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## Review Paper

# Artificial Intelligence in Pharmaceutical Innovation and Research: A Review

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## ABSTRACT

Artificial intelligence (AI) is revolutionizing pharmaceutical research by accelerating and refining drug discovery, development, and clinical practice. This review summarizes the role of AI across key stages of the pharmaceutical pipeline, including target identification and validation, virtual and high-throughput screening, de-novo drug design, structure- and ligand-based approaches, and drug repurposing. In preclinical research, AI enables predictive modeling of pharmacokinetic and pharmacodynamic parameters, toxicity and ADMET profiles, drug–target and drug–drug interactions, and biomarker-driven disease-pathway analysis. In formulation and manufacturing, AI supports rational formulation design, excipient and process-parameter optimization, predictive dissolution models, continuous manufacturing, and real-time release testing within quality-by-design frameworks. AI is also transforming clinical trials and pharmacovigilance through enhanced patient recruitment and stratification, trial-design optimization, real-time safety monitoring, adverse-reaction prediction, and decision-support systems for pharmacists. Nonetheless, several challenges persist, including data quality and bias, regulatory and ethical concerns, lack of standardized validation frameworks, and shortages of skilled workforce and infrastructure. Future perspectives highlight the integration of AI with multi-omics and systems pharmacology, AI-driven personalized and precision medicine, applications in global health and neglected diseases, and emerging trends such as quantum-machine learning, explainable AI, and federated learning. Overall, AI is emerging as a foundational technology in modern pharmaceutical research, promising faster, safer, and more patient-centric drug development.

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## INTRODUCTION

Artificial Intelligence (AI) has emerged as a transformative force in pharmaceutical research, revolutionizing the way drugs are discovered, developed, and delivered. Traditional drug-development pipelines are often time-consuming, costly, and associated with high failure rates, requiring approximately 10–15 years and billions of dollars to bring a single new drug to market. By harnessing large-scale biological, chemical, clinical, and real-world data, AI algorithms can identify patterns, predict molecular behavior, and prioritize promising candidates with higher speed and accuracy than conventional methods.[1]

In recent years, AI and machine learning have been increasingly integrated into virtually every stage of pharmaceutical research, including target identification, virtual screening, de-novo drug design, pharmacokinetic and toxicity prediction, formulation optimization, clinical-trial design, and pharmacovigilance. These tools not only accelerate R&D timelines but also help reduce experimental burden, minimize risks, and support personalized and precision medicine approaches. This review aims to provide a comprehensive overview of the role of artificial intelligence in pharmaceutical research, highlighting key applications, current challenges, and future perspectives for the field.[2]

### 3.1 Definition and evolution of artificial intelligence

Artificial intelligence (AI) is a subfield of computer science that develops systems capable of performing tasks normally associated with human intelligence, such as learning, reasoning, pattern recognition, decision-making, and natural language understanding. The foundations of AI date back to the 1950s, with key milestones including Alan Turing's "Computing Machinery and Intelligence" (1950) and the coinage of the term "artificial intelligence" by John McCarthy at

the Dartmouth workshop in 1956. Over the decades, AI has evolved through symbolic reasoning, expert systems, and, more recently, machine learning and deep-learning-based models, driven by advances in computational power, big data, and improved algorithms.geeksforsci

Today, AI encompasses a wide range of techniques, including supervised, unsupervised, and reinforcement learning, as well as neural networks and natural language processing, which are now widely applied in fields such as medicine, finance, and, importantly, pharmaceutical research. In the pharmaceutical domain, AI systems are trained on large-scale biological, chemical, and clinical datasets to identify patterns, predict molecular behavior, and support decision-making across the drug-development pipeline.

### 3.2 Emergence of AI in pharmaceutical sciences

Artificial intelligence began entering pharmaceutical sciences in the 1990s through early cheminformatics and simple predictive models, but its real momentum came after the 2000s with the rise of machine-learning algorithms and the availability of big data from genomics, proteomics, and electronic health records. Over the past two to three decades, AI-driven tools have been increasingly integrated into drug discovery, target identification, preclinical modeling, clinical-trial design, and pharmacovigilance, significantly reducing development time and cost while improving predictive accuracy.

Modern pharmaceutical research now relies on AI for virtual screening, de-novo drug design, ADMET (absorption, distribution, metabolism, excretion, toxicity) prediction, and formulation optimization, as well as for real-time analysis of clinical trial data and adverse-event signals. Reviews and industry analyses highlight that AI is not only accelerating R&D but also enabling personalized and precision medicine by tailoring



therapies to individual genetic and phenotypic profiles.

### 3.3 Objectives and scope of the review

The primary objective of this review is to systematically examine the role of artificial intelligence in pharmaceutical research, with a focus on current applications, underlying methodologies, and real-world examples. Specifically, the review aims to:

(i) outline how AI techniques are used across the drug-development pipeline, from target discovery to clinical-trial optimization and post-marketing pharmacovigilance; (ii) highlight key benefits such as reduced timelines, improved candidate selection, and enhanced safety prediction; and (iii) discuss persistent challenges including data quality, model interpretability, regulatory-approval pathways, and workforce preparedness. The scope covers peer-reviewed studies and authoritative reviews on AI-driven tools in pharmaceutical sciences, including machine-learning and deep-learning models, generative AI, and data-analysis platforms, while excluding general AI theory without a direct pharmaceutical research context. The review also aims to provide future perspectives on where AI is likely to reshape pharmaceutical innovation, including personalized medicine, multi-omics integration, and next-generation AI-assisted decision-making systems in pharmacy practice and industry.

