Review Article

AI in Drug Delivery Design and Pharmaceutical Technology

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Received: 06-07-2026; **Revised:** 22-09-2026; **Accepted:** 29-09-2026; **Published online:** 20-10-2026.

ABSTRACT

Artificial intelligence (AI) is transforming pharmaceutical sciences by offering innovative approaches to drug discovery, development, and delivery design. Conventional methods of formulation and testing are time-consuming, costly, and often dependent on extensive laboratory experimentation. AI and machine learning algorithms provide the ability to analyze complex biological datasets, predict pharmacokinetic and pharmacodynamic behavior, and guide the optimization of dosage forms. These advances enable researchers to design more efficient delivery systems, reduce experimental errors, and accelerate the regulatory approval of novel therapeutics. Applications of AI extend across multiple domains, including prediction of toxicity, process optimization, personalized medicine, and enhancement of patient adherence strategies. By integrating real-world patient data, AI supports individualized treatment approaches and contributes to the development of safer and more effective formulations. Despite these benefits, challenges such as data integrity, algorithm transparency, and regulatory acceptance continue to limit widespread adoption. Overall, AI presents a significant opportunity to modernize pharmaceutical research and drug delivery design. Its careful integration into current practices holds the potential to reduce costs, improve therapeutic outcomes, and reshape the future of patient-centered healthcare.

Keywords: Artificial Intelligence; Machine Learning; Drug Delivery Systems; Pharmaceutical Formulation; Nanomedicine; 3D Printing.

INTRODUCTION

Numerous sectors are employing various techniques to enhance and satisfy consumer demands. Among them, the pharmaceutical industry is of critical importance because it directly saves lives. In order to address global health issues and react swiftly to medical catastrophes, such as the recent pandemic, this sector relies on ongoing innovation and the application of advanced technologies[1]. Innovation in pharmaceuticals is usually rooted in intensive research and development in areas including production technology, packaging considerations, and patient-centered marketing approaches[2]. To meet unmet medical needs, there is a growing demand for drugs that are more stable, safer, and more effective. However, high toxicity levels associated with newly developed medicines remain a significant concern, necessitating further study and investigation. The overall goal continues to be the development of therapeutic molecules that are both clinically relevant and capable of providing maximum benefit. Despite progress, the pharmaceutical industry still encounters multiple challenges that require novel strategies to satisfy global healthcare demands[3–5].

Another critical aspect of this sector is the need for a trained and skilled workforce. Healthcare professionals must undergo continuous training to keep pace with new systems and therapies. Addressing existing skill gaps is crucial, yet providing adequate training opportunities is often difficult. Workforce shortages remain a pressing issue that limits progress in both research and manufacturing[6]. In addition, supply chain disruptions present one of the most significant challenges for the industry, accounting for nearly 41% of all reported incidents in June 2022[6]. Recent years have seen an increasing focus by pharmaceutical companies on strengthening their supply chains and adopting more resilient models. The global COVID-19 pandemic further exposed the vulnerabilities of existing systems, leading to major disruptions in research, clinical trials, and routine operations worldwide[7].

Supply chain instability can be triggered by various events such as pandemics, natural disasters, price fluctuations, cyberattacks, and logistical failures. For instance, transportation restrictions during the COVID-19 crisis had severe consequences for distribution networks, while trade barriers and unpredictable pricing added to volatility. These circumstances often resulted in manufacturing setbacks, shortages of raw materials, and the need to reconfigure production footprints to meet patient demands. Failures in maintaining cold chain requirements further led to wastage of large quantities of COVID-19 vaccines, reflecting the sector's lack of forecasting accuracy and preparedness [8,9].

Clinical trials, a cornerstone of pharmaceutical development, have also faced significant difficulties. Traditional clinical trial models frequently require heavy manual data entry, repeated tasks, and extensive patient travel to trial sites. Such requirements slow down recruitment, affect patient enrollment and monitoring, and increase dropout rates. These challenges not only delay drug development timelines but also compromise the efficiency and data quality. Additionally, issues such as fragmented systems, data redundancy, and high operational costs add further complexity to trial execution. Patient confidentiality and data security remain pressing concerns, as sensitive information is vulnerable to breaches in conventional systems [10–12].

