REVIEW ARTICLE

# Artificial Intelligence in Pharmacy – Revolutionising, Discovery, Development and Education

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## Abstract

Artificial intelligence (AI) is reshaping the pharmaceutical sciences by introducing data-driven solutions that enhance efficiency, accuracy, and innovation across the entire healthcare spectrum. In drug discovery, AI enables rapid identification of molecular targets, prediction of drug–receptor interactions, and virtual screening of vast compound libraries, significantly reducing the time and cost of identifying novel therapeutics. Within drug development, AI-driven tools support preclinical modeling, optimization of formulation strategies, patient stratification, and clinical trial management, thereby improving safety profiles and regulatory compliance. In pharmacy practice, AI-powered clinical decision support systems, digital adherence monitoring, and personalized therapy recommendations are advancing patient-centered care. Equally transformative is the integration of AI into pharmacy education, where adaptive learning platforms, simulation technologies, and data analytics are preparing future pharmacists to navigate a digitally enabled healthcare landscape. Despite its vast potential, AI adoption in pharmacy faces several challenges, including data quality, algorithmic transparency, ethical concerns, regulatory uncertainties, and the need for workforce training. Addressing these barriers is essential to ensure equitable, responsible, and sustainable implementation of AI technologies. This chapter provides a comprehensive exploration of how AI is revolutionizing pharmaceutical discovery, development, and education, while highlighting the opportunities and challenges that will shape the future of pharmacy in the era of intelligent systems.

**Keywords:** Artificial intelligence, Drug discovery, Drug development, Clinical decision support, Pharmacy education, Personalized medicine.

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## Introduction

Artificial intelligence (AI) has emerged as one of the most transformative technologies of the twenty-first century, with profound implications for healthcare and pharmaceutical sciences. Broadly defined, AI refers to computational systems that mimic human cognitive functions such as learning, reasoning, and decision-making.[1] By leveraging machine learning algorithms, natural language processing, and advanced data analytics, AI has the potential to uncover insights from complex biomedical datasets, automate labour-intensive processes, and enhance the accuracy of decision-making. In the context of pharmacy,[2] AI represents not only a technological advancement but also a paradigm shifts in how drugs are discovered, developed, and delivered to patients.

The relevance of AI to pharmacy becomes clearer when viewed against the historical backdrop of drug development.[3] Traditionally, pharmaceutical research has relied on empirical approaches and trial-and-error experimentation. While these methods yielded many important therapeutics, they were often time-consuming, costly, and inefficient. The introduction of computational chemistry, bioinformatics, and molecular modeling in the late twentieth century marked an important turning point, providing researchers with tools to simulate biological processes and predict drug–target interactions.[4] However, the scale and complexity of modern biomedical data—ranging from genomic sequences to electronic health records—have exceeded the capacity of conventional computational methods. AI now fills this gap by enabling automated pattern recognition and predictive modeling at a scale that was previously unimaginable.[5]

The pharmaceutical sector faces rising R&D costs, slower drug development, and the growing complexity of diseases such as cancer and neurodegenerative disorders. Alongside the global shift toward precision medicine, these challenges demand more efficient and individualized approaches. Artificial intelligence addresses this need by streamlining drug discovery, enhancing clinical trial design, and enabling personalized therapies tailored to patient-specific factors.[6]

The scope of this chapter is to provide a comprehensive overview of how AI is revolutionizing the pharmaceutical sciences across three interconnected domains: discovery, development, and education. In the domain of drug discovery,[7] AI is being utilized to predict protein structures, design new molecular entities, and repurpose existing drugs for novel indications. Within drug development, AI supports preclinical modeling, clinical trial optimization, pharmacovigilance, and manufacturing processes, thereby reducing attrition rates and improving efficiency. Finally, in the sphere of pharmacy education, AI is transforming how future pharmacists are trained by offering adaptive learning platforms, virtual simulations, and data-driven curricula that prepare students for a digitally enabled healthcare environment.[8]

By examining these domains, this chapter aims to illuminate both the transformative potential and the practical challenges of AI integration into pharmacy. While AI presents remarkable opportunities, issues such as data privacy, ethical considerations, regulatory frameworks, and workforce readiness must be carefully addressed. Ultimately, this introduction sets the stage for a detailed exploration of AI's role in reshaping pharmaceutical discovery, development, and education, and its broader implications for global healthcare.[9]

