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REVIEW ARTICLE

Artificial intelligence in pharmacy and medicine: From drug discovery to patient care

Tha'er Ata[1]*, Israa Al-Ani[2]*, Derar H. Abdel-Qader[3], Rana Abu-Huwaij[1], Maisrh Ali Alrubaye[4], Enas Daoud[4], Iman Basheti[5], and Wael Abu Daiyyh[6]

[1]Department of Pharmacy, College of Pharmacy, Amman Arab University, Amman, Jordan

[2]Department of Pharmaceutical Sciences and Pharmaceutics, Faculty of Pharmacy, Middle East University, Amman, Jordan

[3]Department of Clinical Pharmacy and Pharmacy Practice, Faculty of Pharmacy and Medical Sciences, University of Petra, Amman, Jordan

[4]Pharmacological and Diagnostic Research Center, Faculty of Pharmacy, Al-Ahliyya Amman University, Amman, Balqa, Jordan

[5]Department of Doctor of Pharmacy, Faculty of Pharmacy, Jadara University, Irbid, Jordan

[6]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mutah University, Al Karak, Jordan

***Corresponding authors:**
Tha'er Ata
(t.atta@aau.edu.jo)
Israa Al-Ani
(i.alani@meu.edu.jo)

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Abstract

Artificial intelligence (AI) is increasingly reshaping the biomedical continuum, offering new capabilities from early discovery to patient care. This review explores current advances, starting with drug discovery, where AI aids in target identification, virtual screening, lead optimization, and prediction of pharmacokinetic and toxicological profiles, thereby reducing development costs and attrition rates. In preclinical and translational research, AI may support improvements in *in vitro–in vivo* correlations, physiologically based pharmacokinetic modeling, and the development of AI-assisted approaches that could complement selected animal studies. These applications may improve predictive reliability while also helping to address some ethical concerns related to preclinical evaluation. In clinical trials, AI may have a role in patient recruitment, adaptive trial design, dose prediction, and the analysis of real-world evidence. In clinical medicine and pharmacy practice, its use is also increasing across diagnostic support, clinical decision-making, pharmacovigilance, and supply chain management. These applications could improve the delivery of more personalized and accessible care, but this is not always straightforward, since the usefulness of AI depends on the quality of the available data, the validation process, and how the system is applied in real clinical settings. Several concerns, therefore, remain, particularly regarding transparency, algorithmic bias, data privacy, validation, and regulatory compliance. The review also discusses possible future directions, including precision medicine, digital twin technologies, and the integration of AI with emerging biotechnologies, while stressing the need for responsible, validated, and equitable use of AI in healthcare.

Keywords: Artificial intelligence; Pharmaceutical sciences; Drug discovery; Clinical trials; Diagnostics; Pharmacy practice; Precision medicine

1. Introduction

Artificial intelligence (AI) has rapidly emerged as one of the most transformative technologies in contemporary science and medicine.[1] Encompassing fields such as machine learning, deep learning, natural language processing, and reinforcement learning, AI enables the analysis of vast, complex datasets, uncovering patterns and relationships often inaccessible through traditional methods.[2] The integration of AI into healthcare and pharmaceutical sciences reflects a paradigm shift from empirical, experience-driven practices to predictive, data-driven approaches that accelerate discovery, optimize therapy, and personalize patient care.[3]

The pharmaceutical industry faces immense challenges that make it particularly amenable to AI-driven innovation.[4] Drug discovery and development are notoriously costly and time-consuming, often requiring more than a decade of research and billions of dollars to bring a single compound from laboratory to market.[5] Despite these investments, attrition rates remain high, with many candidates failing due to poor efficacy, unexpected toxicity, or unfavorable pharmacokinetics.[6] Beyond discovery, preclinical studies and clinical trials impose additional barriers that slow translation and inflate costs.[7] Traditional approaches, largely based on trial-and-error experimentation, are insufficient to meet the growing demand for safer, more effective, and more affordable medicines.[8] AI offers solutions to these inefficiencies by providing predictive models, generative tools, and decision-support systems that reduce uncertainty, shorten timelines, and enhance the probability of clinical success.[9]

In clinical medicine and pharmacy practice, the demand for precision, safety, and efficiency continues to grow as populations expand and healthcare systems become increasingly complex.[10] Physicians and pharmacists must interpret an ever-expanding volume of information, ranging from genomic data and electronic health records to diagnostic imaging and real-world patient behavior.[11] AI tools can integrate and interpret these datasets to support diagnosis, tailor treatments to individual patients, and monitor adherence and outcomes in real time.[12] At the same time, AI-driven platforms contribute to pharmacovigilance, supply chain management, and telehealth, further broadening their impact across the healthcare ecosystem[13].

Despite these advances, the integration of AI into pharmacy and medicine is accompanied by critical challenges.[14] Issues of algorithm transparency, data privacy, regulatory acceptance, and professional trust must be addressed to ensure safe and equitable adoption.[15] Ethical dilemmas, particularly regarding bias in training data and accountability in clinical decision-making, remain unresolved.[16] Furthermore, disparities in infrastructure and access risk widening global health inequalities if AI-enabled tools remain concentrated in high-resource settings.[17] These challenges highlight the importance of balanced progress, where innovation is guided by ethical, legal, and societal considerations.[18]

This review presents a comprehensive analysis of the role of AI across the pharmaceutical and medical continuum. It first examines the applications of AI in drug discovery and preclinical research, then discusses its involvement in clinical trials, diagnostics, therapy personalization, decision support, and pharmacy practice. The review also considers the regulatory, ethical, and practical barriers that need to be addressed for successful implementation. Finally, future perspectives are discussed, including digital twins, precision medicine, and the integration of AI with emerging biotechnologies. By bringing together developments from these different areas, the review highlights the potential of AI to transform healthcare, while also emphasizing the responsibilities required for its safe and effective use.

Although the main aim of this review is to provide a broad synthesis of AI applications across the biomedical continuum, from drug discovery to patient care, it is guided by a central analytical question: to what extent has AI moved from being mainly a theoretical and experimental tool to becoming a practical and value-adding component within the pharmaceutical pipeline and clinical workflow, and what barriers still limit its full implementation? This question provides the conceptual framework for the review and allows a critical assessment of the current maturity of AI across different stages of pharmaceutical and clinical development, as well as its readiness for wider integration. From this perspective, the discussion not only summarizes the available evidence but also evaluates the translational progress, remaining limitations, and possible future directions of AI in pharmaceutical science and clinical medicine.

2. Methodology

This review used a narrative approach to synthesize the growing body of literature on AI in pharmaceutical science and clinical medicine.

2.1. Literature search strategy

A structured but flexible literature search was performed using PubMed, Scopus, ScienceDirect, and Google Scholar. Publications from 2021 to 2025 were included to ensure that the most current research and recent developments were covered. Search terms were constructed using keywords

and Boolean operators, namely ("AI" OR "machine learning" OR "deep learning") AND ("drug discovery" OR "clinical trials" OR "pharmacy practice" OR "diagnostics" OR "precision medicine").

2.2. Inclusion and exclusion criteria

Included studies were those that:

- Reported applications, evaluations, or methodological developments of AI in any stage of pharmaceutical or medical processes.
- Peer-reviewed articles, reviews, or high-quality conference papers published in English.
- Sufficient methodological transparency or results to support interpretive analysis.

