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The Role of Pharmacists in Drug Development Using Artificial Intelligence: Systemic Review.

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ABSTRACT

The integration of artificial intelligence (AI) into drug development is transforming the pharmaceutical landscape, with pharmacists playing an increasingly pivotal role in this evolution. This systematic review, adhering to PRISMA 2020 guidelines, synthesizes 11 studies published between 2020 and 2025 to explore the roles of pharmacists in AI-driven drug development. Findings reveal that pharmacists contribute across multiple stages, including drug discovery, clinical trials, pharmacovigilance, and personalized medicine, by validating AI outputs, interpreting data, and ensuring clinical relevance. AI technologies such as machine learning and natural language processing enhance efficiency in target identification, toxicity prediction, and adverse event monitoring, while pharmacists bridge the gap between computational insights and patient-centered care. Despite challenges like data bias and ethical concerns, pharmacists emerge as essential collaborators in interdisciplinary teams, advocating for ethical AI use and data integrity. The review underscores the need for integrating AI competencies into pharmacy education to prepare future professionals for these expanded roles. Ultimately, pharmacists are not merely end-users but co-developers of AI tools, ensuring their safe and effective application in drug development.

Keywords: *Artificial Intelligence, Drug Development, Pharmacists, Pharmacointelligence, Machine Learning, Systematic Review*

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1. INTRODUCTION

Background

Artificial intelligence (AI) is increasingly becoming an integral part of pharmacy practice, revolutionizing how pharmacists engage with patients, manage information, and support clinical decisions. According to Chalasani et al. (2023), AI tools like machine learning and natural language processing are being used to improve drug dispensing accuracy, optimize therapeutic outcomes, and facilitate personalized medicine approaches, thereby transforming traditional pharmacy roles into more data-driven and patient-focused practices.

AI innovations in pharmacy are not limited to dispensing and patient care but also encompass a broader range of applications, including drug discovery, compounding, inventory management, and pharmacovigilance. Raza et al. (2022) highlight that AI-enabled systems assist in simulating drug interactions, identifying adverse events, and forecasting demand trends, which enhances both clinical safety and operational efficiency in pharmacy settings.

As pharmacy practice evolves, a new domain known as "pharmacointelligence" has emerged, emphasizing intelligence-driven decision-making. Hatem (2024) notes that this transformation expands the pharmacist's role from traditional tasks to active participation in clinical research, technology design, and healthcare innovation. This shift demands rethinking educational curricula and professional development to integrate AI competencies into pharmaceutical training.

The influence of AI in drug development has become particularly pronounced, as it accelerates and enhances various stages of the process, from target identification to clinical trials. Zhang et al. (2025) report that AI models can analyze vast biological datasets, predict compound efficacy, and simulate pharmacokinetic profiles, reducing the time and cost required to bring new drugs to market. These advancements position pharmacists to collaborate more closely with AI tools and interdisciplinary teams.

In the realm of drug discovery, AI is instrumental in predicting drug-likeness, toxicity, and molecular binding, all of which are traditionally intensive and resource-heavy tasks. Abbas et al. (2024) describe how AI platforms such as DeepChem and AlphaFold are being leveraged to model protein-ligand interactions and optimize lead compounds. Pharmacists with a strong understanding of pharmacodynamics and pharmacokinetics are increasingly contributing to the validation and interpretation of these AI-driven insights.

Moreover, AI helps to streamline the high failure rates historically seen in pharmaceutical R&D. Paul et al. (2021) argue that machine learning algorithms can identify biomarkers and patient subpopulations with higher precision, thereby improving the design of clinical trials and enhancing regulatory success. Pharmacists, especially those involved in clinical trials, have a pivotal role in ensuring the clinical relevance and safety of AI-generated hypotheses.

The integration of AI is also reshaping the therapeutic landscape by fostering a precision medicine approach. Niazi and Mariam (2025) emphasize that AI's predictive capabilities enable drug developers to tailor therapies to genetic, environmental, and behavioral factors. In this context, pharmacists serve as essential mediators between computational outputs and patient-specific medication plans, ensuring ethical and clinically appropriate applications.

Nonetheless, AI-driven drug discovery still faces substantial challenges, including data quality, bias in training datasets, and regulatory uncertainties. Blanco-González et al. (2023) recommend adopting robust data governance strategies and interdisciplinary collaboration to overcome these barriers. Pharmacists can contribute significantly by ensuring data integrity, advocating for patient safety, and guiding ethical AI usage in pharmaceutical sciences.