## AI in Drug Discovery

Drug discovery is one of the most resource-intensive phases of pharmaceutical research, traditionally requiring several years of experimentation and significant financial investment. Artificial intelligence (AI) is redefining this process by enabling rapid analysis of large-scale biological datasets and by supporting predictive modeling for early-stage decision-making. Its application as presented in Table 1 spans multiple stages of discovery, from identifying therapeutic targets to optimizing candidate molecules.[10]

## AI in Drug Development

AI is transforming drug development by improving predictive accuracy and efficiency across the continuum. In preclinical and clinical stages, it integrates multi-omics data, employs digital twins for trial optimization, and enhances safety monitoring through natural language processing, while in manufacturing it enables real-time quality control**.** Various applications and studies of AI in development of drugs are presented in Table 2.

## AI in Pharmacy Practice: Emerging Innovations

Artificial intelligence (AI) is rapidly transforming pharmacy practice by enhancing clinical decision-making, medication management, and patient engagement. Recent advancements have introduced several innovative applications as presented below and in Table 3:

### Predictive Analytics for Medication Therapy Management

AI analyzes patient data to anticipate adverse drug events, supporting proactive pharmacist interventions.

### Virtual Pharmacy Assistants

AI-driven chatbots and voice tools provide continuous access to counselling, reminders, and adherence support.[20]

### Integration of Genomic Data for Personalized Medicine

AI combines genomic and clinical data to design preventive and individualized treatment strategies.

### AI-Enhanced Workflow Automation

AI automates routine pharmacy tasks, reducing administrative load and enhancing patient-centered care.[21]

### Telepharmacy Services

AI enables remote consultations and medication reviews, expanding pharmacy access in underserved regions.

### Pharmacogenomics Integration

AI interprets pharmacogenomic profiles to optimize drug selection, dosing, and therapeutic outcomes. [22]

**Table:** 1: Applications of AI in Drug Discovery

| *Domain* | *Role of AI* | *Key Features/Applications* | *Examples/Case Studies* | *References* |
|---|---|---|---|---|
| Target Identification & Validation | Analysis of genomics, proteomics, and biomarker data | Identifies disease-associated genes/proteins; improves accuracy of therapeutic target selection; reduces false leads | Machine learning on omics datasets | 11 |
| Drug Design | Generative AI and molecular modeling | Creates novel chemical entities; predicts binding affinities, stability, and efficacy; accelerates lead optimization | Generative AI platforms for de novo compound design | 12 |
| Virtual Screening & Repurposing | AI-based docking and deep learning | Screens millions of compounds computationally; identifies promising leads faster; uncovers new indications for existing drugs | AI-driven repurposing (e.g., COVID-19 therapeutics) | 13 |
| Predictive ADMET Models | Simulation of pharmacokinetic and safety profiles | Forecasts absorption, distribution, metabolism, excretion, and toxicity early in discovery; reduces late-stage failures | AI-based ADMET prediction models | 14 |
| Case Studies | Demonstrated impact of AI platforms | Advances in protein structure prediction; novel target identification and drug repurposing | AlphaFold (protein structures), BenevolentAI, Insilico Medicine | 15 |

**Table 2:** Applications and Case Studies of AI in Drug Development

| *Domain* | *Role of AI* | *Key Features/Applications* | *Case Studies / Examples* | *References* |
|---|---|---|---|---|
| Preclinical Studies | Prediction of toxicity and formulation optimization | Uses in silico models to anticipate toxicological effects; designs safer drug candidates; optimizes dosage forms and delivery systems | *Atomwise* uses deep learning for toxicity prediction; *Berg Health* applies AI to analyze metabolomics for early-stage safety insights | 16 |
| Clinical Trials | Streamlining recruitment and adaptive design | Identifies eligible patients via electronic health records (EHRs) and genomics; simulates trial outcomes; enables decentralized and adaptive trial protocols | *Deep6 AI* accelerates patient recruitment by mining EHR data; *Pfizer* used AI-driven trial design during COVID-19 vaccine development | 17 |
| Pharmacovigilance | Monitoring post-market safety and ADR detection | Analyzes structured/unstructured data (EHRs, social media, medical literature) to detect adverse drug reactions; improves reporting accuracy | *FDA's Sentinel Initiative* employs AI for safety signal detection; *MedAware* uses machine learning to prevent prescription errors | 18 |
| Supply Chain & Manufacturing | Automation, quality control, and logistics optimization | Employs predictive analytics to monitor production; detects defects in real time; manages supply chain disruptions and cold-chain storage | *Novartis* integrates AI for predictive maintenance in manufacturing; *UPS Healthcare* applies AI for vaccine cold-chain logistics | 19 |

