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Artificial Intelligence In Drug Discovery And Formulation: Transforming Personalized Medicine

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ABSTRACT
The pharmaceutical drug development process is highly complex, costly, and time-intensive, often taking over a decade and costing billions of dollars to deliver a single drug to market. Artificial intelligence (AI) and machine learning (ML) have emerged as revolutionary forces capable of accelerating this pipeline by enabling data-driven progression in the field of drug discovery, formulation design, and precision medicine. This article overviews the recent advances in AI-based techniques and their integration across key stages of pharmaceutical research and development. In the drug discovery field, AI has improved target identification, virtual screening, and drug design through deep learning architectures. These tools facilitate accurate predictions of drug–target interactions, toxicity, and pharmacokinetic behaviour, thereby reducing attrition rates and experimental burden. AI-driven drug repurposing leverages existing safety and pharmacokinetic profiles to identify new therapeutic uses for approved drugs, offering a faster and cost-effective alternative to traditional drug discovery. AI analyzes large-scale genomic and clinical data to enable the design of personalized therapies tailored to an individual's genetic makeup. AI also plays a critical role in pharmaceutical formulation and drug delivery by optimizing excipient selection, processing parameters, and controlled-release profiles. These applications extend to advanced delivery systems, including nanomedicines, where AI techniques improve bioavailability and targeting efficiency. AI is also reshaping clinical trial design through optimized patient recruitment, adaptive monitoring, and personalized dosing strategies. Despite these advancements, challenges related to model interpretability, algorithmic bias, and ethical governance remain critical barriers to widespread adoption. Overall, this article highlights AI as a central catalyst for innovation in pharmaceutical development, with the potential to enable precision medicine and advance global healthcare through responsible implementation.
Keywords: Artificial Intelligence, Pharmaceutical Development, Drug Discovery, Drug Formulation, Nanomedicine, Precision Medicine

INTRODUCTION:

Artificial Intelligence (AI) is reshaping the future of multiple industries, including finance, education, marketing, manufacturing, and the pharmaceutical sector

Artificial Intelligence(AI) aims to develop computational systems that mimic human intelligence, such as learning, reasoning, perception, and decision-making. It involves methods like optimization algorithms, computer vision for quality checks, and robotics for lab automation. (Aritra et al., 2025) Machine learning (ML) is a subset of AI that focuses on developing algorithms to identify patterns in the data without being explicitly programmed for every task. It is widely used for predictive analysis, for example, predicting drug toxicity, patient responses, and virtual screening for identifying promising drug candidates. Deep Learning (DL) is a subfield of Machine Learning (ML) that employs multi-layered artificial neural networks to derive complex relationships in large datasets. DL architectures, such as convolutional neural networks, recurrent neural networks, and graph neural networks, have demonstrated superior performance in tasks involving images, text, and large-scale biological data. (Fu & Chen, 2025)

Within the pharmaceutical industry, AI has shown great promise to accelerate drug discovery, precision medicine, and clinical workflows. Early applications primarily focused on predicting the performance of conventional dosage forms. More recently, AI-based approaches have also been used to design advanced drug delivery systems and nanoparticles.

Different branches of AI are implemented based on a particular task. Supervised learning is common for predictive modelling with labelled datasets, whereas unsupervised learning helps cluster similar molecules without predefined labels. (Riemer & Freund, 2026)Reinforcement learning is becoming popular for improving sequential decision making, such as adaptive dosing strategies. In addition, AI systems that replicate human decision-making are integrated into clinical workflows as decision support tools. In pharmaceutical sciences, natural language processing is increasingly used

to extract meaningful information from unstructured data sources, such as electronic health records and clinical trial reports.(Kandhare et al., 2025)

This review examines the evolving role of AI across the pharmaceutical development, including drug discovery, formulation development, and clinical trials. By enabling predictive modelling and data-driven optimization at each stage, AI offers a strategic pathway toward more efficient development pipelines and enhanced product quality

2. Role of Artificial Intelligence in Drug Discovery

Drug discovery and development involve identifying and developing new drug molecules for specific therapeutic conditions. A typical drug discovery pipeline involves target identification, hit generation, lead optimisation, followed by preclinical evaluation and clinical trials prior to regulatory approval.