## 4. Fundamental Concepts of Artificial Intelligence and Machine Learning

### 4.1 Basic AI and ML terminologies

Artificial intelligence (AI) refers broadly to systems that can perform tasks normally associated with human intelligence, such as learning, reasoning, pattern recognition, decision-making, and language understanding. Within AI, machine learning (ML) is a core subset that focuses on algorithms that learn from data and

improve their performance on a given task without being explicitly programmed. Common ML terminologies include features (input variables), labels (target outputs in supervised learning), training/validation/test sets, model, accuracy, precision/recall, and overfitting/underfitting, all of which are essential for developing and evaluating predictive models in pharmaceutical applications. [3]

### 4.2 Supervised, unsupervised, and reinforcement learning

In supervised learning, models are trained on labeled data, where each input is paired with the correct output; this approach is widely used in pharmaceutical research for tasks such as classification (e.g., active vs inactive compounds) and regression (e.g., predicting ADMET properties). In unsupervised learning, data are unlabeled and the model discovers hidden patterns or groupings, which is useful for tasks like clustering of similar compounds or signatures, or dimensionality reduction in high-throughput profiling data. Reinforcement learning involves an agent that learns optimal actions by interacting with an environment and receiving rewards or penalties, and it is increasingly explored for optimal-dosing schedules, adaptive trial design, and dynamic treatment-regimen optimization.[3]

### 4.3 Deep learning and neural networks

Deep learning is a specialized branch of machine learning that uses artificial neural networks (ANNs) with multiple layers to process complex, high-dimensional data such as images, sequences, and molecular structures. In pharmaceutical research, deep neural networks, including multilayer perceptrons (MLPs) and graph convolutional networks (GCNs), have been applied to predict pharmacokinetic and pharmacodynamic properties, toxicity, and structure–activity relationships (SAR) from large



cheminformatics datasets. These models learn hierarchical representations of data, enabling them to capture subtle nonlinear patterns that traditional statistical models often miss, thereby improving accuracy in *in silico* drug-design and personalized-dosing tasks.[2,3]

#### **4.4 Natural language processing (NLP) in pharma**

Natural language processing (NLP) is an AI subfield that enables computers to understand, interpret, and generate human language from text or speech. In pharmaceutical sciences, NLP is used to extract structured information from unstructured sources such as research articles, clinical-trial reports, electronic health records (EHRs), and regulatory documents, supporting tasks like adverse-event extraction, drug-label mining, and pharmacovigilance. NLP-based tools also assist in literature-based discovery, hypothesis generation, and summarization of large-scale drug-related knowledge, thereby accelerating evidence-based decision-making for researchers and clinicians.

### **5. Applications of AI in Drug Discovery**

#### **5.1 Target identification and validation**

Target identification is the first critical step in drug discovery, requiring the selection of a biologically relevant and “druggable” protein or pathway that is causally linked to disease. Artificial intelligence supports this process by integrating large-scale multi-omics data (genomics, transcriptomics, proteomics, metabolomics) with disease-pathway networks, clinical-trial data, and pharmacological databases to pinpoint high-probability targets. For example, ensemble-type AI models such as DrugnomeAI use hundreds of gene-level features to rank human protein-coding genes according to their predicted druggability, thereby prioritizing candidates more likely to yield successful drug programs.[6]

AI-based target identification also leverages network medicine and knowledge graphs that connect genes, proteins, diseases, and drugs into a unified graph structure; random-walk, graph-based, or deep-learning models then infer novel target–disease associations that are not obvious from single-omic layer analyses. In target validation, AI tools simulate the biological consequences of target modulation using constraint-based models, flux-balance analysis, and cell-signaling networks, while also cross-referencing phenotypic screening data and clinical-endpoint outcomes to confirm therapeutic relevance. Moreover, AI-assisted virtual screening and *in silico* toxicity prediction can be deployed early to evaluate whether a target is likely to bind small-molecule drugs and to estimate potential off-target effects, thus reducing the risk of late-stage failure[4]

#### **5.2 Virtual screening and high-throughput screening (HTS)**

Classical high-throughput screening (HTS) involves testing hundreds of thousands to millions of compounds in plate-based assays, a process that is resource-intensive, time-consuming, and limited by the physical scope of available libraries. In contrast, virtual screening uses computational methods to dock compounds into a target binding site and rank them by predicted affinity, allowing researchers to interrogate compound spaces far larger than any physical HTS campaign can cover. Recent AI-accelerated platforms, such as RosettaVS and OpenVS, combine classical docking (e.g., VSX for rapid triage and VSH for high-precision ranking) with active-learning neural networks that learn from docking results on-the-fly and prioritize only the most promising candidates for expensive full-flexibility calculations.[4]

These AI-augmented virtual-screening workflows can screen multi-billion-molecule libraries in a



computationally feasible manner, identifying novel hits against challenging targets such as ion channels, E3-ligases, and undrugged GPCRs. Studies testing AI-based virtual HTS across hundreds of targets have shown that such pipelines can match or surpass conventional HTS in hit-discovery performance, while reducing experimental burden and cost. In this way, AI-driven virtual screening has become a powerful complement—or even a partial replacement—for traditional HTS in early-stage drug discovery.

### 5.3 De-novo drug design and generative models

De-novo drug design aims to construct novel, synthetically tractable chemical structures tailored to a given target and desired pharmacological profile, rather than optimizing existing hits. This is often regarded as the “holy grail” of drug discovery because it can open entirely new chemotypes and intellectual-property spaces. Modern AI-driven de-novo pipelines employ generative models that learn the syntax and semantics of chemical space from large datasets of known drugs and pharmacophores, then propose new molecules that satisfy multiple constraints (e.g., potency, selectivity, solubility, metabolic stability).

Key generative architectures include recurrent neural networks (RNNs), autoencoders/variational autoencoders (VAEs), generative adversarial networks (GANs), transformers, and reinforcement-learning-augmented models. Each of these learns either a latent representation of molecules (e.g., SMILES or graphs) or a sequence-generation policy, and then samples new structures that are optimized for user-defined objectives using multi-objective reward functions (e.g., binding affinity, similarity to known actives, synthetic accessibility). Publicly available tools built on these ideas allow medicinal chemists to generate bespoke libraries enriched with drug-like

scaffolds and to explore “dark” chemical space outside traditional screening collections.

Despite these advances, challenges remain in ensuring that generated structures are synthetically accessible, free of toxicophores, and adequately validated in experimental assays; therefore, AI-generated compounds are typically used as starting points that are then refined through iterative medicinal-chemistry cycles.[4]

### 5.4 Structure-based and ligand-based drug design

Structure-based drug design (SBDD) exploits the three-dimensional structure of a target protein, often obtained from X-ray crystallography, cryo-EM, or AI-predicted folds (e.g., AlphaFold), to guide the design of ligands that fit precisely into the binding site. In AI-augmented SBDD, machine-learning scoring functions and deep-learning models improve the accuracy of docking, pose prediction, and binding-affinity estimation over traditional physics-based scoring functions, which tend to be less transferable across targets. AI-based SBDD pipelines can also perform fragment-based design, scaffold-hopping, and binding-site-focused de-novo generation, enabling the rapid optimization of potency, selectivity, and physicochemical properties.