**Table 3:** Applications of AI in Pharmacy Practice

| *Domain / Application* | *Role of AI* | *Key Features / Benefits* | *Case Studies / Examples* | *References* |
|---|---|---|---|---|
| Clinical Decision Support Systems (CDSS) | Assists clinicians in prescribing and treatment decisions | Provides evidence-based recommendations; detects drug–drug interactions; reduces medication errors | *IBM Watson for Health* supports oncology treatment decisions; *MedAware* prevents prescribing errors | 23 |
| Medication Adherence Monitoring | Tracks patient compliance and engagement | Uses smart pill dispensers, wearable devices, and predictive analytics to monitor adherence patterns | *Proteus Digital Health* integrates ingestible sensors with AI for real-time adherence tracking | 24 |
| Personalized Medicine / Therapy Optimization | Tailors drug dosing and treatment plans | Analyzes patient genetics, biomarkers, and lifestyle data to optimize efficacy and minimize adverse effects | *Tempus* uses AI for personalized oncology therapies; *GNS Healthcare* predicts optimal drug response using patient data | 25,26 |
| Chatbots / Virtual Assistants | Patient counseling and support | Provides medication information, reminders, symptom monitoring, and telehealth support | *Ada Health* and *Molly by Sensely* deliver AI-powered patient guidance | 27 |
| Predictive Analytics for Disease Management | Forecasts risk of disease progression or complications | Identifies high-risk patients and recommends preventive interventions | *BlueDot* AI predicts outbreaks; AI-driven diabetes management platforms optimize therapy | 28, 29 |
| Pharmacovigilance Integration | Real-time monitoring of adverse drug reactions in clinical practice | Analyzes EHRs and patient reports to detect early safety signals | *VigiBase* (WHO) enhanced with AI; *Aetion* uses AI to monitor real-world drug safety | 30 |
| Workflow Optimization in Pharmacy Operations | Automates dispensing, inventory, and resource allocation | Reduces human errors and operational costs; improves efficiency | *ScriptPro* and *Swisslog Healthcare* implement AI-driven automation in hospital pharmacies | 31, 32 |

## AI in Pharmacy education

Artificial intelligence (AI) is increasingly integrated into pharmacy education, enhancing both teaching methodologies and student learning experiences. Some applications of AI in education are presented in Figure 1 and Table 4 along with recent developments which include:

### *AI-Driven Virtual Patients*

Provide realistic clinical scenarios, adapt to student responses, and deliver personalized feedback to build diagnostic and critical thinking skills.[33]

### *Adaptive Learning Platforms*

Analyse student performance to customize content, address knowledge gaps, and improve learning outcomes.

### *Automated Assessment Tools*

Enable objective, timely evaluation of complex skills like clinical reasoning and communication.[34,35]

### *Curriculum Enhancement*

Use educational data to identify trends and optimize pharmacy curricula for modern healthcare needs.[36]

