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Review Article

Role of artificial intelligence in pharmaceutical drug development and drug delivery: An updated review

Joshi Ankur[1]*, Priyanka Soni[2], Purva Khemani[1], Gulfisha Shaikh[1], Usha Vishwakarma[1], Shashank Sharma[1], Neelesh Malviya[3], Sapna Malviya[1], Anil Kharia[1]

[1]Modern Institute of Pharmaceutical Sciences, Indore, Madhya Pradesh, India
[2]Sri Aurobindo Institute of Pharmacy, Indore, Madhya Pradesh, India
[3]Smriti College of Pharmaceutical Education, Indore, Madhya Pradesh, India

Abstract

AI accelerates problem-solving by using human knowledge, transforming pharmaceutical development, formulation, and testing. By analyzing genomic and proteomic data, AI identifies disease targets and predicts drug interactions, improving drug discovery efficiency. AI optimizes research, reducing costs, and aids trial design by predicting pharmacokinetics and toxicity, prioritizing lead compounds without animal testing. Personalized medicine using AI improves treatment outcomes and adherence. This study explores AI in PK/PD studies, process optimization, testing, drug delivery, and the advantages and challenges of AI-based pharmaceutical technologies. The pharmaceutical industry funds AI-driven medicine research and patient care.

Keywords: Artificial intelligence (AI); Machine learning; drug discovery; formulation; Dosage form testing; Pharmacokinetics; Pharmacodynamics; Physiologically based pharmacokinetic (PBPK); Quantitative structure-activity relationship (QSAR)

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1. Introduction

The pharmaceutical industry is enhancing performance to meet customer needs and address global healthcare emergencies. Innovations include advanced production, packaging, and customer-focused marketing. Optimal medicinal components are crucial for overcoming toxicity issues.[1-5] Pharma is addressing skill gaps to train healthcare staff, anticipating supply chain changes and new models to boost resilience amid supply chain disruptions and COVID-19-affected clinical studies.[6,7]

Supply chains are impacted by pandemics, natural disasters, price fluctuations, cyber attacks, logistics, and product defects, with COVID-19 transportation concerns, supplier delays, and inefficient vaccine cold chains causing disruptions.[8,9]

AI could improve pharmaceutical supply chain management (**Figure 1**) after decades of research. The article advises more research to improve supply chain management decision-making tools.[10,11]

Pharmaceutical businesses are utilizing AI and VR to restart clinical trials, despite the pandemic's decline. These technologies address high maintenance expenses, skilled labor, data breaches, cyber security concerns, and patient recruitment, enrolment, monitoring, retention, and adherence. AI aids patient-centric research by collecting data and decreasing labour.[12-19]

*Corresponding author: Ankur Joshi
Email: ankurpharmacology@gmail.com

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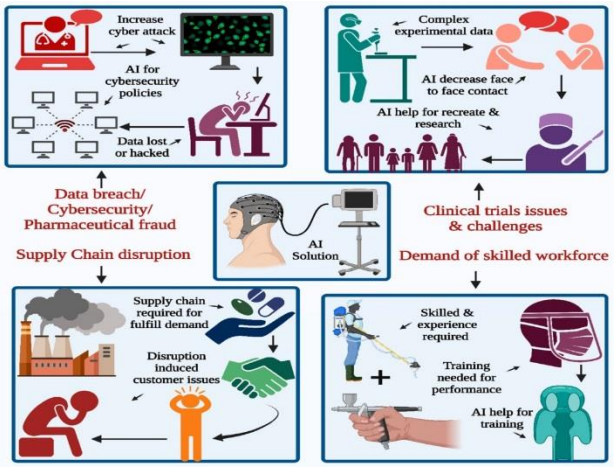

Figure 1: AI-based pharmaceutical business faces challenges like clinical trial difficulties, supply chain disruptions, cyberattacks, data leakage, and security concerns. New technology is needed to combat political fraud and prevent healthcare fraud.

2. Current Pharmaceutical Challenges and the Role of AI

Pharmaceutical companies study small molecules to develop useful products, but generic drugs impede their introduction due to sophisticated data and clinical trials. The bimolecular pharmaceutical business is growing rapidly due to slow discovery. Bio molecules, mostly amino acids and nucleic acid nucleotides, depend on structure and reactivity. AI has potential in pharmaceutical distribution and research, but experts must interpret complex data and address algorithmic bias. Machine, deep, and natural language processing methods, including supervised and unsupervised learning, have been tested to improve pharmaceutical product development. [18,19] **Table 1** and **Figure 2** demonstrate some of the most studied AI models in this subject.

2.1. Supervised AI learning

Supervised learning trains algorithms using labelled data for prediction tasks in image recognition, NLP, and predictive modelling. Its medicinal uses include drug discovery, maintenance, quality control, disease diagnosis, and clinical trial prediction.[20]

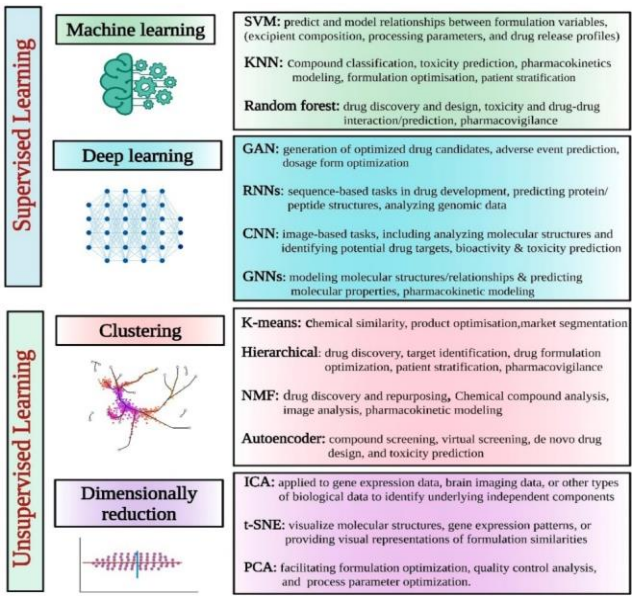

Figure 2: Various artificial intelligence (AI) learning models and tools for pharmaceutical applications, both supervised and unsupervised

2.2. Unsupervised AI learning

Unsupervised learning detects patterns in unlabelled data, aiding in clustering, association rule discovery, and dimensionality reduction, used in pharmaceuticals for data visualization and exploratory analysis.[21]

Table 1: List of the ten most often utilized AI models in the pharmaceutical sector.