Excluded works were non-peer-reviewed materials, commentaries lacking empirical evidence, or reports unrelated to pharmaceutical or clinical contexts.

2.3. Data extraction and analysis

Extracted data mainly focused on the context in which AI was applied, the type of algorithm or model used, the reported therapeutic or operational outcomes, and the main challenges identified in each study. A quantitative meta-analysis was not performed. Instead, a narrative approach was used to compare the available evidence and to show how AI tools may help connect experimental design, translational development, and patient-centered outcomes. The included studies were then grouped thematically into four main domains: drug discovery, preclinical and translational research, clinical trials, and clinical medicine and pharmacy practice.

3. Artificial intelligence in drug discovery and development

Drug discovery and development are still considered among the most resource-intensive and high-risk stages in the pharmaceutical pipeline.[1] In general, bringing a single drug candidate from the early concept stage to regulatory approval may take around 10 to 15 years, with total costs often reaching billions of dollars.[19] Even with this large investment of time and money, almost 90% of compounds that enter clinical trials fail before reaching the market.[20] This high attrition is usually related to limited therapeutic efficacy, unexpected toxicity, poor pharmacokinetic behavior, or more than one of these factors occurring together. As a result, the process remains inefficient, delays the introduction of needed therapies, and adds further pressure to the rising cost of healthcare.[21]

Artificial intelligence has been increasingly explored as a tool that may help address some of these long-standing problems.[22] By integrating machine learning, deep learning, and natural language processing, AI enables rapid analysis of vast chemical and biological datasets, uncovering patterns and relationships previously undetectable with conventional methods.[23] In the earliest stages, AI accelerates molecular discovery by identifying novel druggable targets and predicting compound–target interactions with high accuracy[24]. It also supports virtual screening of immense chemical libraries, significantly reducing the need for resource-intensive laboratory assays.[25] Beyond discovery, AI contributes to lead optimization by predicting absorption, distribution, metabolism, excretion, and toxicity (ADME/Tox) properties, allowing unsuitable candidates to be eliminated earlier in the pipeline.[26,27]

The use of AI in drug discovery may therefore reduce some of the time and cost associated with early development and improve the prioritization of candidates with a better expected efficacy and safety profile.[28] As shown in Figure 1, conventional drug development typically takes 10–15 years and requires substantial financial investment, while nearly 90% of candidates entering clinical development do not reach the market. AI-enhanced workflows may help improve early decision-making and candidate selection, although they should not be viewed as removing the risk of failure completely.

3.1. Target identification and validation

The earliest and perhaps most critical step in drug discovery is the identification and validation of therapeutic targets.[29] These targets are most often proteins, enzymes, or nucleic acids that play a central role in disease mechanisms and can be modulated to restore normal physiological function.[30] Conventional approaches, such as hypothesis-driven biology or high-throughput screening of protein libraries, are laborious, costly, and limited in their ability to reveal novel or unexpected targets.[31] These methods often focus on well-characterized pathways, leaving many disease-related mechanisms underexplored.[32]

Artificial intelligence has emerged as a transformative approach that integrates diverse "multi-omics" datasets, including genomics, transcriptomics, metabolomics, and proteomics, to uncover previously hidden associations between molecular pathways and disease phenotypes.[33] Machine learning algorithms can map vast networks of protein–protein interactions, while deep learning models can recognize structural motifs within proteins that suggest druggability.[34] At the same time, natural language processing applied to biomedical literature and clinical trial repositories accelerates the discovery of drug–gene–disease relationships by mining thousands of articles in a fraction of the time required by traditional review.[35]

Taken together, these approaches may help AI identify

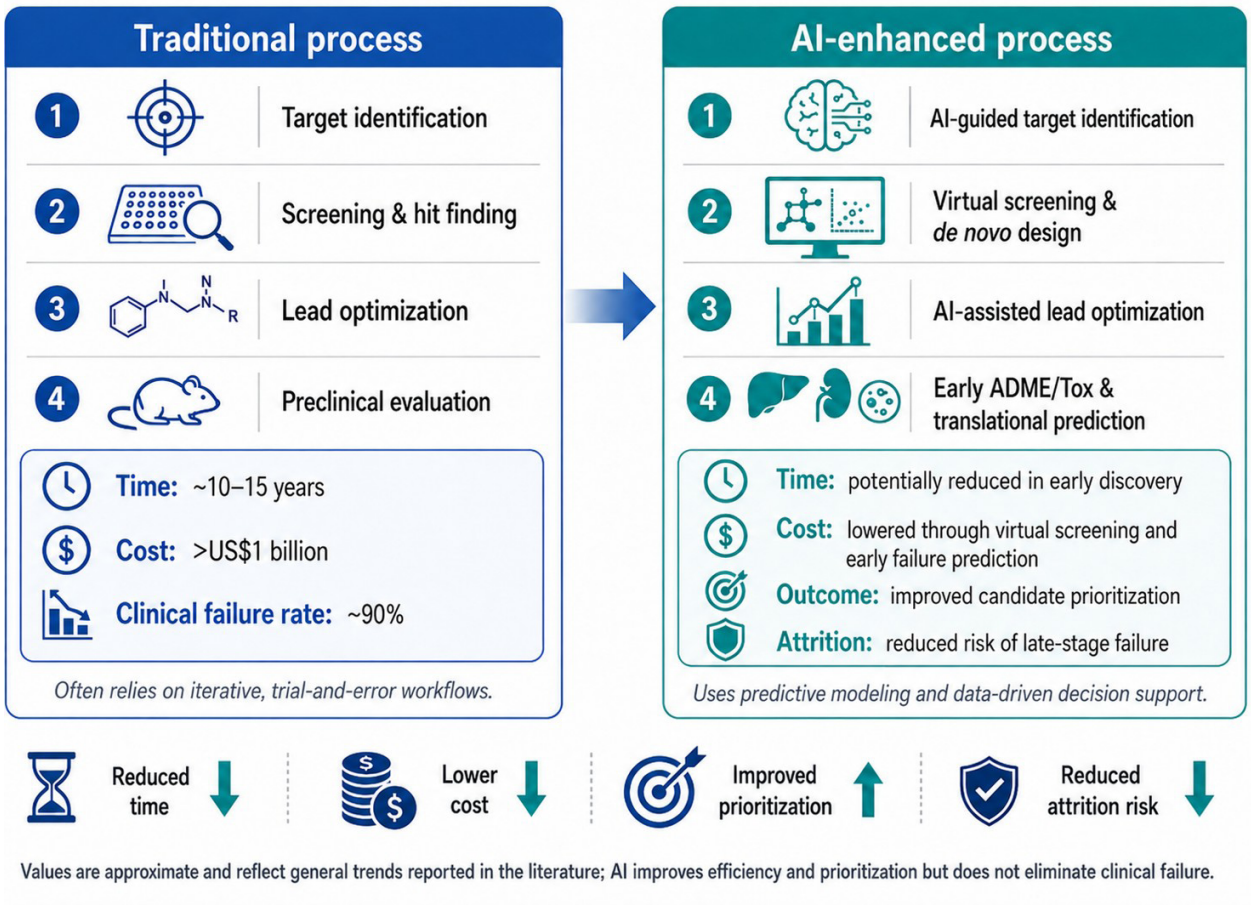

Figure 1. Comparison between the traditional drug discovery process and an AI-enhanced approach. AI may help reduce time and costs, improve candidate prioritization, and lower the risk of attrition during early drug development.
Abbreviations: ADME/Tox: Absorption, distribution, metabolism, excretion, and toxicity; AI: Artificial intelligence.

