defects in the future.<sup>[22]</sup>
- **Real-time Data Integration:** The RNN and LSTM models' incorporation into the pharmaceutical production setting is an essential part of the technique. The trained models will be given data in real time from sensors on the equipment, allowing them to make continuing predictions. By combining these systems, we can detect maintenance issues instantly and respond accordingly.<sup>[5]</sup>
- **Machine learning models for predictive quality management:** Good quality management by the use of machine learning models like Random Forest, Gradient Boosting Machines, and Support Vector Machines (SVM) goes beyond defect detection. These models assimilate production data, which could include values for temperature, pressure, and humidity, to make predictions about quality-related issues. Machine-learning models help manufacturers in mitigating such issues pre-emptively by recognizing trends and anomalies, thus minimizing wastage and ensuring product conformity.<sup>[20]</sup>

### The Role of AI in Detection Technology

The role of artificial intelligence (AI) in the detection of counterfeit drugs is pivotal, leveraging advanced technologies such as machine learning, image recognition, and data analytics. Here's an overview of how each technology contributes to the fight against counterfeit pharmaceuticals.<sup>[23]</sup>

- **Machine Learning (ML):** AI also contains a subfield called machine learning (ML), which uses statistical methods with the ability to learn with or without being explicitly programmed. ML is categorised into supervised, unsupervised and reinforcement learning. Supervised learning comprises classification and regression methods where the predictive model is developed based upon the data from input and output sources. ML can analyze the chemical composition, packaging details, and textual information on drug labels, comparing them against databases of known authentic samples.<sup>[17]</sup>
- **Data analysis (DA):** AI/ML has analysed large volumes of complex and variable RWD from various sources, including sickness registries, medical claims, and EHRs. Predictive modelling and counterfactual simulation utilizing AI/ML are also used to study clinical trial designs. For instance, computer simulation and modeling are used in silico clinical trials to evaluate drug candidates using a virtual cohort of simulated people with traits representing the desired participant population. In these circumstances, AI/ML could help estimate counterfactual simulations and forecast trial results before human trials. Machine learning algorithms can efficiently analyse large and complex clinical datasets. By automating data processing and analysis, AI/ML helps draw quicker insights and aids decision-making.<sup>[24]</sup>
- **Image Recognition:** Image recognition technology employs artificial intelligence to analyse visual data from drug packaging and the drugs themselves. Utilizing convolutional neural networks (CNNs), a type of deep learning algorithm, these systems examine images for inconsistencies in packaging, labelling, and the physical appearance of the pills, such as colour and shape variations that may indicate a counterfeit product. This technology is particularly useful in environments requiring rapid verification, such as customs inspections or pharmacy intake processes.<sup>[23]</sup>

### The Role of AI in Addressing Current Pharmaceutical Challenges

Research on nano molecules is underway in the pharmaceutical sector to improve goods and ensure consumer satisfaction. These molecules have various benefits. Preparing synthetic derivatives is cheap and requires little effort in the chemical synthesis process. Therefore, a

wide variety of stable and effective formulations including tiny molecules, are available in the pharmaceutical industry. Innovative small molecules confront competition from generic molecules, complicated data is necessary for their introduction, and clinical studies are also necessary, except for uncommon illness therapy. As a result of these procedures, businesses are under increasing financial pressure to innovate. Amidst the dilemma caused by molecules being too tiny and advances not being widely disseminated, the biomolecular drug business continues to expand quickly. The shape and reactivity of small molecules constitute the foundation of their effects. The building blocks of proteins, known as amino acids, and the building blocks of nucleic acids, known as nucleotides or ribonucleotides, make up biomolecules. The spatial conformation and supramolecular sequence also impact their stability and function. Products from biomolecules, like insulin and adalimumab, have succeeded wildly. Because infusion is the most practical and preferred method of administering these biomolecules, their pharmacokinetics are intricate. Research based on nucleic acids places a premium on pharmacokinetic regulation and molecular stability.<sup>[25]</sup>

