RESEARCH PAPER

Transforming Drug Discovery And Delivery: An In-Depth Analysis Of Artificial Intelligence Applications, Challenges, And Future Perspective

P. Bharathi[1], Latha Shanmugavadivu S[2], Vadivel Palanisamy[3], R. Sivakumar[4], R. Yasodha[5], Jeevanantham. G[6]

[1] Research Scholar, Department Of Computer Science And Engineering, Tamilnadu College Of Engineering, Coimbatore, India. Email: bharathibrajan@gmail.com

[2] Professor, Department Of Computer Science And Engineering, Tamilnadu College Of Engineering, Coimbatore, India. Email: latha@tnce.in

[3] Assistant Professor, Department Of Mechanical Engineering, Study World College Of Engineering, Coimbatore. Email: vadivelgetit@gmail.com

[4] Professor, Department Of Computer Science And Engineering, Nehru Institute Of Engineering And Technology, Coimbatore, India. Email: rsksivame@gmail.com

[5] Assistant Professor, Department Management Studies, Nehru Institute Of Engineering And Technology, Coimbatore, India. Email: yasodha1507@gmail.com

[6] Assistant Professor, Department Of Computer Science And Engineering, Nehru Institute Of Engineering And Technology, Coimbatore, India. Email: jeevas1984@gmail.com

Received: *20th Feb, 2026;* ***Revised:*** *4th Mar, 2026;* ***Accepted:*** *25th Mar, 2026;* ***Available Online:*** *10th Apr, 2026*

Abstract

Ai has transformed pharmaceutical sciences and altered drug discovery and delivery. It is an overview of the numerous applications of ai in drug research, which involves target discovery, and post-market surveillance. We discuss how machine learning, deep learning, and massive language models are tackling the high costs, time and failures in drug development. The paper summarises the target identification via ai, hit-to-lead optimisation, and medication repurposing, and the enhancement of personalised drug delivery. We contrast the conventional and ai-enabled solutions and find significant time (10-15 years to 5 years), and cost reductions. Such breakthrough technologies as predicting a protein structure with alphafold, generative models of de novo molecular design, and smart medicine delivery systems with ai and nanotechnology and internet of things options are mentioned. The quality of data and standardisation, interpretability of algorithms, regulation, and ethics are also discussed in the review. The last proposals are multimodal foundation models, federated learning frameworks, and safe and reliable ai deployment in the pharmaceutical industry through verified control systems.

Keywords: Artificial Intelligence, Drug Discovery, Drug Delivery Systems, Machine Learning, Deep Learning, Precision Medicine, Computational Pharmacology.

How To Cite This Article: Bharathi P, Latha Shanmugavadivu S, Palanisamy V, Sivakumar R, Yasodha R, Jeevanantham G. Transforming Drug Discovery And Delivery: An In-Depth Analysis Of Artificial Intelligence Applications, Challenges, And Future Perspective. Int J Drug Deliv Technol. 2026;16(26s):141-150. Doi: 10.25258/ijddt.16.26s.14

1. Introduction

The pharmaceutical sector is at a crossroad quite literally and is struggling to create safe, effective and affordable therapeutics like never before. The conventional methods of drug discovery and development have been more and more unsustainable with the rising costs, lengthy cycles and reduced productivity. The overall development of a new drug has crossed the 2 billion mark, and it has taken 10-15 years on average between the discovery and the approval by the regulation authorities (Mak and Pichika, 2019; DiMasi et al., 2016). In addition, about 9 in ten drugs entering clinical trials do not pass the test, mainly because of unexpected toxicity, lack of efficacy, or poor pharmacokinetic characteristics (Chang et al., 2022; Bhinder et al., 2021). Artificial Intelligence has come out as a paradigm-shift solution to these issues. Using the capability to handle massive volumes of biomedical data, detect highly complicated trends, and draw predictive conclusions,

AI has the prospect of transforming all aspects of drug development.

Introducing AI into the field of pharmaceutical sciences is not just a case of a minor enhancement but a complete change in the way we find, develop, and provide therapeutic interventions. The intersecting technology has increased the pace of AI application in drug discovery. These are the exponential threat of biomedical information (genomics, proteomics, clinical records), the tremendous rise of computing and (especially) GPU acceleration, and the algorithmic advances in the system of deep learning (LeCun et al., 2015; Jumper et al., 2021). The release of AI-specific applications like AlphaFold, which predicts protein structures, generative adversarial networks, which generate molecules, and natural language processors, which find the right literature, have allowed showing how much potential AI has to add to human abilities in pharmaceutical research. The objective of this review is to offer an in-depth analysis of the application of AI in the drug discovery and delivery. The introduction initiates the development of the basic ideas of AI in healthcare and then continues to examine AI applications throughout the drug development pipeline. We show comparative data explaining the benefits of AI-based methods, analyze real-world case studies where such methods have already been successfully implemented, and discuss the existing challenges and limitations critically. Lastly, we suggest future paths of incorporating AI in the new technologies to develop more efficient, personalized, and accessible therapeutic solutions.