AI/Machine Learning Models	**Description/Usage**
Generative Adversarial Networks (GANs)	GANs enhance pharmaceutical products by creating unique chemical structures and evaluating them through a discriminator network, resulting in diverse and functionally effective drug candidates.
Recurrent Neural Networks(RNNs)	GANs enhance pharmaceutical products by creating unique chemical structures and evaluating them through a discriminator network, resulting in diverse and functionally effective drug candidates.
Convolutional Neural Networks (CNNs)	CNNs are used for therapeutic target identification and molecular structure analysis, extracting key features from molecular images to aid drug development.
Long Short-Term Memory Networks (LSTMs)	LSTM RNNs are used in pharmacokinetics and pharmacodynamics to model and predict medication efficacy and concentration-time patterns.
Transformer Models	Transformer models like BERT aid pharmaceutical natural language processing by analyzing scholarly publications, patents, and clinical trial data to inform drug development decisions.
Reinforcement Learning(RL)	RL methods optimize drug dosage and personalized treatment plans by learning from interactions and adjusting doses to improve patient outcomes.

Bayesian Models	Gaussian processes and Bayesian networks are used in medication development to assess uncertainty, optimize experimental designs, estimate risk, and make probabilistic predictions.
DeepQ-Networks(DQNs)	Deep Q-Networks (DQNs) using deep learning and reinforcement learning techniques predict chemical activity and suggest potential candidates for further testing, enhancing medication development.
Auto encoders	Auto encoders, as unsupervised learning models, are ideal for drug discovery, dimensionality reduction, and feature extraction. They capture key molecular features, making them valuable for virtual screening and compound analysis.
Graph Neural Networks(GNNs)	GNNs are well-suited for molecular structure drug discovery, as they assess graph-structured data. They excel in molecular graph modeling, property prediction, virtual screening, and de novo drug synthesis.

3. AI for Drug Discovery

Artificial intelligence has transformed drug discovery and research through its significant contributions, including:

3.1. Target identification

AI analyses genomic, proteomic, and clinical data to identify therapeutic targets. Machine learning reveals molecular pathways and disease-linked targets for drug development.

3.2. Virtual screening

AI quickly screens chemical libraries to identify drugs with high target affinity, simulates interactions, estimates binding, and helps prioritize compounds for testing.

3.3. Structure-activity relationship (SAR) modelling

AI models link a compound's biological activity to its structure, helping scientists design compounds with improved pharmacokinetics, selectivity, and potency.

3.4. De novo drug design

Machine learning enables AI to suggest drug-like compounds, expand chemical space, and generate novel candidates using chemical libraries and data.

3.5. Optimization of drug candidates

AI systems evaluate and enhance medication candidates by considering pharmacokinetics, safety, and efficacy, helping researchers improve compound effectiveness and safety.

3.6. Drug repurposing

AI analyzes biomedical data to identify existing drugs with potential for new treatments, speeding up drug discovery by repurposing approved medications.

3.7. Toxicity prediction

Chemical structures and negative outcomes are used by AI systems to forecast pharmaceutical toxicity. This emphasizes low-toxicity chemicals and decreases clinical trial side effects. AI-driven pharmaceutical R&D accelerates the identification, optimization, and creation of new treatment candidates, improving efficacy and efficiency.[22] The pharmaceutical business predicts biological targets from chemical structures using in-silico target fishing (TF) and chemical databases and biological annotations. TF, machine learning, and chem.-informatics study complicated structures to help design drugs for difficult diseases at lower cost. Using 3D features to predict ligand-target binding speeds up phytopharmacology, similarity evaluations, and toxicological prediction. TF helps uncover novel targets, predict drug profiles, and analyze adverse effects for receptor-targeted medicines including methadone, loperamide, and emetine.[23] AI models and technologies have improved drug discovery. **Table 2** shows common pharmaceutical AI tools. New models and strategies to speed drug discovery are continuously evolving, and these are just a handful.

Table 2: Popular AI model tools used for drug discovery

AI Model Tools	Summary
DeepChem	This open-source package offers various tools and models for drug discovery, including molecular property prediction, virtual screening, and generative chemistry.
RDKit	This popular open-source chem.-informatics package offers uses like molecular manipulation, substructure searches, and descriptor calculation. Its integration with machine learning frameworks enhances drug discovery applications.
ChemBERTa	A popular open-source chem.-informatics library with features for molecular manipulation, structure searching, and descriptor calculation. It can be integrated with ML frameworks for drug discovery.
GraphCony	An architecture for deep learning models that processes molecular graphs, effectively using structural information to predict molecular attributes such as bioactivity and toxicity.

AutoDockVina	A popular docking program that uses machine learning algorithms to estimate the binding affinity of small compounds to protein targets, aiding virtual screening and lead optimization in drug discovery.
SMILES Transformer	A deep learning model that generates molecular structures from SMILES strings, useful for both lead optimization and de novo drug design.
Schrödinger Suite	A comprehensive suite of AI-powered drug discovery tools, including predictive modeling, ligand-based and structure-based drug design, virtual screening, and molecular modeling.
BMRXNfor Chemistry	A computer program that predicts chemical reactions using deep learning algorithms and large reaction databases, helping to identify new synthesis methods and potential reaction outcomes.
scape-DB	Scape-DB, or "Extraction of Chemical and Physical Properties from the Literature-DrugBank," is a database that uses NLP and ML to mine scientific articles for biological and chemical information, providing valuable data for drug development research.
GENTRL (Generative Tensorial Reinforcement Learning)	A neural network model that combines generative chemistry and reinforcement learning to create new compounds with specific attributes, used in drug optimization and de novo design.

