DOI: 10.21088/jpmc.2395.6615.11225.2

Journal of Pharmaceutical and Medicinal Chemistry
Volume 11 Number 2, July - December 2025

REVIEW ARTICLE

Artificial Intelligence in Pharmaceutical Research and Development: From Target Identification to Clinical Applications

R. Vinoth[1], D. Senthil Rajan[2], A. Nandhini[3], M. Tamizharasu[4], D. Rajeswari[5]

HOW TO CITE THIS ARTICLE:

R. Vinoth, D. Senthil Rajan, A. Nandhini et al. Artificial Intelligence in Pharmaceutical Research and Development: From Target Identification to Clinical Applications. J Pharmaceut Med Chem. 2025; 11(2): 51-62.

ABSTRACT

Artificial Intelligence (AI) is emerging as a transformational technique in pharmaceutical research and development, enabling the shift from conventional experimental approaches to predictive, data-driven methodologies. This review is a comprehensive overview of the use of AI in the drug development pipeline, such as identifying targets, discovering hits, lead optimization, preclinical trials, clinical trials, and post-marketing surveillance. Machine learning, deep learning, natural language processing, and generative models are advanced methods that assist the integration of data on a multi-dimensional basis and make decisions about data DSSs more efficient. Despite the challenges related to data quality, interpretability, and regulatory compliance, AI demonstrates significant potential in improving translational success and accelerating therapeutic innovation towards precision and patient centric healthcare.

KEYWORDS

• Artificial Intelligence • Pharmaceutical Research • Drug Development • Lead Optimization • Machine Learning

AUTHOR'S AFFILIATION:

[1] Assisant Professor, Department of Pharmaceutics, Swamy Vivekanandha College of Pharmacy, Tiruchengode, Namakkal, Chennai, Tamil Nadu, India.

[2] Professor and Head, Department of Pharmaceutics, Swamy Vivekanandha College of Pharmacy, Tiruchengode, Namakkal, Chennai, Tamil Nadu, India.

[3] Assisant Professor, Department of Pharmaceutics, Swamy Vivekanandha College of Pharmacy, Tiruchengode, Namakkal, Chennai, Tamil Nadu, India.

[4] PG Student, Department of Pharmaceutics, Swamy Vivekanandha College of Pharmacy, Tiruchengode, Namakkal, Chennai, Tamil Nadu, India.

[5] PG Student, Department of Pharmaceutics, Swamy Vivekanandha College of Pharmacy, Tiruchengode, Namakkal, Chennai, Tamil Nadu, India.

CORRESPONDING AUTHOR:

R. Vinoth, Assisant Professor, Department of Pharmaceutics, Swamy Vivekanandha College of Pharmacy, Tiruchengode, Namakkal, Chennai, Tamil Nadu, India.

E-mail: vinothbpharm16@gmail.com

Received: 13.08.2025 **Accepted:** 18.11.2025

INTRODUCTION

The pharmaceutical industry is an important part of promoting worldwide healthcare by creating therapeutic agents that prevent, diagnose and treat diseases. Any chemical substance intended to prevent, diagnose, treat or relieve a condition is called a drug. Drugs can be prophylactic, therapeutic, symptomatic or disease modifying agents and may be of natural or synthetic origin.[1,2] Discovery and development of such agents is a complex and multidisciplinary process that involves the interplay of chemistry, biology, pharmacology, medicine and data science. Drug discovery and development is a stepwise and methodical pipeline, which transforms a biological concept into a therapeutic product that has gone through clinical approvals.[3,4] Drug discovery refers to the procedure of identifying new chemical compounds or biological molecules that have therapeutic applications and drug development involves the procedure of testing the candidates in preclinical and clinical studies and getting regulatory sanctions. This is an important measure to fulfill unmet medical needs, patient outcomes and quality of life.[5]

In the past, drug discovery has been advanced by the use of empirical methods to very high levels of scientific methods. The early drug discovery was based on natural products and observation of the symptoms of a disease without a clear idea of the disease mechanisms.[6] With time, biomedical sciences allowed shifting to the rational design of drugs, which included information on the disease pathway and molecular targets. An example is the development of quinine to treat malaria, which represents the evolution of folk medicine to scientifically proven medicinal treatments.[7,8] This development has formed the basis of contemporary drug discovery methods combining experimental and computational methods. The modern pharmaceutical industry has a structured pipeline of drug discovery, which includes, identification and validation of the targets, discovery of hits, optimization of the lead, preclinical trials, clinical trials, and regulatory approval. Optimization of leads is an important step where medicinal chemists optimize compounds according to the structure-activity relationships (SAR), pharmacokinetics, and toxicity profiles.[9,10] After optimization, promising candidates are taken through preclinical testing to determine their safety, efficacy, and pharmacokinetic characteristics via in vitro and in vivo experiments.

Drug discovery and development is linked with significant challenges even though the process is structured in this pipeline. It is not only time-intensive, with an average of 10-15 years to gain market approval after discovery, but is also linked to significant financial expenditure, which is usually more than 1-2 billion dollars per drug. Moreover, success rates are very low and only a small percentage of compounds make it to all phases to market.[11–13] The lack of efficacy, safety, ineffective pharmacokinetics and regulatory barriers are usually the causes of high rates of attrition. These problems highlight the role of new methods to optimize the efficiency, reduce the costs and enhance the rate of success during drug development.[14]

The pharmaceutical industry has experienced tremendous impacts of technology, which have brought new tools and techniques to deal with these issues. Genomics, proteomics, high-throughput screening, and structure based drug design are innovations that have helped to develop new targets of drugs and design effective therapeutic agents.[15,16] Artificial intelligence (AI) and machine learning (ML) are some of these innovations that have become some of the radical technologies in the history of drug discovery and development. Artificial intelligence refers to a group of computer systems, capable of doing several tasks which require human intelligence, including learning, reasoning, and decision making.[17,18] Machine learning, deep learning, natural language processing, and computer aided drug design are some of the AI technologies that have to be incorporated in the pharmaceutical sector.