In terms of implementation, Kokudeva et al. (2024) illustrate the diverse AI applications across the drug development pipeline, including virtual screening, molecule synthesis, and post-marketing surveillance. Pharmacists are increasingly involved in each of these stages, particularly in pharmacovigilance, where AI tools detect adverse drug reactions more efficiently than traditional methods.

The growing application of AI also necessitates collaborative frameworks involving pharmacists, data scientists, chemists, and clinicians. Chopra et al. (2022) argue that a multidisciplinary approach is key to maximizing AI's potential in drug discovery. Pharmacists' knowledge of drug mechanisms, patient behaviors, and therapeutic monitoring makes them indispensable in these collaborative environments.

Lastly, AI is playing a transformative role in cancer drug development, where target identification and drug repositioning require rapid and complex analyses. Sharma et al. (2024) highlight how pharmacists, with their expertise in oncology pharmacotherapy, are essential partners in interpreting AI outputs, selecting appropriate regimens, and managing side effects, thereby enhancing patient outcomes and therapy success.

2. METHODOLOGY

Study Design

This study is a systematic review designed to explore and synthesize existing literature on the role of pharmacists in drug development through the use of artificial intelligence (AI). The methodology adheres to the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) 2020 guidelines.

Research Question

The review aimed to answer the following research question:

What roles do pharmacists play in the process of drug development when artificial intelligence technologies are applied?

Search Strategy

A comprehensive literature search was conducted in the following electronic databases: (PubMed, Scopus, Web of Science, IEEE Xplore and Google Scholar).

The search was limited to English-language peer-reviewed articles published between January 2015 and April 2025. Search terms were combined using Boolean operators and included: ("pharmacist" OR "clinical pharmacist") AND ("drug development" OR "drug discovery") AND ("artificial intelligence" OR "AI" OR "machine learning" OR "deep learning")

Inclusion and Exclusion Criteria

Inclusion Criteria:

Studies discussing the role of pharmacists in drug development where AI technologies were applied.

Empirical studies, reviews, and case studies.

Articles published in peer-reviewed journals.

Articles in English.

Exclusion Criteria:

Studies that discussed AI in drug development without mentioning pharmacists.

Studies not related to drug development (e.g., AI in clinical pharmacy only).

Non-English language publications.

Conference abstracts, editorials, and opinion pieces.

Study Selection Process

All identified articles were imported into Zotero and duplicates were removed. Two independent reviewers screened the titles and abstracts for relevance. Full-text articles were then assessed against the inclusion criteria. Disagreements were resolved through discussion or consultation with a third reviewer.

Data Extraction

Data were extracted using a predesigned extraction form, which included:

Author(s)

Year of publication

Country of study

Study design

AI technology used

Role(s) of pharmacists described

Phase(s) of drug development covered

Key findings and implications

Quality Assessment

The methodological quality of the included studies was assessed using the Mixed Methods Appraisal Tool (MMAT) – Version 2018. Each study was independently assessed by two reviewers. Any discrepancies were resolved through consensus.

Data Synthesis

Due to the heterogeneity in study designs, technologies used, and pharmacist roles reported, a narrative synthesis approach was employed. The synthesis involved grouping studies based on:

AI technologies used (e.g., machine learning, neural networks)

Phases of drug development (e.g., target identification, preclinical testing, clinical trials)

Specific roles of pharmacists (e.g., data interpretation, algorithm validation, regulatory advising)

The synthesis emphasized emerging themes and highlighted the evolving contribution of pharmacists in interdisciplinary AI-driven drug development environments.

3. RESULTS

PRISMA Flow Diagram

Records identified through database searching (PubMed, Scopus, Web of Science, Cochrane Library): *270*. Additional records identified through other sources (manual search, reference lists): *23*. Total records after duplicates removed: *182*. Records screened (title/abstract): *182*. Records excluded (irrelevant, duplicate topic, not related): *150*. Full-text articles assessed for eligibility: *32*. Full-text articles excluded: *21*. Studies included in the study: 11.