2. AI in Healthcare: Foundational Concepts and Applications

Artificial Intelligence refers to computing systems that mimic activities that are normally performed by human beings. As applied to healthcare and pharmaceutical sciences, AI is revealed in the form of multiple complementary methods: Machine Learning (ML) is a subdivision of AI, where an algorithm learns based on data, not being directly programmed. ML models recognize trends, predict and learn through their experience. The ML algorithms can be used to predict drug-target interactions, optimize chemical structures, and predict pharmacokinetic properties in the pharmaceutical field. Deep Learning (DL) is the continuation of ML by means of artificial neural networks (ANNs) using more than one layer (deep architecture). These models are very good in processing high-dimensional and complex data including molecular structures, genomic sequences and medical images. Convolutional neural networks (CNNs) have shown specific effectiveness when applied to chemical structure analysis and making bioactivity predictions and recurrent neural networks (RNNs) and transformers are used when making sequence-based predictions in genomics and protein engineering. Natural Language Processing (NLP) is a computer application to understand, interpret and produce human language. In pharmaceutical research, NLP algorithms find useful information in scientific sources, clinical notes, and regulatory documents and help discover knowledge faster and process evidence-based decisions (Gibbs et al., 2020; Davenport and Kalakota, 2019).

In addition to the field of drug discovery, AI is changing clinical healthcare in various ways: Diagnostic Imaging: AI algorithms have obtained expert level of performance in identifying different conditions based on medical images. Deep learning is as precise as trained radiologists when detecting diabetic retinopathy and breast, lung nodules, and skin cancers (Esteva et al., 2017). These tools improve the accuracy of the diagnosis, shorten the interpretation time, and provide the possibility to intervene earlier. Predictive Analytics: ML tools use electronic health records, genetic data, and lifestyle data to forecast the disease progression, hospitalization risk, and treatment outcomes. These predictive powers allow interventions to be made proactively and risk management to be customized (Davenport and Kalakota, 2019; Liu et al., 2020). Robotic Surgery: AI-controlled robots improve the precision of the surgery, decrease complications, and hasten the time to reach recovery. These systems combine haptic feedback, predictive algorithms, and real-time imaging to aid the decision-making process in surgery (Esteva et al., 2017). Virtual Health Assistants: Chatbots and virtual assistants, which are AI-based, offer uninterrupted patient care, symptom tracking, medication adherence, and mental health assistance. These tools increase access to healthcare, especially in underserved communities (Gibbs et al., 2020).

The implementation of AI in pharmaceutical sciences resolves the key inefficiencies of drug development: Accelerated Discovery: AI algorithms can screen millions of compounds, make predictions of drug-target interactions, and optimize lead controls in a significantly shorter time, cutting down the time of

hits and lead optimization by several folds (Marques et al., 2024; Schuhmacher et al., 2019). Better Success rates: Predictive models detect potential efficacy and toxicity problems at an earlier stage of development, allowing the elimination of early problematic candidates during expensive clinical trials. It minimizes the attrition rate and also saves resources (Chang et al., 2022; Talat et al., 2023). Personalized Medicine: AI interprets individual patient data (genomic, proteomic, clinical) to predict the most effective treatment plans, providing personalized treatments that are most likely to be effective with the least side effects (Li et al., 2023; Blasiak, 2020). Manufacturing Optimization: Smart manufacturing systems that are powered by AI observe production processes in a real time and guarantee uniform quality, waste reduction, and continuous improvement through predictive maintenance and process control.

3. Traditional Drug Discovery: Challenges and Limitations

The conventional drug development has been one of the most resource-consuming activities in contemporary science. It takes an average of 10-15 years to develop a new drug to be approved by the market, and an average of over 2 billion dollars is spent in this process considering the failures (DiMasi et al., 2016; Marques et al., 2024). These statistics are not reflective of the actual investment, since these are only successful drugs, but the cost of the many failures within the industry is being amortized. The financial and time costs can be attributed to a number of factors: the extensive wet-lab experimentation, the optimization loop, the multi-phase clinical trial of thousands of patients, and the thorough approval process by the regulatory authorities. Every phase presents areas of possible failure, and the cumulative clinical stage success rate is lower than 12% (Bhinder et al., 2021).