These methods allow the examination of large and complex data, which allows detecting patterns and relationships that cannot be easily identified using traditional methods. Among the major strengths of AI is its capacity to incorporate various data sources, such as genomic, proteomic, chemical, and clinical data.[19–21] This feature can be useful especially in the target identification and validation processes, where AI can process biological data to find disease related targets and determine their therapeutic importance. Also, the virtual screening technique (AI-based) enables the high-speed analysis of large chemical libraries, which greatly reduces the amount of time it takes to discover hits.[22,23]

There are a number of challenges that accompany the implementation of AI in the pharmaceutical industry. The quality and availability of data are also the most relevant concerns since AI models need big and high quality data to perform precise forecasts. The use of AI in drug development should be set in clear regulations by the regulatory agencies and these technologies should be created to ensure that they are safe and effective.[24,25] The purpose of this review is to give a detailed discussion of AI applications in the pharmaceutical industry with a special interest in their application to different phases of drug discovery and development. Through exploring the latest developments, issues, and future opportunities, this paper will demonstrate that AI is instrumental in defining the future of pharmaceutical research and innovation.

TRADITIONAL DRUG DISCOVERY PIPELINE AND ITS CHALLENGES

The traditional drug discovery pipeline is a systematic, multi stage process which is used to design, identify, develop, safe and effective therapeutic agents. It starts with the target identification and validation, where the biological components such as receptor, enzyme or gene associated with the disease is selected and confirmed as a viable target.[26] This is followed by the hit molecules discovery, which is achieved through the High throughput screening (HTS) or virtual screening methods to identify the compounds exhibiting the initial biological activity.

Following this, lead optimization process was accomplished to enhance the pharmacological properties of the identified hits with emphasis on enhancing potency, selectivity and pharmacokinetic properties including solubility and metabolic stability.[27] Potential drugs are then exposed to preclinical trials like in vitro and in vivo trials in order to ascertain safety, toxicity and pharmacokinetics. Once they pass through successful preclinical studies, compounds progress to clinical trial (Phase I-III) which determines the safety, efficacy, dose and long-term of the compound in human being.[28,29] Lastly, it needs to be approved by the regulators and this should be followed by post-marketing surveillance to ascertain its continued safety.

This traditional drug discovery pipeline, is characterized by high challenges, although it is structured. It is a lengthy process that can take many years to complete drug discovery and this process is associated with high expenses, which is usually in the billions of dollars.[30] Also, the success rate is very low and most candidates fail because they are ineffective, toxic or have poor pharmacokinetics. Weaknesses in predictive performance, especially in the translation of preclinical results to human performance, regulatory issues and constraints of clinical trials, further reduce efficiency, which requires the integration of new technologies, including AI, to address these obstacles.

ROLE OF ARTIFICIAL INTELLIGENCE IN PHARMACEUTICALS

Artificial Intelligence (AI) is transforming the pharmaceutical industry by shifting the traditional empirical approaches to predictive, data-centric, and systems-driven approaches. AI makes it possible to optimize many parameters simultaneously as compared to the traditional approaches, which involve a series of experiments, incorporating biological, chemical, and clinical factors into coherent computational models.[31–33] One of the most significant improvements made possible by AI is the shift to in silico hypothesis generation, where artificial intelligence autonomously identifies targets of therapeutics, drug-drug interactions, and propose the optimized drug molecules before successful experimental validation.[34] This minimizes the reliance on trial and error modeling and increases the accuracy of decisions. Also, AI can be used to create network pharmacology models, where researchers learn about the complex disease pathways and polypharmacological effects instead of targeting unique interventions.

Translational medicine is another field where AI is important to help bridge the gap between laboratory observations and clinical results. With the help of real world data, electronic health records and multi-omics data, AI facilitates the identification of patient centric responses to therapeutic interventions, thus promoting precision and personalized medicine. Also, AI based solutions make adaptive learning systems, which means that models evolve continuously by integrating data throughout the drug lifecycle. The Figure 1 shows the multidimensional approach of

AI in pharmaceuticals.[35–37] The idea of AI use in predictive safety pharmacology is another emerging dimension whereby early dysfunction and toxicity are predicted by use of computational modeling and resultant failures in the later stages are reduced. Together, AI is not just an auxiliary tool, it is the strategic engine of innovation that will fundamentally change the nature of pharmaceutical research, making it more efficient, predictive, and patient-centered.