4. AI Tool Application in Dosage Form Designs

Pharmacological effects are explained by biological membranes simplifying bodily compartments. Drug distribution pathway determines physicochemical obstacles. Monitoring route-specific penetration aids medicine delivery. Following ingestion, drugs enter the bloodstream through the stomach or intestines. Distribution sends drugs to tissues and cells.[24] Drugs can enter cells intracellularly. Active or passive biological barriers absorb most medicines. Drugs facilitate passive diffusion. Actual drug distribution may differ from in-silico models and computer analysis. Drug destiny in the body depends on biological interactions and is available in biological contexts. Drug molecular properties govern this. For many small molecules and physiologically active compounds, passive diffusion is insufficient for medicine administration. Complex biological processes include active permeation and membrane transfer. Computational techniques, models, and attributes help explain this process. New computer models study drug delivery system pharmacokinetics. Pharmaceutical R&D struggles with preclinical model predictability, especially in complex in-silico models. Choosing parameters is critical. The simulated environment can better investigate membrane drug interactions for AI exploration and appraisal (**Figure 3**).[25] Multilayer data analysis is enhanced by AI for research units. AI can automate model and parameter evaluation stages like simulation, scoring, and refining to improve forecasts and data refinement. Drug-biological interactions are important for AI training, says the system biology database. Pharmacokinetic research uses cutting-edge AI like artificial neural networks. AI analyzes complicated molecular capabilities using chemical, genetic, and phenotypic databases. A study of how pharmaceutical delivery systems affect pharmacokinetics can reveal drug disposition and toxicity. Innovative drug delivery methods are developed, described, and tested before trials.AI evaluates pharmaceutical delivery systems using multiple data sources. AI finds the optimal medications for individual illnesses or patient needs by analyzing molecular, patient, and pharmacokinetic data. Compare chemical entities to known molecules to choose pharmaceutical delivery strategies with passive AI. AI aids drug discovery and repurposing for novel diseases. AI impacts patient needs, sickness characteristics, formulation, pharmacokinetics, and drug development. Without rich datasets for unbiased model validation, AI-driven delivery system development is limited. AI applies current knowledge to new issues. **Figure 4** shows how AI systems leverage massive data volumes to rationalize product design, with self-supervised experiments and dependable parameter recording codifying knowledge.[26]

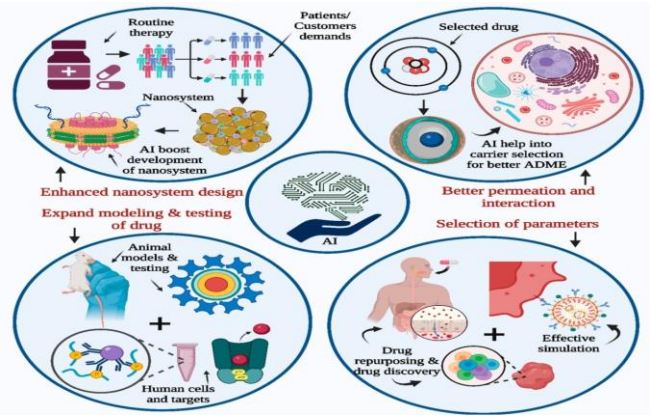

Figure 3: AI's contribution to Drug development and research. In drug design, drug discovery, and drug repurposing, AI can improve nano system design, enhance drug testing models, and increase the accuracy of parameter and factor selection. By analysing drug permeability, modeling, and human cell targets, AI provides a clearer understanding of how the simulated human environment interacts with the membrane.

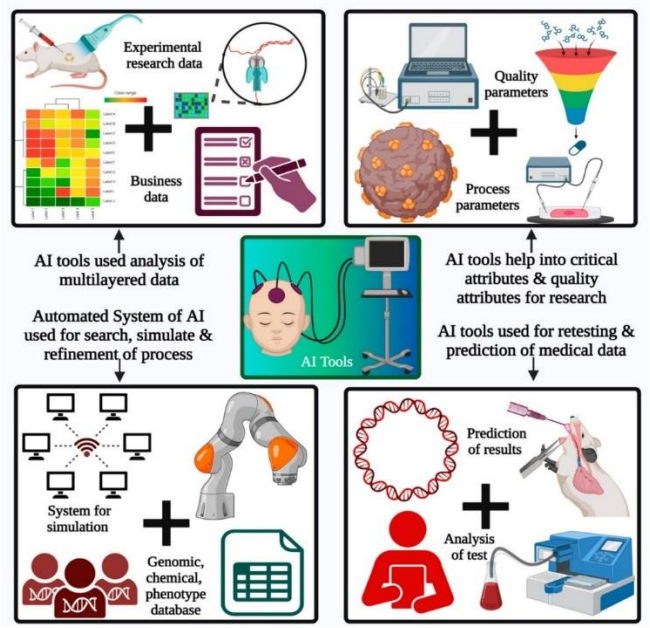

Figure 4: Artificial intelligence applications in the pharmaceutical industry. AI techniques assist in analyzing complex data layers, making automated AI systems invaluable for research and product development, including efficient searches, simulations, and process modifications. AI bots, along with chemical, genomic, phenotypic, and systems biology databases, enhance drug release and activity predictions and provide recommendations for effective drug delivery systems.

5. AI for Drug Delivery

Big data and AI are revolutionizing computational pharmaceutics by enhancing drug distribution through multiscale modelling, reducing costs, and improving efficiency. This method predicts drug activity, stability, release, and physicochemical qualities, enabling preventive drug performance improvements.[27]

5.1. AI for oral solid dosage form development

Artificial intelligence is revolutionizing pharmaceutical companies by enhancing production efficiency, supply chain accuracy, and understanding process characteristics. Machine learning has been used to predict solid dispersion stability and maintain drug release over time. Artificial neural networks (ANNs), fuzzy logic, and evolutionary algorithms are used to analyze attributes for optimal tablet formulations, requiring regulators to adjust cGMP policies.[28]

Table 3: List of commonly explored AI models in pharmaceutical product development.