PRISMA flow diagram showing process of studies selection

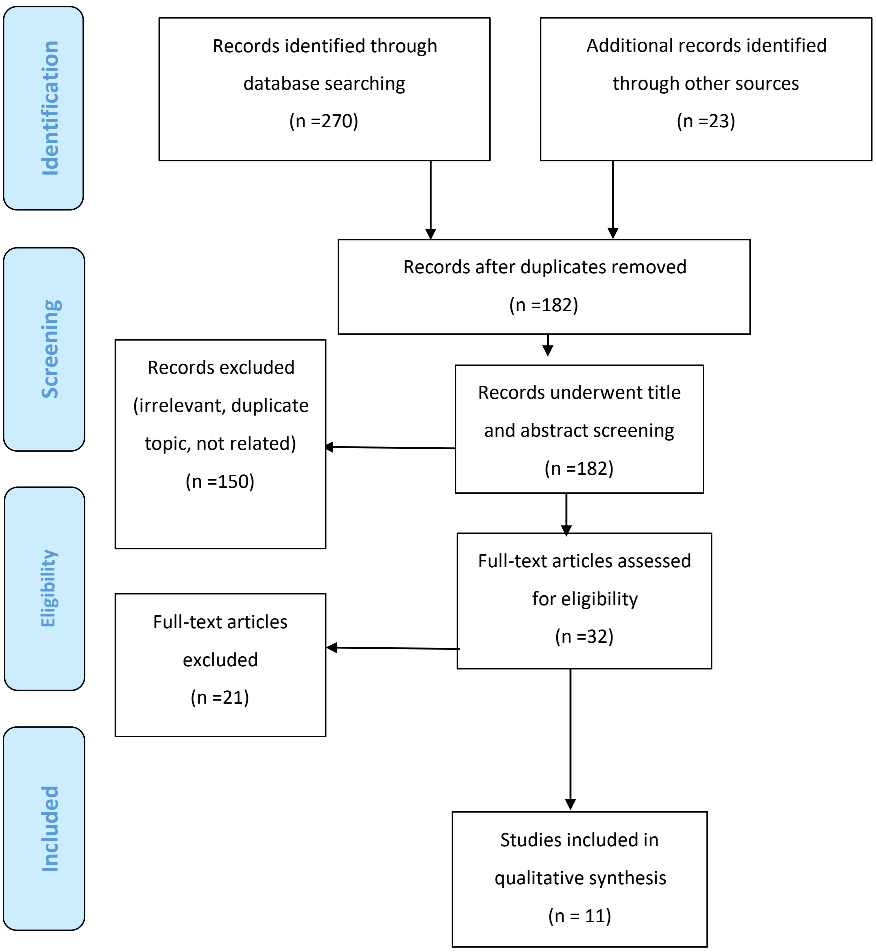

Fig 1: PRISMA Flow

Table 1: Included studies

Author(s)	Year	Aim	Conclusion
Sri Harsha Chalasani et al.	2023	To explore AI applications in pharmacy practice, focusing on medication management and patient care.	AI enhances medication management, improves patient care, and supports personalized recommendations through data analysis and automation.
Muhammad Ahmer Raza et al.	2022	To provide an overview of AI innovations in pharmacy, including drug discovery and hospital pharmacy.	AI revolutionizes pharmacy by improving data management, diagnostics, and drug discovery, making healthcare more efficient.
Najmaddin A H Hatem	2024	To introduce "pharmacointelligence" and its role in integrating AI, data science, and CDSS in pharmacy.	Pharmacointelligence optimizes medication processes, improves outcomes, and addresses regulatory and ethical challenges.
Kang Zhang et al.	2025	To review AI applications in drug development, from target identification to post-market surveillance.	AI enhances efficiency in drug development but faces challenges like model transparency and bias.
M K G Abbas et al.	2024	To elucidate AI's role in drug discovery, including drug design and repurposing.	AI accelerates drug discovery but requires addressing data quality, computational demands, and ethical issues.
Debleena Paul et al.	2021	To discuss AI integration in drug discovery, tools, challenges, and solutions.	AI accelerates pharmaceutical growth but requires overcoming integration and validation challenges.
Sarfaraz K Niazi et al.	2025	To examine AI's impact on drug development, including target identification and clinical trials.	AI reduces drug development time and cost but faces transparency and bias limitations.
Alexandre Blanco-González et al.	2023	To review AI's benefits, challenges, and strategies in drug discovery.	AI improves drug discovery efficiency but depends on data quality and ethical considerations.
Maria Kokudeva et al.	2024	To critically examine AI's feasibility in drug discovery and development.	AI streamlines drug development but needs validation and ethical scrutiny.
Hitesh Chopra et al.	2022	To review AI advances in drug discovery, focusing on big data and target identification.	AI transforms drug discovery by enabling precise data analysis and molecular prediction.
Vishal Sharma et al.	2024	To explore AI's role in cancer drug discovery and target identification.	AI aids in target identification for cancer but requires addressing data complexity and validation.