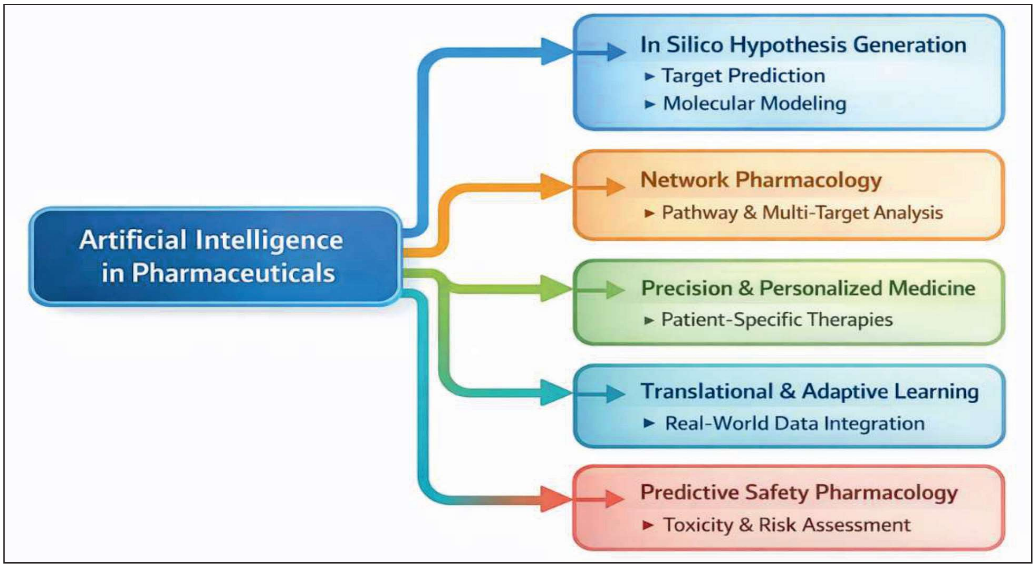

Figure 1: AI in Pharmaceuticals

AI TOOLS AND TECHNIQUES USED IN THE PHARMACEUTICAL SECTOR

The use of Artificial Intelligence (AI) in pharmaceuticals is driven by highly specialized computational frameworks aimed at capturing the complexity of biology and accelerating the therapeutic drug innovation. The figure 2 explains the AI tools and its techniques in pharmaceutical industry. Neural networks, reinforcement learning, and knowledge graph based systems are advanced methods that allow interpreting multidimensional biomedical data and providing insights into omics profiles and real life clinical evidence.[38,39] They are extensively used in the fields of molecular design, drug repurposing, biomarker discovery and systems level simulation of biological interactions. AI techniques can facilitate better informed decision making processes in the research and development sphere, aiding in more specific, efficient, and clinically relevant in drug development strategies.

1. Machine Learning (ML)

In the pharmaceutical sector, machine learning (ML) can be used to provide predictive insights out of heterogeneous biomedical data, which assists in hypothesis refinement and decision prioritization. The models such as unsupervised and supervised learning models provides a broad application in biomarker discovery, patient stratification, and drug repurposing. As an example, ML-based systems like IBM Watson to Drug Discovery have been applied to discover new therapeutic targets using a combination of genomic and clinical data. Algorithms such as random forests and support vector machines also support early predicting of drug efficacy and safety to allow informed selection of candidates.[40,41] ML therefore increases the translational efficiency by matching the computation predictions with the clinically relevant results.

2. Deep Learning (DL)

Deep learning (DL) is a branch of machine learning that uses multi layered neural networks to approximate complex biological systems and nonlinear interactions. DL has also been successfully applied in pharmaceutical research in analyzing high dimensional data including imaging, genomics, and proteomics.[42–44] Another notable instance is AlphaFold, the invention of DeepMind that has transformed protein structure prediction by near experimental accuracy. Predicting drug target actions and disease progression are also accomplished with the help of DL architectures such as convolutional and recurrent neural networks. These functions make it possible to gain a more mechanistic insight into the dynamics of biology in general, which will allow developing more specific and targeted therapeutic approaches.

3. Natural Language Processing (NLP)

Natural Language Processing (NLP) helps to extract and interpret unstructured biomedical information in scientific literature, clinical documentation, and regulatory documents.[45] The NLP based algorithms facilitate automatic synthesis of knowledge, which helps in the pharmacovigilance and drug repurposing. As an example, BioBERT and PubMedBERT are trained on biomedical corporate in particular to detect drug disease interactions and drug adverse reactions. NLP can also assist real time monitoring of clinical outcomes through analysis of electronic health records.[46] NLP can improve the evidence based decision making process and speed up the generation of pharmaceutical innovations based on knowledge by transforming textual data into actionable insights.

4. Computer Aided Drug Design (CADD)

Computer Aided Drug Design (CADD) is a combination of computational chemistry and structural biology that seeks to maximize drug discovery at the molecular scale. Molecular docking, molecular dynamics simulations and pharmacophore modeling techniques allow the accurate assessment of ligand target interactions. As an example, prediction of binding affinities and rational drug design are heavily dependent on software platforms such as Schrodinger Suite, and AutoDock. CADD is also useful in structure based and ligand based methods, which eliminate the use of experimental screening.[47] CADD allows optimization of drug candidates in silico, which can boost efficiency, reduce resource use, and increase chances of clinical success.

5. Generative AI Models

Generative AI models are an innovative method in pharmaceutical research, which allows the generation of new chemical compounds with preferred pharmacological activity using de novo drug design methods. The production of optimized molecular structures is done through techniques like variational autoencoders (VAEs), generative adversarial network (GANs), and transformer based models. As an example, Insilico Medicine has been able to apply generative AI to generate drug candidates in the case of fibrosis in much shorter timeframes.[48] These models have the capability to co-optimize various parameters such as potency, selectivity and ADMET profiles. Generative AI, therefore, makes drug discovery a more proactive and design focused process to develop next generation therapeutics more quickly.