AI/Machine Learning Models	Description/Usage
Genetic Algorithms	Genetic algorithms are optimization techniques inspired by genetics and evolution principles. They optimize formulation composition, drug release profiles, and process parameters to achieve desired dosage form characteristics.
Artificial Neural Networks (ANNs)	Artificial neural networks (ANNs) have been used to model and optimize drug release kinetics from various dosage forms. They improve predictions of optimal formulations and API release behavior under different conditions.
Support Vector Machines (SVMs)	Support vector machines (SVMs) are used to model and predict correlations between formulation factors such as drug release patterns, processing parameters, excipient composition, and variables. They aid in optimizing the formulation design space.
Particle Swarm Optimization (PSO)	Particle Swarm Optimization (PSO), a population-based algorithm, is used to optimize dosage forms. It has been applied to refine formulation characteristics like particle size distribution and dissolution profiles.
Artificial Intelligence-based Expert Systems	Expert systems mimic human decision-making using AI techniques like fuzzy logic and rule-based systems. They optimize dosage forms by considering various formulation and process characteristics.
Monte Carlo Simulation	Monte Carlo simulation techniques optimize medicinal product performance by accounting for uncertainties and variability in formulation and process parameters. They support robust formulation and process design.
Computational Fluid Dynamics (CFD)	Computational fluid dynamics (CFD) simulations optimize fluid flow and mixing in dosage form manufacturing processes, such as coating, drying, and granulation. They help design more efficient and consistent processes.
Response Surface Methodology (RSM)	Response Surface Methodology (RSM) is a statistical approach that models and analyzes the relationship between variables and their impact on formulation responses, aiding in the optimization of dosage form formulations. It provides insights into and optimizes formulation parameters.

Artificial Neural Network–Genetic Algorithm (ANN-GA) Hybrid Models	Hybrid models combining ANN and GA methods are used to optimize dosage forms. These models efficiently search the formulation space, making it easier to find optimal solutions and predict formulation properties.
Multivariate analysis Techniques	Multivariate analysis techniques like partial least squares (PLS) and principal component analysis (PCA) are used to optimize dosage forms. They help optimize formulation performance, reduce dimensionality, and identify key formulation factors.

Common dose forms like tablets dominate medicine delivery. APIs and excipients are moulded or compressed to the desired shape and size. Patient-selected excipients control disintegration, dissolution, and medication release. Glidants and lubricants ease manufacturing. AI can anticipate drug absorption and assess tablet manufacture to improve quality control. It also detects tablet faults.[29]

5.1.1. Prediction of dug release through formulations

Drug release prediction is crucial for quality control and product development. Spectrophotometry is used for extensive studies, while AI can reduce batch optimization and production costs. Artificial neural networks predict dissolution profiles and particle size distribution, while key material characteristics and PAT are used to collect data for drug release modelling.[30]

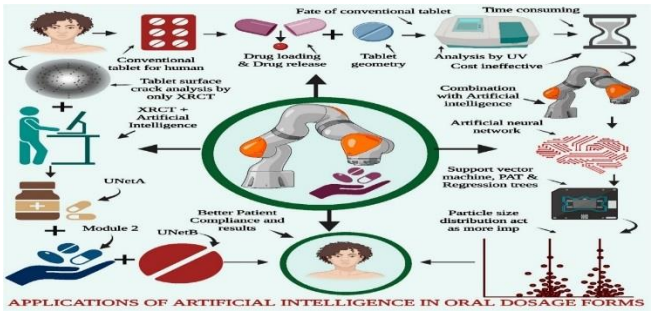

Figure 5: Oral dosage form AI. Traditional tablet analysis methods are time-consuming and costly. AI can integrate these methods with ANN, SVM, PAT, and regression trees to analyze tablet cracks, finding potential healthcare applications.

5.1.2. Application of AI for 3D-printed dosage forms

Artificial intelligence in 3D-printed dosage forms is revolutionizing drug administration and personalized therapy. It can customize doses based on patient data, optimize dosage strengths, and address production challenges. AI-driven feedback systems enhance 3D printing accuracy, repeatability, and scalability, improving patient outcomes and enabling more tailored treatments.[31]

3D-printed tablets, produced using methods like pressure micro syringe, laser sintering, and fused-filament manufacturing, are studied using an artificial neural network model. The study found that infill density and surface area-to-volume ratio are critical factors for proper drug release, enhancing solubility.[32]

5.1.3. Application of AI for the detection of tablet defects

AI-based tablet fault detection has revolutionized pharmaceutical quality control by identifying issues like cracks, chips, and discoloration in images. This technology, combined with X-ray computed tomography and deep learning, saves time, reduces costs, and enhances defect detection accuracy. Real-time monitoring allows AI systems to quickly detect faults and correct them, ensuring defective tablets don't reach store shelves. This AI-driven approach improves product quality, productivity, safety, and efficacy, contributing to more consistent manufacturing processes and improved product standards.

5.1.4. AI for the prediction of physicochemical stability

AI can predict the physicochemical stability of oral dosage forms, a crucial area in pharmaceutical research. By analyzing vast datasets, AI can assess factors like drug breakdown, excipient interactions, and environmental impact. This allows researchers to optimize formulations, detect stability issues early, and make informed decisions, improving drug development efficiency and cost-effectiveness.[33] LightGBM, a free, open-source distributed gradient boosting system, leverages machine learning for tasks like ranking and classification. It was trained using data from around fifty pharmacological compounds, with 646 public physical stability data points. The database construction included molecular models and characteristics such as molecular weight, hydrogen bond acceptors, melting point, and heavy atom count. The model was evaluated using a three-month accelerated stability study, and it achieved 82% accuracy in predicting physical stability. This performance demonstrates the potential of machine learning models like LightGBM in pharmaceutical stability prediction, aiding in the optimization of drug formulations.[34]

5.1.5. Contribution of AI to dissolution rate predictions

Artificial intelligence (AI) has significantly improved the prediction of dissolution rates, aiding in the optimization of pharmaceutical formulations and dosage forms. By analyzing large sets of experimental data, AI models can identify key physicochemical properties and molecular characteristics influencing the dissolution process. This advancement empowers researchers to accelerate drug development, refine formulation methods, and improve patient outcomes. Studies have explored the dissolution profiles of conventional

pharmaceuticals, highlighting the importance of recrystallization and precipitation.