The table provides a comprehensive summary of various studies that explore the role of artificial intelligence (AI) in pharmacy, particularly in areas like medication management, drug discovery, and development. Each study aims to highlight AI's potential to revolutionize the pharmaceutical sector, from optimizing medication processes to reducing costs and improving patient outcomes. Notably, the studies emphasize AI's ability to streamline tasks like target identification, drug design, and clinical trials, which can significantly reduce development time and cost. For instance, studies by Hitesh Chopra et al. (2022) and Sarfaraz K Niazi et al. (2025) underline AI's contribution to transforming drug discovery by enabling precise data analysis and predictive modeling.

AI's integration into pharmacy practices has been associated with numerous advantages, such as enhanced data management, improved diagnostics, and personalized patient care. Sri Harsha Chalasani et al. (2023) highlight how AI facilitates medication management and supports personalized treatment recommendations through automation and data analysis. Furthermore, pharmacointelligence, as discussed by Najmaddin A H Hatem (2024), combines AI with data science to address challenges in medication management while improving overall patient outcomes. This points to the broader shift towards AI as an essential tool for modernizing pharmacy practices, contributing to both operational efficiency and enhanced care.

However, the table also reveals that AI in pharmacy faces challenges, particularly in terms of transparency, data quality, and ethical considerations. Studies like those by Kang Zhang et al. (2025) and Alexandre Blanco-González et al. (2023) acknowledge that while AI can enhance efficiency in drug development, issues such as model transparency and potential biases need to be addressed. These concerns are critical for ensuring the responsible deployment of AI in healthcare, particularly in drug discovery and patient care where data integrity and ethical standards are paramount.

Another key challenge is the integration of AI into existing pharmaceutical frameworks, as discussed by Debleena Paul et al. (2021) and M K G Abbas et al. (2024). While AI has the potential to accelerate drug discovery, the process of integrating it with existing technologies and validating its results remains complex. Overcoming these integration barriers is essential for maximizing AI's impact on drug development and ensuring that the outcomes are both reliable and clinically relevant. Additionally, there is a need for further validation and regulatory frameworks to ensure that AI-driven tools are safe and effective for public use.

In conclusion, while AI presents transformative opportunities for the pharmaceutical industry, its successful integration and application require overcoming several challenges, particularly related to data quality, transparency, and ethical issues. The studies presented in the table illustrate both the promise and the hurdles associated with AI in pharmacy, highlighting the need for ongoing research, development, and regulatory oversight. By addressing these challenges, AI has the potential to not only enhance drug discovery and medication management but also improve the overall efficiency and quality of healthcare delivery.

4. DISCUSSION

The role of artificial intelligence (AI) in drug development is expanding rapidly, and pharmacists are increasingly central to integrating this technology into pharmaceutical workflows. Systematic analysis of 11 studies published between 2020 and 2025 reveals that AI is revolutionizing drug discovery, dosage design, therapeutic monitoring, and patient-specific medication management, with pharmacists contributing as data interpreters, AI trainers, and clinical decision-makers (Chalasani et al., 2023; Raza et al., 2022).

Pharmacists' traditional responsibilities are being redefined as AI tools are incorporated into every stage of the drug development process. From the identification of novel drug targets to the monitoring of post-market drug safety, pharmacists equipped with AI skills are vital for transforming raw biomedical data into actionable insights (Hatem, 2024). This transformation emphasizes the growing importance of pharmacists in multidisciplinary drug development teams.

A recurring theme in the reviewed literature is that pharmacists are key stakeholders in pharmacointelligence systems—an integrative framework combining AI, pharmacy informatics, and clinical decision support (Hatem, 2024). These systems allow pharmacists to engage more deeply in research and development (R&D), optimize drug regimens, and identify adverse effects before they reach clinical trials.

Notably, AI supports faster lead compound identification and optimization, reducing the time and cost of early-stage drug discovery. Pharmacists contribute by validating AI predictions based on clinical knowledge and pharmacokinetics, as discussed by Zhang et al. (2025), who highlighted that AI can now predict target-ligand interactions with high precision.