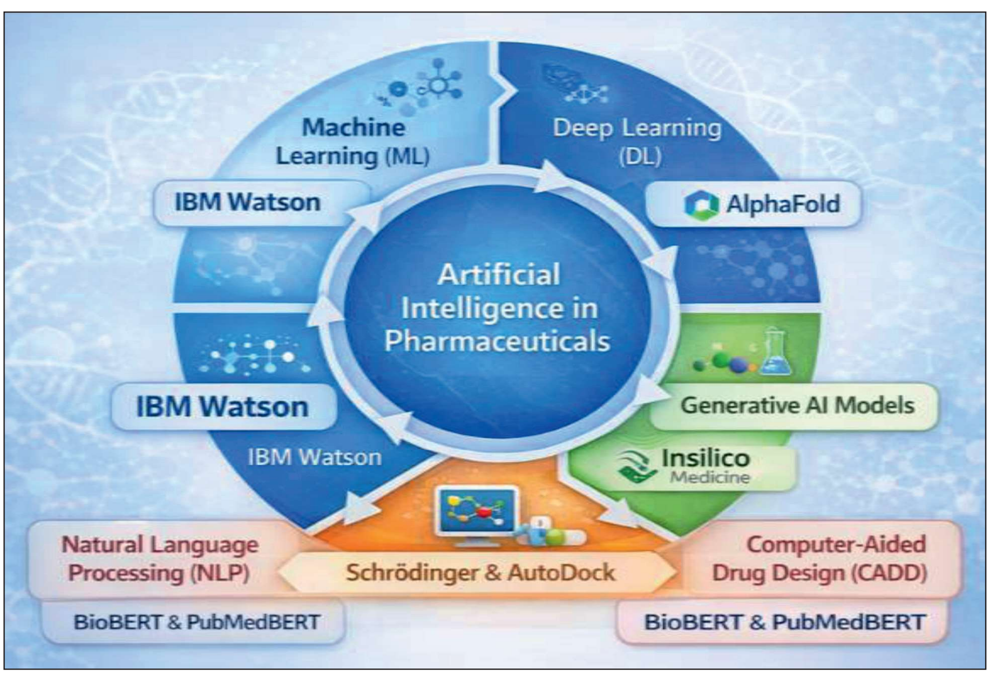

Figure 2: AI Tools in Pharmaceuticals

AI USE IN THE DRUG DEVELOPMENT PIPELINE

Artificial Intelligence (AI) is currently integrated across the drug development cycle, allowing a shift from linear workflows to interconnected and data driven processes. AI supports the smooth transition between target detection and post marketing surveillance by improving the accuracy of prediction, eliminating redundancy in experiments, and making decisions in real time. It facilitates the identification of biologically relevant targets, optimization of candidate molecules, and prediction of pharmacokinetic and safety profiles. Moreover, clinical trial efficiency is enhanced with the help of AI based analytics, which includes patient stratification and adaptive study designs.[49] The Table 1 shows the various AI tools in drug discovery process and its applications. This broad based application of AI throughout the pipeline quickens the drug development process and provides higher precision, scalability and translational relevance in pharmaceutical research.

1. Target Identification and validation.

The development of AI based identification of targets has shifted to systems biology and multi-omics integration to allow the identification of disease driving pathways as opposed to single targets. The advanced models are used to analyze the genomic, transcriptomic and proteomic data to identify new therapeutic nodes. As an example, neurodegenerative diseases targets have been identified in platforms such as Benevolent AI through biological network mining.[50] It is also possible to have in silico validation by AI using causal inference and gene disease association modelling, avoiding the need to perform expensive experimental validation. This strategy increases the reliability of the targets and helps in the creation of mechanism based therapies that have better translation potential.

2. Hit Discovery

AI has changed the concept of hit discovery to be a computationally guided selection algorithm and reduced the necessity of doing exhaustive experimental screening. Virtual screening models using deep learning are used to predict binding affinities between a ligand and a target with high accuracy. To give an example, a successful use of AtomNet has found novel small molecule hits on undruggable targets.[51,52] AI can also be used to prioritize chemically diverse scaffolds and can enhance innovation in the early stage discovery. Combining structural biology and cheminformatics, AI enhances the speed of identifying hits, and the likelihood of getting biologically relevant hits.

3. Lead Optimization

Multi objective AI models are becoming the trend in optimization of lead, focusing on improving efficacy, selectivity, and pharmacokinetics at the same time. Reinforcement learning frameworks are used to systematically develop molecules as parameters like lipophilicity, solubility and toxicity are optimized. As an example, the AI driven systems of DeepChem and Schrodinger allow quick structural activity relationship (SAR) modeling and optimization of compounds. AI is also accurate to predict ADMET properties, minimizing late stage failures. This combined optimization scheme enables acceleration to clinically viable candidates with balanced drugs.[53]

4. Preclinical Studies

AI is used in preclinical research to conduct predictive toxicology and translational models to enhance the accuracy of early stage studies. Machine learning algorithms are used to predict organ specific toxicity, drug metabolism, and pharmacokinetics using in vitro and in vivo data. Indicatively, DeepTox has been shown to be very efficient in predicting toxicity using chemical descriptors. AI can also be used in modeling virtual organs, and simulation of biological behavior, eliminating the need to subject animals to testing. AI boosts predictive validity and increases candidate selection and reduces attrition later in the development.[54]

5. Clinical Trials

The adaptive design, patient stratification, and real time analytics improve trial efficiency using AI. Through the analysis of electronic patient record data and genomic data, AI can determine the appropriate groups of patients, enhance recruitment and minimize variability. As an example, Tempus AI applies to pair cancer patients with specific clinical trials according to their molecular profiles.[55] The AI based surveillance allows detecting the safety indicators and protocol violation early. Also, predictive modeling facilitates dose optimization and outcome prediction, thus enhancing the success rates of trials and speeding up the clinical development life cycles.

5. Regulatory and Post Marketing Surveillance.

Regulatory science and pharmacovigilance are increasingly using AI to facilitate proactive safety monitoring and decision making using data. The systems based on NLP examine adverse event reports, clinical data, and real world evidence to identify safety signals. As an illustration, the FDA Sentinel Initiative uses AI tools to track post-market drug safety. AI also enables automated regulatory reporting and evaluation of compliance.[56] With an ongoing data integration in post-marketing surveillance, it is possible to identify rare adverse effects early in the course of patient safety, and lifecycle management of pharmaceutical products.