### Advantages of AI Technology

The potential advantages of AI technology are as follows,

- 1) **Error minimization**— AI assists to decrease the errors and increase the accuracy with more precision. Intelligent robots are made of resistant metal bodies and capable of tolerating the aggressive atmospheric space, therefore, they are sent to explore space.<sup>[1]</sup>
- 2) **Speeds up finding promising molecules** — discovering new drug molecules is slow. Scientists have to test thousands of compounds in the lab, which can take years. AI can analyse huge amounts of chemical and biological data much faster than humans. It predicts which molecules are likely to work as drugs, helping researchers focus only on the most promising candidates. This reduces time, cost, and effort in early drug discovery.<sup>[26]</sup>
- 3) **Reduces early experimental cost** — In traditional drug discovery, researchers need to run many lab experiments to test potential drug molecules, which is expensive and time-consuming. AI can predict which molecules are most likely to succeed before any lab work. By focusing only on the promising candidates, companies spend less money on unnecessary experiments, saving a lot of cost in the early stages of drug development.<sup>[27]</sup>
- 4) **Improves target identification and validation** — A drug target is usually a protein or gene involved in a disease. Identifying the right target is crucial because the drug must interact with it to be effective. Traditionally, finding targets involves years of

experiments. AI can analyse large datasets—like genetic data, protein structures, and disease pathways—to identify which targets are most likely involved in a disease.<sup>[28]</sup>

- 5) **Better ADMET / toxicity prediction earlier** — Short Explanation: AI can quickly predict how a drug will behave in the body and if it might be toxic, helping scientists avoid unsafe or ineffective compounds early and save time and money.<sup>[29]</sup>
- 6) **Improves clinical trial design and patient selection** — AI can analyze patient data, genetics, and disease patterns to identify the right patients for a trial and design more effective studies. This increases the chances of success, reduces costs, and speeds up drug development.<sup>[26]</sup>
- 7) **Combines diverse data** — AI can integrate many types of data—like genetics, chemical structures, clinical records, and research papers—into a single analysis. This helps researchers see patterns and insights that humans might miss, improving decision-making in drug discovery.<sup>[30]</sup>
- 8) **Shortens timeline from idea to clinic** — AI speeds up drug development by quickly identifying targets, predicting promising molecules, checking safety early, and optimizing clinical trials, allowing drugs to reach patients faster.<sup>[31]</sup>

### Disadvantage of AI Technology

The potential disadvantage of AI technology are as follows,

- 1) **Data quality and availability problems** —If the AI is trained on incorrect, outdated, or incomplete information, it might make wrong suggestions for drugs, leading to wasted time, cost, and effort. Also, some important data may be unavailable due to privacy, regulatory, or proprietary reasons, limiting AI's ability to learn.<sup>[26]</sup>
- 2) **Poor model interpretability** — If the AI is trained on incorrect, outdated, or incomplete information, it might make wrong suggestions for drugs, leading to wasted time, cost, and effort. Also, some important data may be unavailable due to privacy, regulatory, or proprietary reasons, limiting AI's ability to learn.<sup>[32]</sup>
- 3) **Overfitting and reproducibility concerns** — These issues make AI models unreliable because they may work perfectly on known data but fail on new data, and their results cannot always be trusted or repeated.<sup>[28]</sup>
- 4) **Regulatory and validation hurdles** — AI may suggest a new medicine, but it must pass many tests and government approvals before people can use it.<sup>[29]</sup>
- 5) **Data sharing and privacy issues** — companies often keep data private, limiting AI training.<sup>[26]</sup>

- 6) **Risk of false predictions** — An AI model predicts that a certain chemical compound will be effective against a disease, but lab tests show it doesn't work. This leads to wasted time, cost, and effort in the drug development process.<sup>[30]</sup>
- 7) **Security concerns** — AI could be misused to design harmful compounds.<sup>[26]</sup>

## CONCLUSION

Artificial Intelligence (AI) is changing how we discover and develop drugs by making the process faster, cheaper, and more accurate. In drug discovery, AI helps find new drug candidates, predict how molecules interact, and improve potential drugs. In drug development, it helps design better clinical trials, select the right patients, and predict safety and effectiveness, saving time and money. In pharmaceutical manufacturing, AI improves production, ensures quality, and predicts equipment problems. AI in detection technologies helps diagnose diseases early, find biomarkers, and monitor treatment in real time. It also helps solve current challenges like high failure rates, complex regulations, and the need for personalized medicine.