When the target structure is unknown or poorly resolved, ligand-based drug design (LBDD) becomes the primary strategy. Here, AI models focus on known active compounds, extracting pharmacophores, 3D-shape similarity, electrostatic properties, and QSAR-type relationships to predict the activity of new analogs. Techniques such as pharmacophore-guided virtual screening, matched-molecular-pair analysis, and deep-learning-based QSAR models allow medicinal chemists to propose new scaffolds, modify functional groups, and improve ADMET profiles while staying within the chemical space of known actives. Hybrid workflows that combine



SBDD and LBDD—with AI models trained on both structural and ligand-property data—are increasingly used to balance novelty and target-specific activity, yielding optimized leads more rapidly than either approach alone.[12]

### 5.5 Drug repurposing using AI

Drug repurposing—finding new indications for approved or clinical-stage drugs—offers a faster, lower-risk alternative to de-novo drug development because safety, pharmacokinetic, and manufacturing data are already available. AI dramatically expands the scope of repurposing by mining heterogeneous biomedical data, including genomic associations, gene-expression profiles, protein–protein interactions, clinical-trial outcomes, adverse-event databases, and electronic health records, to infer non-obvious drug–disease relationships. For example, frameworks such as DeepDrug construct heterogeneous biomedical graphs connecting genes, proteins, drugs, and disease pathways, then apply graph neural networks (GNNs) to embed nodes and compute drug–disease association scores, ultimately proposing effective drug combinations for complex diseases like Alzheimer’s.

AI-based repurposing strategies include network-based inference, where shared pathways or disease signatures link drugs to new indications; similarity-based methods, which match drug-response profiles across diseases; and deep-learning-assisted text-mining of scientific literature and clinical-trial registries to extract hidden patterns. Case studies have successfully repurposed existing drugs for oncology, neurodegenerative disorders, infections, and rare diseases, demonstrating that AI can identify promising candidates for experimental validation and clinical-phase testing. By lowering development time and cost, AI-driven drug repurposing is becoming a core component of pharmaceutical innovation, especially in areas

where de-novo discovery is particularly challenging.[10]

## 6. AI in Preclinical Research

### 6.1. Prediction of pharmacokinetic and pharmacodynamic (PK/PD) parameters

AI is increasingly used in preclinical research to predict pharmacokinetic (PK) and pharmacodynamic (PD) parameters of drug candidates, allowing early optimization of dosing regimens and exposure–response relationships. Machine-learning and deep-learning models are integrated with physiologically based pharmacokinetic (PBPK) frameworks to simulate drug absorption, distribution, metabolism, and excretion (ADME) and to forecast time-dependent concentration profiles in different organs. These AI-PBPK platforms can predict PK and PD outcomes from limited in vitro and animal-data inputs, enabling virtual “first-in-human” simulations and reducing the number of costly and time-consuming in vivo experiments.

AI-driven PK/PD modeling is also applied to personalized dosing, where models trained on patient-specific factors (e.g., age, weight, renal/hepatic function, genetics) generate individualized PK/PD curves that help optimize efficacy while minimizing toxicity. Techniques such as graph neural networks (GNNs) and Bayesian/ensemble-based learners further improve uncertainty quantification, allowing researchers to assess the robustness of predicted PK/PD parameters and guide design of subsequent preclinical and clinical studies.[5]

### 6.2. Toxicity and ADMET prediction

Toxicity and ADMET (absorption, distribution, metabolism, excretion, toxicity) prediction is a critical stage in preclinical research, since many drug candidates fail due to poor safety or pharmacokinetic profiles. AI-based platforms such as ADMET-AI and ADMETLab 3.0 use graph



neural networks (GNNs) and other deep-learning architectures to predict hundreds of ADMET-related endpoints, including hERG inhibition, hepatotoxicity, carcinogenicity, and respiratory toxicity. These models are trained on large-scale chemical and biological datasets, learning molecular substructures and physicochemical properties associated with adverse effects.

AI-enabled ADMET predictors are substantially faster and more accurate than traditional rule-based or statistical models, allowing chemists to virtually screen compound libraries and prioritize candidates with favorable safety and PK properties. Moreover, many modern ADMET platforms include uncertainty estimation, highlighting when predictions are less reliable so that borderline compounds can be flagged for additional experimental testing. In this way, AI-based toxicity and ADMET prediction reduces late-stage attrition, minimizes animal testing, and supports early-stage lead optimization. [5]

### 6.3. In silico models for drug–target and drug–drug interactions

AI-powered in silico models are widely used in preclinical research to predict drug–target interactions (DTIs) and drug–drug interactions (DDIs), which are essential for understanding efficacy and safety. DTI prediction leverages machine-learning and deep-learning approaches that combine chemical fingerprints of drugs with protein-sequence or structural features of targets to score the likelihood of binding or modulation. Techniques such as random-walk on networks, random forests, and graph-based models integrate protein–protein interaction (PPI) and drug–drug networks to infer novel interactions, including off-target effects and polypharmacology patterns.

For drug–drug interactions, AI models analyze pharmacokinetic and pharmacodynamic data, cytochrome-P450 inhibition profiles, and

concomitant-drug usage patterns to flag potential DDIs that may alter exposure or toxicity. These in silico models can be run early in preclinical development to screen combinations and identify high-risk scenarios before moving to animal or clinical testing. By providing a comprehensive interaction map across multiple targets and co-administered drugs, AI-driven DTI/DDI platforms support safer drug design and regimen selection. [5]

### 6.4. Biomarker discovery and disease-pathway analysis

AI is transforming biomarker discovery and disease-pathway analysis in preclinical research by integrating multi-omics and heterogeneous datasets to identify molecular signatures associated with disease subtypes, drug response, and resistance. Deep-learning and graph-based models analyze genomic, transcriptomic, proteomic, epigenomic, and imaging data to extract patterns that are not easily detected by classical statistical methods. These AI-driven analyses can pinpoint novel biomarkers, such as circulating antibodies, nucleic acids, or protein panels, that correlate with disease onset, progression, or therapeutic outcome.