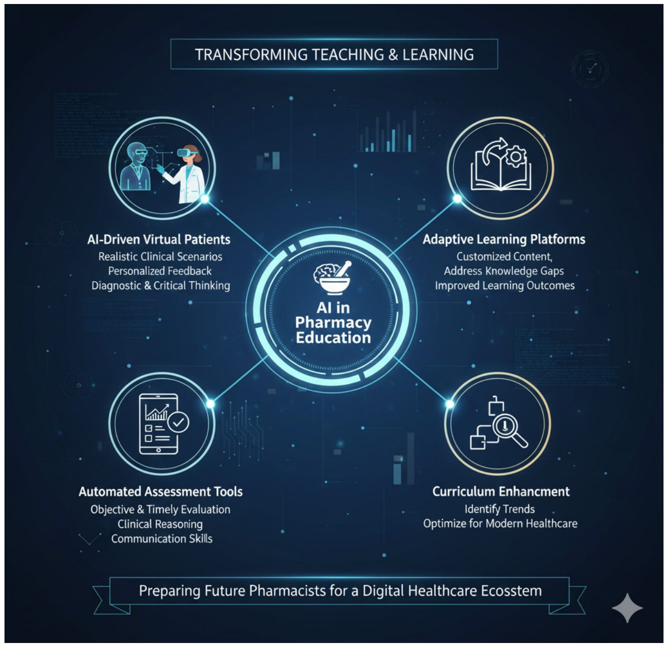


**Figure 1:** AI in Pharmacy education

## AI in Regulatory Science Beyond Explainability

Although explainable AI (XAI) has emerged as a promising solution for enhancing transparency, the broader regulatory ecosystem surrounding AI in pharmacy remains underexplored. Research is limited on regulatory sandboxes, adaptive approval pathways, and mechanisms for post-market surveillance of AI-based technologies. Comparative analyses of how agencies such as the FDA, EMA, CDSCO, PMDA, and WHO evaluate AI tools are still lacking, creating uncertainty regarding global harmonization.[46]

## Socio-Economic and Ethical Dimensions

While ethical challenges are acknowledged, the socio-economic implications of AI integration require deeper investigation. Concerns around equitable access in low- and middle-income countries, data ownership, privacy, and digital colonialism remain insufficiently addressed. Furthermore, the environmental sustainability of AI systems—particularly the high energy demands of large-scale model training—has yet to be adequately studied in the context of pharmaceutical research.[47]

## AI in Pharmacoepidemiology and Real-World Evidence (RWE)

The application of AI in analyzing large-scale healthcare data, including electronic health records and insurance claims, represents an underdeveloped domain. AI could significantly improve pharmacoepidemiological studies, post-marketing surveillance, and health economics evaluations, yet few systematic investigations exist. Standardized frameworks for validating AI-driven real-world evidence are also absent.[48]

## AI in Formulation and Advanced Drug Delivery Systems

Most current discourse centres on drug discovery and development, with minimal emphasis on formulation sciences. AI has the potential to optimize nanomedicine design, tailor personalized formulations, and accelerate 3D printing of drugs and drug-device combination products. However, research in this domain is nascent, leaving a substantial gap in leveraging AI for advanced pharmaceutical technologies. [49]

## Integration with Other Emerging Technologies

The synergistic application of AI with other disruptive technologies remains largely unexplored. Blockchain could enhance the traceability and security of pharmaceutical supply chains, while the Internet of Things (IoT) and wearable biosensors could enable continuous patient monitoring. Moreover, quantum computing holds potential to exponentially accelerate molecular simulations. These cross-technology integrations demand systematic academic and industrial investigation.[50]

## Workforce Transformation and Curriculum Standardization

Although AI integration into pharmacy education is progressing, a lack of globally standardized frameworks for AI-related competencies persists. Research into strategies for upskilling practicing pharmacists, who may not have received formal training in digital health technologies, is limited. Without structured workforce development programs, adoption barriers may increase, perpetuating digital divides within the profession.[51]

**Table 4:** Applications of AI in Pharmacy Education

| *Domain / Application* | *Role of AI* | *Key Features / Benefits* | *Examples / Case Studies* | *References* |
|---|---|---|---|---|
| Curriculum Transformation | Integrates AI, data science, and digital health into pharmacy education | Introduces students to machine learning, bioinformatics, digital therapeutics, and AI-driven decision support systems | Universities such as *University of California, San Francisco* and *King's College London* incorporate AI modules in pharmacy programs | 37, 38 |
| AI-Based Simulation and Virtual Labs | Provides immersive, interactive learning experiences | Simulates drug formulation, dispensing, and clinical scenarios; allows risk-free experimentation and skill development | *MyDispense* platform enables virtual pharmacy practice; *SimPharm* virtual lab for medication management | 39 |
| Personalized Learning with Adaptive AI Tutors | Tailors learning to individual student needs | Analyzes student performance data to provide customized feedback, adaptive quizzes, and targeted learning pathways | AI tutors integrated in platforms like *Coursera for Health* and *Smart Sparrow* | 40, 41 |
| Clinical Case-Based Learning | Enhances critical thinking and clinical decision-making | Uses AI-driven case studies and virtual patients to simulate real-world clinical challenges | *Body Interact* and *vSim for Pharmacy* platforms for interactive clinical education | 42 |
| Assessment and Feedback Automation | Optimizes evaluation and progress tracking | AI evaluates student performance on assignments, simulations, and exams; identifies learning gaps | *Gradescope* AI-assisted grading; *ExamSoft* with analytics for competency tracking | 43, 44 |
| Preparation for Digital Healthcare | Prepares students for AI-driven healthcare environment | Teaches integration of AI in clinical decision support, telepharmacy, and digital therapeutics | Curriculum examples at *University of Toronto* and *Monash University* emphasize AI competencies in pharmacy practice | 45 |

