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Review Article

Artificial Intelligence in Pharmaceutics: Current Applications, Methodological Challenges, and Translational Potential—A Review

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Abstract

Background: Artificial intelligence (AI), designed to emulate human cognitive processes, has rapidly become an integral component of contemporary pharmaceutical research. Advances in machine learning (ML) and deep learning (DL) have significantly enhanced efficiency across the drug development pipeline, including target identification, formulation design, and drug delivery optimization.

Objective: This systematic review aims to synthesize recent evidence on the application of AI in pharmaceutical technology and drug delivery design, with particular emphasis on drug discovery, dosage form optimization, manufacturing processes, and pharmacokinetic/pharmacodynamic (PK/PD) modeling.

Methodology: A systematic literature review was conducted in accordance with PRISMA 2020 guidelines. Peer-reviewed studies examining AI-driven approaches in pharmaceutics were identified, screened, and analyzed, focusing on their methodological frameworks, applications, and reported outcomes.

Results: AI-based systems enabled the analysis of large-scale genomic, proteomic, and chemical datasets, facilitating the identification of disease-relevant biomarkers and potential drug candidates. Modeling and simulation approaches improved preclinical predictions of pharmacokinetics, pharmacodynamics, and toxicity, supporting candidate prioritization and experimental design. Applications were particularly prominent in antitumor drug discovery, formulation optimization, manufacturing process enhancement, and PK/PD modeling. Despite these advances, significant challenges persist, including data bias, limited model interpretability, insufficient external validation, and regulatory uncertainty.

Conclusion: AI offers substantial opportunities for automation, precision, and innovation in pharmaceutical sciences. However, addressing methodological limitations, improving transparency, and establishing ethically guided and regulatory-compliant AI frameworks are essential for successful clinical translation. Continued interdisciplinary collaboration will be critical to the safe and effective integration of AI into pharmaceutical technology and drug delivery systems.

Keywords: Artificial Intelligence, Deep Learning, Drug Discovery, Drug Delivery Systems, Machine Learning, Pharmaceutical Technology, Pharmacokinetics, Pharmacodynamics.

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Introduction

The rapid digital transformation of the pharmaceutical sector has intensified the need to integrate artificial intelligence (AI) tools across drug discovery, formulation optimization, and drug delivery design [1,2]. As a cornerstone of global healthcare, the pharmaceutical industry must continuously adopt innovative technologies to address evolving health challenges, including the recent surge in large-scale medical emergencies [3]. In response, contemporary pharmaceutical research increasingly emphasizes computational modeling and AI-driven analytics to enhance formulation design, manufacturing efficiency, and decision-making throughout the drug development pipeline.

The development of diverse pharmaceutical products including small-molecule drugs and biologics requires achieving an optimal balance between stability, potency, and safety to meet therapeutic demands. Among the most persistent challenges in preclinical development is the accurate assessment of toxicity and pharmacological safety. AI-based predictive modeling has emerged as a promising approach to address these challenges by enabling data-driven toxicity prediction, reducing reliance on trial-and-error experimentation, and improving early candidate screening [4].

Beyond drug development, AI-driven predictive analytics are increasingly being explored to mitigate post-pandemic challenges such as supply chain disruptions, logistics inefficiencies, and demand forecasting uncertainties [5]. Pharmaceutical companies are actively seeking innovative and disruptive AI-enabled supply chain models to build more resilient and adaptive business frameworks [6]. Several studies have highlighted that the COVID-19 pandemic substantially disrupted pharmaceutical operations, with clinical trials, manufacturing timelines, and distribution networks among the most affected domains [7].

Supply chain disruptions arise from multiple interconnected factors, including pandemics, natural disasters, price volatility, cybersecurity threats, transportation delays, and interruptions in raw material availability. Transportation bottlenecks became particularly pronounced during the COVID-19 pandemic, significantly impacting pharmaceutical supply chains worldwide and exerting pressure on both economies and healthcare systems [8]. Price variation delays often caused by uncertainty in supplier pricing updates further complicate procurement and inventory planning. Additional challenges stem from evolving cross-border trade regulations, increased criminal activity, and fluctuations in access to essential manufacturing and operational resources. These factors collectively influence infrastructure planning, manufacturing footprint requirements, regulatory compliance, and the industry's ability to meet patient needs effectively.