Fig.1 Schematic representation of key stages involved in drug discovery and drug development

Traditional drug discovery is costly and time-consuming, relying heavily on repetitive experimental methods with limited scalability. AI has transformed this process by enabling systematic analysis of large biomedical datasets, improving efficiency across discovery stages.(Wang et al., 2025)

The drug discovery process involves the following steps:

2.1. Target Identification and Validation:

The process begins with the identification and validation of suitable biological targets, such as proteins, genes, or molecular pathways involved in disease progression. Artificial intelligence (AI) enables the analysis of large text-based and multi-omics data to identify disease-relevant targets. Analysis of multi-omics data, including genomic, proteomic, metabolomics, and transcriptomic datasets, facilitates the identification of altered metabolic pathways and biomarkers. (Knox et al., 2024) For target validation, targets are analysed based on criteria like druggability, toxicity, novelty, protein family classification, disease conditions, etc. (Pun et al., 2023). PandaOmics is a deep learning-based platform used for target discovery, target validation, and biomarker identification. (Kamya et al., 2024)

2.2. Hit Identification:

Following target identification and validation, **hit identification** involves screening large chemical libraries to find compounds that interact with the target. This can be performed using high-throughput experimental screening or computational methods such as virtual screening. Use of AI speeds up the screening process and improves the accuracy. Databases such as DrugBank and ChEMBL are commonly analyzed using AI-based tools. Deep Docking (DD), a deep learning-based platform, accelerates virtual screening by docking only a subset of compounds and predicting scores for the rest, allowing efficient screening of vast libraries. (Dreiman et al., 2021) In addition to screening existing compounds, **de novo drug design** focuses on creating new molecules that bind to specific targets without using predefined templates. Generative adversarial networks (GANs) are widely used for this purpose and enable the design of novel drug candidates with desired properties. (Visan & Negut, 2024)

2.3. Lead Optimisation:

Next step is lead candidate optimisation, where promising hit compounds are chemically modified to improve potency, selectivity, and drug-like characteristics. At this stage, absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties are evaluated to ensure an acceptable pharmacokinetic and safety profile. (Pun et al., 2023)Several generative deep learning models, including recurrent neural networks, variational autoencoders, GANs, graph convolution networks, and transformer-based models, have been used to generate and optimize drug molecules.(Li et al., 2022)

2.4. Prediction of Pharmacokinetic Properties:

AI also supports early prediction of drug toxicity and pharmacokinetic properties by analyzing data from toxicology studies, clinical trials, and chemical databases. AI tools are used to predict absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties of drugs. Experimentally measured pharmacokinetic data is integrated into machine learning models, which are then coupled to physiologically-based pharmacokinetic (PBPK) models to estimate key pharmacokinetic parameters. (Chou & Lin, 2023) AI-driven pharmacokinetic platforms, including pkCSM (aProximate), ADMET Predictor (Property Prediction, 2024), GastroPlus (L. Wang et al., 2023), and XGBoost(Wiens et al., 2025), predict absorption, metabolism, clearance, and drug-drug interactions with high accuracy.

Prediction of drug bioactivity relies on the drug–target binding affinity (DTBA), which is the strength of interaction between the drug and the target. AI techniques used in DTBA evaluation include WideDTA, DeepDTA, GraphDTA and DeepAffinity (Zhu et al., 2023) AI techniques are also used to predict the potential toxicity of the drug candidates. Models trained on historical data from clinical trials, toxicology studies, and chemical databases are used to predict the toxicity, mutagenicity, carcinogenicity, and other adverse effects. Tools such as Toxtree, DeepTox (Banerjee et al., 2018), PrOCTOR, ChemProp, and ProTox-II help identify the likelihood of drug toxicity before clinical testing. (Mayr et al., 2016)

A notable example of AI-driven drug discovery is INS018_055, an AI-designed inhibitor of TNIK for idiopathic pulmonary fibrosis. Using platforms such as PandaOmics and Chemistry42, the entire discovery process - from target identification to preclinical candidate selection was completed in approximately 18 months, far faster than traditional methods, which take more than a decade. (Ren et al., 2024)