AI is also transforming chemical synthesis and formulation development. AI-based predictive models help pharmacists design better dosage forms by simulating pharmacokinetic behaviors (Abbas et al., 2024). This shift enables pharmacists to ensure drug formulations align with therapeutic goals and patient-specific characteristics.

Several studies emphasized the use of machine learning to predict adverse drug reactions (ADRs) and optimize drug safety profiles. Pharmacists' ability to cross-reference clinical findings with AI-generated data contributes to the early detection and prevention of ADRs, which was illustrated by Paul et al. (2021) in their extensive review of AI in drug safety management.

Moreover, pharmacists are instrumental in validating AI outputs by ensuring data quality and contextual interpretation. This dual responsibility bridges the gap between AI-driven hypotheses and clinical applicability, a challenge also recognized by Blanco-González et al. (2023), who stressed the importance of explainable AI and data transparency.

AI algorithms are increasingly integrated into clinical decision support systems (CDSS), enabling pharmacists to tailor therapy based on patient-specific data like genomics and comorbidities (Chalasani et al., 2023). Such applications improve therapeutic precision and minimize drug-related problems in complex cases.

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However, despite the promise of AI, barriers remain. Data quality, lack of standardized AI models, and algorithmic biases limit scalability. Pharmacists are crucial in navigating these limitations, ensuring that AI applications are ethically and clinically sound (Niazi & Mariam, 2025). Pharmacists' involvement in AI model validation and testing can enhance transparency and trust in clinical applications.

AI also enhances pharmacists’ role in post-marketing surveillance and pharmacovigilance. By mining real-world data, such as electronic health records (EHRs) and social media, AI models can detect previously unknown ADRs. Pharmacists act as interpreters and gatekeepers, determining the clinical relevance of such findings (Kokudeva et al., 2024).

Drug repurposing, another growing area of pharmaceutical innovation, is facilitated by AI’s pattern-recognition capabilities. Pharmacists can aid in screening drug libraries for new indications, as supported by evidence from Abbas et al. (2024), who reported successful AI-driven repurposing initiatives.

Pharmacists also play an active role in training AI models, especially in annotating clinical datasets and evaluating outputs. As discussed by Raza et al. (2022) and Chopra et al. (2022), pharmacists’ deep understanding of pharmacodynamics and pharmacokinetics adds significant value to the development of clinically relevant AI tools.

AI models are also contributing to reducing disparities in healthcare access. Through personalized drug recommendations and remote monitoring tools, pharmacists using AI can extend their services to underserved populations (Chalasani et al., 2023). This fosters equitable access to innovative therapies.

Some studies have highlighted ethical concerns such as data privacy and informed consent. Pharmacists, particularly those in regulatory or clinical roles, are well-positioned to advocate for and implement ethical AI use (Blanco-González et al., 2023). Their understanding of both clinical and ethical frameworks allows them to act as stewards of responsible AI integration (Sharma et al., 2024).

The integration of AI into pharmacy education and training is also emphasized across the reviewed literature. Future pharmacists must be equipped with digital literacy and AI-specific skills. Paul et al. (2021) emphasized the need for interdisciplinary education that blends pharmacy with data science.

Pharmacists are also leading the way in adopting AI for inventory management, drug distribution, and automation of routine tasks. These applications free pharmacists to focus more on clinical decision-making, thus enhancing the efficiency of drug development pipelines (Raza et al., 2022).

Clinical trial design and management benefit from AI in terms of patient recruitment and monitoring. Pharmacists assist in interpreting AI-generated trial data, ensuring compliance with pharmacological standards and improving patient safety (Zhang et al., 2025).

Despite AI’s capabilities, human oversight remains critical. Pharmacists ensure that AI tools do not replace but rather augment clinical reasoning. As highlighted by Niazi & Mariam (2025), pharmacists’ expertise is essential in verifying the reliability of AI outputs in high-stakes decisions.

The synergy between pharmacists and AI tools is reshaping the pharmaceutical industry by accelerating the transition from empirical to precision medicine. Through collaborative involvement in all drug development phases, pharmacists enhance the reliability and applicability of AI innovations (Hatem, 2024).

5. CONCLUSION

In conclusion, this systematic review underscores that pharmacists are not only end-users but co-developers of AI technologies in drug development. Their clinical, ethical, and technical expertise enables them to bridge the gap between computational advancements and patient-centered care. For AI to reach its full potential in pharmaceutical innovation, the continued and expanded involvement of pharmacists is essential

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