Beyond logistics and operations, AI demonstrates transformative potential across drug design, formulation development, and advanced drug delivery systems. Over the past decades, AI-based approaches have been increasingly investigated for their ability to generate integrated solutions to complex pharmaceutical challenges, including interconnected supply chain management and evidence-based decision support [5]. Moreover, these advances open new avenues for future research aimed at developing intelligent, adaptive, and sustainable pharmaceutical ecosystems.

In this context, the present study systematically reviews recent advances in AI-driven pharmaceutical technology and drug delivery design, with a focus on emerging applications, current limitations, and future research directions.

Methodology

Eligibility criteria

This systematic review included peer-reviewed original research articles published between January 2020 and June 2025 that investigated the application of artificial intelligence (AI), machine learning, or deep learning in pharmaceutical technology, drug design, formulation development, or drug delivery systems. Eligible studies were required to report empirical findings, computational modeling, predictive analytics, or validated AI-based frameworks relevant to pharmaceutical sciences. Studies focusing on non-pharmaceutical or non-biomedical applications of AI were excluded. Conference abstracts, editorials, commentaries, letters to the editor, review articles, and non-peer-reviewed publications were also excluded to ensure methodological rigor and data reliability.

Information sources

A comprehensive literature search was conducted across major electronic databases, including PubMed, Scopus, Web of Science, IEEE Xplore, ScienceDirect, and SpringerLink. These databases were selected to ensure broad coverage of biomedical, pharmaceutical, and computational research. The search period spanned from January 2020 to June 2025 to capture recent and relevant advances in AI-driven pharmaceutical research.

Search strategy

The search strategy employed predefined Boolean operators and controlled vocabulary terms tailored to each database. The primary search string consisted of combinations of AI-related and pharmaceutical-related keywords: ("Artificial Intelligence" OR "Machine Learning" OR "Deep Learning" OR "Neural Networks" OR "Computational Modeling") AND ("Pharmaceutical Technology" OR "Drug Delivery" OR "Drug Design" OR "Dosage Form" OR "Pharmacokinetics" OR "Pharmacodynamics"). Variations and database-specific indexing terms were applied to maximize retrieval sensitivity while maintaining relevance.

Selection process

All retrieved records were exported into Zotero reference management software for organization and duplicate removal. Following de-duplication, titles and abstracts were independently screened for relevance to the study objectives. Full-text articles were then assessed for eligibility based on the predefined inclusion and exclusion criteria. Discrepancies during the screening process were resolved through consensus discussion. The study selection process adhered to the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2021)[9] guidelines.

Data collection process

Data extraction was performed using a standardized data collection form designed to capture essential methodological and outcome-related information from each included study. Extracted data included study objectives, AI methodology, pharmaceutical application domain, datasets used, validation approaches, and key findings. Data extraction was cross-checked to ensure consistency and accuracy across studies.

Data items

Key data items extracted from each study comprised study design, AI model type, pharmaceutical application area (e.g., drug discovery, formulation optimization, pharmacokinetics/pharmacodynamics modeling, or drug delivery), input data sources, performance metrics, validation techniques, and reported limitations. These variables were selected to allow systematic comparison across heterogeneous AI-based studies.

Study risk of bias assessment

The methodological quality and risk of bias of the included studies were assessed using tailored evaluation criteria based on study design and AI methodology. AI-based modeling studies were evaluated for data quality, transparency of model development, validation procedures, reproducibility, and reporting completeness. Only studies meeting minimum quality thresholds were included in the final synthesis to reduce methodological bias and enhance reliability.

Effect measures

Given the heterogeneity of study designs and outcome measures, effect measures were reported descriptively. Performance indicators such as prediction accuracy, sensitivity, specificity, area under the curve (AUC), and validation outcomes were extracted where available. Qualitative assessments of model robustness, interpretability, and clinical or industrial relevance were also considered.

Synthesis methods

A narrative synthesis approach was employed to integrate findings across studies due to substantial methodological and outcome heterogeneity. Studies were grouped according to pharmaceutical application domains and AI techniques. Comparative analysis focused on identifying common trends, methodological strengths, technological limitations, and emerging research directions within AI-driven pharmaceutical technology and drug delivery design.

Reporting bias assessment

Potential reporting bias was evaluated by examining selective outcome reporting, transparency of methodological descriptions, and consistency between stated objectives and reported results. Publication bias could not be formally assessed due to the absence of quantitative meta-analysis; however, restricting inclusion to peer-reviewed studies and applying strict eligibility criteria helped mitigate the risk of selective reporting.