In addition, AI frameworks such as graph neural-network-based embeddings and pathway-aware models connect biomarkers to underlying disease-pathway networks, revealing how dysregulated pathways drive phenotypes and how drugs might modulate them. This enables target prioritization, patient stratification, and rational design of combination therapies in preclinical models. By linking biomarkers to mechanistic pathways, AI-based biomarker discovery enhances the biological plausibility of preclinical findings and supports more precise translation into clinical development. [11]

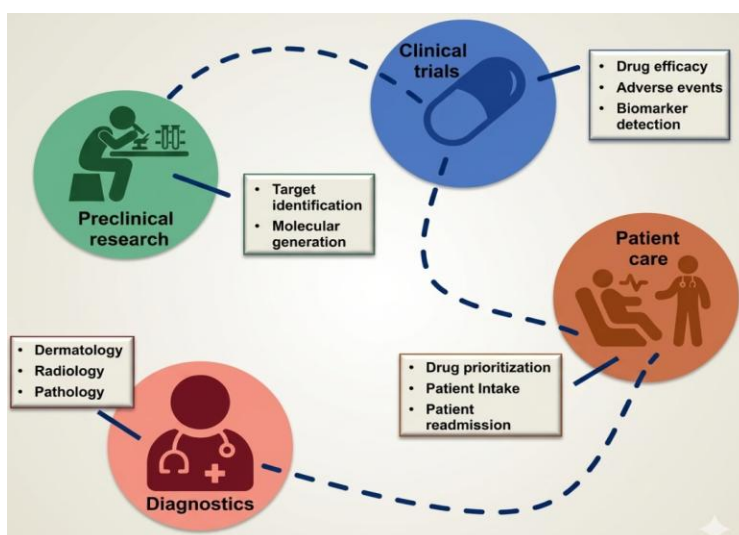


Fig. No. 01

## 7. AI in Pharmaceutical Development and Formulation

### 7.1. AI-assisted formulation design (solid, liquid, and nano-formulations)

Artificial intelligence is increasingly embedded into formulation development workflows, enabling data-driven design of solid, liquid, and nano-formulations rather than relying solely on empirical trial-and-error approaches. Machine-learning and deep-learning models screen large numbers of active pharmaceutical ingredient (API)–excipient combinations, predict compatibility, and narrow down optimal candidates before any laboratory experiments are conducted. Public and industrial platforms such as FormulationAI provide web-based tools that, given only basic drug and excipient inputs, can predict key formulation properties (e.g., solubility, stability, dose-form behavior) and suggest promising formulations for further testing.

For solid dosage forms (tablets, pellets, granules), AI helps design robust, high-performance formulations by modeling tablet-compression behavior, disintegration, and stability under different environmental conditions. In liquid formulations, models predict miscibility, solubility, viscosity, and phase separation, supporting the design of stable oral liquids,

injectables, and self-emulsifying systems. For nano-formulations (liposomes, polymeric nanoparticles, lipid-based systems), AI assists in selecting surfactants, stabilizers, and processing routes by learning from historical formulation data and physicochemical parameters, thereby accelerating development of nanocarriers with improved bioavailability and controlled release.[8,9]

### 7.2. Optimization of excipients and process parameters

Excipient selection and process-parameter optimization are critical for achieving desired stability, manufacturability, and in-vivo performance, and AI has become a powerful tool for these tasks. Supervised models such as random forests, gradient-boosting machines, and deep neural networks classify excipients by compatibility with APIs and predict ideal excipient ratios to meet targets such as dissolution rate, compressibility, and disintegration time. Iterative optimization techniques like Bayesian optimization (BO) and reinforcement learning (RL) further refine excipient concentrations by dynamically updating model parameters based on real-time experimental feedback, capturing complex nonlinear interactions that classical

design-of-experiments (DoE) often misses academic.

AI-integrated high-throughput experimentation (HTE) and robotics allow automated labs to generate hundreds of mini-formulations per day, with AI continuously learning from the data to narrow the search space toward the most promising formulations. This creates a self-learning excipient-optimization system that can tailor formulations to patient-specific needs (e.g., lactose-free, low-taste-masking, pediatric- vs geriatric-adapted dosage forms), aligning formulation design with the principles of precision medicine.[9]

### 7.3. Predictive modeling for dissolution and release profiles

Predictive modeling of dissolution and release profiles enables virtual optimization of drug release behavior and facilitates the design of controlled-release and modified-release systems. Artificial neural networks (ANNs), genetic programming, and other nonlinear modeling approaches have been used to develop mathematical models that describe drug release from solid-lipid extrudates and other complex dosage forms, outperforming traditional linear fits in accuracy. These models relate formulation variables (e.g., particle size, tablet geometry, polymer-type, porosity) and process conditions to the percentage of drug released over time, allowing in-silico screening of formulations before costly dissolution-testing campaigns.

More advanced platforms combine near-infrared (NIR) or other process-analytical signals with AI-based predictive dissolution models (PDMs) to support real-time release testing, where the dissolution profile is predicted from process data instead of waiting for physical dissolution tests. Such models are calibrated on historical and experimental data and then deployed on-line to monitor batch-to-batch variability and detect

deviations early, thereby improving batch release decisions and overall product quality.[10]

### 7.4. AI in quality by design (QbD) and process analytical technology (PAT)

AI is naturally aligned with Quality by Design (QbD) and Process Analytical Technology (PAT), which emphasize product-quality understanding through systematic design, analysis, and control of manufacturing processes. In QbD, AI-driven DoE substitutes or enhances classical experimental designs by dynamically proposing new experimental runs based on prior outcomes, reducing the total number of experiments by up to about 70% while maintaining robustness. This adaptive-DoE approach allows formulators to map critical material attributes (CMAs) and critical process parameters (CPPs) that affect critical quality attributes (CQAs) such as dissolution, content uniformity, and stability more efficiently.[9]