2.5. Drug Repurposing:

Drug repurposing aims to identify new therapeutic uses for existing drugs by leveraging their established safety, pharmacokinetic, and manufacturing profiles, offering a faster and more cost-effective alternative to de novo drug discovery. This approach has gained increased attention for treating rare diseases and responding to emerging health challenges, such as the COVID-19 pandemic. Traditional repurposing methods, including literature mining, high-throughput screening, and molecular docking, have led to successful examples such as sildenafil (earlier for hypertension, now repurposed for erectile dysfunction) and thalidomide (repurposed for multiple myeloma). (Vemula et al., 2024)

However, conventional approaches such as literature-based reviews can take several months, and high-throughput screening can require substantial financial investment. In addition, reliance on manual selection and predefined targets restricts scalability. These limitations underscore the need for AI-driven drug repurposing strategies capable of rapidly analysing large-scale biomedical data and accelerating therapeutic discovery.

DeepDrug and DeepPurpose are deep learning frameworks that support sequence-based drug repurposing. (Huang et al., 2021) Database-driven platforms such as RepurposeDB and CMap (Shameer et al., 2018) use gene expression data for mechanism-based repurposing but are limited by data availability. High-throughput tools, including TensorFlow Drug Repurposer and DeepDrugRepurposing (Pang et al., 2020), enable large-scale predictions by analyzing multi-drug screening datasets, particularly in oncology.

AI-driven models, including graph neural network (GNN) based DeepDrug and electronic health record-based approaches, have further advanced drug repurposing. GNNs combined with multi-omics data have supported drug repurposing for rare diseases, including Amyotrophic Lateral Sclerosis (ALS) and Alzheimer's disease. (Sharifi-Noghabi et al., 2019)

During the COVID-19 pandemic, BenevolentAI, a UK-based company, applied AI techniques to examine gene expression profiles, protein interactions, and repurposed existing drugs to identify Baricitinib as a potential treatment against inflammatory reactions caused by SARS-CoV-2. Baricitinib was granted an Emergency Use Authorization by the FDA after being validated in clinical trials. (Richardson et al., 2022)

2.6. Personalised Medicine:

Selection of an effective treatment and dosage for patients is challenging due to individual variability in drug response, combination therapies, and changing disease conditions.AI supports personalized medicine by analyzing genetic, molecular, and clinical data to tailor treatments to individual patients, thus improving therapeutic outcomes and reducing adverse effects. (Visan & Negut, 2024)

CURATE.AI is an example of an AI platform designed for personalized dosing. It creates a unique patient profile by mapping treatment inputs to clinical outcomes. Its effectiveness has been demonstrated in optimizing dosages for chronic diseases, including hypertension and diabetes (Mukhopadhyay et al., 2022)

Another personalized medicine platform is the quadratic phenotypic optimization platform

(QPOP), which identifies optimal drug combinations using experimental data from patient samples. This approach is particularly important in oncology, where addressing tumor heterogeneity is critical for effective therapy. (Goh et al., 2022) AI-driven platforms can predict patient-specific drug responses, enabling the development of personalized treatment strategies. For example, Tempus, an AI and data analytics company, applies precision oncology approaches to match cancer patients with the most effective treatments based on their individual genomic profiles. (Hasseleren and Oprea, 2024).

Table 1: Various AI-based tools used across different stages of drug discovery

No.	Tool / Software	Key Application in Drug Discovery	Ref
	Target Identification and validation		
1	**PandaOmics (Insilico Medicine)**	Discover new therapeutic targets by analysing multi-omics data	(Kamya et al., 2024)
2	**Precision Target (Exscientia)**	Identify disease-relevant targets from available data	(Exscientia)
3	**AlphaFold (DeepMind)**	Protein structure prediction for structure-based drug design	(Jumper et al., 2021)
	Drug Screening		
4	**Chemistry42 (Insilico Medicine)**	Structure and Ligand-based drug design, lead optimisation	(Ren et al., 2024)
5	**AtomNet (Atomwise)**	Uses deep learning to identify the binding affinity of drugs to target proteins	(Chen et al., 2023)
6	**DeepChem**	Virtual screening, molecular	(Sharma and Sharma,