There is a consistent problem of high attrition rates in the pharmaceutical industry during the development process. Only about 90 percent of drug candidates undergoing clinical trials get approved (Chang et al., 2022). Failure modes include: Unexpected Toxicity: It is common to find that many candidates show satisfactory safety profiles during preclinical testing, but exhibit safety profiles different than expected during human testing, usually because of differences between species or complicated interactions that are not well represented in animal models. Poor Efficacy: Candidates can be found to lack adequate therapeutic effect in the target populations and this can be due to ineffective preclinical efficacy models or incomplete knowledge of the disease mechanism. Poor Pharmacokinetics: Suboptimal absorption, distribution, metabolism or excretion characteristics may impair the performance of a drug resulting in either inadequate target exposure or over-accumulation in non-target tissues. Commercial Viability: Market factors, such as competition, pricing force, or lack of differentiation over current therapies can kill even technically successful candidates.

Conventional drug discovery experiences disjointed data ecosystems. Vital data genomic profiles, chemical structures, clinical results, real-world results are lies in different databases with minimal interoperability. This fragmentation does not allow the holistic analysis that is required to extract the multifaceted patterns and relationships that are needed to develop drugs successfully (Mukherjee et al., 2024). The lack of incorporation of the multi-omics data, chemical properties, and clinical outcomes is a basic drawback of the traditional approaches. The cognitive ability of humans cannot handle the high-dimensional datasets that are currently present, so computational methods are needed that will be able to extract meaningful information out of the complex biological systems.

4. AI-Driven Drug Discovery: A Transformative Paradigm

The ways in which AI has been applied in drug discovery were outlined. AI presents a completely new concept of drug discovery, where it is driven by data, predictive modeling, and optimization. Table 1 can be used to summarize the major AI applications throughout the discovery pipeline.

Table 1: Key Applications of AI in Drug Discovery

AI Application	Description	Key Tools/Technologies	Notable Examples
Target Identification	Identifies disease-related genes, proteins, or pathways	Graph Convolutional Networks, Deep Neural Networks, Digital Twins	DeepMind (AlphaFold)
Hit and Lead Optimization	Discovers and refines potential drug candidates	CNNs, GANs, Predictive Models	Exscientia (DSP-1181)
Drug Repurposing	Finds new therapeutic uses for existing drugs	NLP, ML on Clinical Records	BenevolentAI (Baricitinib)
Drug-Target Interaction Prediction	Predicts interactions between molecules and biological targets	SVMs, Transformers, GCNs	Atomwise
Precision Medicine	Tailors therapies using individual patient data	Wearable Tech, In Silico Modeling	Flatiron Health, Healx

4.1 AI Workflow in Drug Discovery

Figure 1 displays an AI-driven workflow of drug discovery, which combines various computational strategies to hasten the development. It involves start with the genomic, proteomic, and literature data analysis to identify the target.

The AI algorithms rank targets based on the association with the disease, drugability, and safety. After target selection, AI-based virtual screening quickly interacts with millions of compounds against the target structure. Deep learning models are used to predict binding affinities, selectivity, and pharmacokinetic properties and rank lists of promising candidates. Generative models are then used to suggest new molecular structures that are optimized to satisfy desired properties, which search chemical space beyond current libraries. The process of lead optimization uses iterative cycles wherein AI models use structure-activity relationships to make predictions on synthetic priorities and predict possible toxicity concerns. In this process experimental data are used through feedback loops to improve predictor models to form continuous improvement loops.

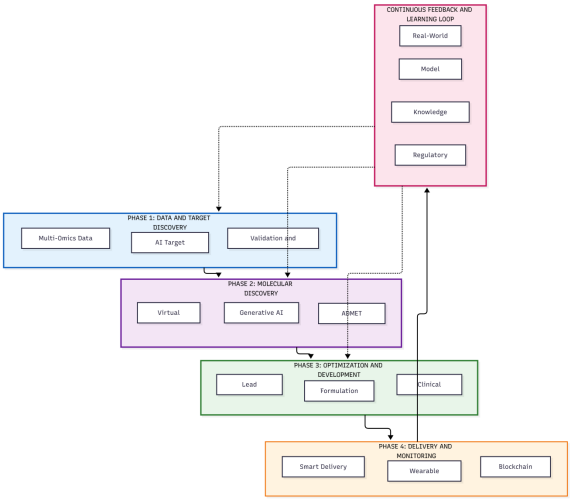

Figure 1: Integrated AI-Driven Drug Discovery and Delivery Ecosystem.