The AI techniques employed in this study include Support Vector Machine (SVM), LightGBM, and Extreme Gradient Boosting (XGBoost).[35] XGBoost is a scalable machine learning framework featuring a distributed gradient-boosted decision tree, which helps predict issues related to unstructured data, such as images and text. In this study, the artificial neural network outperformed all other existing algorithms and frameworks. The same team also used molecular computational software to analyze the descriptors of both the active pharmaceutical ingredients (APIs) and the polymers. The selected input variables for the study included temperature, drug loading, and volume, while dissolution was identified as the binary outcome, encompassing precipitation or super saturation. The dissolution rate was considered the research outcome, leading to improved accuracy in predicting the dissolution profiles of the chosen APIs and polymers.[36]

5.2. AI for nanomedicine

AI can accelerate nanoscale interventions, diagnostics, drug delivery, and personalized medicine by improving precision and efficiency. It enhances nanoparticle development for precision medication delivery, imaging, and sensing. AI algorithms predict physicochemical properties, stability, and efficacy, aiding in creating nanoparticles with desired characteristics. In cancer treatment, AI aids in selecting the right drug, dosage, and stimuli-responsive materials, leading to more accurate and personalized treatments.[37,38] AI programs predict nanoparticle behavior, drug release kinetics, and toxicity for safe nanomedicine formulations. AI-powered nanosensors monitor biomarkers, drug concentrations, and disease progression, providing real-time feedback for personalized treatment.[39,40]

AI-driven databases automate nanocarrier scaling and optimize drug delivery systems, enhancing cell-type-specific nanocarriers for tumor treatment. Machine learning predicts nanocrystal production, and simulations quantify key experiments. AI aids in identifying heterogeneous vascular permeability in nanoparticle-based drug delivery systems, potentially leading to the design of protein nanoparticle systems for cancer treatment.[41]

5.3. AI Application for parenteral, transdermal and mucosal route products

AI can improve injectables, biologics, and formulations by predicting physicochemical features, analyzing components, and enhancing solubility, stability, and viscosity. It can detect patterns, detect quality issues early, and aid in real-time monitoring and machinery maintenance.[42]

AI was utilized to monitor particle behavior, analyze suspended particles, isolate particles, and analyze images. Deep learning was used for image processing, while Surface Qualifies 7500 analyzed millions of data points per second.[43] Machine learning (ML) in pharmaceutical research can improve product performance, reduce production risks, and ensure safe, effective pharmaceuticals. Despite limitations, tree-based models like LGBM reduce LAI formulation time and cost, demonstrating its value.[44] Traditional trial-and-error methods for drug delivery systems are inefficient due to lack of understanding. Advances in computational pharmaceutics, machine learning, and multiscale simulations enhance product development efficiency, improving formulation design in Pharma 4.0.[45]

5.4. AI Tools for biologics product development

AI helps develop new proteins, peptides, nucleic acid biologics, and immunotherapeutics.[46] AI algorithms may help build specific proteins and peptides By analyzing protein structure and function datasets, AI models can create therapeutic sequences with improved stability, binding affinity, or immunogenicity. This helps produce personalized biologics with improved efficacy and safety.[47]

AI algorithms can find treatment targets using genetic, proteomic, and clinical data. By identifying illness targets, AI helps researchers design protein and peptide biologics that change biological pathways or target pathogenic proteins. Protein folding can be predicted by AI models using amino acid sequences. Understanding protein function and designing optimum biologics requires protein folding. Deep learning and molecular dynamics simulations predict protein folding patterns, helping create stable and functional biologics (**Figure 6**).[48]

AI algorithms predict protein/peptide-target molecule binding affinity. Training AI models with large protein–protein or protein–peptide datasets can properly predict binding strength. Selecting or creating biologics with high target affinity and specificity improves therapeutic efficacy. Artificial intelligence may improve protein and peptide biologic compositions. Formulation, stability, and aggregation tendency affect biological quality and efficacy. By examining protein physicochemical qualities, formulation components, and manufacturing processes, AI algorithms can improve formulation conditions, biological stability, and shelf life.[49]

AI algorithms predict protein and peptide biological toxicity. AI systems trained on toxicological datasets can predict biological side effects and immunogenicity using structure–activity correlations. This lets researchers find and alter harmful sequences or structures. Artificial intelligence improves protein and peptide biologics clinical studies. AI algorithms can predict patient reactions and improve trial methods using patient data, disease features, and therapy outcomes. Patient enrollment, research design, and personalized treatment are optimized.[50] AI can improve exosome, CAR T-cell, and CRISPR/Cas9 research, diagnostics, and therapeutics.

AI's data analysis, pattern recognition, and predictive modelling help speed up protein/peptide and gene therapy biologic development and improve therapeutic molecule design and optimization. AI has the ability to change the area by creating novel biologics with improved characteristics and increasing biologic development success.[51]

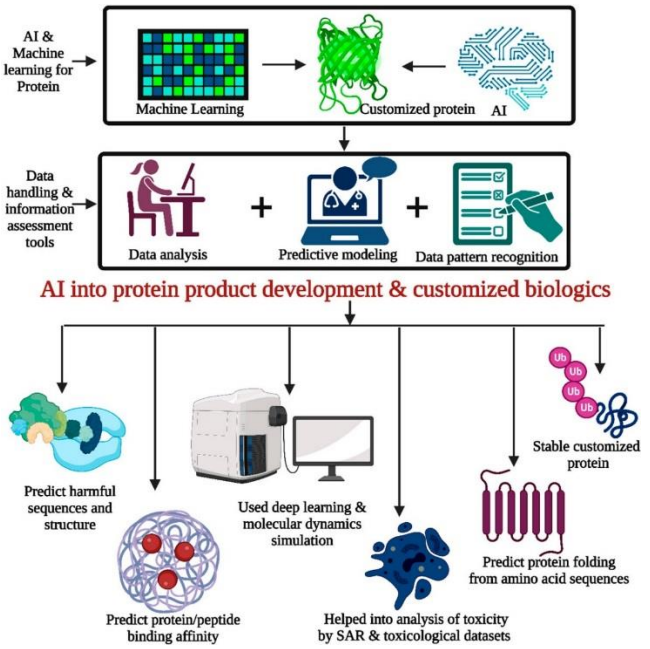

Figure 6: AI aids in protein development and customized biologics through data analysis, predictive modeling, and pattern recognition. It helps identify disease targets, understand altered biological pathways, and predict protein folding and binding affinity. AI uses deep learning and molecular dynamics simulations to enhance protein folding understanding and utilizes SAR and toxicological datasets to predict binding strength and toxicity.