For PAT, AI models integrate in-line, on-line, and at-line sensor data (e.g., NIR, Raman, temperature, pressure, flow-rate) to monitor unit operations such as blending, granulation, drying, coating, and compression in real time. These models detect abnormal patterns that may indicate defects (e.g., over-wet granulation, segregation, insufficient mixing) and can trigger automatic corrective actions or flag batches for additional testing. By embedding AI within QbD and PAT frameworks, pharmaceutical companies can move from reactive quality control toward predictive and preventive quality assurance, ensuring consistent product quality, regulatory compliance, and efficient scale-up from lab to commercial manufacturing.[11]

## 8. AI in Clinical Trials and Drug Development

### 8.1. Patient recruitment and stratification

Patient recruitment is one of the most time-consuming and costly aspects of clinical trials, with many studies failing to meet enrollment



targets or suffering from significant delays. Artificial intelligence accelerates recruitment by analyzing large-scale electronic health records (EHRs), insurance claims, and other health-data sources to identify patients who match protocol-specific eligibility criteria. AI-enabled matching tools can screen thousands of potential participants, flagging those with suitable disease-stage, prior-treatment history, and comorbidities, thereby reducing screening workload and shrinking recruitment timelines.

Beyond simple matching, AI also supports patient stratification, using machine-learning models to subgroup patients based on molecular profiles, imaging features, or clinical trajectories. This enables enrichment of trial populations with individuals most likely to respond to a therapy, improving statistical power and reducing sample-size requirements. Stratified recruitment strategies powered by AI are increasingly used in oncology, neurological disorders, and rare-disease trials, where identifying the right patient population is critical for demonstrating efficacy.[12]

## **8.2. Trial design optimization and endpoint prediction**

AI contributes to trial design optimization by simulating protocol scenarios, predicting enrollment rates, and identifying potential operational bottlenecks before the first patient is enrolled. Simulation-based tools use historical trial-data repositories to forecast recruitment curves, dropout rates, and required site-numbers, helping sponsors design feasible and efficient protocols. AI can also recommend optimal endpoint selection, inclusion–exclusion criteria, and dose-levels by mining prior-trials data and pharmacological knowledge, thereby improving the likelihood of a successful outcome.

Adaptive and AI-optimized trial designs leverage Bayesian and reinforcement-learning algorithms to dynamically adjust trial parameters (e.g., cohort

size, randomization ratio, or even endpoints) based on interim analyses. These approaches allow mid-trial reallocation of patients to more promising arms, early termination of ineffective treatments, and focus of resources on the most promising regimens, leading to shorter development timelines, lower costs, and improved ethical standards.[14]

## **8.3. Real-time monitoring and adverse-event detection**

AI-driven systems are transforming real-time monitoring of clinical-trial participants by integrating data from EHRs, wearables, mobile apps, and central-laboratory reports to detect early safety signals and protocol deviations. Natural language processing (NLP) and anomaly-detection algorithms scan clinical-narrative notes and structured data to flag adverse events (AEs) that might otherwise be missed or underreported by manual chart review. Patient-reported outcome (PRO) platforms that use AI-enabled prompts and adaptive questionnaires further enhance self-reported AE capture, enabling continuous surveillance outside scheduled clinic visits.

AI-based monitoring tools can also identify outliers in vital signs, lab values, or medication-use patterns, triggering automated alerts to site staff or central monitors so that interventions occur before events escalate. This real-time surveillance not only improves patient safety but also maintains data integrity and supports regulatory compliance, as AI-assisted AE-detection systems can standardize coding and expedite reporting workflows.[15]

## **8.4. Use of AI in real-world data (RWD) and real-world evidence (RWE)**

AI plays a central role in extracting real-world data (RWD) from diverse sources such as routine clinical care, pharmacy claims, registries, and digital-health platforms and converting it into



structured real-world evidence (RWE) that supports regulatory and commercial decisions. Machine-learning and NLP models process unstructured clinical narratives and heterogeneous databases to infer diagnoses, treatments, and outcomes, enabling large-scale analyses of drug-utilization patterns, long-term safety, and comparative-effectiveness. RWD-based AI analyses can complement randomized clinical-trial data by characterizing how drugs perform in broader, more diverse populations outside tightly controlled settings.

Regulators and industry increasingly use AI-generated RWE for post-marketing safety surveillance, label-expansion studies, and health-technology assessments. AI-powered RWE platforms can also support trial design by identifying untreated or under-treated patient populations and suggesting optimal comparator regimens or endpoints derived from routine-care patterns. By bridging the gap between clinical-trial evidence and everyday practice, AI-driven RWD and RWE enhance decision-making across the drug-development lifecycle.[16]

## 9. AI in Pharmacovigilance and Clinical Pharmacy

### 9.1. Adverse drug reaction (ADR) prediction and signal detection

Artificial intelligence is transforming pharmacovigilance by enabling earlier and more accurate detection of adverse drug reactions (ADRs) than traditional spontaneous-reporting systems. Machine-learning models trained on electronic health records (EHRs), spontaneous-ADR databases (e.g., FAERS, EudraVigilance), and unstructured clinical narratives can identify patterns associated with specific ADRs and detect “signals” that may be missed by manual review. Ensemble methods such as gradient-boosting, deep neural networks, and LSTM-based models

have demonstrated high performance (AUC-ROC >0.85–0.90) in predicting ADRs using features like age, drug type, dose, and comorbidities.

AI-based signal-detection platforms scan millions of adverse-event reports and clinical-data entries to flag unusual risk increases for specific drug–event combinations, shortening the time from drug launch to safety signal confirmation. In addition, natural language processing (NLP) extracts ADR-related phrases from case-reports, social-media discussions, and clinician notes, enriching structured databases and improving completeness of pharmacovigilance records. These tools support not only post-marketing surveillance but also proactive risk prediction, allowing clinicians and regulators to implement monitoring strategies for high-risk patients or drug classes. [16]

### 9.2. AI-based decision support systems for pharmacists

AI-enabled clinical decision support systems (AI-CDSS) are increasingly integrated into pharmacy workflows to assist pharmacists with complex prescribing and medication-management decisions. These systems ingest patient-specific data (e.g., diagnosis, lab values, concomitant drugs, and genetic profiles) and compare them against large-scale drug-interaction and guideline databases to generate real-time alerts and evidence-based recommendations. AI-CDSS platforms such as Lexicomp and Micromedex use advanced algorithms to predict drug–drug interactions, assess toxicity risks, and suggest dose adjustments, improving both safety and therapeutic precision.