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In summary, the pharmaceutical sector is confronted with a wide spectrum of obstacles ranging from workforce shortages and supply chain instability to inefficiencies in clinical trials and increasing demands for safer, more effective therapies. These barriers underscore the necessity of developing advanced, technology-driven approaches to sustain growth, ensure global preparedness, and meet rising healthcare expectations [13–15].

SIGNIFICANCE OF AI IN DRUG DELIVERY DESIGN

Researchers can identify any hazards and difficulties associated with drug delivery systems beforehand in the situation process by employing the applicable set of AI technologies. This makes it possible to make visionary changes and adjustments to reduce pitfalls and improve drug performance. By reducing the need for expensive and time-consuming trial-and-error experiments, artificial intelligence (AI) and computational modeling lower the risk of unexpected outcomes. It helps predict the physicochemical properties, stability, and in vitro drug release profile of a medicine. Without extensive trial-and-error testing, researchers can evaluate different scenarios and improve drug delivery systems by modeling the composition and transport behavior of drugs. AI systems can predict drug performance at every scale by analyzing complex correlations between pharmacological characteristics, formulation components, and physiological parameters. By simulating drug formulation and delivery processes, researchers can estimate various scenarios and enhance drug delivery systems without extensive trial-and-error experiments. Computational pharmaceutics analyzes large volumes of data and predicts drug performance using AI algorithms and machine learning approaches [16,17].

Applications of AI for:

i. For the Physicochemical Stability Prediction.
ii. Developing an Oral Solid Dosage Form.
iii. Creation of 3D-Printed Oral Solid Dosage Forms.
iv. Biologics for Nanomedicine.
v. Product Design and Health Services Innovation.

For the Physicochemical Stability Prediction-

By using machine learning algorithms to study the stability of oral formulations, artificial intelligence (AI) can analyze and interpret large datasets, including pharmacological characteristics, formulation parameters, and environmental factors, using computational models. Factors such as drug degradation, interactions with excipients, and environmental impacts on formulation stability can all be estimated using AI models. Using these predictive capabilities, researchers can improve formulation designs, identify possible stability problems early in the development process, and make well-informed choices that increase the effectiveness and shelf life of oral dosage forms. The use of AI for stability prediction helps make drug development processes more efficient and cost-effective, ultimately resulting in the provision of safe and effective medicines to patients. Several researchers have investigated the use of machine learning to determine solid dispersion using a variety of approaches. Han et al. explored the use of artificial neural networks (ANN) in conjunction with K-nearest neighbor (KNN) to predict solid dispersion. It was applied to individual data points to classify or complete the predictions of the group [18]. LightGBM, a free and open-source distributed gradient boosting framework based on machine learning, was also used together with individual data points to classify or complete the group's predictions [19]. This study made use of both the KNN and LightGBM (light gradient boosting machine) algorithms. In addition, SVM was applied, which is generally used for classification and ranking tasks besides other machine learning applications. About fifty pharmacological compounds with 646 physical stability data points were gathered from a public database to build the training model for this study. The dataset was built using descriptors such as the number of hydrogen bond acceptors, fingerprint representations, and molecular properties such as molecular weight, melting point, and the number of heavy atoms. A stability study was conducted over three months to evaluate the model's performance against the actual physical stability results, and among the machine learning approaches compared, the random forest model achieved the best prediction accuracy of 82.5%. [20,21].

Building an Oral Solid Dosage Form-

The regulatory bodies are also faced with the difficulty of redefining current good manufacturing practice (cGMP) rules in light of the deployment of AI. For the formation of solid dosage forms and a better comprehension of the inputs and outputs for operations, many AI technologies are used, including artificial neural networks (ANNs), fuzzy logics, neural networks, and genetic algorithms. An artificial neural network (ANN) is employed to improve prediction capabilities for solid dosage forms, and genetic algorithms are used to forecast the outcomes of using input parameters[22].

Table 1: Common AI/ML Models in Pharmaceutical Product Development.