5.5. AI in medical devices

Medical devices, either standalone or integrated with software or associated systems in vitro, address patient medical needs. AI has significantly transformed medical technologies and healthcare, with the pandemic accelerating the adoption of personalized treatment and remote health monitoring. The following are key AI applications in medical devices:

5.5.1. Diagnostic assistance

AI algorithms aid healthcare professionals in diagnosing conditions by analyzing medical imaging data, identifying malignant tumors and irregularities in ECGs.

5.5.2. Remote monitoring

AI-powered medical devices enable remote health monitoring, especially for chronic conditions, providing personalized care at home. AI algorithms analyze data, providing alerts and insights to healthcare providers.[52]

5.5.3. Wearable devices

AI is integrated into wearable technologies like smartwatches, fitness trackers, and biosensors, monitoring health metrics and providing actionable insights to improve users' well-being.[53]

5.5.4. Prosthetics and rehabilitation

AI improves prosthetic devices' functionality and natural movement, utilizing machine learning algorithms to align with user intentions and aid in rehabilitation through motion analysis and patient feedback.[54]

5.5.5. Surgical assistance

AI is being integrated into surgical instruments, supporting surgeons during operations, and improving surgical accuracy and outcomes through real-time guidance based on preoperative and intraoperative data analysis.[55]

5.5.6. Medication management

AI-powered devices assist patients in managing their medications, ensuring timely pill intake, correct dose distribution, and monitoring adherence, while analyzing patient data for personalized recommendations.[56]

AI improves medical diagnosis, monitoring, therapy, and patient care by analyzing large datasets, identifying trends, and offering personalized insights. It drives innovative products, engages new client groups, and boosts healthcare industry commercial potential.

Medtronic has developed AI-powered applications like the Guardian Connect system and Sugar IQ app to help diabetics manage their condition. The Guardian Connect system offers real-time insights, while Sugar IQ, a Watson-created app, provides personalized insights, glycemic assistance, and food logging.[57]

6. AI for Pharmacokinetics and Pharmacodynamics

Drug development involves discovery, preclinical studies, clinical trials, and regulatory approval, relying on pharmacokinetics and pharmacodynamics to determine optimal dosage, administration route, and safety profile.[58]

Traditional animal studies and clinical trials in pharmacokinetics and pharmacodynamics research face ethical issues, sample size limitations, and variability, while computational models and AI improve predictions faster and more cost-effectively.[59,60]

AI, powered by advanced computing and machine learning, is promising in pharmacokinetics, pharmacodynamics, and drug development, improving prediction accuracy, efficiency, and cost-effectiveness despite data challenges.[61]

6.1. AI-Based Methods to Predict Pharmacokinetic Parameters

ML and DL predict pharmacokinetic parameters like ADME using Bayesian, random forests, SVMs, ANNs, decision trees, deep learning, and QSAR, aiding in ADME property predictions.[62]

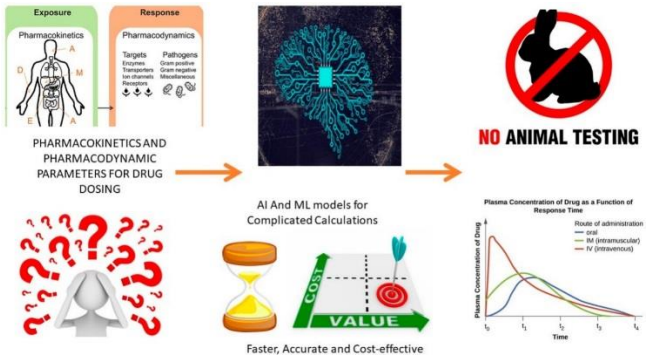

Figure 7: AI in pharmacokinetics and pharmacodynamics studies aids in drug absorption, distribution, metabolism, and excretion analysis. AI accelerates complex calculations, ensuring dataset integrity for precise, rapid, and cost-effective results. It converts data into graphs, helping identify core issues. AI also reduces animal testing by evaluating multiple factors like enzymes, dosage, and patient data across species.

6.2. AI-based computational method for PBPK

AI enhances PBPK models by identifying key features and optimizing parameters, reducing the need for animal and human clinical trials in drug distribution and clearance simulations.[63] **Table 4**

Pharmacokinetics is crucial for drug safety and efficacy, involving in vivo and in vitro studies. Preclinical data, PBPK modeling, and AI/ML aid in drug discovery, optimization, and prediction.[64] **Table 4**

6.3. Prediction of drug release and absorption parameters

AI algorithms predict drug release and absorption by analyzing physicochemical properties, formulation, and delivery system mechanisms, estimating kinetics from oral tablets, transdermal patches, and inhalers.[65]

AI models predict bioavailability and absorption by assessing drug solubility, permeability, lipophilicity, and molecular weight. These algorithms enhance medication formulations and drug delivery systems by analyzing parameters and applying machine learning techniques.[66]

6.4. Prediction of metabolism and excretion parameters

AI models predict drug metabolism and excretion by analyzing molecular structure and physicochemical properties. They identify structural features linked to metabolic changes and predict metabolites and metabolism enzymes.[67]

AI models predict drug metabolic pathways by analyzing enzyme kinetics, expression, genetic polymorphisms, and drug interactions, optimizing dosage and predicting interactions.[68]

AI models predict drug clearance using molecular weight, lipophilicity, ionization, and clearance route data, aiding in dosing regimens and ensuring safety.[69]

AI models predict drug-transporter interactions and drug–drug interactions by analyzing physicochemical properties, aiding in understanding drug dispersion and improving formulations.[70]

AI models assess drug metabolism and excretion to predict drug disposition, optimize dosing, identify interactions, and design safer treatments, improving drug development efficiency.