A total of 456 records were initially identified through database searching. After removal of duplicates and non-relevant studies, 95 full-text articles were assessed for eligibility, of which 45 studies met the inclusion criteria and were included in the final synthesis. The study selection process is summarized using a PRISMA 20219 flow diagram (Figure 1), illustrating the number of records identified, screened, excluded, and included at each stage of the review.

The methodological quality of the included studies was assessed using relevant checklists depending on study type (e.g., AI-based modeling papers were evaluated for data validation, reproducibility, and methodological transparency). Only studies meeting minimum quality thresholds were retained in the final synthesis.

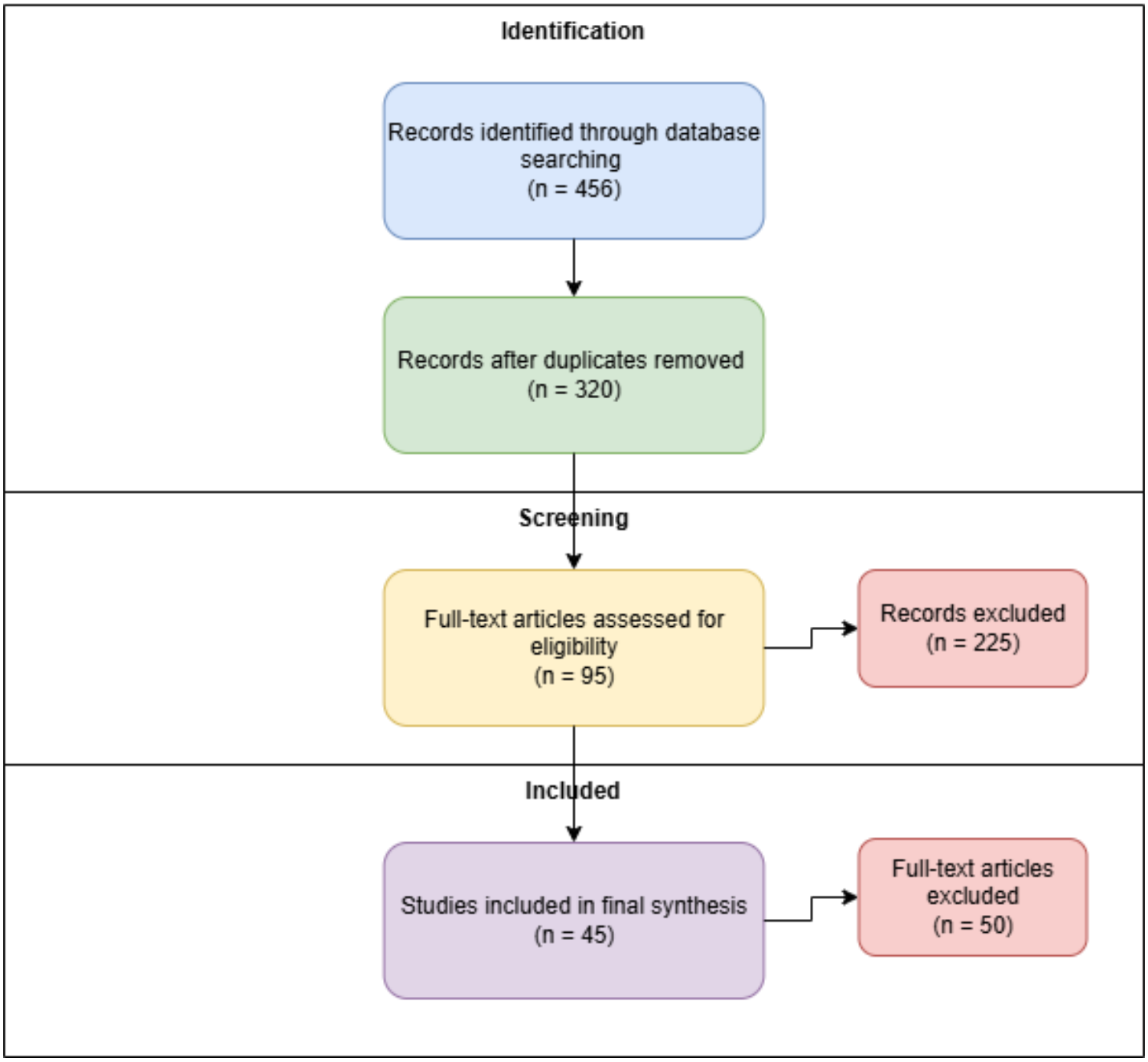


Figure 1: PRISMA flow diagram

Results

Study selection

The systematic review identified studies addressing major pharmaceutical challenges and the role of artificial intelligence (AI) across drug discovery, formulation development, drug delivery systems, medical devices, and pharmacokinetics/pharmacodynamics (PK/PD). The selected studies collectively represent advances in small-molecule therapeutics, biomolecular drugs, supervised and unsupervised AI learning models, computational pharmaceutics, and AI-enabled medical technologies. These studies formed the evidentiary basis for evaluating how AI is being applied to address current pharmaceutical limitations and innovation demands.