Model	Usage
Genetic Algorithms	Optimize formulation composition, drug release, process parameters
Artificial Neural Networks	Model & predict drug release kinetics, formulation behavior
Support Vector Machines	Optimize formulation design space; predict relationships of variables
Particle Swarm Optimization	Optimize particle size, dissolution profiles, formulations
Expert Systems (AI Based)	Rule-based/fuzzy logic for formulation & process optimization
Monte Carlo Stimulation	Optimize drug performance under variability/uncertainty
Computational Fluid Dynamics	Model mixing & flow in dosage manufacturing
Response Surface Methodology	Study variable relationships & optimize formulation
ANN-GA Hybrid Models	Search formulation space, predict optimal outcomes

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Tablets are one of the most common solid dose forms in the pharmaceutical industry. Several factors, depending on the type of tablet, go into its preparation. Searching for the best formulation and researching the desired qualities involved can be aided by AI. AI is anticipated to use automated algorithms and technology to process duties as well. collection of AI models that are frequently investigated in the creation of pharmaceutical products. Given below in table 1, are the common AI/ML Models in Pharmaceutical Product management.

Biologics for Nanomedicine-

The possibilities for use of nanoparticles tend to involve monitoring, visual analysis, and targeted medication delivery. due to the fact that AI algorithms can forecast the physicochemical characteristics, stability, and effectiveness of nanoparticles, they can help with their design and optimization. Researchers can use this to create nanoparticles with the desired properties for particular uses. Especially for treating cancer patients, nanomedicines are used as efficient drug delivery vehicles for medications or therapeutic combinations based on the idea of drug synergy. The development of new nanoscale interventions, better diagnostics, better medication delivery, and the advancement of customized medicine can all be accelerated by nanomedicine researchers by utilizing AI's strengths in data analysis, pattern classification, and optimization. Artificial Intelligence (AI) in nanomedicine has the potential to completely transform healthcare by facilitating tailored and accurate therapeutic techniques at the nanoscale [23]. The selection of drugs, doses, and stimuli-responsive materials are among the significant and influential inputs they contain. When utilized to treat melanoma, the deep learning algorithm has demonstrated remarkable accuracy in patient care and aiding in diagnostic processes [24,25]. Nano sensors and biosensors that use AI can track drug levels, disease development, and biomarkers in real time. By giving healthcare professionals ongoing input, these sensors can facilitate prompt interventions and individualized treatment modifications [26]. AI systems are able to simulate how nanoscale materials behave and interact with biological systems. The creation of safe and efficient nanomedicine formulations is made easier by the ability to predict the behavior of nanoparticles, drug release kinetics, and possible toxicity. An automated system is used to scale up nanocarriers with the help of an AI-based database. AI is also utilized in medication delivery systems that use nanocarriers, specifically in the computational optimization of nanocarriers and drug compatibility testing. Evaluations of drug loading, filling, formulation stability, and drug retention are conducted by using these methods. Consequently, the application of AI to the treatment of malignancies helps to improve the therapeutic nanocarriers needed for particular cell types. Yuan He and colleagues conducted research on the use of machine learning techniques for the prediction of nanocrystals made using the wet ball milling process in conjunction with high-pressure homogenization. For quantitative measurements in crucial investigations, the simulation techniques are useful. Another study by Lutz Nuhn on the use of AI for improved analysis discovered that, through an examination of individual blood vessels, AI assisted in revealing the heterogeneous vascular permeability for developed nanoparticle-based drug delivery systems. The development of a drug delivery system using protein nanoparticles to provide an active form of trans endothelial permeability into tumors may benefit from these discoveries [27]. In order to investigate cancer medicine successfully, Zhoumeng Lin et al. employed AI for improved assessment using a PBPK modeling approach. Gaining a deeper comprehension of the reasons behind low nanoparticle tumor delivery effectiveness is also aided by this [28].

Creation of 3D-Printed Oral Solid Dosage Forms-

Based on patient-specific variables like gender, height, and medical history, AI algorithms can optimize the formulation and design of 3D-printed dosage forms, resulting in customized medication regimens. Pharmaceutical manufacturing has undergone a revolution thanks to the use of AI in 3D-printed dosage forms, which offers tailored treatment and improves drug delivery methods. Drug release profiles, dose strengths, and geometries can be quickly prototyped and optimized by using AI to examine massive datasets and model the behavior of 3D-printed dosage forms with the use of machine learning and computational modeling.