**Table 5:** Challenges and Limitations associated with AI

| *Category* | *Recent Developments (2024–2025)* | *References* |
|---|---|---|
| Data Issues | Recent studies highlight that AI medical tools often exhibit biases, downplaying symptoms in women and ethnic minorities, leading to under-treatment and misdiagnosis. These biases are largely attributed to the datasets used in training, many of which reflect societal stereotypes found online. Additionally, the accuracy of race and ethnicity data in electronic health records remains a significant concern, affecting the performance of AI systems across different patient groups. | 56 |
| Ethical & Legal Concerns | The integration of AI into healthcare raises significant ethical and legal challenges, including issues of autonomy, beneficence, non-maleficence, justice, transparency, and accountability. These concerns are particularly pressing as AI systems can perpetuate or even exacerbate existing biases, often resulting from non-representative datasets and opaque model development processes. Moreover, the potential benefits of AI must be balanced against legal-ethical issues such as bias, consent, access, privacy, and cost. | 57 |
| Regulatory Hurdles | The European Medicines Agency (EMA) has taken significant steps towards integrating AI into pharmacovigilance processes. In 2024, the EMA published tools and guidelines to incorporate AI into pharmacovigilance, emphasizing the importance of transparency, accessibility, validation, and monitoring of AI systems to ensure patient safety and data integrity. Similarly, the U.S. Food and Drug Administration (FDA) has released guidance on marketing submission recommendations for AI-enabled device software functions, focusing on transparency and predetermined change control plans. | 58 |
| Workforce Adoption | Healthcare organizations should invest in training and upskilling programs to prepare a workforce for the integration of AI into healthcare delivery. Additionally, a study conducted by Writer reveals that nearly half of surveyed executives feel that AI integration is leading to internal discord, with employees expressing concerns over job obsolescence and ineffective AI tools. These findings underscore the importance of addressing workforce readiness and support for AI adoption. | 59 |

## Health Economics and Cost-Benefit Analysis

The economic evaluation of AI adoption in pharmacy has not been comprehensively studied. Rigorous cost-benefit analyses are required to quantify return on investment, cost savings in R&D, and broader economic impacts on healthcare systems. Such evidence is essential for policy-makers and industry leaders to justify large-scale AI deployment.[52]

## Patient-Centric AI and Human–AI Interaction

Patient perceptions of AI-driven recommendations and their implications for trust and adherence have been underexplored. Issues of informed consent, transparency in patient–AI communication, and barriers related to digital literacy need empirical examination. Research on designing human–AI interactions that

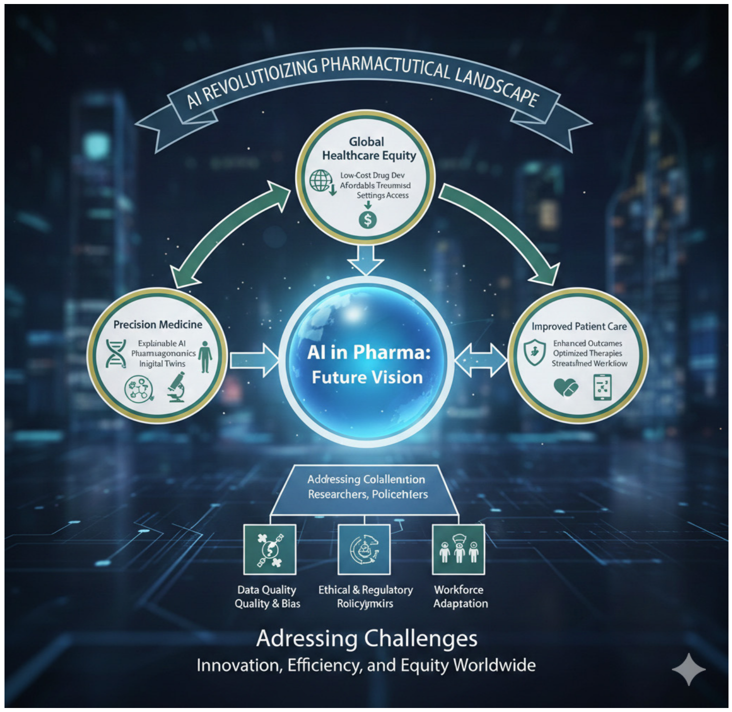


**Figure 2:** AI applications in Pharma and its Future Vision.

prioritize patient autonomy and shared decision-making is still in its infancy.[53]