Table 4: Algorithms used for the development of AI models for various PKPD studies along withtheir advantages and limitations

Algorithm/Software	Aim/Target	Advantage	Limitation	PK/ PD/ Both
Bayesian/WinBUGS	To handle data below the limit of quantification	Prior information from the literature can be directly used for model-fitting Easy implementation	Long computational time Negative data in certain PK/PD model swhich are not possible	Both
Bayesian/PKBUGS (v 1.1)/WinBUGS (v 1.3)	Pharmacokinetic analysis of sirolimus concentration data for therapeutic drug monitoring	Easy incorporation of prior information with current data Identification of possible covariate relationship	A limited number of datasets and poorly informative data	PK
Support Vector Machine/Least Square-SVM	Drug concentration analysis of sample drug based on individual patient profile	Personalized model for every new patient SVM-based approaches are more accurate than the PK modelling method for	Out liersin samples greatly affect the model, limiting its accuracy	PK

		predicting drug concentration		
Support Vector Machine/Drug Administration Decision Support System (DADSS) and Random Sample Consensus RANSAC	Prediction of drug concentration, ideal dose, and dose intervals for a new patient	More flexible and structurally adjustable	The noise of datasets impacts the overall predictability of the algorithm	PK
Support Vector Machine/Profile Dependent SVM	Therapeutic drug monitoring of kidney transplant recipient	Critical dosing and cost-effective Effective for nonlinear models	Time-consuming Large datasets	PK
Support Vector System + Random Forrest Model	Pharmacodynamic drug interaction based on Side-Effect Similarity (SES), Chemical Similarity (CS), and Target Protein Connectedness (TPC)	PDI was predicted with an accuracy of 89.93% and an AUC value of 79.96%	Requires larger data processing and filtration	PD
Linear Regressions (LASSO)/Gradient Boosting Machines/ XGBoost/Random Forest	Prediction of the Plasma concentration–time series and area under the concentration versus-time curve from 0 to 24 h after repeated dosing of Rifampicin	Time-efficient analysis Improves method for covariate selections	Risk of results being not clinically relevant	PK
XGBoost	Estimation of drug area under the curve (AUC) of tacrolimus or mycophenolate mofetil (MMF)	Pharmacokinetic (PK) datasets from renal, liver, and heart transplant patients were Predicted accurately	Not possible to calculate the probability of target attainment and accurate dosing	PK
Simulated Annealing k-Nearest-Neighbor (SA-kNN)/Partial Least-Square (PLS)/ Multiple Linear Regression (MLR)/ Sybyl version 6.7	Prediction of Pharmacokinetic parameters of antimicrobial agents in humans based on their molecular structure	Cost-effective Requires less sample size	Requires multiple model generation methods Interpretation of individual descriptors is almost impossible	Both
Drug Target Interaction Convolutional Neural Network (DTICNN)	Identification of the drug-target interactions and predict potential drug molecules	Cost-effective Time-saving	Large datasets are required	PD
Deep Long Short-Term Memory (DeepLSTM)	Computational methods to validate the interaction between drugs and target	Based on Position Specific Scoring Matrix (PSSM) and Legendre Moment (LM) (drug molecular substructure fingerprints)	Large datasets are required	PD

7. Limitations of AI Tools

AI-based models offer many benefits but require large datasets, can be biased, and are often hard to interpret. Therefore, they should complement traditional experimental methods to ensure drug safety and efficacy. Key constraints include:

7.1. Lack of transparency

AI models, often called "black boxes," are difficult to understand, making it hard to validate their accuracy and trustworthiness. This lack of transparency can hinder approval and reduce trust, especially when predictions conflict with expectations.[70]

7.2. Limited availability of data

AI models require extensive data for accuracy. Insufficient or biased data, especially for rare diseases or unrepresentative populations, can lead to inaccurate results. Limited access to data like real-world evidence makes it crucial to assess data quality and representativeness.

7.3. Biases in data

AI model performance depends on data quality. Biased or incomplete data can lead to inaccurate predictions, especially if certain populations are underrepresented. Reliable, complete, and unbiased training data is essential for accurate healthcare decisions.[71]

7.4. Inability to incorporate new data

AI model performance depends on data quality. Biased or incomplete data can lead to inaccurate predictions, especially if certain populations are underrepresented. Reliable, complete, and unbiased training data is essential for accurate healthcare decisions.

7.5. Limited ability to account for variability

AI models in medication development face challenges in updating with new data, leading to inaccurate predictions and poor decisions. Continuous improvement strategies, such as creating updatable models or integrating them into a framework, are crucial.

7.6. Interpretation of results

AI models can be complex and challenging to interpret, making them ineffective in clinical practice or pharmaceutical research. To ensure clear and practical predictions, they must be more interpretable and explainable.[72]

7.7. Ethical considerations

The FDA's discussion paper on AI in drug development addresses ethical issues, including patient privacy and data ownership. It emphasizes the need for regulatory agencies to establish protocols, standards, and assessment procedures, considering animal welfare and patient safety. The paper also highlights the importance of validating AI models for reliability and accuracy.[73]

7.8. Complex biological systems

AI models struggle to replicate complex biological systems due to their numerous feedback loops and molecular interactions, genetic, environmental, and individual variations, and the difficulty in predicting emergent properties and integrating AI models.

7.9. Lack of clinical expertise

AI can identify similarities, but treatments may vary for individual patients. Statistical AI algorithms may struggle with complex variables and their impact, limiting their ability to handle treatment decisions. AI's ability to fully understand the fundamental aspects and repercussions of specific parameters may be limited.

7.10. Inactive molecules

AI predicts binding interactions between small molecules and target proteins, but may identify inactive molecules. Docking methods can lead to false positives and negatives, and experimental validation is crucial for drug efficacy.[74]

AI technologies have potential in pharmaceutical research, but challenges like data misreporting need to be addressed. Implementing FAIR data and aligning with ALCOA concepts can improve data quality and reliability. Despite AI's potential, human expertise is still essential. AI should be used cautiously in pharmaceutical research, acknowledging its limitations and confirming results with scientific methods.

8. Current Trend: Fairy Tale to the Holy Grail

Current trends show AI's broad impact on pharmaceuticals, including drug discovery, precision medicine, formulation optimization, clinical trials, safety monitoring, and supply chain management. Here are some key trends:

8.1. Drug discovery and development

AI is revolutionizing drug discovery through virtual screening, molecular modelling, and predictive analytics. AI algorithms analyze large chemical and biological datasets to identify potential therapeutic candidates, optimize lead compounds, and predict their properties, speeding up the development of new treatments.

8.2. Precision medicine

AI enhances precision medicine by analyzing patient data, including genomes, proteomics, and clinical records, to identify subgroups, predict therapy responses, and support personalized treatment. It also helps advance biomarkers for disease diagnosis and prognosis.

8.3. Drug repurposing

AI is used in drug repurposing by analyzing datasets to identify new drug-disease connections, enabling existing medications to be applied to new therapeutic uses. This offers a faster, cost-effective route to pharmaceutical development.