Table 1: Various AI Tools and its applications

AI Tool / Technique	Key Applications (Uses)	Industry / Sector
Machine Learning (ML)	Predictive modeling, biomarker identification, drug repurposing, patient stratification	Pharmaceuticals, Biotechnology, Clinical Research
Deep Learning (DL)	Protein structure prediction, imaging analysis, drug–target interaction prediction	Pharmaceuticals, Medical Imaging, Genomics
Natural Language Processing (NLP)	Literature mining, clinical data extraction, pharmacovigilance, regulatory documentation	Pharmaceuticals, Healthcare IT, Regulatory Affairs
Computer-Aided Drug Design (CADD)	Molecular docking, virtual screening, pharmacophore modeling, SAR analysis	Pharmaceuticals, Medicinal Chemistry
Generative AI Models (GANs, VAEs, Transformers)	De novo drug design, molecular optimization, ADMET prediction	Pharmaceuticals, Drug Discovery Startups
AlphaFold (DeepMind)	Protein structure prediction, target validation	Biotechnology, Structural Biology
IBM Watson for Drug Discovery	Knowledge mining, target identification, drug repurposing	Pharmaceuticals, Healthcare Analytics
Insilico Medicine	AI-driven drug design, fibrosis and oncology drug development	Biotech, AI-driven Pharma
DeepChem	Molecular modeling, QSAR analysis, predictive toxicology	Pharmaceuticals, Computational Chemistry
AtomNet	Structure-based drug discovery, ligand binding prediction	Biotechnology, Drug Discovery
BioBERT/ PubMedBERT	Biomedical text mining, adverse event detection, knowledge extraction	Healthcare, Pharmacovigilance
Schrödinger Suite	Molecular simulation, lead optimization, binding affinity prediction	Pharmaceuticals, Medicinal Chemistry
AutoDock	Molecular docking, ligand–receptor interaction analysis	Academic Research, Drug Discovery
Tempus AI	Clinical data analytics, precision medicine, trial matching	Oncology, Clinical Research
FDA Sentinel (AI-enabled systems)	Post-marketing surveillance, adverse drug reaction monitoring	Regulatory Agencies, Public Health

ADVANTAGES OF AI IN THE PHARMACEUTICAL SECTOR

Artificial Intelligence (AI) provides a revolutionary benefit to the pharmaceutical industry by making it possible to transition to predictive, precision based, and scalable research models. Among its strengths, it is able to combine and analyze complex, high dimensional data, such as multi omics data and real world clinical evidence, which can further aid in mechanistic insights into diseases and responses to therapy.[57,58] This can help to create patient specific and targeted interventions, which are in line with the concept of precision medicine.

Multi objective optimization is also the field where AI can be utilized, with such important aspects as efficacy, safety, and pharmacokinetics being taken into account at the same time, in the course of drug design. This minimizes the use of workflow sequential experimentation and boosts the effectiveness of decision making.[59] Moreover, simulation models powered by AI enable the formation of virtual biological systems, where the behavior of a drug in question can be predicted early on, and the uncertainty of the experiment can be reduced.

The other valuable benefit is the improvement of the success of translation, where AI models are more likely to predict human reactions to integrated preclinical and clinical information. This minimizes the failure at late stages and enhances efficiency in overall development.[60] Adaptive learning systems are also assisted by AI, as models are constantly improved based on new data, and they improve dynamically throughout the entire drug lifecycle.

In addition, AI can synthesize and automate knowledge and streamline the complicated processes of data interpretation, trial optimization and safety supervision. The fact that it is able to unveil concealed patterns and speeds up the innovation process and aids the discovery of new therapeutic opportunities.[61] These benefits together establish AI as one of the key facilitators of the future of pharmaceutical research, one that is more efficient, accurate, and focused on patients.

CHALLENGES AND LIMITATIONS

Although Artificial Intelligence (AI) has a transformative potential, its application in the pharmaceutical industry is limited by a number of essential issues. The biggest constraint is the incompleteness and heterogeneity of biomedical data, in which discrepancies between datasets may undermine model reliability and reproducibility.[62] AI models are very sensitive to quality and curated data, but real world data can be biased, have missing values, and variable experimental conditions, and this can result in inaccurate predictions.

The interpretability and transparency of complex AI models, especially in deep learning, is another crucial issue that must be taken into consideration. These models remain a black box and they present a challenge in comprehending the decision pathways and, therefore, their applicability to regulatory contexts where clarification is needed.[63,64] Also, the problem of model generalizability is still to be addressed since the results of algorithms trained on particular datasets might not be predictable across different populations and disease states.

There are also regulatory and ethical impediments to the adoption of AI. The lack of unified models for verifying the results of AI usage throws a dark cloud over the approval procedures. Besides, data privacy, data security and informed consent are important issues that must be addressed particularly when dealing with sensitive patient data. The implementation of AI in current pharmaceutical processes necessitates a large upfront investment in infrastructure and across the board skills as well.[65] All of these restrictions point to the necessity to include an efficient validation strategy, regulatory convergence, and ethical regulation in order to implement AI technologies safely and efficiently.

FUTURE PERSPECTIVES

The future of Artificial Intelligence in the pharmaceutical industry is set to move to more integrated, autonomous and patient centric drug development ecosystems. The newest methods, like digital twins, the virtual patient representations, are likely to allow simulating disease progression and individual therapeutic reactions, which will greatly boost the precision medicine.[66] Moreover, AI and multi omics platforms will be combined in order to gain a more indepth insight into the functioning of the intricate biological systems and reveal new therapeutic targets and pathways. The development of explainable AI (XAI) is expected to overcome the existing restrictions on explanations of models, enhance regulatory acceptance, and clinical trust. Moreover, the integration of AI with the upcoming technologies like quantum computing and organ on chip systems can transform the face of the predictive modeling and preclinical trials as highly precise simulations of biological processes may become a reality.[67] The development of adaptive and decentralized clinical trials, in which adaptable and real time data analysis and remote monitoring can support trial efficiency and patient engagement, will also be propelled by AI. AI powered systems could be used in regulatory science to facilitate approval procedures by evaluating data automatically and monitoring safety. Finally, AI in pharmaceuticals is going to develop through the joint work of academia, industry, and regulatory authorities and create an ecosystem focused on innovation, transparency, and ethical conduct that will help prevent time loss by speeding up the process of obtaining safe and effective treatments.