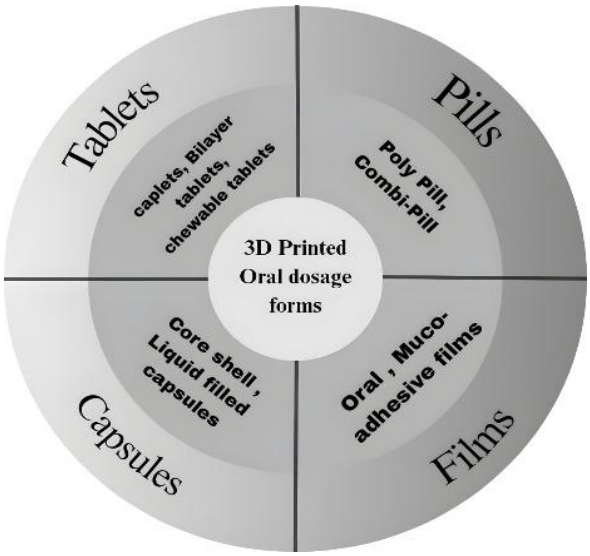


Figure 1: Types of 3D printed oral dosage forms

Additionally, AI helps with quality monitoring, printing parameter optimization, and anticipating and resolving possible production issues. Personalized medicine and patient outcomes could be greatly enhanced by the use of AI in 3D-printed dose forms[29-30]. There are various types of 3D printed Oral Dosage forms used in the field; some of them are illustrated in the figure 1 below.

Product Design and Health Services Innovation-

AI programs can use clinical, proteomic, and genomic data to identify potential treatment targets. By identifying

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disease targets, AI assists researchers in formation or creation of protein and peptide biologics that modifies the biological pathways and also target proteins that cause disease. Artificial intelligence algorithms can use amino acid sequences to anticipate how proteins will fold. Understanding protein function and creating optimal biology require an understanding of protein folding. Protein folding patterns can be predicted by deep learning and molecular dynamics simulations, which aids in the creation of stable and effective biologics [31]. An apparatus, instrument, implant, machine, or reagent used for a particular medical purpose is called a medical device. It can be used either on its own or together with software or supporting equipment to diagnose or treat patients' medical conditions, including in vitro applications. AI has significantly advanced the field of medical devices, transforming healthcare in a number of ways. The pandemic has increased the use of AI and machine learning in the healthcare industry by making tailored medicine and remote health monitoring necessary and widely accepted in many nations. In the given **figure 2** below are some instances in which AI is being applied to medical devices:

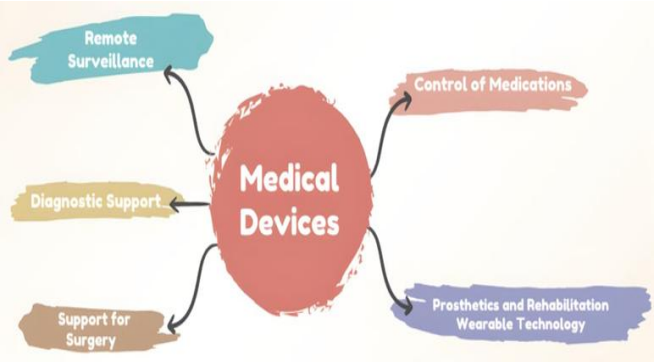


Figure 2: AI applied in medical devices

ADVANTAGES OF AI IN PHARMACEUTICAL INDUSTRY

Small molecules are still being investigated by the pharmaceutical industry due to their benefits, which include stable formulations, cost effectiveness, and ease of production. Many small molecules, however, have drawbacks despite these advantages, such as low solubility, poor bioavailability, and a lack of clinical success because of safety and efficacy issues [32-38]. On the other hand, biomolecular medications like proteins and nucleic acids are becoming more and more significant. Despite their great specificity and efficacy, these compounds have drawbacks, including complex pharmacokinetics, structural instability, and challenging administration methods (e.g., insulin, monoclonal antibodies) [39]. Important objectives still include stabilization, pharmacokinetic exposure regulation, and nucleic acid-based research improvement [40–45]. By predicting molecular attributes, improving medication design, and speeding up candidate molecule screening, artificial intelligence (AI) presents new potential to address these problems. AI-based algorithms lessen the need for trial-and-error by supporting pharmacokinetic modeling, dose prediction, and stability assessment [40–45]. However, there are still certain restrictions or limitations on AI. Its predictions frequently need to be interpreted by experts, and issues like algorithm bias, overfitting, or the production of false-positive outcomes in docking simulations are still prevalent [46]. Consequently, ongoing human involvement in this field is required for decision-making and validation. AI has the potential to significantly lower pharmaceutical research and medication development failure rates, costs, and time despite these obstacles [47].