		property prediction	2018)
	Drug design		
7	**GENTRL (Insilico Medicine), PaccMan (IBM)**	Generation of new molecular structures	(Zhavoronkov et al., 2019) (Born et al., 2021)
8	**GraphInvent (Astrazeneca)**	De novo drug design	(Mercado et al., 2021)
9	**AIDDISON**	Structure and ligand-based drug design	(Rusinko et al., 2024)
	Drug–Target Interaction Prediction		
10	**PotentialNet**	Prediction of protein-ligand binding affinity	(Feinberg et al., 2018)
11	**Schrödinger Maestro**	Molecular docking, QSAR modelling	(Bordoloi et al., 2023)
12	**DeepDTA, WideDTA,**	Prediction of binding affinity, analysis of the interaction between the drug and the target protein	(Zhu et al., 2023)
	Pharmacokinetics Prediction		
13	**pkCSM, ADMET predictor**	In-silico prediction and evaluation of ADMET properties	(aProximate), (Property Prediction, 2024)
14	**Simcyp (Certara Inc.)**	Predicts human pharmacokinetics, PBPK modelling	(Notwell and Wood, 2023)
15	**GastroPlus, XGBoost**	Predicts pharmacokinetics of drugs, PBPK modelling	(Wang et al., 2023), (Wiens et al., 2025)
	Drug Toxicity prediction		
16	**DeepTox, PrOCTOR**	Toxicity and safety assessment of drug candidates	(Hao et al., 2023)
17	**Toxtree, ProTox-II**	Prediction of toxicity using decision tree methods, Prediction of LD50, and organ toxicity	(Banerjee et al., 2018)
18	**Drug repurposing**		
19	**DeepPurpose, DeepDrug**	Drug-target interaction and drug repurposing	(Huang et al., 2021)
20	**TensorFlow Drug Repurposer**	Large-scale screening for drug repurposing	(Pang et al., 2020)
21	**RepurposeDB, CMap**	Drug repurposing by analysing gene expression data	(Shameer et al., 2018)

3. The Role of AI in Optimisation Formulation and Drug Delivery

Pharmaceutical formulation development is a critical stage in the drug development process. AI algorithms analyse experimental data and uncover relationships between formulation composition, process parameters, and product quality attributes. These models can also predict formulation parameters, such as the effects of excipients on drug solubility, sustained-release profiles of drugs from dosage forms, and the long-term physical stability of pharmaceutical products.(Ali et al., 2024)

3.1 Conventional Dosage Forms:

AI has been used to predict key aspects of drug behaviour, including mechanical properties, dissolution profiles, bioavailability, and stability. By learning the effects of excipients and processing conditions, these computational models enable efficient formulation optimization and significantly reduce development timelines.

Djuris et al., 2021 used an artificial neural network to identify factors such as compression load, excipient co-processing, and paracetamol addition, that affect tablet tensile strength and the tableting process. For the colon-targeted delivery of Chlorogenic acid, 3D-printed capsules were developed using ANN. Parameters such as nozzle diameter, temperature, and printing speed were optimised for optimal results (Y. Wang et al., 2023). Multilayer 3D-printed capsules were designed using genetic algorithms, with the arrangement of capsule

geometry, as per specific dissolution profiles.(Hu et al., 2024)

Jiang et al., 2022 used machine learning models to assess the performance of a dry powder inhaler formulation prepared by Thin-Film-Freezing technology. Different models were used to compare median aerodynamic diameter and fine particle fraction. Amongst all, Artificial neural networks and Random Forest were selected as the best models for predicting these parameters. Convolutional neural networks were used to predict SEM images of formulations.