Such tools help pharmacists prioritize high-risk prescriptions, manage polypharmacy, and tailor therapy for special populations (e.g., elderly, renal-impaired, pediatric, or oncology patients). Importantly, successful AI-CDSS deployment requires human-centered design, appropriate alert-filtering, and explainable outputs so that



pharmacists retain clinical autonomy while leveraging AI-generated insights. Well-designed AI-CDSS not only reduce cognitive load but also enhance guideline adherence, medication-appropriateness, and patient-outcomes in hospital and community-pharmacy settings.[17,18]

### **9.3. Medication-error reduction and prescription-verification tools**

AI is playing a growing role in reducing medication errors across the medication-use process—prescribing, dispensing, administration, and monitoring. AI-driven models analyze prescribing patterns, EHR data, and prior-error databases to predict patients at highest risk for medication discrepancies or adverse events, enabling targeted pharmacist interventions. For example, machine-learning tools that prioritize patients for medication-reconciliation upon admission have been shown to identify more error-exposed patients than conventional methods, improving pharmacist-efficiency and error-detection rates.

AI-powered prescription-verification tools and automated dispensing systems compare orders against institutional rules, allergy lists, and interaction-databases, flagging illegible or ambiguous prescriptions, dose-outliers, and potential duplications. In hospital settings, AI-integrated workflows such as intelligent infusion pumps, barcode-assisted dispensing, and computerized provider order-entry (CPOE) with AI-CDSS have reduced various types of medication errors by up to 55–95% in some studies, depending on the context. By combining predictive analytics, real-time alerts, and workflow automation, AI-assisted medication-safety tools help pharmacists shift from reactive correction to proactive prevention of errors, thereby improving patient safety and the overall efficiency of clinical-pharmacy practice. [18]

## **10. AI in Pharmaceutical Manufacturing and Quality Control**

### **10.1. Process optimization and predictive maintenance**

Artificial intelligence is increasingly used to optimize pharmaceutical manufacturing processes by analyzing large-scale sensor data, batch histories, and equipment logs to identify critical process parameters (CPPs) and sources of variability. Machine-learning models establish relationships between raw-material attributes, process conditions (e.g., temperature, humidity, mixing speed), and critical quality attributes (CQAs) such as tablet hardness, dissolution, or purity, enabling data-driven process optimization rather than empirical fine-tuning. By correlating historical batch outcomes with real-time process data, AI tools can recommend optimal set-points, reduce batch failures, and narrow the design space for robust commercial-scale production.

AI also supports predictive maintenance of manufacturing equipment such as mixers, granulators, tablet presses, and lyophilizers by monitoring vibration, temperature, pressure, and power-consumption patterns. Anomaly-detection and failure-prediction models flag early signs of wear or malfunction, allowing maintenance to be scheduled proactively instead of waiting for breakdowns. This reduces unplanned downtime, improves overall equipment effectiveness (OEE), and helps maintain consistent product quality across successive batches, which is essential for GxP-compliant facilities. [13]

### **10.2. AI-based image recognition for defect detection**

AI-based **computer-vision systems** are now widely deployed for automated visual inspection of tablets, capsules, vials, syringes, and packaging, detecting defects that may be missed during manual inspection. Convolutional neural networks



(CNNs) and other deep-learning models are trained on large image datasets of acceptable and defective products (e.g., broken tablets, double-weight tablets, color-spot defects, cracked vials, incorrect labeling), enabling high-speed, real-time classification on production lines. These systems can inspect thousands of units per minute, far exceeding human-operator speed, while maintaining high sensitivity and specificity.

Automated visual-inspection tools can distinguish between critical defects (e.g., broken tablets, contaminated vials) and cosmetic variations (e.g., minor color differences), reducing unnecessary batch rejections and improving yield. Integration with **process-analytical technology (PAT)** platforms allows image-based defect signals to be combined with other in-line data (e.g., weight, thickness, or moisture content) for root-cause analysis and closed-loop process control, further strengthening quality assurance.[19]

### **10.3. Continuous manufacturing and real-time release testing**

AI is a key enabler of continuous pharmaceutical manufacturing (CM), where raw materials are fed continuously into an integrated series of unit operations instead of being processed in discrete batches. In CM, AI models process real-time data streams from sensors to maintain stable operating conditions, adjust flows and mixing parameters on-the-fly, and ensure consistent product quality across the entire run. Predictive models link process variables to dissolution, content-uniformity, and other CQAs, allowing operators to anticipate and correct drifts before they impact product specifications.

AI-based predictive dissolution models and other mathematical frameworks support real-time release testing (RTRT), where product quality is inferred from in-line and at-line process data rather than waiting for off-line dissolution or stability tests. By correlating NIR, Raman, or other

process-analytical signals with reference-method measurements, these models can predict release profiles and other key parameters during ongoing production, enabling faster batch-release decisions and reducing laboratory-workload. In combination with quality-by-design (QbD) principles, AI-driven continuous manufacturing and RTRT reduce variability, shorten cycle times, and improve supply-chain resilience. [20]

### **10.4. Regulatory-compliance and data-integrity support**

AI supports regulatory compliance and data integrity by automating documentation workflows, flagging deviations, and ensuring adherence to GxP standards throughout manufacturing and QC. AI-enabled systems monitor batch records, electronic logs, and audit trails to detect missing entries, inconsistent timestamps, or unauthorized changes that may compromise data integrity. Natural-language-processing (NLP) tools can also scan standard-operating-procedure (SOP) documents and deviation reports, automatically tagging regulatory-relevant sections and suggesting corrective-and-preventive-action (CAPA) measures.