CONCLUSION

The pharmaceutical industry is currently undergoing a fundamental transformation with Artificial Intelligence (AI) transitioning drug discovery and development, from traditional and sequential approaches, to data driven and integrated paradigm. AI increases the accuracy and effectiveness of therapeutic innovation by allowing high level predictive modeling, multidimensional integration of data, and analysis on a systems level. Its application across the drug development pipeline, starting with target identification to post marketing surveillance, has shown that it has a huge potential to enhance decision making, resource utilization and speed up the process of translation through its results. Notably, AI allows transition to a more mechanism oriented and patient centric model and thus it helps to promote precision medicine and personalized therapeutics. In the future, the integration of AI with new technologies, including multi-omics, digital health tools, and advanced simulation systems is likely to boost its effects. Researchers, industry players, and regulators will have to work together in order to create strong validation frameworks and promote responsible innovation. Altogether, AI is a revolutionary input, which can dramatically enhance the effectiveness, accuracy, and clinical applicability of pharmaceutical research and eventually the speedup the process of drug discovery and development of precision medicine.

REFERENCES

1. Askin S, Burkhalter D, Calado G, Dakrouni SE. Artificial Intelligence Applied to clinical trials: opportunities and challenges. Health technology. 2023. doi:10.1007/S12553-023-00738-2
2. Ali KA, Mohin S, Mondal P, Goswami S, Ghosh S, Choudhuri S. Influence of artificial intelligence in modern pharmaceutical formulation and drug development. Future Journal of Pharmaceutical Sciences (Print). 2024. doi:10.1186/S43094-024-00625-1
3. Bhatia N, Khan MMU, Arora S. The Role of Artificial Intelligence in Revolutionizing Pharmacological Research. Current Pharmacology Reports. 2024. doi:10.1007/S40495-024-00367-X
4. Bhatt P, Singh S, Kumar V, Nagarajan K, Mishra SK, Dixit PK, et al. Artificial Intelligence in Pharmaceutical Industry: Revolutionizing Drug Development and Delivery. The Chinese Journal of Artificial Intelligence. 2023. doi:10.2174/0129503752250813231124092946.
5. Bhattamisra SK, Banerjee P, Gupta P, Mayuren J, Patra S, Candasamy M. Artificial Intelligence in Pharmaceutical and Healthcare Research. Big Data and Cognitive Computing. 2023. doi:10.3390/BDCC7010010.
6. Boniolo F, Dorigatti E, Ohnmacht AJ, Saur D, Schubert B, Menden MP. Artificial intelligence in early drug discovery enabling precision medicine. Expert opinion on drug discovery. 2021. doi:10.1080/17460441.2021.1918096.
7. Chen H, Lu DX, Xiao Z, Li S, Zhang W, Luan X, et al. Comprehensive applications of the artificial intelligence technology in new drug research and development. Health Information Science and Systems. 2024. doi:10.1007/S13755-024-00300-Y.
8. Chen W, Liu X, Zhang S, Chen S. Artificial intelligence for drug discovery: Resources, methods, and applications. Molecular Therapy: Nucleic Acids. 2023. doi:10.1016/J.OMTN.2023.02.019.
9. Chen Z, Liu X, Hogan WR, Shenkman E, Bian J. Applications of artificial intelligence in drug development using real-world data. Drug Discovery Today. 2021. doi:10.1016/J.DRUDIS.2020.12.013.
10. Chinnaiyan K, Mugundhan SL, Narayanasamy D., Mohan M. Revolutionizing Healthcare and Drug Discovery: The Impact of Artificial Intelligence on Pharmaceutical Development. Current Drug Therapy. 2024. doi:10.2174/0115748855313948240711043701.
11. Chopra H, Baig AA, Gautam RK, Kamal MA. Application of Artificial intelligence in Drug Discovery. Current pharmaceutical design. 2022. doi:10.2174/1381612828666220608141049
12. Colombo S. Applications of artificial intelligence in drug delivery and pharmaceutical development. Elsevier eBooks. 2020. doi:10.1016/B978-0-12-818438-7.00004-6
13. Dermawan D, Alotaiq N. From Lab to Clinic: How Artificial Intelligence (AI) Is Reshaping Drug Discovery Timelines and Industry Outcomes. Pharmaceuticals. 2025. doi:10.3390/PH18070981