AI supports quality by design (QbD) in pharmaceutical manufacturing by improving data analysis, process optimization, and predictive modeling. Artificial neural networks were used to predict hardness and *in-vitro* dissolution characteristics of extended-release tablets prepared by direct compression. Spectroscopic and manufacturing data from pilot-scale batches were used to predict, critical quality attributes to ensure batch-to-batch consistency. (Nagy et al., 2023)

Khan et al., 2023 used an artificial neural network (ANN) to evaluate drug release from orodispersible moxifloxacin tablets. The ANN model was trained using formulation data generated through a central composite design, enabling efficient optimization of tablet performance. Currently, the evaluation of tablet coating quality relies only on the visual observation by operators. Image-based AI methods were applied to accurately assess tablet coating time and ensure product quality.(Hirschberg et al., 2020)

3.2 Advanced Drug Delivery:

AI techniques have been applied in the design and evaluation of novel dosage forms such as nanoemulsions, transdermal patches, and solid dispersions.

Water-in-oil emulsions were formulated using microfluidics and machine learning models. Different ML models like ANN, support vector machines, and XGBoost were integrated into a single model for improved prediction. Monodisperse emulsions with optimal droplet size were generated using a Microfluidic chip. (Damiati et al., 2025)

Bagde et al., 2023 developed an AI-optimized 3D-printed sustained-release transdermal microneedle patch using digital light processing technology. A semi-supervised machine learning model was applied to optimize print fidelity and microneedle morphology for effective delivery of lipophilic drugs. Amorphous solid dispersions consist of one or more APIs dispersed in a solid matrix. They are used to improve the solubility and dissolution of hydrophobic drugs. et al used AI and PBPK modelling to predict in-vitro dissolution and systemic absorption of solid dispersions. Multiple formulations with a large set of dissolution time points were used to train the model.(Zhu et al., 2025)

Microparticles of Poly(lactic-co-glycolic acid)(PLGA) were fabricated using machine learning models and microfluidics. The concentration of PLGA and the flow rates of aqueous and dispersed phases were the key parameters influencing the particle sizes of microparticles. Five artificial neural networks were designed using these factors, which ultimately led to the construction of a single in silico model capable of predicting particle sizes of microparticles produced from different microfluidic systems. (Damiati et al., 2020)

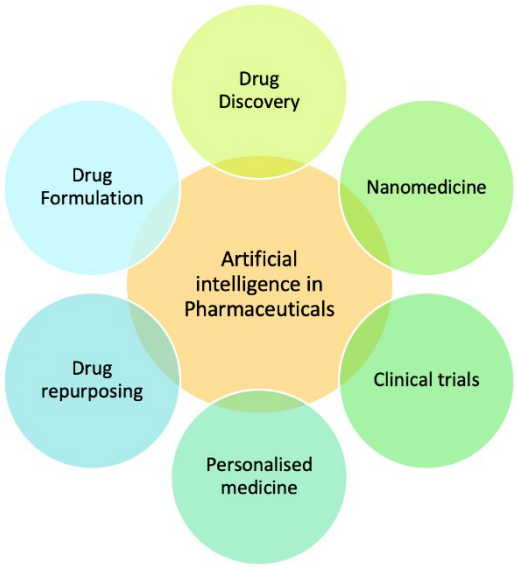

Fig.2 Applications of Artificial intelligence based techniques in Pharmaceuticals

3.3 Nanomedicine:

Optimizing nanomedicines requires careful control of interconnected factors such as particle size, shape, surface chemistry, and drug loading. Traditional trial-and-error methods are time-consuming, costly, and poorly scalable. As a result, these approaches are limited in efficiently exploring large design spaces and identifying optimal nanomedicine formulations. Recent advances in AI and machine learning have transformed the rational design of nanomedicine formulations.(Chou et al., 2025)

In lipid nanoparticle (LNP) research, AI is widely used to optimize ionizable lipids for RNA delivery, reducing reliance on trial-and-error methods. Machine learning-based screening has been shown to significantly improve mRNA delivery efficiency. (Li et al.,2024 ; Shan et al.,2024) Notably, large-scale in silico screening of nearly 20 million ionizable lipids identified new candidates that outperformed benchmark lipids such as MC3 (First FDA-approved RNAi therapy Onpattro) and SM-102 (Moderna's COVID-19 mRNA vaccines), leading to enhanced RNA delivery. (Wang et al., 2022)

Xue et al., (2024) introduced the AGILE platform, which uses a graph neural network to screen ionizable lipids and predict thousands of optimized variants with improved mRNA transfection. Such AI pipelines reduce development time and reveal structure-function relationships, enabling precise tuning of lipid composition, pKa, and chain length to improve delivery efficiency.