In pharmaceutical sciences, artificial intelligence (AI) techniques such as machine learning (ML), deep learning, and natural language processing have grown in significance. Learning can be either supervised (with known inputs and outputs) or unsupervised (with uncertain outputs), depending on the data and goals. Unsupervised models categorize data into homogeneous groups, whereas supervised models use various attributes to predict outcomes like labels or objectives [48]. Various AI models are used in pharmaceutical product development to enhance procedures including pharmacovigilance, drug discovery, formulation design, and toxicity prediction. AI is a useful tool for developing the pharmaceutical industry because of these uses, which improve accuracy and efficiency.

Figure 3 describes a collection of frequently investigated AI models in this field.

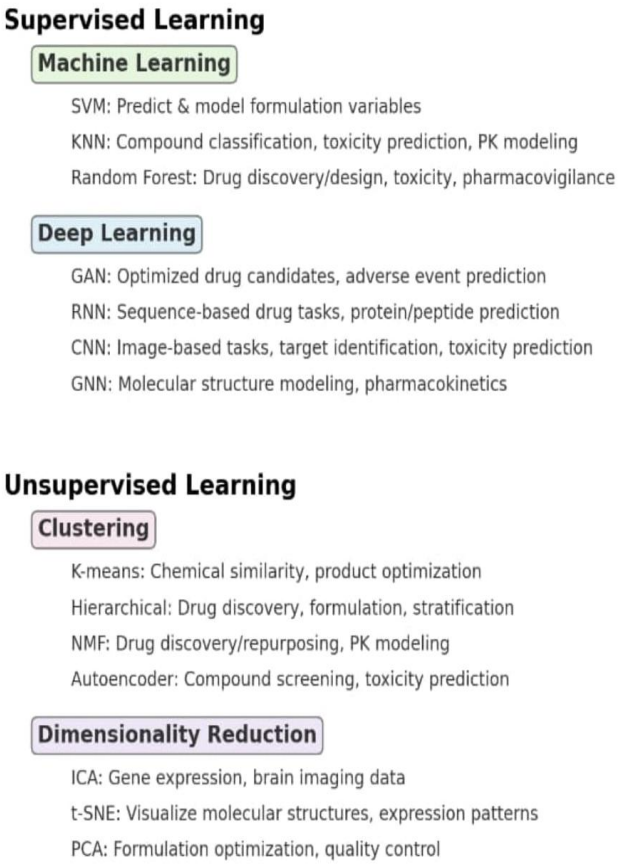


Figure 3: Frequently investigated AI models.

Several AI/ML models have been successfully adapted for pharmaceutical research, each with unique strengths. **Table 2** summarizes the most common models, their applications, and relevant literature.

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Table 2: Common AI/ML models used in pharmaceutical R&D

AI/ML MODEL	ADVANTAGES
Generative Adversarial Networks (GANs)	Novel molecule/structure generation; candidate optimization; chemical-space exploration
Recurrent Neural networks (RNNs)	Sequence tasks (genomics, protein/peptide design); pattern learning from biological sequences
Convolutional neural Networks (CNNs)	Image-based analysis; molecular structure features; target identification
Long Short-Term Memory (LSTM)	Temporal modeling; PK concentration-time profiles; efficacy prediction
Transformer models	NLP on literature/patents/clinical notes; property prediction from sequences
Reinforcement Learning (RL)	Strategy optimization in design; dosing/sequential decision making; personalized plans
Bayesian Models	Uncertainty quantification; risk/decision support; experimental design optimization
Deep Q-Networks (DQNs)	Active learning for discovery; next-experiment suggestion and activity prediction
Autoencoders	Dimensionality reduction; feature extraction; virtual screening/ compound profiling
Graph Neural Networks (GNNs)	Molecular graph modeling; property prediction; de novo design/screening

DISADVANTAGES OF AI TOOLS

Despite their many advantages, AI models have drawbacks, such as the requirement for huge datasets, potential biases, and restricted interpretability. Thus, it's critical to combine AI models with conventional experimental techniques to guarantee the efficacy and safety of drugs.