The framework illustrates the end-to-end integration of artificial intelligence across four interconnected phases of pharmaceutical development: (1) Data and Target Discovery, (2) Molecular Discovery, (3) Optimization and Development, and (4) Delivery and Monitoring. A continuous feedback loop enables real-world data integration and model refinement. Key AI technologies employed include deep neural networks, graph convolutional networks, generative adversarial networks, and reinforcement learning algorithms.

4.2 Comparative Advantages of AI-Driven Approaches

The benefits of AI-mediated drug development in comparison with more conventional approaches are enormous and can be summarized as in Table 2.

Table 2: Comparative Advantages of AI in Drug Development

Parameter	Traditional Methods	AI-Driven Methods	Key Achievement
Development Timeline	10-15 years	~5 years	50-70% reduction
Development Cost	$2+ billion	~$500 million	75% reduction
Data Utilization	Limited, manual review	Comprehensive, big data models	Enhanced pattern recognition
Clinical Trial Success	10-12%	20-30% projected	2-3x improvement

These benefits are linked to the fact that AI helps to work with large amounts of data, detect small trends, and make predictions which can be used to prioritize experiments. AI saves resources by eliminating the need to screen candidates exhaustively by using wet-labs, and enhances the quality of candidates.

4.4 Investment Trends and Industry Adoption

There has been growing interest in AI adoption in the pharmaceutical industry. The amount of money invested globally in AI to discover drugs in 2025 was 12.5 billion, marking a growth of over 30% as compared to the previous five years (Roche et al., 2023; FDA, 2024). This is the investment in the existing pharmaceutical entities, specialized AI drug discovery firms, and in academic-industry collaboration. Big pharmaceutical firms have set up special divisions to handle AI, with smaller firms, such as Exscientia, BenevolentAI and Atomwise, basing their business model purely on AI-enabled discovery. The regulatory organizations, such as FDA, have established strategies to assess AI-generated evidence, and computational methods are increasingly accepted in regulatory submissions as time passes (Liu et al., 2023; Niazi, 2023).

4.5 Real-World Case Studies

Case Study 1: AlphaFold and Prediction of Protein Structure. AlphaFold by DeepMind is an innovative breakthrough in AI-related drug discovery. AlphaFold has solved one of the most difficult problems in biology, namely, predicting atomic-resolution protein structures given amino acid sequences (Jumper et al., 2021). The deep learning system takes evolutionary data and physical laws to create three-dimensional assemblies that are close to the experiment in most instances. The effect of AlphaFold is felt in drug discovery. Proper structures of proteins allow the structure-based drug design, virtual screening and mechanistic insights of disease-related proteins. The prediction AlphaFold has been used to find new inhibitors of targets such as CDK20, and has proven useful in drug discovery pipelines (Ren et al., 2023). Exscientia and DSP-1181

Case Study: 2. The DSP-1181 of Exscientia is the first AI-designed molecule to be put into clinical trials. DSP-1181 was developed to treat obsessive-compulsive disorder and was developed on the basis of a generative design, property prediction and experimental validation AI platform (Exscientia, 2023). It only took the molecule 12 months to go through concept to clinical candidate, whereas it would be 4-5 years to go through comparable projects in the more traditional timelines.

Case Study 3: Baricitinib Repurposing and BenevolentAI. In response to the COVID-19 pandemic, the BenevolentAI showed that AI could be used to quickly re-purpose drugs. The platform examined scientific literature and biomedical data and found a potential treatment of severe COVID-19 in baricitinib, an approved JAK inhibitor (Stebbing et al., 2020). This theory resulted in clinical trials, which proved efficacy and led to regulatory approval and proved that AI can find therapeutic opportunities within the first few hours based on a public health crisis.

5. AI in Drug Delivery Systems

5.1 Personalized Drug Delivery

Conventional mode of drug delivery is based on one-size-fits-all dosing systems with consideration of population averages, which fails to address interindividual differences in the absorption, metabolic and response of drugs. AI changes the delivery of drugs, with the personal approach, which would maximize the timing, dose, and route of delivery in each patient. Machine learning techniques utilize patient-specific data, such as genetic profiles, metabolic data, and clinical history to produce personalized dosing schedules. Reinforcement learning methods allow developing a continuous optimization strategy in response to patient reactions, modifying treatments in response to new conditions (Liu et al., 2021; Gallego et al., 2021). The application of oncology is a good example of personalized delivery. Patients AI platforms keep track of tumor markers, patient response, and genetic predictors to optimise the dose of chemotherapy, which maximizes efficacy and minimises toxicity. The applications of chronotherapy rely on AI to determine the best times of administration through circadian rhythms, which improves therapy (Sarkar et al., 2023).