Beyond lipid nanoparticles, AI-based techniques are also applied to polymeric micelles, inorganic nanocarriers, and dendrimers. Algorithms and deep generative models

efficiently optimise design space for parameters like polymer composition, surface chemistry, and core-shell structure, thus improving stability and drug-loading capacity of the nanocarriers (Rezvantalab et al., 2024). Yacoub et al.,2022 explored the AI-assisted design of in-situ forming Piroxicam-loaded nanoparticles for arthritis via intra-articular delivery. AI techniques help determine the drug release and encapsulation efficiency of nanoparticles. Li et al., (2020) made use of supervised machine learning for the prediction of liposomal properties and found enhanced accuracy than conventional models in the prediction of encapsulation efficiency and particle size.

Efficient delivery of nanoparticles to the tumor site is a challenging task. Lin et al., 2022 applied AI techniques to improve the same. The nano-tumor database, consisting of 376 datasets, was generated from a physiologically based pharmacokinetic model. A variety of AI techniques, including deep neural networks, regression, and support vector machines, were applied, out of which the deep neural network showed promising results. Nuhn et al., 2023 have applied AI techniques for the analysis of a single blood vessel, which revealed the presence of heterogeneous vascular permeability in several tumors

The in silico designs are further assessed using multiscale tumor or tissue simulations combined with reinforcement learning. Optimization of nanoparticle properties has been used to improve colloidal stability, tumor penetration, and controlled drug release. (Kim et al., 2024) Results and insights from the models are shared through online platforms such as FormulationAI, where researchers can submit nanoparticle descriptors, share datasets, and receive AI-based performance predictions. (Ding et al., 2023)

AI-based protein structure prediction tools, such as AlphaFold, enable the rational design of protein and peptide targeting ligands for nanomedicine. These ligands are designed to adopt specific 3D structures that bind cellular receptors with high affinity, improving receptor-mediated uptake. AI-guided design increases binding efficiency before synthesis, and when attached to nanocarriers, these ligands enhance tumor targeting, cellular uptake, and reduce off-target effects. (Yang et al., 2023)

AI has shown promise in drug delivery for rare genetic disorders such as Duchenne muscular dystrophy. Using a combination of experimental knowledge and AI, novel non-toxic peptides were generated to attach to the Phosphonodiamidite Morpholino Oligomers (PMO), improving permeation to cell nuclei and dystrophin gene modulation. (Wilton-Clark & Yokota, 2022) Animal models often fail to predict nanoparticle behaviour *in vivo* due to species-specific biological differences. AI-PBPK approaches improve the prediction of tumor delivery and tissue distribution while reducing reliance on animal studies. (Chou et al., 2023)

4. Use of Artificial Intelligence in Clinical Trials

In clinical trials, the use of AI enables real-time data analysis, trial monitoring, and improved patient recruitment. Advanced AI algorithms stratify patients based on phenotypic and genotypic characteristics, ensuring that trials are conducted with the most suitable cohort of participants. (Chopra et al., 2023)

Natural language processing (NLP) tools analyze prior protocols to generate inclusion and exclusion criteria, shifting trial design from intuition-based to evidence-informed planning. Machine learning models evaluate the protocol feasibility and identify eligible participants through demographic, geographic, and clinical information. AI-assisted virtual screening and continuous monitoring systems improve patient assessment and the detection of adverse events. AI also assists in the development of adaptive trials by modifying randomization and dosing based on real-time information. ML models discover patient subgroups by combining multi-omics and clinical data, thus enhancing personalized treatment approaches. (Olawade et al., 2026)