The following lists the main restrictions.

Lack of transparency

Since it is difficult to comprehend how AI models create predictions, they are frequently referred to as "black boxes." Because it is difficult to prove the accuracy and dependability of AI-based drug development tools, this lack of clarity makes it difficult to obtain regulatory approval. Additionally, it can erode confidence in the model's output, particularly if projections don't match what researchers or physicians had in mind [49-50].

Limited availability of Data

Multiple or larger volumes of data are necessary for AI algorithms to produce precise predictions. However, data may be scarce for some medications or particular demographics, producing results that are biased or less trustworthy. For instance, developing models for rare diseases can be difficult due to a lack of enough data and furthermore, forecasts could be distorted if the training data is not representative of the target population. The inability to gather certain crucial data types, such as real-world or long-term evidence, may further restrict the performance of the model and therefore, it is crucial to ensure that the data utilized to build AI models is high-quality and representative.

Inability to Incorporate New Data

AI models can be challenging to update with fresh data once they have been trained. In drug development, where fresh information is always being discovered, this is a significant restriction. For instance, the model needs to be updated to preserve accuracy whenever new medications are released or more information is obtained from clinical studies. But it frequently takes a lot of effort and money to retrain AI models. These models must adapt as medication development changes in order to prevent poor decision-making and erroneous forecasts. Thus, methods for simple updating are crucial, including creating adaptable models or incorporating them into systems that can be improved over time.

Limited Ability to Account for Variability

Large datasets that frequently concentrate on average answers are used to train AI algorithms. For patients whose reactions deviate significantly from the norm, this may result in erroneous predictions. When it comes to medications, such as those used to treat cancer, where patient reactions can differ greatly, this problem is crucial [51].

Interpretation of Results

Even for specialists, interpreting the results of AI models can be challenging due to their frequent complexity. They might not provide a clear explanation of how predictions are made, which could make it challenging for researchers and doctors to comprehend and use the findings. Sometimes it is difficult to turn these forecasts into useful applications for drug development or clinical practice. Furthermore, the usability of such models may be limited by the technical skills required to use them, which not all specialists possess. To guarantee that AI models' predictions are comprehensible and useful, it is crucial to enhance their interpretability and explainability [52-53].

Ethical Considerations

Several ethical issues are brought up by the use of AI in medicine development. Patient privacy is a major concern because these models are frequently trained using sensitive health data. Protecting patients' rights requires implementing robust data security and handling procedures. Data ownership is an additional concern. Uncertainty over data ownership and usage may arise from the collection of patient information in some situations without explicit authorization. Pharmaceutical corporations, researchers, and patients may clash over these problems [54-55]. Strict procedures, rules, and uniform assessment techniques must be established by regulatory bodies in order to safely include AI into medication development. A number of issues should be covered by these policies, including moral ones like patient safety and

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animal welfare. Given the significance of animal research in drug development, every attempt should be made to minimize, improve, or eliminate the use of animals whenever feasible while adhering to ethical standards. AI models must also undergo rigorous testing and validation to guarantee their accuracy and dependability in order to safeguard patients. The publication of the U.S. Food and Drug Administration's (FDA) discussion paper, "Using Artificial Intelligence & Machine Learning in the Development of Drug and Biological Products," is a significant step in addressing the ethical and regulatory implications of AI in drug research. It examines the use of AI in clinical research, nonclinical investigations, and drug discovery. It also offers recommendations for the most effective ways to use machine learning and artificial intelligence. By addressing the potential advantages and difficulties of AI in drug development, this FDA initiative marks a significant turning point in the regulation of AI in healthcare and opens the door for further advancements in the area [56].

Lack of Clinical Expertise

Although AI is capable of identifying correlations, patient treatments frequently deviate from these trends. AI mostly uses statistical models, which might not adequately account for the many unique and complex variables affecting treatment choices. AI finds it difficult to comprehend deeper clinical nuances due to this intricacy, which goes beyond statistical relationships [57]. Consequently, AI's capacity to fully figure out the aspects and implications that accompany specific parameters may be bound up.

Following figure 4 below summarizes the limitations of AI tools.