AI-based analytics further assist in regulatory-readiness by generating summary reports, identifying batches that deviate from historical norms, and highlighting recurring issues for root-cause analysis. By embedding traceability and consistency-checks into the manufacturing data-pipeline, AI helps organizations meet expectations from regulatory agencies such as the FDA and EMA concerning data integrity, change-control, and continuous-improvement. In this way, AI not only improves product quality and safety but also strengthens the digital foundation needed for regulatory submissions, inspections, and post-approval surveillance. [21]



## 11. Data Infrastructure and Tools for AI in Pharmaceutical Research

### 11.1. Big data sources (genomics, proteomics, clinical databases)

Pharmaceutical AI-driven research depends on large-scale, heterogeneous data gathered from multiple domains. Genomic data (e.g., whole-genome sequencing, transcriptomics) and proteomic datasets (e.g., protein-expression profiles, post-translational modifications) provide insights into disease mechanisms, target identification, and biomarker discovery. These omics datasets are often combined with pharmacogenomics information from preclinical models (e.g., cancer-cell-line panels) to predict drug response and resistance patterns.

Additional critical sources include clinical trial databases (e.g., ClinicalTrials.gov, internal sponsor databases), electronic health records (EHRs), adverse-event reporting systems (FAERS, EudraVigilance), and real-world data (RWD) platforms such as insurance claims and disease registries. Open-data initiatives and consortia have made many of these datasets publicly accessible, enabling AI models to learn from shared, large-scale evidence across diseases and drug classes. Integration of such big data is essential for training robust AI models that generalize well across indications and populations rather than being confined to single-study silos. [22]

### 11.2. Data preprocessing, integration, and standardization

Before AI models can be trained, raw data must undergo preprocessing, integration, and standardization because pharma datasets are often noisy, incomplete, and stored in different formats and ontologies. Typical preprocessing steps include missing-value imputation, outlier detection, normalization, and feature engineering

(e.g., deriving ADMET-relevant descriptors from chemical structures or extracting structured flags from unstructured clinical notes using NLP).

Data integration involves merging genomics, proteomics, chemistry, imaging, and clinical-variable data into unified, patient- or compound-level feature matrices while preserving temporal and contextual relationships (e.g., treatment sequence, dose-time courses). Standardization efforts follow FAIR principles (Findable, Accessible, Interoperable, Reusable) and domain-specific standards such as SDTM for clinical data or InChI/SMILES for chemical structures to ensure that diverse data sources can be harmonized and reused across AI pipelines. Well-designed data-integration frameworks are now considered prerequisites for scalable, reproducible AI-enabled drug discovery.[24]

### 11.3. Commonly used AI platforms and software tools

Several AI-driven platforms and tools are commonly deployed across pharmaceutical research, from target discovery to clinical-trial analytics. In drug discovery, platforms such as Atomwise, Insilico Medicine, and other AI-drug-discovery engines use deep-learning models for virtual screening, de-novo molecule generation, and ADMET prediction. These tools integrate cheminformatics libraries, docking simulations, and proprietary AI models to propose novel leads and optimize properties such as potency and toxicity.

For clinical-trial and commercial analytics, companies use augmented-analytics platforms (e.g., Tellius, ThoughtSpot, Tableau, Power BI, and others) that combine AI-driven insight generation with visualization dashboards for sales, market-access, and real-world-evidence analyses. In-house or cloud-based machine-learning pipelines built on frameworks such as Scikit-learn, TensorFlow, PyTorch, and R packages support



custom model development for pharmacokinetic prediction, adverse-event detection, and biomarker-discovery workflows. These platforms are often embedded into larger R&D data-infrastructure stacks so that AI models can be versioned, monitored, and updated without disrupting ongoing studies.[9]

#### 11.4. Cloud computing and high-performance computing (HPC)

Cloud computing and high-performance computing (HPC) provide the computational backbone necessary to store, process, and analyze the vast datasets generated in AI-enabled pharmaceutical research. Cloud-based data warehouses and lakehouse architectures allow organizations to scale storage and compute on demand, integrate data from internal systems, external partners, and public repositories, and maintain regulatory-compliant environments (e.g.,

HIPAA, GDPR, 21 CFR Part 11) through robust access controls and audit trails.

HPC clusters and GPU-accelerated infrastructure are essential for tasks such as molecular-dynamics simulations, deep-neural-network training, and large-scale virtual screening of compound libraries, which require intensive parallel computation. Cloud-native HPC offerings enable global collaboration among research teams, CROs, and contract-research sites by providing shared, secure environments for federated learning and multi-site data analysis without unnecessary data duplication. By combining scalable cloud storage, managed HPC resources, and standardized analytical platforms, pharmaceutical companies create an “AI-ready” infrastructure that accelerates the transition from hypothesis to data-driven decision-making across the R&D pipeline. [25]

#### 12. Challenges and Limitations

Sub-section	Key Issue	Main Points (1–2 lines)
<b>Data quality, bias, and interpretability</b>	Poor-quality, incomplete, or biased datasets	Pharmaceutical AI models often rely on heterogeneous, noisy data (e.g., EHRs, spontaneous-report databases, or proprietary assays), which can lead to inaccurate or unstable predictions; biases in training data (e.g., population-, disease-, or drug-class-specific biases) may propagate into clinical- or development-level decisions.
	Model “black-box” behavior	Many deep-learning models lack clear interpretability, making it difficult for researchers and regulators to understand <i>why</i> a specific prediction (e.g., toxicity, PK profile, or target association) is made, which undermines trust and hinders mechanistic-driven drug-design.
<b>Regulatory and ethical concerns</b>	Evolving regulatory landscape	Current guidelines (e.g., FDA, EMA) for AI in drug development and clinical decision support are still maturing; agencies emphasize validation, transparency, and auditability, but clear, harmonized standards for AI-driven submissions are lacking.
	Ethical and privacy issues	Use of sensitive patient data (e.g., genomics, EHRs, or social-media traces) raises privacy and informed-consent concerns; improper deployment of AI could amplify health-inequity or support off-label-driven commercial decisions without robust clinical-evidence backing.
<b>Lack of standardized validation frameworks</b>	No universal AI-validation guidelines	Pharmaceutical AI models are often validated in narrow contexts, using proprietary or single-source datasets, leading to poor generalizability; there is no widely accepted, cross-industry framework for benchmarking

		performance across different targets, indications, or dosage-forms.
	Model drift and reproducibility	AI models can degrade over time (“model drift”) as new data, formulations, or clinical-practices emerge; without standardized re-training, re-validation, and version-control procedures, reproducibility across organizations and academic groups remains a major challenge.
<b>Shortage of skilled workforce and infrastructure</b>	Talent gap	There is a global shortage of professionals who combine expertise in AI/ML, statistics, and pharmaceutical sciences; this gap limits the design, implementation, and critical evaluation of AI-driven projects in drug discovery and clinical-pharmacy.
	Infrastructure limitations	Many mid-size and educational institutions lack the cloud-scale data-storage, HPC, or GPU-based clusters needed for large-scale AI training, hindering local AI adoption in preclinical and clinical-research settings.