Study characteristics

The included studies covered a wide range of pharmaceutical applications, including small-molecule synthesis, biomolecular drug development, AI-based drug design, dosage form optimization, delivery system modeling, medical device innovation, and PK/PD prediction. Methodologically, the studies employed supervised learning, unsupervised learning, artificial neural networks, computational modeling, and multiscale simulations. Applications ranged from predicting drug activity, toxicity, and pharmacokinetic behavior to optimizing formulation stability, drug delivery performance, and clinical trial outcomes [10–13].

Risk of bias in studies

Across the included studies, several sources of potential bias were identified. Algorithmic bias emerged as a recurring concern, particularly in studies relying on limited, non-diverse, or proprietary datasets, which may influence prediction accuracy and hypothesis evaluation [14-17]. Docking simulations and AI-based screening occasionally reported inactive molecules as active, reflecting limitations in training data and model assumptions [17]. In addition, heterogeneity in validation strategies and limited external dataset testing contributed to uncertainty regarding model robustness and reproducibility [17,18].

Results of individual studies

Studies focusing on small-molecule pharmaceuticals reported advantages such as chemical stability, cost-effective synthesis, and formulation versatility [10,11]. However, these studies also highlighted increasing competitive pressure from generic drugs, necessitating accelerated innovation and rapid clinical data generation to maintain market viability [12]. In contrast, biomolecular drug studies emphasized the complexity of macromolecular therapeutics, where stability, supramolecular conformation, and pharmacokinetic behavior are critical determinants of efficacy [6,13,14]. Examples such as insulin and adalimumab illustrated the need for specialized delivery routes due to structural and pharmacokinetic constraints.

Research on supervised AI learning demonstrated successful application of classification and regression techniques for drug discovery, quality control, drug target identification, disease prognosis, and clinical trial prediction [18-20,21–25]. Algorithms such as Support Vector Machines, Random Forests, K-Nearest Neighbors, Decision Trees, and Linear Regression were frequently employed to predict drug activity, toxicity, equipment failure, and patient outcomes. These studies reported improved decision-making efficiency when labeled datasets were available and appropriately curated.

Unsupervised learning studies focused on clustering, dimensionality reduction, anomaly detection, and association rule mining to uncover hidden patterns in unlabeled pharmaceutical data [26–28]. Clustering techniques were used to group drugs, genes, or patients based on similarity profiles [29], while dimensionality reduction methods such as PCA and t-SNE supported visualization and interpretation of high-dimensional datasets [30]. Anomaly detection algorithms were applied to identify adverse events and data irregularities [24,31], and association rule mining revealed drug–drug interactions and pharmacovigilance signals [21,31].

Studies addressing dosage form design and drug delivery highlighted the importance of biological barriers, membrane permeability, and route-specific pharmacokinetics [32–35]. Computational and AI-based models were used to simulate drug–membrane interactions, predict permeation behavior, and evaluate pharmacokinetic parameters under modeled conditions [19,21]. AI-assisted modeling enhanced the analysis of complex multilayered biological data and supported iterative optimization of delivery systems.

Computational pharmaceutics studies demonstrated that AI-enabled multiscale modeling can predict physicochemical properties, release profiles, stability, and in vivo–in vitro correlations of drug delivery systems [36–38]. These approaches reduced experimental iterations, development time, and cost while improving formulation selection and risk mitigation [15,39,40]. AI applications in medical devices showed improvements in diagnostic

imaging, wearable health monitoring, prosthetics, surgical assistance, and medication management [40–44]. PK/PD-focused studies reported limitations of traditional experimental methods, including ethical constraints, small sample sizes, and poor human predictability [43,45-47]. AI-based PK/PD models demonstrated improved accuracy, faster prediction, and cost efficiency in simulating drug behavior and toxicity [48–50], although data availability and dataset quality remained key constraints [6,28].