a wider range of possible therapeutic targets.[36] This is not limited to the usual protein targets. It may also include non-coding RNAs, epigenetic regulators, and microbial genes that have a role in host–pathogen interactions. Target validation is another area where AI can be useful, although it is still not a complete substitute for experimental confirmation. Predictive models may provide an early indication of whether changing a candidate target is likely to yield a useful therapeutic effect, and whether this could be associated with unacceptable toxicity.[37] Therefore, AI can support target selection in a more data-based way, but the final value of these predictions still depends on biological validation and clinical relevance.[38]

3.2. Virtual screening and hit identification

After a promising target has been validated, the next step is usually to identify small molecules that can interact with it in a useful pharmacological way.[39] Traditionally, this step has relied mainly on virtual screening and molecular docking. Docking methods estimate how a molecule may fit within a protein binding site and interact with key amino acid residues.[40] Although these methods are useful, they can be computationally demanding, especially when very large compound libraries are screened. Their predictions are also not always consistent with experimental results. For this reason, many compounds selected through docking do not show the expected activity when tested *in vitro* or *in vivo*.[41]

Artificial intelligence may help improve this stage by supporting large-scale screening and, in some cases, the design of new chemical structures.[42] Deep generative models, including variational autoencoders and generative adversarial networks, can be used to generate molecular structures with predicted binding affinity, acceptable

pharmacokinetic properties, and suitable drug-likeness features.[43] This means that the search is not limited only to existing chemical libraries. Instead, these models may propose new candidate molecules that are designed around the selected target, although their activity and safety still need to be confirmed experimentally.[44]

Artificial intelligence-based quantitative structure–activity relationship (QSAR) models are also increasingly used at this stage.[45] Compared with classical QSAR approaches, newer AI models may provide better predictions of biological activity, especially when trained on large, well-curated datasets. These models can combine chemical descriptors, molecular fingerprints, and biological assay data to rank candidate compounds before synthesis and experimental testing.[46] In practice, some AI systems can screen very large chemical spaces in a relatively short time, including libraries containing billions of molecules. This would be much slower using only conventional computational or laboratory-based methods[47] (Figure 2).

This faster screening process may reduce some early development costs and help researchers focus on candidates that appear more promising.[48] Table 1 compares traditional and AI-supported approaches in early drug discovery, including target identification, virtual screening, and hit selection. It also shows how data-based tools may improve decision-making at these early stages, although experimental confirmation remains necessary.

It should be emphasized that AI-based prediction does not replace experimental validation. Candidate molecules identified through QSAR models or generative chemistry approaches must still undergo chemical synthesis, *in vitro* biological testing, *in vivo* evaluation, and regulatory assessment before clinical translation.

3.3. Lead optimization and molecular design

Once the first hit compounds are found, they usually need further optimization before they can be considered as stronger candidates. In this step, the chemical structure is adjusted to improve activity, selectivity, and pharmacokinetic behavior, while trying to reduce off-target toxicity.[49] Traditionally, this phase is one of the most resource-intensive, involving repeated cycles of chemical synthesis, biological testing, and incremental adjustments to molecular scaffolds.[50] Despite extensive effort, this iterative approach often results in late-stage failures when optimized compounds fail to translate successfully into clinical settings.[51]

Artificial intelligence has introduced a paradigm shift in lead optimization by employing predictive modeling and intelligent search techniques to explore chemical space more efficiently.[52] Reinforcement learning and Bayesian optimization methods allow algorithms to balance

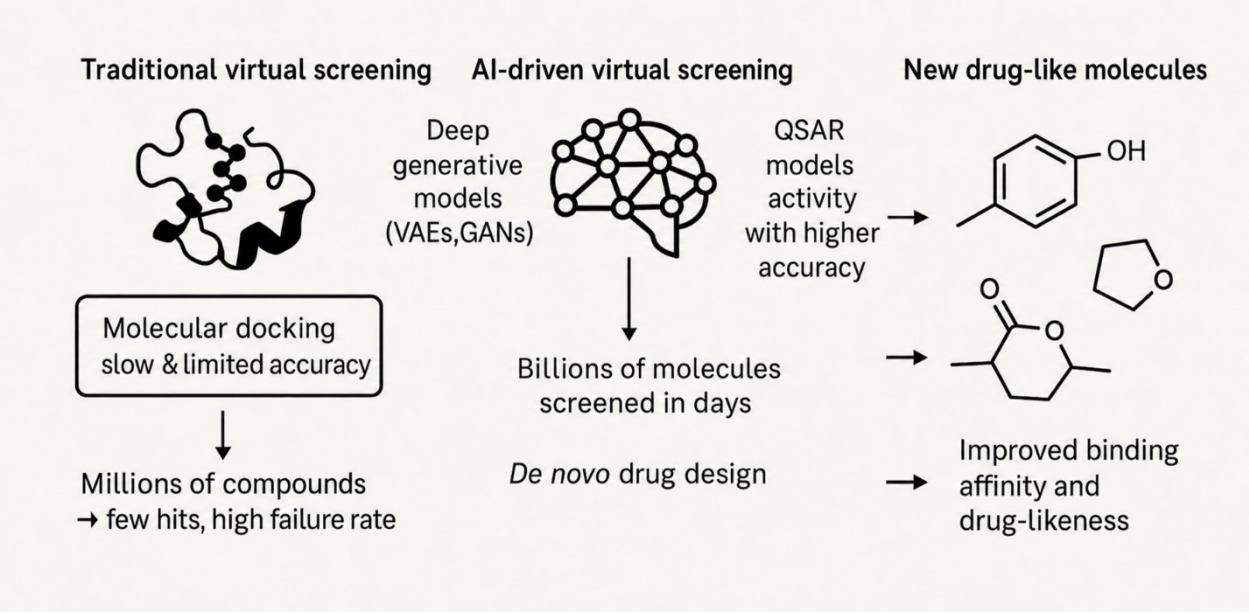

Figure 2. AI transforms virtual screening by moving beyond docking to large-scale screening
Abbreviations: AI: Artificial intelligence; GANs: Generative adversarial networks; QSAR: Quantitative structure–activity relationship; VAEs: Variational autoencoders.