### 13. Future Perspectives

#### 13.1. Integration of AI with multi-omics and systems pharmacology

In the near future, AI will increasingly be integrated with multi-omics (genomics, transcriptomics, proteomics, metabolomics, epigenomics) and systems-pharmacology frameworks to build holistic, dynamic models of drug action and disease progression. By combining AI-powered pattern recognition with mechanistic pathway models, researchers can simulate how drugs perturb biological networks across multiple scales (from genes to organs), enabling more rational target selection and combination-therapy design. Such integrated platforms will help bridge the gap between in-silico predictions and in-vivo outcomes, improving the translation of preclinical findings into clinically meaningful effects.

These systems-pharmacology-plus-AI workflows are especially promising for complex polygenic diseases (e.g., cancer, neurodegenerative and autoimmune disorders), where multiple targets and feedback loops operate simultaneously. As multi-omics datasets grow and standardized ontologies improve, AI-driven systems-pharmacology is

expected to become a core component of modern drug-development pipelines, supporting hypothesis-generation, mechanism-of-action elucidation, and biomarker-driven trial design.[25]

#### 13.2. AI-driven personalized and precision medicine

AI will play a central role in advancing personalized and precision medicine, tailoring drug therapy to individual patients based on their genetic background, comorbidities, environmental factors, and real-time physiological data. Machine-learning models trained on large-scale genomic and electronic-health-record data can predict drug response, adverse-reaction risk, and optimal dosing regimens for specific subpopulations, moving beyond “one-size-fits-all” approaches. In oncology, psychiatry, and rare diseases, such personalized models can guide the selection of therapies most likely to benefit a given patient while minimizing toxicity.

Wearable-device-derived data, continuous-monitoring platforms, and AI-enabled decision support systems will allow adaptive treatment regimens that evolve as new patient-specific information becomes available. By embedding AI-based personalization tools into clinical-pharmacy



workflows and electronic prescribing systems, healthcare providers can move toward safer, more effective, patient-centric therapy, reducing trial-and-error prescribing and improving long-term outcomes. [24]

### **14.3. Role of AI in global health and neglected diseases**

AI has significant potential to address challenges in global health and neglected tropical, infectious, and orphan diseases, where conventional R&D is often economically unattractive. AI-enabled virtual screening and de-novo drug design can rapidly identify hit compounds against poorly explored targets, while repurposing AI tools can uncover new uses for existing, low-cost, off-patent drugs relevant to resource-limited settings. These approaches can shorten discovery timelines and reduce costs, making it feasible to develop treatments for diseases that disproportionately affect low- and middle-income countries.

In addition, AI-driven diagnostics, predictive-epidemiology models, and supply-chain-optimization tools can support early-outbreak detection, treatment-allocation strategies, and more efficient drug-distribution networks in underserved regions. As global-data-sharing initiatives and open-source AI platforms expand, AI-assisted research can democratize access to cutting-edge tools, allowing local scientists and institutions to participate in drug-discovery programs for diseases that have long received inadequate investment.[23]

### **14.4. Emerging trends: quantum-machine learning, explainable AI, and federated learning**

Several emerging AI trends are expected to reshape pharmaceutical research. Quantum-machine learning (QML) promises to accelerate optimization problems such as molecular-conformation search and combinatorial-

chemistry-space exploration by leveraging quantum-computing principles, although practical deployment will depend on the maturation of quantum-hardware platforms. In parallel, explainable AI (XAI) methods—such as attention-mechanism visualizations, SHAP-values, and counterfactual explanations—are being developed to make black-box models more transparent and interpretable for regulators, clinicians, and medicinal chemists, thereby improving trust and adoption.

Federated learning represents another key trend, enabling AI models to be trained across multiple institutions (e.g., hospitals, universities, and companies) without sharing raw patient data. This approach preserves privacy and data-ownership while allowing collaborative model-building for rare-disease cohorts or cross-border pharmacovigilance systems. Together, quantum-machine learning, explainable AI, and federated-learning frameworks are likely to drive the next generation of secure, efficient, and transparent AI applications in drug discovery, clinical-trials management, and post-marketing surveillance.[25]

## **CONCLUSION**

Artificial intelligence is rapidly transforming pharmaceutical research, spanning from early-stage drug discovery and preclinical development through formulation design, clinical-trial management, pharmacovigilance, and manufacturing. By leveraging large-scale biological, chemical, clinical, and real-world data, AI-driven tools are accelerating target identification, enabling virtual screening and de-novo drug design, predicting pharmacokinetic and toxicological profiles, and supporting biomarker-driven personalized medicine. In clinical-pharmacy and pharmacovigilance, AI-based decision support systems and adverse-event-prediction models are enhancing patient safety and



reducing medication-errors, while in manufacturing, AI-powered process optimization, image-based quality control, and real-time release testing are improving product consistency and efficiency.

Despite these advances, significant challenges remain, including issues of data quality, bias, model interpretability, regulatory-uncertainty, lack of standardized validation frameworks, and shortages of skilled AI-capable personnel and infrastructure. Addressing these limitations will require concerted efforts in data-governance, interdisciplinary training, and harmonized guidelines across academia, industry, and regulatory agencies. Looking ahead, the integration of AI with multi-omics, systems-pharmacology, quantum-machine learning, explainable AI, and federated-learning approaches promises to further deepen mechanistic understanding, drive precision medicine, and expand the impact of AI-enabled research to global health and neglected diseases. In sum, AI is not merely an adjunct to pharmaceutical research but an increasingly central pillar shaping the future of safer, faster, and more personalized drug development.

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