Results of syntheses

Across domains, the synthesized evidence indicates that AI consistently enhances pharmaceutical research efficiency, predictive accuracy, and system-level understanding. AI applications were most effective when integrated with computational modeling, large-scale datasets, and iterative validation frameworks. While supervised learning dominated predictive tasks, unsupervised learning provided critical exploratory insights. AI-driven approaches collectively supported improved drug discovery pipelines, optimized delivery systems, and advanced PK/PD modeling [15,18,36–40].

Reporting biases

Reporting bias was observed in the preferential emphasis on successful AI implementations, with limited discussion of negative results or failed models. Some studies relied on controlled or proprietary datasets, potentially overstating real-world applicability. Nonetheless, several studies acknowledged limitations related to dataset size, bias, and interpretability, partially mitigating selective reporting concerns [6,28].

Certainty of evidence

The overall certainty of evidence was assessed as moderate. While the reviewed studies demonstrated consistent methodological innovation and promising performance outcomes, variability in validation rigor, dataset transparency, and external generalizability limited confidence in large-scale clinical or industrial adoption.

Continued advancements in standardized datasets, explainable AI, and regulatory alignment are required to strengthen the evidence base and support broader implementation [15,18,28].

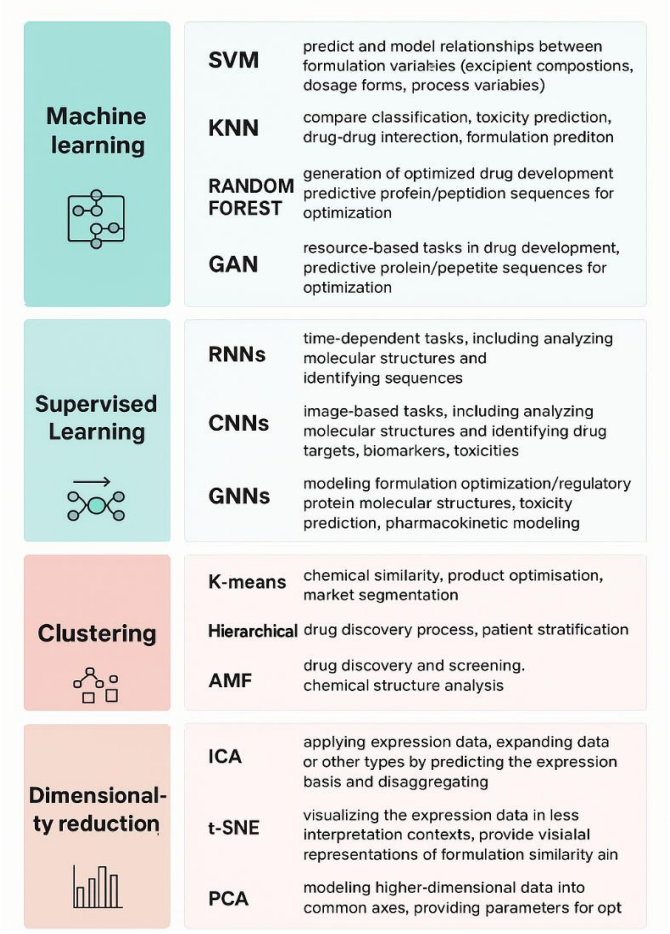


Figure 2: Different supervised and unsupervised AI learning models/tools for Pharmaceutical applications.

Discussion

The present review underscores the growing role of artificial intelligence (AI) as a transformative force in pharmaceutical technology, particularly across drug discovery, formulation design, and drug delivery optimization. The reviewed evidence demonstrates that AI-driven approaches have achieved promising levels of accuracy in virtual screening, pharmacokinetic modeling, and dosage optimization. Nevertheless, a critical appraisal of the literature indicates that much of the existing evidence remains preliminary and is frequently constrained by methodological shortcomings and data-related limitations. In particular, reproducibility and external validation across independent datasets remain limited, which restricts the translational and regulatory utility of many proposed models [7,51]. Moreover, the frequent reliance on proprietary or non-standardized datasets reduces model generalizability and poses challenges for regulatory acceptance.

A major methodological concern highlighted in this review is the limited interpretability and transparency of deep learning systems. While these models are capable of identifying complex, nonlinear relationships underlying drug design and delivery processes, their "black-box" nature hampers scientific validation, regulatory scrutiny, and clinical trust [23,29]. Consequently, the integration of explainable artificial intelligence (XAI) frameworks is increasingly recognized as essential for improving model interpretability, enhancing confidence in AI-assisted decisions, and ensuring alignment with ethical and regulatory expectations in pharmaceutical research.