Collaboration between the Pharmaceutical industries and AI firms is accelerating the drug discovery process. Companies such as BenevolentAI, DeepMatter, Medidata AI, Saama, and Recursion have partnered with major pharmaceutical companies like Astrazeneca, Bristol-Myers-Squibb, Pfizer, and Roche to facilitate the clinical trials. Intelligent Trials is an AI-based system from Medidata to speed up clinical trial design and monitoring with predictive capabilities. (Chopra et al., 2023)

5. Ethical and Regulatory Considerations

As AI is integrated into the Pharmaceutical industry, regulatory and ethical oversight is important to ensure fairness and transparency of these techniques. This necessitates the implementation of a rigid regulatory framework to address the key challenges, such as algorithmic bias, data privacy, and validation of results (Fu & Chen, 2025)

Data minimization tools are essential to remove unnecessary information. Critical data should be encrypted and accessible only to authorized users. Protecting patient privacy is critical when training AI on sensitive health data, requiring strict safeguards to ensure ethical and secure use of personal information. AI systems, especially those affecting public safety, must be transparent and interpretable. (Riemer & Freund, 2026)

Regulatory agencies are establishing guidelines for AI in drug development, prioritizing patient safety and ethical use by reducing, refining, or replacing animal testing with validated AI models. In the United States, HIPAA Privacy Regulations and the Digital Health Innovation Action Plan ensure secure medical records and promote the responsible use of AI in the pharmaceutical and healthcare systems. The European Council adopted a new AI regulation in 2024 to establish standards for the safe use of AI across member states.(Ali et al., 2024)

6. Challenges in the Implementation of AI

AI can speed up drug discovery by rapidly identifying lead compounds through virtual screening. However, many ML models lack interpretability and function as ‘black boxes’; therefore, developing more transparent AI models is essential. AI models can be limited by data bias, as their predictions depend on the quality of training data. Incomplete or unbalanced datasets may lead to inaccurate predictions of drug efficacy, especially when certain

diseases or populations are underrepresented. Ensuring high-quality, diverse, and unbiased training data is therefore essential. (Visan & Negut, 2024)

AI systems struggle to adapt quickly to new data, and outdated models can produce inaccurate predictions. Strategies are needed to continuously update AI tools with new data to maintain reliability. In addition, AI often favours average patterns, limiting its ability to capture individual variability, which can reduce prediction accuracy for patients with diverse or complex responses, such as those with cancer. AI struggles to capture the complexity of biological systems and interindividual variability, limiting its predictive power in personalized medicine. Improved modelling of microenvironments and patient-specific factors is essential for accurate outcomes.(Chou et al., 2025)

Another challenge is the need for substantial investments and skilled professionals for the effective adoption of AI technologies. Addressing these issues through strategic partnerships between pharmaceutical companies and technology partners is essential to improving efficiency and success in drug development. (Joshi & Sheth, 2025)

7. Future Perspective and Conclusion

Drug development is a cost-intensive, time-consuming, and multi-stage process. It often takes many years to deliver a safe, efficacious, optimised formulation to market. Recent progress in AI-based techniques have transformed pharmaceutical development by providing data-driven strategies to overcome these obstacles. IT enhances the speed and accuracy across multiple stages of drug development, ranging from target identification, hit generation, lead optimisation, formulation development, preclinical and clinical testing. A wide range of AI-driven platforms, including AlphaFold, GastroPlus, AtomNet, ProTox-II, and Chemistry42, have been developed to support drug development and clinical translation.

Several AI-discovered drugs have advanced to clinical trials. For instance, DSP-1181, developed by Exscientia for obsessive–compulsive disorder, was the first entirely AI-designed drug to enter Phase I trials. Similarly, INS018_055 by Insilico Medicine for idiopathic pulmonary fibrosis has progressed to clinical testing. AI-driven drug repurposing has contributed to the emergency use authorization of Baricitinib for COVID-19 treatment.

Despite these advances, challenges remain, including data quality, model interpretability, and ethical concerns such as algorithmic bias and patient privacy. Addressing these issues through diverse training datasets, transparent models, and robust data-security frameworks will be critical. Overall, AI holds substantial promise for accelerating a data-driven revolution across the pharmaceutical development stages, addressing unmet medical needs, and improving global access to effective therapies

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