5.2 Smart Drug Delivery Devices

Closed-loop drug delivery systems and self-regulatory dosing can be achieved through AI integration, where the dosing dose depends on real-time physiological measurements. The examples of AI-based delivery devices are provided in Table 3.

Table 3: AI-Enabled Smart Drug Delivery Systems

Device Type	Application	AI Function	Outcome
AI-Powered Insulin	Diabetes management	Predictive glucose modeling, automated	Improved glycemic control

Device Type	Application	AI Function	Outcome
Pumps		insulin delivery	
Smart Inhalers	Respiratory diseases	Breath pattern analysis, medication adherence monitoring	Reduced exacerbations
Wearable Drug Delivery	Chronic conditions	Real-time dosing adjustment, adverse event prediction	Enhanced therapeutic outcomes
Ingestible Sensors	Medication monitoring	Adherence tracking, physiological response monitoring	Improved compliance

Figure 2 represents a closed-loop architecture that incorporates continuous measurement, AI-driven decision making, and automated response to ensure therapeutic goals. In insulin administration, the continuous glucose monitors send real-time data to AI algorithms forecasting glucose trends and estimating the optimal dose of insulin, which are administered by automated pumps. The method provides greater levels of glycemic control when compared to traditional therapy (Aundhia et al., 2024).

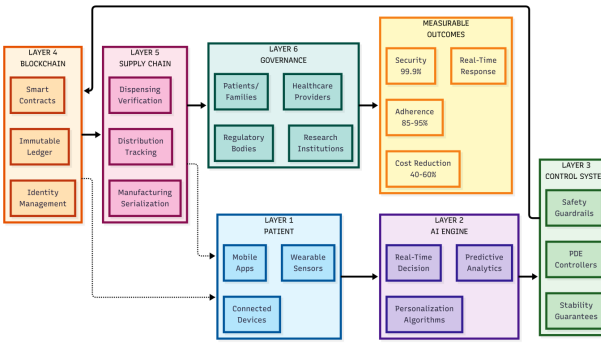

Figure 2: AI-Enabled Precision Drug Delivery Framework.

This architecture presents a secure, personalized drug delivery system integrating seven functional layers: patient layer (wearable sensors and connected devices), AI intelligence engine (predictive analytics and personalization), certified control system (PDE controllers with stability guarantees), blockchain security layer (immutable ledgers and smart contracts), supply chain layer (end-to-end traceability), governance layer (stakeholder access), and measurable outcomes demonstrating significant improvements in adherence, cost reduction, and security

5.3 Nanotechnology and AI Integration

Nanotechnology allows the delivery of drugs by advancing nanoparticles that are designed to concentrate in tissues or cells. The use of AI improves nanoparticle development by: Selection of Material: Machine learning methods predict the best nanoparticle materials, surface engineering, and targeting ligands according to the desired properties and target properties (Gallego et al., 2021; Hao et al., 2023). Property Prediction: Deep learning models are used to predict the behavior of nanoparticles in biology, such as biodistribution, cellular uptake, and release kinetics, eliminating the necessity of large-scale experimental studies. Optimization of Manufacturing: AI is used to control the production of nanoparticles, and the quality attributes of a specific nanoparticle (size, shape, surface properties) that are essential to regulatory acceptance and therapeutic effectiveness can be maintained.

5.4 Predictive Analytics and Pharmacovigilance

The use of AI predictive analytics changes post-market surveillance and safety monitoring. NLP algorithms are used to analyze clinical notes, social media, and spontaneous reports to recognize adverse drug reaction earlier than the conventional pharmacovigilance approaches (Schuhmacher et al., 2021; Roche et al., 2023). Predictive models are used to find patients who are at high risk of certain adverse events, and it is possible to monitor and intervene. The machine learning solutions combine the multi-omics data and clinical features to predict individual responses, which can be used to calculate personalized risk-benefit.

6. Integration with Emerging Technologies

Genomics can be combined with AI to provide a complex study of the genetic diversity and its connection with the response to drugs. Machine learning models detect disease-related polymorphisms, calculate polygenic risk scores, and predict drug responses in individuals depending on the genetic profiles (Marques et al., 2024; Bhinder et al., 2021). One area where precision medicine is heading is the integration of genomics, transcriptomics, proteomics, and metabolomics known as multi-omics. AI models combine different forms of omics data to produce pervasive biological understanding, discovering new therapeutic targets and making future treatment choices with an accuracy never observed before.