Ethical and data governance considerations also represent critical challenges in the deployment of AI-based pharmaceutical technologies. The utilization of patient-derived genomic, clinical, and real-world datasets raises concerns related to data privacy, informed consent, and bias propagation. Algorithmic bias, particularly when training data inadequately represent diverse patient populations, can lead to inequitable therapeutic predictions and outcomes [3,41,45]. These risks underscore the importance of adhering to robust data governance frameworks, implementing bias mitigation strategies, and maintaining transparency in model development and reporting.

From an implementation standpoint, several practical barriers hinder the seamless integration of AI into existing pharmaceutical research and development workflows. These include limited interoperability between computational platforms, substantial computational resource requirements, and a shortage of professionals with interdisciplinary expertise spanning pharmacology, data science, and artificial intelligence. Furthermore, regulatory pathways for AI-enabled drug discovery, formulation, and delivery systems remain under development, with limited consensus on validation standards and performance benchmarks for algorithmic models. Addressing these challenges will be essential for the successful translation of AI innovations from experimental settings to routine pharmaceutical practice.

Despite these limitations, the collective findings of the reviewed studies point to the substantial potential of AI to reshape pharmaceutical innovation. When synergistically combined with systems biology, high-throughput screening technologies, and real-world data analytics, AI can accelerate hypothesis generation, reduce experimental costs, optimize development timelines, and facilitate patient-specific therapeutic strategies. Realizing these benefits, however, requires the establishment of robust validation pipelines, standardized and shareable datasets, and ethically guided implementation frameworks.

Limitations

This systematic review has several limitations that should be acknowledged. First, substantial heterogeneity was observed across the included studies in terms of AI methodologies, pharmaceutical application domains, datasets, validation strategies, and outcome measures, which precluded quantitative meta-analysis and limited direct comparison of results. Second, many studies relied on proprietary, simulated, or relatively small datasets, reducing external validity and limiting the generalizability of AI model performance to real-world pharmaceutical settings.

Third, inconsistencies in reporting model development, training procedures, and validation frameworks hindered reproducibility assessment and risk-of-bias evaluation across studies. Additionally, publication bias cannot be excluded, as studies demonstrating positive AI performance were more frequently reported, while negative or null findings were often underrepresented. Finally, the rapidly evolving nature of AI technologies means that recently developed models and regulatory frameworks may not have been fully captured within the defined search period. These limitations highlight the need for standardized reporting guidelines, transparent data sharing practices, and robust external validation to strengthen future evidence on AI integration in pharmaceutical technology and drug delivery design.

Conclusion

Artificial intelligence (AI) has emerged as a powerful and versatile tool in pharmaceutical research and development, enabling data-driven decision-making across drug discovery, formulation optimization, and drug delivery system design. The reviewed literature demonstrates that AI techniques particularly machine learning, deep learning, and computational modeling have contributed to improved prediction of pharmacokinetic and pharmacodynamic behaviors, enhanced formulation stability assessment, and accelerated virtual screening of drug candidates. However, most existing studies remain at experimental or preclinical stages, with limited large-scale clinical validation. Key barriers to broader implementation include the absence of standardized datasets, persistent challenges related to model interpretability, and evolving regulatory frameworks governing AI-assisted pharmaceutical development. Overcoming these obstacles will require stronger interdisciplinary collaboration among computer scientists, pharmacologists, clinicians, and regulatory authorities. Future research should prioritize the development of transparent, explainable, and reproducible AI systems that adhere to ethical, safety, and regulatory standards. Ultimately, the integration of AI in pharmaceutics holds significant promise not as a replacement for human expertise, but as a complementary tool that enhances innovation, precision, and patient-centered care.

Authors' Contributions:

All authors meet the ICMJE criteria for authorship.

Author 1: Substantial contribution to conception and design, drafting the manuscript, final approval, agreed to be accountable for all the work.

Author 2: Substantial contribution to conception and design, data acquisition, drafting the manuscript, final approval, agreed to be accountable for all the work.

Author 3: Analysis and interpretation of data, drafting the manuscript, final approval, agreed to be accountable for all the work.

Author 4: Analysis and interpretation of data, critical revision, final approval, agreed to be accountable for all the work.

Author 5: Substantial contribution to conception and design, drafting the manuscript, final approval, agreed to be accountable for all the work.

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