AI has many benefits, including faster drug development, lower costs, and more precise treatments, but challenges like data quality, ethical issues, and regulatory hurdles remain.

In the future, AI will work with more data, virtual trials, and smart manufacturing to improve personalized medicine, reduce failures, and provide faster solutions, ultimately improving patient care worldwide.

## REFERENCES

1. C. Souljah, C. Bejjani, N. Adra, L. Blackburn. "Artificial intelligence as a drug information Resources: Limitations and Strategies to Optimize in pharmacy practice." *Hospital Pharmacy*, 00185787251, 372-424, 2025.
2. S. Das, R. Dey, A. K. Nayak. "Artificial intelligence in pharmacy." *Indian J Pharma Educ Res*. Kumar Nayak.
3. V. Kaul, S. Enslin, S. A. Gross. "History of Artificial intelligence in medicine." *Gastrointestinal endoscopy*, 2020; 92(4): 807-812.
4. K.K. Mak, Y. H. Wong, M. R. Pichika. "Artificial intelligence in drug discovery and development." *Drug discovery and evaluation: safety and Pharmacokinetic assay*, 2024; 1461-1498.

5. A. K. Mehta, P. Lanjewar, D. S. Murthy, P. Ghildiyal, R. Faldu. "AI and lean management principles based pharmaceutical manufacturing process." 2023 10th IEEE Uttar Pradesh section International Conference on Electrical, Electronic and Computer engineering (UPCON), 2023; 10: 1599-1604.
6. H. Allam. "Prescribing the future: The role of artificial intelligence in pharmacy." *Information*, 2025; 16(2): 131.
7. M. J. Lamberti, M. Wilkinson, B. A. Donzanti, G. E. Wohlhieter, et al. " A study on the application and use of artificial intelligence to support drug development." *Clinical therapeutics*, 2019; 41(8): 1414-1426.
8. P. Agrawal. "Artificial intelligence in drug discovery and development." *Journal of Pharmacovigilance*, 2018; 6(2): 1000e 173.
9. F. Bai, S. Li, H. Li. "AI enhances drug discovery and development." *National science review*, 2024; 11(3): nwad303.
10. H. Jessica, R. Brithey, E. D. Sarira, et al. "Applications of Artificial intelligence in current Pharmacy Practice: A scoping review." *Research in social and administrative pharmacy*, 2025; 21(3): 134-141.
11. M. H. A. Aziz, C. Rowe, R. Southwood, et al. "A scoping review of artificial intelligence within pharmacy education American." *Journal of pharmaceutical education*, 2024; 88(1): 100615.
12. Bowen Lou, Lynn Wu. "AI on drugs: Can artificial intelligence accelerate drug development? Evidence from a large-scale examination of bio-pharma firms." *MIS quarterly*, 2021; 45(3): 1451-1482.
13. A.B. Gonzalez, A. Cabezon, Alejandro Seco-Gonzalez, Daniel Conde-Torres, Paula Antelo-Riveiro, Angel Pineiro, Rebeca Garcia-Fandino. "The role of AI in drug discovery: challenges, opportunities, and strategies." *Pharmaceuticals*, 2023; 16(6): 891.
14. V. Patel, M. Shah. "Artificial intelligence and machine learning in drug discovery and development." *Intelligent Medicine*, 2022; 2(3): 134-140.
15. B.S. Mahajan, B.S.P Mahale, A.R. Pawar, V.V. Patil, P.S. Patil, J. Songire. "A Review on Artificial Intelligence in Pharmacy." *Research Journal of Science and Technology*, 2024; 16(2): 129-136.
16. Z. Chen, X. Liu, W. Hogan, E. Shenkman, J. Bian. "Applications of artificial intelligence in drug development using real-world data." *Drug discovery today*, 2021; 26(5): 1256-1264.