8.4. Drug formulation and delivery

AI enhances pharmaceutical formulations and delivery systems by predicting drug release kinetics and absorption patterns, improving efficacy and targeted delivery, and designing devices for patient compliance and convenience.

8.5. Clinical trial optimization

AI improves clinical studies by enhancing efficiency, reducing costs, and enabling real-time data monitoring, enabling faster decision-making and adaptive trial designs.

8.6. Regulatory compliance and safety

AI enhances pharmaceutical safety by analyzing real-world data, adverse event reports, and literature, identifying safety concerns, monitoring post-marketing drug safety, aiding in pharmacovigilance, signal detection, and predicting adverse events.

8.7. Supply chain optimization

AI improves pharmaceutical supply chains by optimizing manufacturing, inventory, and delivery. It forecasts demand, manages production schedules, and enhances quality control, leading to more efficient, cost-effective operations.

Pharmaceutical companies like GNS, AstraZeneca, Atom wise, Recursion, and Insilico Medicines are utilizing AI in pharmacokinetics and pharmacodynamics to improve dosage form development, predict drug interactions, and enhance patient outcomes. **Table 5**

Table 5: List of companies using AI and ML technologies in pharmaceutical research.

S.No.	Domain	Technology and Outcome	Industry and Collaborations
1	Drug design	Novel therapeutic antibodies	Exscientia
2	Molecular drug discovery	AtomNet–deep learning-driven computational platform for structure-based drug design	AtomWise
3	Gene mutation related disease	Machine learning based recursion operating system for biological and chemical datasets	Recursion
4	Drug design	Ligand-and structure-based de-novo drug design, especially in multi parametric optimization	Iktos
5	Drug discovery	Generative modeling AI technology	IktosandGalapagos
6	Drug development	Potential preclinical candidates	IktosandOnoPharma
7	Drug design	Rapid drug design by software “Makya”	IktosandSygnatureDiscovery
8	Drug discovery and Drug development	Pharma.AI, PandaMics, ALS.AI	Insilico Medicine
9	Drug target and Drug development	ChatPandaGPT	Insilico Medicine
10	Drug development	Protein motion in drug development lie RLY-4008 (Novel allosteric, pan mutant and isoform selective inhibitor of PI3Kα	Relay therapeutics
11	Drug discovery	AI and machine learning for selection of drug target	BenevolentAI
12	Drug target	Drug target selection for chronic kidney disease and idiopathic pulmonary fibrosis	BenevolentAI and AstraZeneca, GlaxoSmithKline, Pfizer
13	Clinical trials	AI in clinical trials	Pfizer and Vysioneer
14	Disease treatment	AI and supercomputing for oral COVID-19 treatment Paxloid	Pfizer
15	Drug discovery	NASH drugs and sequencing behemoth Illumina	AstraZeneca and Viking therapeutics
16	Drug development	Trials360.ai platform in clinical trials for site feasibility, site engagement and patient recruitment	Janssen
17	Drug research	Automate medical literature review by using natural language processing	Sanofi
18	Drug development	AI in drug development	BioMed X and Sanofi
19	Drug research and Drug development	AI empowerment and AI exploration platforms	Novartis and Microsoft
20	Drug discovery	AI drug discovery platform	Bayer

9. Futuristic Overview

AI can revolutionize drug R&D by accelerating virtual screening, precision medicine, and personalized dose formulations. It can also predict drug side effects and toxicity, improve safety evaluation, and enable remote patient care. AI-powered monitoring systems and wearable's can also optimize clinical trial design, patient selection, and recruitment.[75]

AI models are revolutionizing manufacturing, regulatory assistance, and clinical risk prediction. They monitor key factors in real-time, standardize production, and improve safety. In medicine, AI can address challenges in drug delivery, improve decision-making, and optimize dosage ratios. However, its application in pharmaceutical distribution remains limited, with methods like decision trees and ANN not fully evaluated in clinical settings.

AI integration with PBPK modelling is crucial for drug development and environmental risk assessments. Neural-ODE algorithms improve pharmacokinetic data learning. Collaboration among pharmaceutical companies, regulators, and healthcare professionals is needed for successful AI applications. Addressing data quality, legal frameworks, and ethical considerations could improve patient outcomes.[76,77,78]

10. Conclusions

AI is significantly transforming drug delivery by facilitating targeted and personalized medicine, enhancing drug efficacy, and improving patient outcomes. Its capabilities in analyzing data and optimizing pharmacokinetics and pharmacodynamics lead to more efficient drug development processes, reducing reliance on animal testing and clinical trials. By making computational pharmaceutics more efficient and cost-effective, AI is poised to advance the pharmaceutical industry into a new era, ultimately expediting drug development and improving manufacturing processes.

11. Abbreviation

AI-Artificial Intelligence, ANN-GA-Artificial Neural Network–Genetic Algorithm, ANNs-Artificial Neural Networks, BERT-Bidirectional Encoder Representations from Transformers, CFD-Computational Fluid Dynamics, CNNs-Convolutional Neural Networks, COVID-Coronavirus Disease, DQNs-Deep Q-Networks, GANs-Generative Adversarial Networks, GENTRL-Generative Tensorial Reinforcement Learning, GNNs-Graph Neural Networks, LAI-Long-Acting Injectable, LDA-Latent Dirichlet Allocation, LOF-Local Outlier Factor, LSTMs-Long Short-Term Memory Networks, ML-Machine Learning, Neural-ODE-Neural-ordinary differential equation, NLP-Natural Language Processing, PAT-Process Analytical Technology, PBPK-Physiologically Based Pharmacokinetic, PCA-Principal Component Analysis, PK/PD-Pharmacokinetic/ Pharmacodynamics, PSO-Particle Swarm Optimization, QSAR-Quantitative Structure-Activity Relationship, R&D-Research and Development, RL-Reinforcement Learning, RNNs-Recurrent Neural Networks, RSM-Response Surface Methodology, SAR-Structure-Activity Relationship, SVMs-Support Vector Machines, TF-Target Fishing, t-SNE-t-Distributed Stochastic Neighbour Embedding, XGBoost-Extreme Gradient Boosting.

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None.

13. Conflict of Interest

None.

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