Table 1. Traditional versus artificial intelligence (AI)-driven drug discovery approaches

Stage	Traditional approach	AI-driven approach	Key advantages
Target identification	High-throughput screening and conventional bioinformatics	Multi-omics integration with machine learning/deep learning and natural language processing-based literature mining	Faster identification of potential and novel targets
Virtual screening	Docking-based screening of limited compound libraries	AI-assisted virtual screening and *de novo* molecular design	Larger chemical-space exploration and faster hit prioritization
Hit identification	Empirical synthesis followed by biological testing	Quantitative structure–activity relationship-based activity prediction and generative models to prioritize compounds before experimental validation	Lower experimental burden, improved candidate ranking, and more focused synthesis/testing

multiple objectives simultaneously, such as improving solubility while preserving potency and ensuring metabolic stability.[53] By leveraging these models, structural modifications can be guided toward combinations of properties that maximize therapeutic potential rather than being driven by trial and error.[54]

Deep generative models further extend this capability by designing novel analogs of promising hits that maintain essential pharmacophores while introducing structural diversity.[55] This approach enhances the chances of identifying molecules with improved activity profiles and lower toxicity.[56] AI also supports predicting ADME/Tox properties during optimization, ensuring that compounds likely to fail in later stages are deprioritized early.[57]

As a result, lead optimization cycles that previously required months of laboratory work can be condensed into weeks, with fewer experimental iterations and higher overall success rates.[58] The integration of AI into this stage is therefore central to modern drug discovery, providing a powerful bridge between virtual screening and preclinical evaluation.[59]

3.4. Prediction of pharmacokinetics and toxicology

Failures in late-stage drug development are frequently attributable to unfavorable pharmacokinetic or toxicity profiles that were not identified earlier in the pipeline.[20] These failures are expensive and may also create safety concerns, especially when a compound reaches advanced clinical trials before its limitations are clear.[60] AI may help at the preclinical stage by predicting ADME/Tox properties before full experimental testing.[61] Machine learning and deep learning models trained on experimental and clinical datasets can give an early indication of whether a compound is likely to have poor ADME/Tox behavior.[62] These predictions are useful for prioritizing candidates, but they still need experimental confirmation.

One of the key contributions of AI in this domain is the prediction of drug absorption and bioavailability.[63] Algorithms can anticipate whether a compound will permeate biological membranes, cross the blood–brain barrier, or be absorbed in the gastrointestinal tract, providing valuable insights for oral and central nervous system drug candidates.[64] Similarly, AI models enhance the prediction of drug distribution by estimating tissue partitioning and plasma protein binding, which are critical for understanding drug exposure and therapeutic windows.[65] In metabolism, AI-driven platforms predict interactions with cytochrome P450 enzymes, allowing early detection of potential drug–drug interactions and metabolic liabilities.[66] Predictions of renal clearance and biliary excretion further improve understanding of elimination pathways.[67]

Toxicity prediction is perhaps the most critical and impactful application of AI in this space.[68] Deep learning models trained on toxicogenomic and clinical datasets can detect signals of hepatotoxicity, cardiotoxicity, and immunotoxicity with high sensitivity.[69] For example, predictive models of hERG channel inhibition are essential in avoiding compounds with cardiac safety risks.[70] By incorporating toxicology insights early, AI reduces the number of unsafe candidates that progress into animal studies or clinical testing, saving time, costs, and ethical burden.[71]

In silico physiologically based pharmacokinetic (PBPK) models further enhance predictive accuracy by simulating drug behavior in virtual human systems.[72] When combined with AI, these models improve the extrapolation of *in vitro* findings into *in vivo* contexts, strengthening *in vitro–in vivo* correlations and bridging the translational gap.[73] Such hybrid approaches are particularly valuable for predicting human responses from limited preclinical datasets.[74]

3.5. Case studies and applications

The practical utility of AI in drug discovery is already evident in several high-profile examples.[75] DeepMind's AlphaFold has revolutionized protein structure prediction, enabling rational drug design at a pace and accuracy previously unattainable.[76] Insilico Medicine reported discovering a fibrosis drug candidate in less than 18 months, an achievement made possible by AI-driven generative chemistry. Exscientia has advanced AI-designed compounds for psychiatric disorders and oncology into clinical trials, demonstrating the clinical viability of this approach.[77] Furthermore, major pharmaceutical companies, including Pfizer, Novartis, and AstraZeneca, have established collaborations with AI startups to enhance their discovery pipelines.[78]

Artificial intelligence is useful in early drug discovery, mainly in target identification, virtual screening, and ADME/Tox prediction. However, its results depend strongly on the training data and on whether the model can still perform well when applied to new datasets. This point is important because limited or biased data may lead to predictions that look better than they really are. In some cases, the model may also miss rare toxicity signals. Therefore, AI can reduce part of the uncertainty in early development, but it cannot prevent failure in later stages. Its predictions should be used as supportive information before moving to preclinical and translational studies, where experimental validation is still required.

4. Artificial intelligence in preclinical and translational research

Preclinical studies serve as the bridge between discovery and clinical testing, providing the data required to assess the pharmacological activity, pharmacokinetics, and safety of new compounds.[79] This stage relies heavily on *in vitro* assays, animal models, and early pharmacokinetic studies, which are costly, time-intensive, and frequently limited in their ability to predict human outcomes.[80] The high rate of clinical trial failures reflects the persistent translational gap, whereby compounds that appear promising in preclinical settings fail to deliver efficacy or safety in human studies.[81] AI is reshaping this stage of development by improving predictions of pharmacokinetics and toxicity, enhancing *in vitro*-to-*in vivo* correlation (IVIVC), and supporting the development of ethical alternatives to animal testing.[82]

4.1. Enhancing the *in vitro*-to-*in vivo* correlation

Establishing a robust IVIVC is critical for translating preclinical findings into meaningful human outcomes. Conventional approaches depend on extensive validation with animal data, which is often poorly predictive. AI strengthens IVIVC by combining *in vitro* dissolution profiles with PBPK models to generate more reliable forecasts of human absorption, distribution, and bioavailability. Neural networks trained on historical datasets further improve correlations between laboratory assays and clinical performance, thereby reducing the need for exhaustive animal studies.

4.2. Potential alternatives and complementary approaches to animal testing

Although animal models remain an essential component of preclinical drug development and are generally required before progression to clinical trials, increasing attention has been paid to approaches that may reduce, refine, or partially replace selected animal experiments.[83] AI-enabled platforms, including organ-on-chip systems, three-dimensional (3D) bioprinted tissues, toxicogenomic models, and *in silico* disease simulations, offer promising complementary tools for improving the human relevance of preclinical testing.[84] For example, organ-on-chip systems combined with AI-driven imaging may support real-time monitoring of drug responses in human-relevant microphysiological environments. Similarly, AI can assist in optimizing 3D tissue models and predicting tissue-level responses with improved reproducibility.[85] Computational disease models may also provide early insight into disease progression and therapeutic effects. However, these approaches should currently be viewed as supportive rather than fully substitutive, as they still require experimental validation and regulatory acceptance.[86] Therefore, AI-enabled alternatives may contribute to the principles of replacement, reduction, and refinement, but they do not eliminate the need for animal testing in most translational drug development pathways.[87] Table 2 summarizes AI-enabled alternatives to traditional animal models.