17. K.K. Mak, M.R. Pichika." Artificial intelligence in drug development: present status and future prospects." *Drug discovery today*, 2019; 24(3): 773-780.
18. H. Farghali, N.K. Canová, M. Arora. "The potential applications of artificial intelligence in drug discovery and development." *Physiological Research*, 2021; 70(Suppl 4): S715.
19. R. Alizadehsani, S.S. Oyelere, S.Hussain, S.K. Jagathesaperumal, R.R. Calixto, M. Rahouti, M. Roshanzamir, V.H.C.D. Albuquerque. "Explainable artificial intelligence for drug discovery and development: a comprehensive survey." *IEEE Access*, 2024; 12: 35796-35812.
20. M.V. Rajesh, K. Elumalai. "The transformative power of artificial intelligence in pharmaceutical manufacturing: Enhancing efficiency, product quality, and safety." *Journal of Holistic Integrative Pharmacy*, 2025; 6(2): 125-135.
21. C. Sarkar, B. Das, V.S. Rawat, J.B. Wahlang, A. Nongpiur, I. Tiewsoh, N.M. Lyngdoh, D. Das, M. Bidarolli, H.T. Sony. "Artificial intelligence and machine learning technology driven modern drug discovery and development." *International Journal of Molecular Sciences*, 2023; 24(3): 2026.
22. G.C. Saha, L.N. Eni, H. Saha, P.K. Parida, R. Rathinavelu, S.K. Jain, B. Haldar. "Artificial intelligence in pharmaceutical Manufacturing: Enhancing quality control and decision making." *Rivista Italiana di Filosofia Analitica Junior*, 2023; 14(2): 2023.
23. R.O. Joseph, W.O. Abiodun, D.U. Oboite, E.O. Oyeniyi, Q.D. Hakeem."The Role of AI in Combating Counterfeit Drugs." *Journal of Clinical and Metabolism Studies*, 2024.
24. S.K Niazi. "The coming of age of AI/ML in drug discovery, development, clinical testing, and manufacturing: the FDA perspectives." *Drug Design, Development and Therapy*, 2023; 2691-2725.
25. R.J. Alanazi. " Role of artificial intelligence in pharmacy practice: A systematic review." *Archives of Pharmacy Practice*, 2024; 15(2-2024): 34-42.
26. Vamathevan J. et al., 'Applications of machine learning in drug discovery and development', *Nature Reviews Drug Discovery*, 2019. Link: <https://www.nature.com/articles/s41573-019-0024-5>
27. Kim H. et al., 'Artificial Intelligence in Drug Discovery: A Comprehensive Review', *Pharmaceuticals*, 2021. Link: <https://www.mdpi.com/1424-8247/14/8/806>
28. Blanco-González A. et al., 'The Role of AI in Drug Discovery: Challenges and Opportunities'; *Frontiers*, 2023. Link: <https://www.frontiersin.org/articles/10.3389/fdgth.2023.1119282/full>

29. Jiménez-Luna J. et al., 'Artificial intelligence in drug discovery: recent advances and future perspectives', Drug Discovery Today, 2021. Link: <https://www.sciencedirect.com/science/article/pii/S1359644620304427>
30. Dara S., 'Machine Learning in Drug Discovery: A Review', Springer, 2021. Link: <https://link.springer.com/article/10.1007/s10989-021-10125-5>
31. Annual Review 2024. Link: <https://www.annualreviews.org/journal/drugdisc>
32. Bender A., 'Artificial intelligence in drug discovery: what is realistic?', 2021. Link: <https://pubs.acs.org/doi/10.1021/acs.jmedchem.0c01222>