14. Frusciante L, Visibelli A, Geminiani M, Santucci A, Spiga O. Artificial Intelligence approaches in drug discovery: Towards the laboratory of the future. Current topics in medicinal chemistry. 2022. doi:10.2174/1568026622666221006140825
15. Gupta R, Srivastava D, Sahu M, Tiwari S, Ambasta RK, Kumar P. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. Molecular diversity. 2021. doi:10.1007/S11030-021-10217-3
16. Han R, Yoon H, Kim G, Lee H, Lee Y. Revolutionizing Medicinal Chemistry: The Application of Artificial Intelligence (AI) in Early Drug Discovery. Pharmaceuticals. 2023. doi:10.3390/PH16091259
17. Hassan-Farghali, Canová NK, Arora M. The potential applications of artificial intelligence in drug discovery and development. Physiological Research. 2021. doi:10.33549/PHYSIOLRES.934765
18. Husnain A, Rasool S, Saeed A, Hussain HK. Revolutionizing Pharmaceutical Research: Harnessing Machine Learning for a Paradigm Shift in Drug Discovery. International Journal of Multidisciplinary Sciences and Arts. 2023. doi:10.47709/IJMDSA.V2I2.2897
19. Irissarry C, Burger Helmchen T. Using Artificial Intelligence to Advance the Research and Development of Orphan Drugs. Businesses. 2024. doi:10.3390/Businesses4030028
20. Jung YL, Yoo HS, Hwang J. Artificial intelligence-based decision support model for new drug development planning. Expert systems with applications. 2022. doi:10.1016/J.ESWA.2022.116825
21. Khadela A, Popat S, Ajabiya J, Valu D, Savale S, Chavda VP, et al. AI, ML and Other Bioinformatics Tools for Preclinical and Clinical Development of Drug Products. 2023. doi:10.1002/9781119865728.CH12
22. Kokudeva M, Vichev M, Naseva E, Miteva DG, Velikova T. Artificial intelligence as a tool in drug discovery and development. World Journal of Experimental Medicine. 2024. doi:10.5493/WJEM.V14.I3.96042.
23. Kolluri S, Lin J, Liu R, Zhang Y, Zhang W. Machine Learning and Artificial Intelligence in Pharmaceutical Research and Development: a Review. AAPS Journal. 2022. doi:10.1208/S12248-021-00644-3.
24. Koromina M, Pandi M, Patrinos GP. Rethinking Drug Repositioning and Development with Artificial Intelligence, Machine Learning, and Omics. Omics. 2019. doi:10.1089/OMI.2019.0151.
25. Kumar M, Nguyen TPN, Kaur J, Singh TG, Soni D, Singh R, et al. Opportunities and challenges in application of artificial intelligence in pharmacology. Pharmacological Reports. 2023. doi:10.1007/S43440-022-00445-1
26. Lamberti MJ, Wilkinson M, Donzanti BA, Wohlhieter GE, Parikh S, Wilkins R, et al. A Study on the Application and Use of Artificial Intelligence to Support Drug Development. Clinical Therapeutics. 2019. doi:10.1016/J.CLINTHERA.2019.05.018
27. Liebman M. The Role of Artificial Intelligence in Drug Discovery and Development. Chemistry International. 2022. doi:10.1515/CI-2022-0105
28. Liu Y, Zhang L, Jiang Z, Xia T, Li P, Wu P, et al. Applications of Artificial Intelligence in Biotech Drug Discovery and Product Development. MedComm. 2025. doi:10.1002/MCO2.70317
29. Mak K, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discovery Today. 2019. doi:10.1016/J.DRUDIS.2018.11.014
30. Malandraki-Miller S, Riley PR. Use of artificial intelligence to enhance phenotypic drug discovery. Drug Discovery Today. 2021. doi:10.1016/J.DRUDIS.2021.01.013.
31. Malheiro V, Santos B, Figueiras A, Mascarenhas-Melo F. The Potential of Artificial Intelligence in Pharmaceutical Innovation: From Drug Discovery to Clinical Trials. Pharmaceuticals. 2025. doi:10.3390/PH18060788.
32. Mohapatra M, Sahu C, Mohapatra S. Trends of Artificial Intelligence (AI) Use in Drug Targets, Discovery and Development: Current Status and Future Perspectives. Current Drug Targets. 2024. doi:10.2174/0113894501322734241008163304.
33. Moingeon P, Kuenemann MA, Guedj M. Artificial intelligence-enhanced drug design and development: Toward a computational precision medicine. Drug Discovery Today. 2021. doi:10.1016/J.DRUDIS.2021.09.006.
34. Morishita EC, Nakamura S. Recent applications of artificial intelligence in RNA-targeted small molecule drug discovery. Expert Opinion on Drug Discovery. 2024. doi:10.1080/17460441.2024.2313455.
35. Mottaghi-Dastjerdi N, Soltany Rezaee Rad M. Advancements and Applications of Artificial Intelligence in Pharmaceutical Sciences: A Comprehensive Review. Iranian journal of pharmaceutical research. 2024. doi:10.5812/

IJPR-150510.

36. Nagasundaram N, Yee EYK, Le NQK, Kamaraj B, Al Subaie AM, Yeh H. Application of Computational Biology and Artificial Intelligence Technologies in Cancer Precision Drug Discovery. BioMed Research International. 2019. doi:10.1155/2019/8427042

37. Naik K, Goyal RK, Foschini L, Chak CM, Thielscher C, Zhu H, et al. Current Status and Future Directions: The Application of Artificial Intelligence/Machine Learning for Precision Medicine. Clinical pharmacology and therapy. 2023. doi:10.1002/CPT.3152.

38. Napolitano G, Has C, Schwerk A, Yuan JH, Ullrich C. Potential of Artificial Intelligence to Accelerate Drug Development for Rare Diseases. Pharmaceutical Medicine. 2024. doi:10.1007/S40290-023-00504-9.

39. Narayan A, Chanana A, Shanker O, Kulkarni YR, Gupta P, Patel A, et al. Role of Artificial Intelligence in Pharmaceutical Drug Development. Current Indian science. 2024. do i:10.2174/012210299X313252240521111358.

40. Niazi SK. The Coming of Age of AI/ML in Drug Discovery, Development, Clinical Testing, and Manufacturing: The FDA Perspectives. Drug Design, Development and Therapy. 2023. doi:10.2147/DDDT.S424991

41. Niazi SK, Mariam Z. Artificial intelligence in drug development: reshaping the therapeutic landscape. Therapeutic Advances in Drug Safety. 2025. doi:10.1177/20420986251321704

42. Ocaña A, Pandiella A, Privat C, Bravo I, Luengo-Oroz M, Amir E, et al. Integrating artificial intelligence in drug discovery and early drug development: a transformative approach. Biomarker Research. 2025. doi:10.1186/S40364-025-00758-2.

43. Odah M. Artificial Intelligence Meets Drug Discovery: A Systematic Review on AI-Powered Target Identification and Molecular Design. 2025. doi:10.20944/Preprints202503.0912.V1

44. Paliwal A, Alam MdA, Sharma P, Jain S, Dhoundiyal S. Revolutionizing Cancer Research and Drug Discovery: The Role of Artificial Intelligence and Machine Learning. Current Cancer Therapy Reviews. 2024. doi:10.2174/0115733947288355240305080236.