Figure 4: Disadvantages/limitations of AI tools

FUTURE SCOPE

Through its ability to speed up drug discovery and development, artificial intelligence (AI) holds the potential to completely transform the pharmaceutical sector. Virtual screening speeds up lead compound selection by quickly analyzing large chemical libraries to find medicinal possibilities. Through analysis of genomes, proteomes, and clinical data, AI-driven precision medicine makes it possible to classify patients, predict therapeutic responses, and provide individualized treatments. Innovative drugs with enhanced target binding can be designed using deep learning and generative models, increasing efficacy and reducing side effects. By taking into account individual characteristics like age, genetics, weight, and illness state, AI can also optimize medicine compositions and customize dosage formulations.

In drug safety, AI algorithms predict the side effects and toxicity of drug candidates, while AI-powered monitoring systems ensure remote patient care and medication adherence. Wearable devices and sensors continuously gather data to guide AI-based personalized therapy. Clinical trial processes also benefit, as AI optimizes trial design, patient selection, and recruitment using electronic health records, biomarkers, and genetic profiles—reducing costs and accelerating approvals. AI also enhances pharmaceutical manufacturing by providing feedback control and real-time monitoring, which guarantees consistent and effective production. Large-scale data analysis can improve the knowledge of regulatory judgments, enable quicker approvals while uphold safety regulations.

Due to the high expenses and time involved in medication research and development, artificial intelligence (AI) offers novel approaches such as multivariate data analysis, dosage ratio optimization, drug bioactivity and interaction prediction, and cellular response modeling. AI helps in the creation of drug delivery systems, the prediction of therapy outcomes, and the optimization of combination therapies in the treatment of infectious diseases. Nevertheless, there are still few real-world uses of AI in drug administration, particularly in clinical settings.

Integrating AI with physiologically based pharmacokinetic (PBPK) modeling is proving valuable in drug development and environmental chemical risk assessment. PBPK models describe drug absorption, distribution, metabolism, and excretion, but constructing mechanistically valid models for novel compounds remains difficult. Advances like Neural-ODE algorithms now enable the creation of PBPK simulations directly from pharmacokinetic data without prior detailed knowledge. Such developments, combined with deep neural networks, enhance the accuracy of PK and PBPK modeling, improving drug discovery and toxicity assessment [58]. Mechanistically valid models for new substances are still hard to create, but PBPK models explain drug absorption, distribution, metabolism, and excretion. It is now possible to create PBPK simulations directly from pharmacokinetic data without the need for prior extensive knowledge thanks to developments like neural-ODE algorithms. When paired with deep neural networks, these advancements improve drug discovery and toxicity

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evaluation by increasing the accuracy of PK and PBPK modeling [58]. AI in pharmacokinetics and pharmacodynamics (PKPD) cannot be fully realized without a solid grasp of scientific principles and the implementation of stringent yet helpful restrictions. It is crucial that pharmaceutical corporations, regulators, and medical professionals work together. Future pharmaceutical research and better patient outcomes could be greatly impacted by AI advancements, even while issues with data quality, ethics, and legal frameworks still exist.

CONCLUSION

Artificial intelligence (AI) integration and technological breakthroughs are causing a radical change in the pharmaceutical industry. Persistent challenges such as supply chain disruptions, rising development costs, and the limitations of conventional drug discovery approaches underscore the critical need for innovation. AI offers practical solutions by accelerating target identification, enabling virtual screening, optimizing clinical trials, and strengthening pharmacovigilance systems. These applications not only reduce timelines and costs but also promote patient-centric, data-driven decision-making. Still, the widespread adoption of AI remains constrained by data privacy concerns, regulatory complications, workforce skill gaps, and high implementation costs. Overcoming these barriers will require interdisciplinary collaboration, robust ethical frameworks, and supportive regulatory programs.

ACKNOWLEDGEMENT

The authors are deeply grateful to their guide, Ms. Sakshi Wankhade, for her invaluable guidance, constant encouragement, and mentorship throughout this work. The authors also thank Dr. Rajendra Gode College of Pharmacy, Amravati (affiliated to Dr. Babasaheb Ambedkar Technological University, Lonere, Raigad) for providing the necessary facilities and support.

Source of Support: The author(s) received no financial support for the research, authorship, and/or publication of this article

Conflict of Interest: The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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