## AI for Rare Diseases and Neglected Tropical Diseases

Current AI applications are disproportionately concentrated on oncology, cardiology, and other high-income country disease priorities. Limited research addresses the potential of AI in accelerating drug development for rare diseases, orphan drugs, and neglected tropical diseases. This gap highlights a pressing equity concern, as these therapeutic areas often lack commercial incentives for innovation.[54]

## Research Methodologies and Standardization

Finally, there is a need for methodological advancements to evaluate AI applications in pharmacy. The absence of standardized datasets, benchmarking protocols, and validation frameworks hampers the reproducibility and comparability of AI studies. Future research should focus on developing transparent, reproducible, and globally accepted methodologies to assess AI effectiveness and safety.[55]

### *Challenges and Limitations*

No technology is perfect. Here are few challenges and limitations of Artificial Intelligence along with recent developments in those field as presented in Table 5.

## Future Perspectives of AI in Pharmacy

### *Explainable AI (XAI) in Regulatory Approval*

Explainable AI is increasingly recognized as essential for regulatory compliance. By providing transparent and interpretable decision-making processes, XAI enhances trust among clinicians, regulators, and patients, facilitating smoother approval of AI-driven tools and therapeutics.[60]

### *Integration with Pharmacogenomics*

AI can analyze complex genomic datasets to predict individual drug responses, supporting personalized medicine. The integration of AI with pharmacogenomics enables tailored therapy regimens, reduces adverse drug reactions, and improves therapeutic efficacy.[61]

### *Digital Twins in Precision Health*

AI-powered digital twin models simulate patient physiology and disease progression, allowing clinicians to test treatment strategies virtually before clinical application. This approach improves patient outcomes, optimizes therapy selection, and reduces trial-and-error interventions.[62]

### *Global Healthcare Equity*

AI offers the potential to democratize access to medicines through low-cost drug discovery and development. AI-driven platforms can identify novel therapeutics efficiently, lower R&D costs, and provide affordable treatments in resource-limited settings, contributing to equitable healthcare delivery worldwide.[63]

### *Future Research and Collaboration*

Continuous collaboration between AI developers, pharmacists, clinicians, and regulators is essential to harness AI's full potential while addressing ethical, legal, and technical challenges.[64]

## Conclusion

Artificial intelligence (AI) has emerged as a transformative force across the pharmaceutical sciences, profoundly impacting drug discovery, development, pharmacy practice, and education as shown in Figure 2. In drug discovery, AI accelerates target identification, molecular design, virtual screening, and predictive modeling, thereby reducing costs and improving the efficiency of therapeutic innovation. During drug development, AI enhances preclinical testing, clinical trial design, pharmacovigilance, and manufacturing processes, supporting safer and more effective therapies. In pharmacy practice, AI-driven clinical decision support systems, personalized medicine platforms, adherence monitoring tools, and virtual assistants improve patient outcomes, optimize therapy, and streamline workflow. Simultaneously, AI is reshaping pharmacy education by integrating data science, virtual simulations, adaptive learning platforms, and AI also offer the potential to democratize access to medicines through low-cost drug discovery and development. AI-driven platforms can identify novel therapeutics efficiently, lower R&D costs, and provide affordable treatments in resource-limited settings, contributing to equitable healthcare delivery worldwide dictive analytics to prepare future pharmacists for a digital healthcare ecosystem. Despite these advances, challenges such as data quality, bias, ethical concerns, regulatory compliance, and workforce adaptation remain critical considerations. Looking ahead, explainable AI, integration with pharmacogenomics and digital twins, and AI-enabled low-cost drug development offer promising avenues for precision medicine and global healthcare equity. By addressing existing limitations and fostering collaboration among researchers, clinicians, and policymakers, AI has the potential to revolutionize the pharmaceutical landscape, driving innovation, efficiency, and improved patient care worldwide.

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