5. Artificial intelligence in clinical trials

Clinical trials are costly and have a high risk of failure. Many drug candidates still fail during clinical evaluation, even after large investments in earlier stages. This may be related to poor patient recruitment, problems with dose selection, or safety findings that emerge only after human testing. The usual clinical trial model is also quite rigid and requires substantial time and resources. In many cases, promising preclinical results are not enough to achieve regulatory approval.[88] AI is being explored to support some parts of trial design and conduct.[89] It may help in finding eligible patients, adjusting trial designs, selecting doses, and monitoring patients during the study. These uses can improve some operational decisions in clinical development, but they still cannot remove the possibility of trial failure.[90]

Table 2. Artificial intelligence and emerging alternatives to animal testing

Alternative model	Artificial intelligence's role	Benefits
Organs-on-chips	Imaging analysis, biomarker prediction	Human-relevant, real-time monitoring
Three-dimensional bioprinted tissues	Optimization of design and response modeling	Personalized, reproducible outcomes
In silico disease models	Simulation of disease progression	Ethical, scalable, predictive
Toxicogenomics	Integration of transcriptomic data	Early biomarker detection

5.1. Patient recruitment and stratification

Finding eligible participants is still a major problem in many clinical trials. Slow recruitment can delay the study and may also reduce statistical power if the required sample size is not reached.[91] In many cases, recruitment depends on clinician referrals or registry databases, but these sources may not identify sufficient suitable patients within a reasonable time.[92] AI addresses this by mining electronic health records, integrating genomic data, and analyzing real-world patient characteristics to match individuals with specific trial eligibility criteria.[93] It may also give an early estimate of which patients are more likely to follow the protocol and continue in the study.[94] This is useful not only for recruitment, but also for patient stratification, especially in trials where molecular markers or specific clinical features are part of the selection process.[95]

5.2. Trial design and simulation

Many clinical trials are designed in a fixed way, which makes later changes difficult once the study has started. With AI-based tools, some trial decisions can be adjusted based on data collected during the study, including sample size, dose selection, or even selected endpoints.[90,96,97] Synthetic control arms are one example of this approach. In these designs, historical data are used to estimate part of the control response, which may reduce the need for a large placebo or control group.[98] Digital twins are another related tool. They use individual-level data to simulate possible patient outcomes and may help investigators judge the protocol before testing it in a real trial.[99] Overall, these methods can make trial planning more flexible and may reduce certain ethical concerns linked to placebo use, but they still depend on the quality and relevance of the data used.[100] Table 3 illustrates differences between conventional and AI-driven clinical trial processes.

5.3. Dose optimization and response prediction

Choosing the dose in early-phase trials is a sensitive step. The dose should be sufficient to demonstrate a potential therapeutic effect, but not expose participants to avoidable safety risks.[101] In many trials, dose selection is based on pharmacokinetic and pharmacodynamic modeling, followed by gradual dose escalation. This approach is useful, but it may still lead to doses that are too low to give a clear effect or too high for some participants.[102] AI may provide support here by integrating preclinical findings, genomic information, and early clinical data.[103] These data can help estimate dose–response patterns, predict dose-limiting toxicity, and guide dose selection based on patient factors such as age, genetics, and comorbidities.[104,105]

5.4. Monitoring and real-world data integration

Patient safety and treatment response need to be followed carefully during clinical trials. Traditionally, this has relied mainly on scheduled site visits and manual reporting, which may miss changes occurring between visits.[106] AI enhances monitoring through wearable devices, smartphones, and biosensors that collect continuous physiological and behavioral data.[107] When analyzed properly, these data may show early changes in patient status or possible adverse events, allowing investigators to respond earlier.[108] Real-world evidence can also be added from sources such as insurance claims, registries, and post-marketing surveillance.[109] Automated data cleaning and error detection further improve data integrity, ensuring more reliable trial outcomes.[110]

5.5. Regulatory and ethical considerations

Regulatory bodies such as the United States Food and Drug Administration and the European Medicines Agency have expressed growing interest in AI-enabled clinical trials, particularly in adaptive trial designs and synthetic control arms.[3,111,112] However, the integration of AI raises concerns regarding transparency, interpretability, and fairness.[113] Algorithms must be validated to ensure they do not introduce bias or disproportionately exclude underrepresented populations.[114] Furthermore, the use of electronic health data in recruitment requires careful attention to privacy and informed consent.[115] Addressing these issues is critical to gaining regulatory acceptance and maintaining public trust.[116] Table 4 provides examples of AI-driven clinical trial applications and their impact.

Artificial intelligence can speed up certain parts of clinical trials, especially recruitment and adaptive design.

Table 3. Traditional versus artificial intelligence-driven clinical trials

Aspect	Traditional approach	Artificial intelligence-driven approach	Advantages
Patient recruitment	Advertising, clinician referrals	Electronic health record mining, natural language processing-based eligibility matching	Faster, more precise, more diverse
Trial design	Fixed protocol, large control arms	Adaptive design, synthetic controls, digital twins	Flexible, ethical, cost-saving
Dose optimization	Manual pharmacokinetics/pharmacodynamics and toxicity assessment	Artificial intelligence-based modeling and predictive toxicology	Personalized, safer, more efficient
Monitoring	Periodic site visits	Continuous monitoring via wearables and sensors	Early detection of adverse events
Data integration	Manual and fragmented systems	Automated artificial intelligence-driven harmonization	Higher accuracy, real-time insights

Table 4. Case studies of artificial intelligence in clinical trials

Organization/tool	Application	Impact
Deep6 AI	Electronic health record mining for patient recruitment	Reduced recruitment time by over 50%
Exscientia	Artificial intelligence-designed compounds in Phase I/II trials	Shortened early development timelines
BenevolentAI	Rare disease trial design and patient matching	Improved patient targeting and outcomes
United States Food and Drug Administration (synthetic control arms)	Artificial intelligence-based virtual placebo groups	Reduced sample size, ethical benefits
Fitbit/Apple AI Tools	Wearable-based monitoring in decentralized trials	Continuous monitoring, better adherence

This does not mean that its use is free of problems. Electronic health record data, for example, may be incomplete or may reflect existing demographic and socioeconomic differences. If these data are used without careful checking, they can affect which patients are selected and how the trial outcomes are understood. For this reason, AI tools need human review and clear reporting of how the data and models were used. They may support trial planning, but they should not replace methodological judgment. The same concern applies as AI is introduced into clinical practice and pharmacy operations.

6. Artificial intelligence in clinical medicine and pharmacy practice

Artificial intelligence is now being used not only in research laboratories and clinical trials, but also in daily medical and pharmacy practice.[117] In routine care, it may support clinicians and pharmacists in tasks such as early diagnosis, therapy selection, medication management, and patient counseling.[118] For patients, these applications may appear through decision-support tools, digital health platforms, or systems that help monitor treatment and medication use. This shows that AI is gradually moving from a mainly research-based tool to a technology used in healthcare delivery, although its role still depends on proper validation and careful clinical use.[119]

6.1. Artificial intelligence in clinical diagnostics

Diagnosis is one of the areas where AI has been used early in healthcare, especially in medical imaging.[120] Deep learning and computer vision systems are now applied to different imaging methods, including computed tomography, magnetic resonance imaging, and mammography.[121] These systems can help detect abnormalities in images, and in some studies, their performance has been close to that of specialist radiologists. They may also be useful for finding small or early changes that are difficult to notice during routine image review.[122] Another use is image triage. AI tools can help prioritize urgent cases, such as stroke, pulmonary embolism, or intracranial hemorrhage, so that

they are reviewed more quickly in emergency settings[123,124] (Figure 3).