Wearables provide real-time physiological signal streams which artificial intelligence algorithms convert into practical clinical information. Applications include: • Disease Prediction: Model of machine learning based on wearable data predicts the occurrence of such conditions as type 2 diabetes and heart-related events (Lam et al., 2021). • Parkinson's Monitoring: With the help of deep learning analysis of movement patterns, it becomes possible to assess the severity of the disease objectively (Schalkamp et al., 2023). • Mental Health: The AI algorithms identify trends based on anxiety, depression, and stress based on physiological signals (Kargarandehkordi et al., 2024).

The virtual models of biology, which are computer-generated using AI, known as digital twins, facilitate exploration of treatment options in silico. Digital twins can predict the response to treatment by combining patient-specific data with mechanistic models, which allows optimizing it prior to clinical implementation (Blasiak, 2020; Dercle et al., 2020). An example of the digital twin uses is cancer treatment. Genomic and imaging tumor models support the prediction of the response to different therapies, which is used to choose the best sequence of treatment and combination.

New innovations in foundation models and large language models (LLMs) are transforming drug discovery by: Knowledge Integration: LLMs that are trained on biomedical sources and databases allow quick synthesizing of the current knowledge to aid in hypothesis generation and designing experiments (Marques et al., 2024; Mesko and Topol, 2023). Molecular Design: Generative models Transformer-based and diffusion architectures design new molecules with optimized properties, which explore chemical space beyond conventional libraries (Lloyd, 2024) Property Prediction: Foundation models are used to predict ADMET properties (absorption, distribution, metabolism, excretion, toxicity) with enhanced accuracy and facilitate early candidate selection.

7. Challenges and Limitations

Data quality is a basic factor in the execution of AI models. Healthcare data poses a number of problems: Heterogeneity: Biomedical data is different across institutions and is thus of different formats and thus difficult to integrate and compare. Incompleteness: Lack of data points and inconsistency in the recording can decrease the utility of a dataset and can also impact bias. Bias and Representation: Training data usually represents minority groups unequally, and this results in models that are poor performers with respect to different groups of patients (Vora et al., 2023). Privacy Limitations: Data sharing can prevent thorough datasets access, which hinders model creation and validation.

Algorithmic Interpretability Face recognition is a black box model that can create faces which humans are unable to reproduce. Most AI models are black boxes, which pose a problem with applications in healthcare that need to make explainable decisions. Clinicians and regulators need to know factors that motivate AI recommendations especially where high-stakes decisions are involved that impact patient safety. The Explainable AI (XAI) strategies put forward seek to provide explanations using attention to interpretability, analysis of feature importance, and rule extraction. Nevertheless, existing XAI approaches tend to give post-hoc explanations that do not fully give a picture of model reasoning (LeCun et al., 2015; Russell and Norvig, 2016).

The current regulations were not set to handle AI systems which develop through continuous learning. Key challenges include: • Validation Requirements: Determining evidence standards of AI systems that can be enhanced by more data. • Algorithmic Drift: Assuring the performance consistency as models are presented with new data distributions. • Liability: How to be responsible in case AI-driven recommendations result in such negative outcomes? • Post-Market Surveillance: Measuring the progress of AI systems after implementation. Regulatory bodies

are also coming up with dynamic frameworks to deal with such challenges. Digital Health Innovation Plans like the one developed by the FDA are geared towards creating a balance between innovation and safety (FDA, 2024; Mesko and Topol, 2023).

The use of AI in drug development causes serious ethical concerns: Equity: Making AI beneficial to all populations, not only in well-resourced healthcare systems. Autonomy: Educating AI-driven decisions by human influence and control. Data Ownership: Deciding patient data rights in AI model development. Informed Consent: making patients aware of the role of AI in their treatment and its risks.