45. Parvathaneni M, Awol AK, Kumari M, Lan K, Lingam M. Application of Artificial Intelligence and Machine Learning in Drug Discovery and Development. Journal of Drug Delivery and Therapeutics. 2023. doi:10.22270/JDDT.V13I1.5867.

46. Pun FW, Ozerov IV, Zhavoronkov A. AI-powered therapeutic target discovery. TIPS - Trends in Pharmacological Sciences. 2023. doi:10.1016/J.TIPS.2023.06.010.

47. Qureshi R, Irfan M, Gondal TM, Khan S, Wu J, Hadi MU, et al. AI in drug discovery and its clinical relevance. Heliyon. 2023. doi:10.1016/J.Heliyon.2023.E17575.

48. Sahoo A, Dar GM. A comprehensive review on the application of artificial intelligence in drug discovery. 2021. doi:10.52679/TABCJ.2021.0007.

49. Sampene AK, Nyirenda F. Evaluating the effect of artificial intelligence on pharmaceutical product and drug discovery in China. Future Journal of Pharmaceutical Sciences. 2024. doi:10.1186/S43094-024-00632-2.

50. Sarkar C, Das B, Rawat VS, Wahlang JB, Nongpiur A, Tiewsoh I, et al. Artificial Intelligence and Machine Learning Technology Driven Modern Drug Discovery and Development. International Journal of Molecular Sciences. 2023. doi:10.3390/IJMS24032026.

51. Sarvepalli S, Vadarevu S. Role Of Artificial Intelligence In Cancer Drug Discovery And Development. Cancer Letters. 2025. doi:10.1016/J.Canlet.2025.217821.

52. Selvaraj C, Chandra I, Singh SK. Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. Molecular diversity. 2021. doi:10.1007/S11030-021-10326-Z.

53. Sharma A, Virmani T, Pathak V, Sharma A, Pathak K, Kumar G, et al. Artificial Intelligence-Based Data-Driven Strategy to Accelerate Research, Development, and Clinical Trials of COVID Vaccine. BioMed Research International. 2022. doi:10.1155/2022/7205241

54. Sharma P, Jain V, Tailang M. How Artificial Intelligence is Transforming Medicine: The Future of Pharmaceutical Research. Advanced technologies and societal change. 2023. doi:10.1007/978-981-99-1949-9_7

55. Sharma V, Singh AK, Chauhan S, Sharma PK, Chaudhary S, Sharma A, et al. Role of Artificial Intelligence in Drug Discovery and Target Identification in Cancer. Current Drug Delivery. 2023. doi:10.2174/1567201821666230905090621

56. Shiammala PN, Duraimutharasan N, Vaseeharan B, Alothaim AS, Al Malki ES, Snekaa B, et al. Exploring the Artificial

Intelligence and Machine Learning Models in the Context of Drug Design Difficulties and Future Potential for the Pharmaceutical Sectors. Methods. 2023. doi:10.1016/J.YMETH.2023.09.010

57. Singh S, Kumar R, Payra S, Singh SK. Artificial Intelligence and Machine Learning in Pharmacological Research: Bridging the Gap Between Data and Drug Discovery. Cureus. 2023. doi:10.7759/CUREUS.44359

58. Suriyaamporn P, Pamornpathomkul B, Patrojanasophon P, Ngawhirunpat T, Rojanarata T, Opanasopit P. The Artificial Intelligence-Powered New Era in Pharmaceutical Research and Development: A Review. AAPS PharmSciTech. 2024. doi:10.1208/S12249-024-02901-Y

59. T S, Ali HM, Kumar BV. AI - Driven Drug Discovery and Therapeutic Target Identification for Rare Genetic Diseases. 2024 International Conference on Advancements in Smart, Secure and Intelligent Computing (ASSIC). 2024. doi:10.1109/ASSIC60049.2024.10507989

60. Tiwari P, Pal R, Chaudhary MJ, Nath R. Artificial intelligence revolutionizing drug development: Exploring opportunities and challenges. Drug development research (Print). 2023. doi:10.1002/DDR.22115

61. Unogwu OJ, Ike M, Joktan OO. Employing Artificial Intelligence Methods in Drug Development: A New Era in Medicine. Mesopotamian Journal of Artificial Intelligence in Healthcare. 2023. doi:10.58496/MJAIH/2023/010

62. Vamathevan J, Clark DA, Czodrowski P, Dunham I, Ferrán EA, Lee G, et al. Applications of machine learning in drug discovery and development. Nature reviews Drug discovery. 2019. doi:10.1038/S41573-019-0024-5

63. Vidiyala N, Sunkishala P, Parupathi P, Nyavanandi D. The Role of Artificial Intelligence in Drug Discovery and Pharmaceutical Development: A Paradigm Shift in the History of Pharmaceutical Industries. AAPS PharmSciTech. 2025. doi:10.1208/S12249-025-03134-3

64. Vora LK, Gholap AD, Jetha K, Singh TRR, Solanki HK, Chavda VP. Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. Pharmaceutics. 2023. doi:10.3390/Pharmaceutics15071916.

65. Wang B, Zhang T, Liu Q, Sutcharitchan C, Zhou Z, Zhang D, et al. Elucidating the role of artificial intelligence in drug development from the perspective of drug-target interactions. Journal of Pharmaceutical Analysis. 2024. doi:10.1016/J.JPHA.2024.101144

66. You Y, Lai X, Pan Y, Zheng H, Vera J, Liu S, et al. Artificial intelligence in cancer target identification and drug discovery. Signal Transduction and Targeted Therapy. 2022. doi:10.1038/S41392-022-00994-0

67. Zhang K, Yang X, Wang Y, Yu Y, Huang N, Li G, et al. Artificial intelligence in drug development. Nature Network Boston. 2025. doi:10.1038/S41591-024-03434-4