Pathology has also undergone substantial transformation through the adoption of AI-based digital pathology platforms.[125] By analyzing whole-slide images, AI models can classify tumor subtypes, quantify biomarker expression, and provide reproducible cancer grading, reducing inter-observer variability and enhancing diagnostic consistency.[125] These systems are also being combined with molecular and genomic data to enable integrated diagnostics, which not only provide histopathological assessments but also predict treatment response and patient outcomes with high precision.[126]

In dermatology, AI-powered image classifiers have emerged as effective tools for detecting malignant skin lesions, including melanoma, basal cell carcinoma, and squamous cell carcinoma.[127,128] Smartphone-based applications integrated with AI further extend diagnostic capabilities to patients themselves, offering rapid pre-screening in primary care or remote areas where dermatological expertise may be limited.[129] This democratization of diagnostic support has the potential to reduce disparities in skin cancer outcomes, especially in underserved populations.[130]

Cardiology has equally benefited from AI through algorithms that analyze electrocardiograms and echocardiograms.[131] These tools improve the early recognition of arrhythmias, such as atrial fibrillation, and provide accurate assessments of ventricular function, valve disorders, and heart failure risk.[132] Beyond static interpretation, AI-enabled wearable devices can continuously monitor cardiac activity, identifying silent arrhythmias or ischemic events in real time and alerting patients or clinicians before complications arise.[133,134]

Emerging applications of AI in diagnostics extend beyond imaging. In ophthalmology, deep learning systems have demonstrated high accuracy in detecting diabetic retinopathy, age-related macular degeneration, and glaucoma from retinal fundus photographs and optical coherence tomography scans.[135,136] Similarly, in gastroenterology, AI-assisted endoscopy improves polyp detection during colonoscopy, supporting early

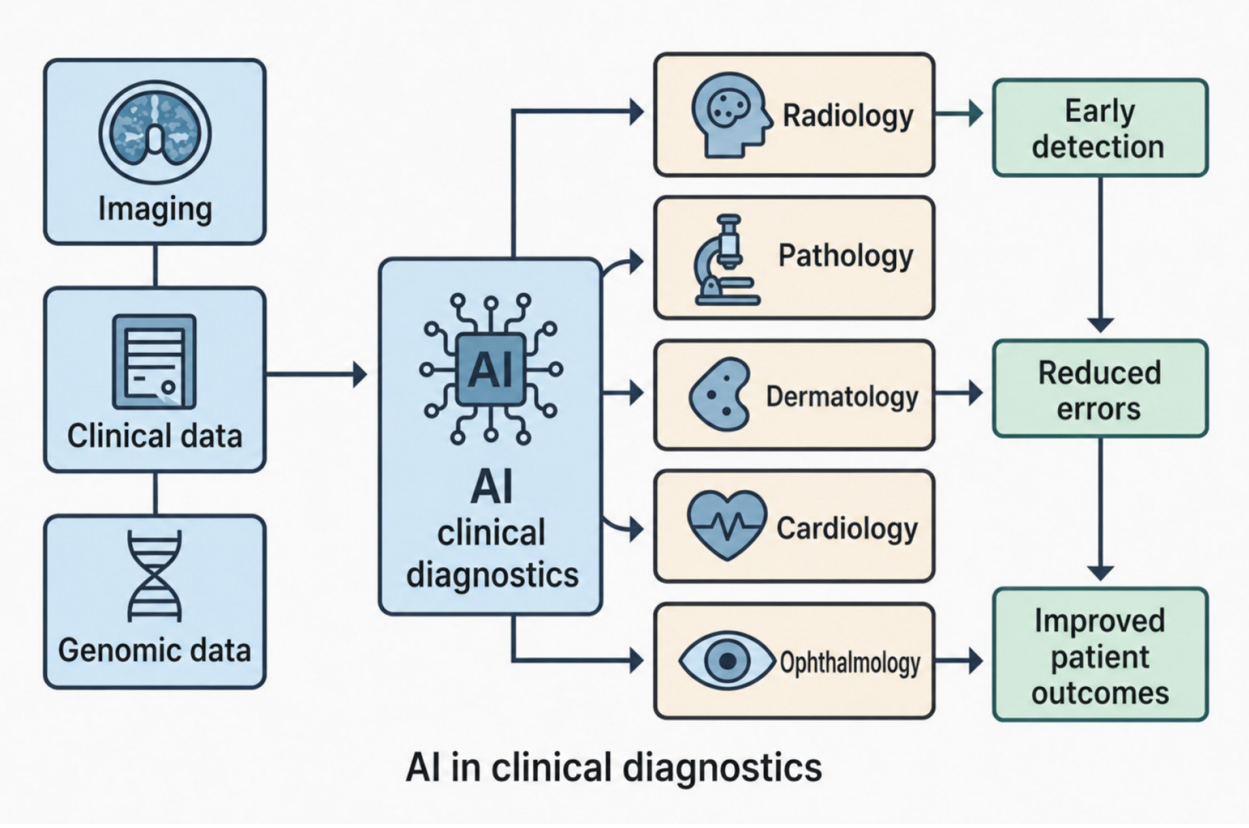

Figure 3. Flowchart showing how artificial intelligence (AI) uses imaging, clinical, and genomic data to support diagnostic specialties, leading to early detection, fewer errors, and better patient outcomes

identification of colorectal cancer.[137,138] In infectious disease diagnostics, machine learning models are being used to detect pathogens in microscopy slides, analyze sequencing data, and even predict antimicrobial resistance patterns, providing critical support in the fight against global health threats such as multidrug-resistant bacteria.[139,140]

Collectively, these advances enhance diagnostic speed, reduce human error, and expand access to expert-level analysis in resource-limited settings.[141,142] Importantly, AI is not intended to replace clinicians but to augment their expertise, functioning as a decision-support system that improves accuracy, efficiency, and patient outcomes.[143] As regulatory frameworks mature and validation studies continue to demonstrate safety and reliability, AI-enabled diagnostic systems are expected to become an integral component of routine clinical practice, reshaping the future of precision medicine.[15]

6.2. Artificial intelligence in decision support and pharmacy practice

Artificial intelligence is transforming both clinical decision-making and pharmacy practice, creating a unified ecosystem where patient safety, therapeutic effectiveness, and healthcare efficiency are enhanced simultaneously.[144,145] Rather than operating as separate domains, AI-driven decision support and pharmacy innovations now converge to provide clinicians and pharmacists with actionable insights that optimize care delivery across diverse healthcare settings.[146,147]

At the clinical level, AI-augmented decision support systems have progressed beyond static, rule-based alerts to highly adaptive, predictive platforms.[148] Embedded into electronic health records, they generate real-time safety warnings about drug–drug interactions, contraindications, dosing errors, and allergy risks.[149] Advanced predictive models can anticipate adverse clinical events, such as hospital readmission, sepsis, or medication-related complications, enabling early intervention before harm occurs.[150] In telemedicine, AI-powered chatbots and virtual assistants triage patients, deliver guideline-based recommendations, and support clinician–patient communication, reducing the administrative burden on providers while ensuring more consistent, standardized care.[151,152]

In parallel, AI is profoundly reshaping pharmacy practice, particularly at the intersection of medication management and patient engagement.[153] Predictive adherence algorithms identify patients at high risk of missing doses, empowering pharmacists to deliver timely interventions that improve therapeutic outcomes in chronic disease management.[154] In pharmacovigilance, AI mines vast amounts of data—from electronic health records and pharmacovigilance databases to social media platforms—to detect adverse drug reactions faster and more reliably than traditional methods. This strengthens drug safety monitoring and accelerates regulatory response.[155,156]

Artificial intelligence has a role in pharmaceutical supply chains, mainly in demand forecasting, inventory control, and detecting possible medicine shortages earlier. This can help keep essential medicines available during periods when healthcare services are under pressure. In clinical pharmacy, the same tools may also use patient-related data, such as age, renal function, and pharmacogenomic information, to support more individualized therapy selection, as shown in Figure 4. Telepharmacy is another example. It uses AI to assist with patient counseling, remote dispensing, and adherence follow-up, which may be useful for rural or underserved communities. These uses are promising, but they still require suitable infrastructure, reliable data, and pharmacist supervision.