9. Conclusion

AI is radically changing the pharmaceutical sciences, providing answers to the perennial problems of drug discovery and delivery. Through its use of sophisticated computing techniques, AI can expedite discovery, lower development expenses, enhance success rates, and provide personalized therapeutic treatments that were once out of reach. The reviewed evidence shows that AI-driven solutions can lead to significant gains throughout the development pipeline. Multi-omic data analysis can help identify our targets more accurately. Optimization of leads is made faster by predictive modeling of structure-activity relationship. AI-enabled devices can deliver drugs more personally, as they adjust to the needs of individual patients. Predictive patient selection and adaptive design are aspects that make clinical trials more efficient. Such breakthrough results as AlphaFold predicting protein structures, Exscientia predicting clinical candidates using AI, and BenevolentAI rediscovering drugs in a matter of days during the COVID-19 pandemic demonstrate the practical effects of AI. These achievements confirm the possibilities of AI and emphasize existing issues that have to be addressed. Effective implementation of AI requires solving such critical issues as data quality and standardization, algorithmic interpretability, regulatory frameworks, and ethical issues. Advancements in these fields need data scientists, pharmaceutical researchers, clinicians, regulators and ethicists to work together. The intersection of AI and new technologies such as genomics, wearables, digital twins, nanotechnology, and so forth holds even more potentially game-changing opportunities. Multimodal foundation models will incorporate multiple types of data to get whole insights. The federated learning will provide a way of collaborative model development without violating privacy. Formal safety will be given by certified control systems to AI-driven delivery. To achieve the potential of AI, it is imperative to adhere to strict validation and transparency of the methodology, and to a fair implementation of AI. Properly developed AI would have the potential to democratize access to high-tech therapeutics, quicken the response to new health risks, and allow truly personalized medicine. The future of drug discovery and delivery is in the establishment of effective cooperation between machine intelligence and human expertise, and the leveraging of the advantages of both in enhancing human health.

References

1. Mak, K. K., & Pichika, M. R. (2019). Artificial intelligence in drug development: Present status and future prospects. Drug Discovery Today, 24(3), 773-780.
2. DiMasi, J. A., Grabowski, H. G., & Hansen, R. W. (2016). Innovation in the pharmaceutical industry: New estimates of R&D costs. Journal of Health Economics, 47, 20-33.
3. Chang, W. T., et al. (2022). An artificial intelligence approach for predicting cardiotoxicity in breast cancer patients receiving anthracycline. Archives of Toxicology, 96, 2731-2737.
4. Bhinder, B., Gilvary, C., Madhukar, N. S., & Elemento, O. (2021). Artificial intelligence in cancer research and precision medicine. Cancer Discovery, 11, 900-915.
5. LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. Nature, 521(7553), 436-444.
6. Jumper, J., et al. (2021). Highly accurate protein structure prediction with AlphaFold. Nature, 596(7873), 583-589.
7. Liu, S., Wang, Y., & He, H. (2020). A new playing method of the guessing football lottery. IOP Conference Series: Materials Science and Engineering, 790(1), 012100.
8. Bansal, V., et al. (2022). Machine learning in medical imaging. Journal of Clinical Imaging Science, 12(1), 23.
9. Esteva, A., et al. (2017). Dermatologist-level classification of skin cancer with deep neural networks. Nature, 542(7639), 115-118.
10. Haeberle, H. S., et al. (2019). Artificial intelligence in medical imaging and