Artificial intelligence can help bring some research findings into clinical decision-making and pharmacy practice, but its use is not straightforward. There are ethical and professional issues to consider. Predictive algorithms may be useful in diagnosis and drug safety monitoring, although their results depend heavily on the data used to build them. If the training data are incomplete, poor in quality, or biased, the output may not be appropriate for all patient groups. A further concern is that some AI models are difficult to interpret. Clinicians and pharmacists may not fully trust a recommendation if the system does not explain how it reached it. Because of this, professional review is still needed. Pharmacists and clinicians should assess whether the output makes clinical sense and fits the patient's situation. AI should be used to support clinical judgment, not to replace it.

7. Regulatory, ethical, and practical obstacles

7.1. Ethical challenges

The most urgent concerns are ethical in character, directly affecting the trust of clinicians, pharmacists, and patients.[157] A significant issue is the "black-box" dilemma, wherein numerous AI systems, particularly those utilizing deep learning, provide results without transparent explanations of the reasoning behind their conclusions.[158-160] This opacity contradicts the principles of medical decision-making, in which transparency and rationale are essential to ensure accountability and informed consent. In the absence of interpretability, even exceptionally accurate systems may be perceived as unreliable, hence constraining their use in clinical practice.[161,162]

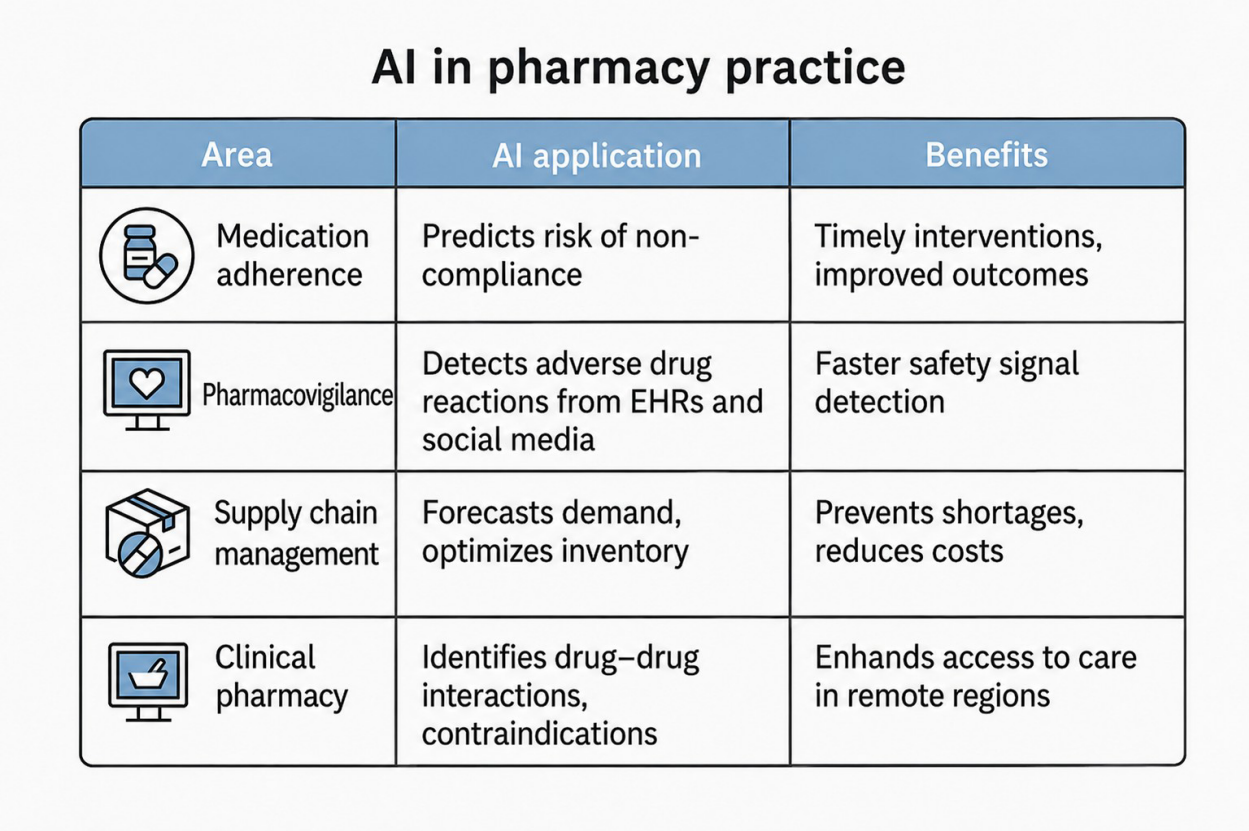

Figure 4. AI in pharmacy practice
Abbreviations: AI: Artificial intelligence; EHRs: Electronic health records.

Explainable artificial intelligence (XAI) has emerged as a key response to the "black-box" dilemma in modern AI systems.[163] Techniques such as Shapley additive explanations and local interpretable model-agnostic explanations enable users to understand how input variables—such as demographic or clinical parameters—affect algorithmic predictions, thus enhancing transparency and clinician trust.[164] These models are increasingly applied to identify biases and ensure fairness in predictive healthcare analytics.[165] Nevertheless, interpretability remains an evolving field; current XAI frameworks can oversimplify relationships or yield inconsistent explanations across models.[166] Consequently, while XAI tools represent a crucial step toward accountable and ethically aligned AI in medicine, they should complement—not replace—rigorous model validation and regulatory oversight.[167]

The matter of bias and equity is intricately connected to trust. If AI is trained on datasets that inadequately represent specific populations, its performance may differ markedly among demographic groups, thus sustaining or intensifying health inequities.[168,169] Diagnostic models created predominantly from data in affluent contexts may not generalize successfully to marginalized populations. Ensuring equity requires using diverse, representative training datasets and conducting continuous audits to detect and mitigate bias.[170,171] A further ethical dilemma pertains to data privacy and security. AI applications depend significantly on sensitive patient data obtained from electronic health records, wearable devices, and various digital sources.[172,173] The aggregation, retention, and examination of these extensive databases raise concerns about confidentiality, informed consent, and susceptibility to breaches.[174] An isolated data breach can undermine public confidence in both the technology and the healthcare organizations utilizing it.[175]

Issues of accountability remain unaddressed. When AI-assisted judgments result in negative consequences, accountability may be dispersed across developers, clinicians, healthcare organizations, and regulatory bodies.[176] In contrast to conventional medical errors, which carry more direct liability, AI presents additional complexities that necessitate explicit frameworks for

determining guilt and establishing legal accountability.

7.2. Regulatory challenges

The regulatory framework for AI in healthcare remains unclear and raises several ethical concerns.[177] One difficult issue is how to validate adaptive algorithms that continue to change when new data are added. This differs from conventional medicines or medical devices, which are usually expected to maintain stable performance once approved. AI systems may evolve over time, raising questions about how their long-term safety, efficacy, and clinical reliability should be evaluated.[178,179]

Regulators are usually cautious with AI systems that are hard to interpret. This is mainly because black-box models make it difficult to assess reliability, accountability, and the reason behind a given output.[180] Another problem is that regulatory rules differ between countries and regions. This can slow the broader adoption of AI in healthcare, especially when the same system requires approval in multiple settings. Clearer rules are needed, but they should also be flexible enough to accommodate AI systems that may evolve as new data become available.[181,182]

7.3. Practical challenges

Even if ethical and regulatory points are clarified, the use of AI in healthcare still faces practical barriers.[183] Many health systems, particularly in low- and middle-income countries, do not yet have the digital infrastructure needed to run advanced AI tools.[184] Another problem is the connection with existing electronic health records. In practice, systems often use different interoperability standards, and many platforms were not built to communicate smoothly with each other.[185,186]

Moreover, AI systems require ongoing retraining and updates to remain therapeutically relevant.[187] This procedure is resource-demanding, requiring financial commitment, technical proficiency, and continuous oversight to maintain quality.[188] These standards present considerable difficulties for underfunded or overextended healthcare systems.

Professional readiness is equally significant. Inadequate training may lead doctors and pharmacists to either underutilize AI due to a lack of confidence or to over-rely on it without thoroughly assessing its outcomes.[189,190] Workflow integration is crucial; if AI technologies complicate processes rather than simplify them, they may unintentionally increase workload rather than reduce it.[191,192]

Artificial intelligence technologies are often developed and used first in well-resourced settings. This may increase the risk that existing global health inequalities widen rather than narrow. For these tools to be useful in different healthcare systems, they need to be affordable, scalable, and accessible, not only available in high-income settings.[193,194]

8. Future perspectives

The use of AI in pharmaceutical science and clinical medicine is expected to increase in the coming years. Current applications of AI mainly focus on drug discovery, preclinical research, and support for clinical practice. In the coming years, its use may become more closely connected with precision medicine, real-world patient data, and emerging biotechnologies.[195] This transformation promises to redefine how drugs are discovered, manufactured, prescribed, and monitored, paving the way toward a healthcare system that is more predictive, personalized, and efficient.[196]

8.1. Artificial intelligence and precision medicine

Precision medicine is one of the main areas where AI may have an important role in the future. AI can combine different types of patient data, such as genomic, proteomic, metabolomic, and lifestyle information, to support more individualized treatment decisions.[197,198] In oncology, this may help match drug combinations with the molecular profile of the patient's tumor.[199] In chronic diseases, AI may also support treatment plans that evolve over time in response to patient behavior, disease status, or physiological changes. The aim is to move toward more individualized therapy, in which drug selection, formulation, and dose are adjusted more closely to each patient's needs.[200,201]

8.2. Digital twins and virtual clinical trials

Digital twin technology, which creates a virtual replica of a patient based on real-world physiological and clinical data, represents another transformative opportunity.[202] These models can simulate drug responses, predict adverse effects, and optimize treatment strategies without exposing patients to unnecessary risk. In the clinical trial context, digital twins may reduce the need for large control arms by generating virtual comparators, accelerating the evaluation of new drugs while lowering ethical and financial barriers.[203,204]

Despite their transformative potential, digital twin technologies remain in the early stages of practical implementation.[205] Major technical and regulatory barriers hinder their immediate translation into healthcare and pharmaceutical practice. On the technical side, creating physiologically accurate digital replicas requires vast, high-quality multimodal datasets that integrate genomic, clinical, imaging, and behavioral information—data that

are rarely standardized or interoperable across systems.[206] Moreover, ensuring continuous synchronization between the virtual and physical patient involves complex computational modeling and real-time data validation.[207] From a regulatory perspective, there are no universally accepted frameworks for evaluating or approving digital twin-based medical tools.[208] Concerns regarding patient data protection, model validation, and accountability further complicate their clinical adoption.[209] As a result, while digital twins represent an exciting frontier for personalized medicine and clinical trial innovation, their safe and reliable use will depend on significant advancements in data governance, model standardization, and regulatory oversight.

8.3. Integration with emerging biotechnologies

Artificial intelligence is likely to become more closely linked to gene editing, advanced nanomedicine, and regenerative therapies.[210,211] Machine learning is already being used in areas such as CRISPR guide RNA design, nanoparticle formulation for targeted delivery, and prediction of stem cell differentiation outcomes.[212] As these fields continue to develop, AI may help connect some of these approaches and support more integrated therapeutic strategies. This may be relevant for complex diseases that involve molecular and cellular changes. However, these applications still require careful validation before they can be used more widely in clinical practice.

8.4. Artificial intelligence in sustainable and equitable healthcare

Sustainability and equity will become central themes in the future deployment of AI. The pharmaceutical industry faces growing pressure to adopt environmentally responsible manufacturing practices, and AI can contribute by minimizing waste, improving process efficiency, and supporting green chemistry approaches.[213,214] At the same time, ensuring equitable access to AI-driven healthcare remains a critical priority. Without deliberate strategies, the benefits of AI may disproportionately favor high-resource settings.[215] Future frameworks must therefore emphasize the global distribution of AI-enabled tools to reduce, rather than widen, health disparities.[216]

9. Conclusion

Artificial intelligence is no longer a peripheral innovation in pharmacy and medicine; it is becoming an important component of the modern biomedical continuum, from early drug discovery to patient-centered care. The evidence reviewed in this article shows that AI can support target identification, virtual screening, lead optimization, pharmacokinetic and toxicological prediction, preclinical modeling, clinical trial design, diagnostic support, pharmacovigilance, supply chain management, and individualized therapy. Its greatest value lies in its ability to analyze complex datasets, identify patterns that may be missed by conventional approaches, and support faster and more informed decisions. However, the practical impact of AI depends not only on technical performance, but also on clinical relevance, reproducibility, transparency, and appropriate human oversight. AI should therefore be viewed as a complementary tool that strengthens the work of researchers, clinicians, and pharmacists, rather than as a repl

For AI to deliver its full potential, future implementation must be guided by strong validation standards, explainable models, representative datasets, data privacy safeguards, and clear regulatory pathways. Particular attention is needed to prevent algorithmic bias, ensure equitable access across different healthcare settings, and maintain accountability when AI-assisted decisions influence patient outcomes. If these challenges are addressed responsibly, AI has the potential to improve the efficiency of pharmaceutical development, reduce late-stage failure, enhance treatment personalization, strengthen medication safety, and expand access to high-quality care. The central message of this review is that the future of AI in pharmacy and medicine will depend on balanced integration: innovation must be matched with ethical governance, rigorous evidence, and sustained professional involvement. Under these conditions, AI can move from a promising analytical technology to a trusted and value-adding partner across

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Author contributions

Conceptualization: Tha'er Ata, Israa Al-Ani
Data curation: Tha'er Ata, Israa Al-Ani, Derar H. Abdel-Qader
Formal analysis: Tha'er Ata, Maisrh Alrubaye, Enas Daoud
Methodology: Tha'er Ata, Derar H. Abdel-Qader, Rana Abu-Huwaij
Project administration: Tha'er Ata, Israa Al-Ani
Supervision: Israa Al-Ani
Writing–original draft: Tha'er Ata, Israa Al-Ani
Writing–review & editing: All authors

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