surgery. Journal of Healthcare Engineering, 2019.
11. Gibbs, B., et al. (2020). NLP in clinical documentation and decision-making. Journal of Biomedical Informatics, 102, 103356.
12. Davenport, T., & Kalakota, R. (2019). The potential for AI in healthcare. Future Healthcare Journal, 6(2), 94-98.
13. Marques, L., et al. (2024). Advancing precision medicine: A review of in silico approaches. Pharmaceutics, 16, 332.
14. Schuhmacher, A., et al. (2019). AI in pharmaceutical R&D management. Drug Discovery Today, 24(4), 892-898.
15. Talat, M., et al. (2023). AI for antimicrobial drug discovery. Journal of Antimicrobial Chemotherapy, 78(1), 15-27.
16. Li, H., et al. (2023). AI-enabled delivery of mRNA for Alzheimer's disease treatment. Neuroscience Bulletin, 39(4), 563-574.
17. Blasiak, A. (2020). CURATE.AI: Optimizing personalized medicine with artificial intelligence. SLAS Technology, 25(2), 95-105.
18. Arden, N. S., et al. (2021). Industry 4.0 for pharmaceutical manufacturing: Preparing for the smart factories of the future. International Journal of Pharmaceutics, 602, 120554.
19. Grangeia, H. B., et al. (2020). Quality by design (QbD) in pharmaceutical development. European Journal of Pharmaceutics and Biopharmaceutics, 156, 85-95.
20. Mukherjee, D., Roy, D., & Thakur, S. (2024). Transforming cancer care: The impact of AI-driven strategies. Current Cancer Drug Targets, 24, 1-4.
21. Liu, Z., Roberts, R. A., Lal-Nag, M., Chen, X., Huang, R., & Tong, W. (2021). AI-based language models powering drug discovery and development. Drug Discovery Today, 26(11), 2593-2607.
22. Gallego, V., Naveiro, R., Roca, C., Rios Insua, D., & Campillo, N. E. (2021). AI in drug development: A multidisciplinary perspective. Molecular Diversity, 25, 1461-1479.
23. Sarkar, C., Das, B., Rawat, V. S., Wahlang, J. B., Nongpiur, A., Tiewsoh, I., et al. (2023). Artificial intelligence and machine learning technology driven modern drug discovery and development. International Journal of Molecular Sciences, 24(3), 2026.
24. Aundhia, C., et al. (2024). Smart insulin pumps and AI integration for diabetes management. Journal of Diabetes Science and Technology, 18(2), 234-245.
25. Hao, Y., Lynch, K., Fan, P., Jutschenko, C., Cid, M., Zhao, Z., & Yang, H. S. (2023). Development of a machine learning algorithm for drug screening analysis on high-resolution UPLC-MSE/QTOF mass spectrometry. Journal of Applied Laboratory Medicine, 8(1), 53-66.
26. Schuhmacher, A., et al. (2021). AI-driven pharmacovigilance systems. Expert Opinion on Drug Safety, 20(10), 1231-1240.
27. Roche, V., Robert, J. P., & Salam, H. (2023). A holistic AI-based approach for pharmacovigilance optimization from patients' behavior on social media. Artificial Intelligence in Medicine, 144, 102638.
28. Lam, B., et al. (2021). Using wearable activity trackers to predict type 2 diabetes: Machine learning-based study. JMIR Diabetes, 6, e23364.
29. Schalkamp, A. K., et al. (2023). Wearable-based Parkinson's disease severity monitoring using deep learning. Nature Medicine, 29, 135-144.
30. Kargarandehkordi, A., et al. (2024). Real-time modeling of stress-related blood pressure fluctuations using wearable devices and AI. Journal of Hypertension, 42(3), 456-465.
31. Dercle, L., et al. (2020). Identification of non-small cell lung cancer sensitive to systemic cancer therapies using radiomics. Clinical Cancer Research, 26, 2151-2162.
32. Mesko, B., & Topol, E. J. (2023). The imperative for regulatory oversight of large language models (or generative AI) in healthcare. NPJ Digital Medicine, 6, 120.
33. Lloyd, L. (2024). AI for drug discovery. Nature Reviews Urology, 21, 517.
34. Vora, L. K., et al. (2023). Artificial intelligence in pharmaceutical technology and drug delivery design. Pharmaceutics, 15(7), 1916.
35. Russell, S. J., & Norvig, P. (2016). Artificial intelligence: A modern approach. Pearson.
36. Liu, Q., Huang, R., Hsieh, J., Zhu, H., Tiwari, M., Liu, G., Jean, D., ElZarrad, M. K., Fakhouri, T., Berman, S., & Wang, Y. (2023).

Landscape analysis of the application of artificial intelligence and machine learning in regulatory submissions for drug development from 2016 to 2021. Clinical Pharmacology & Therapeutics, 113(4), 771-774.

37. Niazi, S. K. (2023). The coming of age of AI/ML in drug discovery, development, clinical testing, and manufacturing: The FDA perspectives. Drug Design, Development and Therapy, 17, 2691-2725.
38. FDA. (2024). FDA's digital health innovation plan. U.S. Food and Drug Administration.
39. Exscientia. (2023). Advancements in AI-designed molecules. Exscientia Press Release.
40. Stebbing, J., et al. (2020). Baricitinib in COVID-19 treatment. The Lancet, 395(10238), 1322-1325.
41. Ren, F., Ding, X., Zheng, M., Korzinkin, M., Cai, X., Zhu, W., et al. (2023). AlphaFold accelerates artificial intelligence powered drug discovery: Efficient discovery of a novel CDK20 small molecule inhibitor. Chemical Science, 14(6), 1443-1452.
42. Cai, X., Lin, Y., Li, Y., Wang, R., & Ke, C. (2025a). Set point regulation control for KdVB equation. 37th Chinese Control and Decision Conference, 5716-5720.
43. Cai, X., Lin, Y., Li, Y., Zhang, L., & Ke, C. (2025b). Inverse optimal adaptive boundary control for heat PDE. 37th Chinese Control and Decision Conference, 1825-1828.
44. Cai, X., Li, Y., Wang, P., Lin, Y., Zhang, L., & Liu, L. (2025c). Adaptive inverse optimal control for unstable reaction-diffusion PDE system. Kybernetika, 61(4), 537-553.