# Artificial Intelligence in Pharmacy

*submitted in partial fulfilment*

*of the requirements of the*

*Degree of Master of Pharmacy*

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**2025**

# Acknowledgement

I would like to extend my heartfelt gratitude to my thesis supervisor, Professor Lilian Azzopardi, for her invaluable guidance, continuous support, and encouragement throughout the course of this research. Your insight, feedback, and expertise have been instrumental in shaping this dissertation.

I am equally thankful to my co-supervisor, Dr. Nicolette Sammut Bartolo, whose constructive suggestions and thoughtful input enriched the depth and direction of my work. Your mentorship has been deeply appreciated.

I would also like to extend my heartfelt thanks to the faculty and staff at University of Malta, whose academic support and resources made this research possible.

To my family and friends, thank you for your unconditional love, patience, and unwavering support. Your belief in me has been a constant source of strength and motivation. This achievement would not have been possible without your presence in my life.

I offer my profound gratitude to God for his grace and mercy that sustained me throughout this phase.

Lastly, I am grateful to everyone who contributed directly or indirectly to this work. Your contributions, whether academic or emotional, are deeply appreciated and never forgotten.

Sneha George

# Abstract

Artificial intelligence (AI) has emerged as a transformative technology within the pharmaceutical sciences, offering innovative solutions across drug discovery, personalised medicine, clinical trials, and pharmacy operations. The increasing complexity of healthcare demands more efficient, accurate, and patient-centred approaches, and AI provides tools capable of analysing vast datasets, predicting therapeutic outcomes, and optimizing decision-making processes.

This thesis explores the application of AI in pharmacy, with a specific focus on its roles in drug discovery and development, personalised medicine predictive analytics, patient-centred care, pharmaceutical operations and pharmacy practice. It also examines the challenges surrounding AI adoption, including regulatory, ethical, and data-related concerns.

This research used a literature review to gather relevant studies on AI application in pharmacy. The search included articles published between 2015 and 2024, sourced from databases such as PubMed, Scopus and Google scholar. Keywords included Artificial intelligence in pharmacy, AI in drug discovery, personalised medicine.

AI has shown measurable benefits in accelerating drug target identification, optimizing clinical trials, and tailoring therapies using genomic data. Notable tools such as DeepMind's AlphaFold and IBM Watson for Oncology exemplify AI's potential in reducing development time and supporting personalized treatment. In pharmacy practice, AI-enabled clinical decision support systems (CDSS), chatbots, and computerized prescriber order entry (CPOE) have reduced medication errors and improved patient counselling. Nevertheless, concerns persist around data privacy, algorithmic bias, model interpretability, and cost of implementation

AI presents substantial opportunities for enhancing efficiency, safety, and innovation within pharmacy practice. By addressing current challenges through interdisciplinary collaboration and regulatory advancements, AI can further revolutionize pharmaceutical research, development, and patient care, ultimately improving health outcomes and operational efficiency across the sector.

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## List of Abbreviations

| | |
|---|---|
| AI | Artificial Intelligence |
| CDSS | Clinical Decision Support System |
| EHR | Electronic Health Record |
| GDPR | General Data Protection Regulation |
| HIPAA | Health Insurance Portability and Accountability |
| NLP | National Language Processing |

# Chapter 1

# Introduction

## 1.1 Introduction overview

Artificial intelligence (AI) is a “multidisciplinary field whose goal is automate activities that presently require human intelligence” (William, 1983). Artificial intelligence including machine learning, deep learning, and other data driven algorithms is rapidly reshaping pharmaceutical research by harnessing vast biomedical data to guide drug discovery and development. AI- powered predictive analytics involve training computational models on large datasets to predict outcomes of interest such as drug-target interactions, efficacy, and safety (Ferreira and Carneiro, 2025). In the pharmaceutical industries, these tools accelerate tasks that were traditionally laborious and empirical: identifying promising targets, screening chemical libraries, optimising lead compounds, and designing clinical trials. As one review notes, AI has created “unprecedented opportunities for the acceleration of drug discovery and delivery, the optimisation of treatment regimens, and the improvement of patient outcomes,” effectively revolutionising processes from target identification and validation through to supply chain optimisation (Burki ,2020).

The application of AI across various sectors has accelerated dramatically in the past decade due to the availability of big data, improvements in computational power, and advances in algorithms. In healthcare, AI is revolutionising diagnostics, therapeutics, and decision-making. Within pharmacy, AI has emerged as a transformative force, enabling innovations in drug discovery, personalised medicine, clinical decision support, medication adherence, and operational efficiencies.

## 1.2 The Need for AI in Pharmacy

The pharmacy profession in undergoing a paradigm shift- from a product- oriented model to a patient- centered approach. This shift increases the demand for decision support systems that are accurate, responsive, and data driven. AI provides a robust platform for handling complex datasets such as electronic health records, genomic sequences, chemical compound databases, and real- world evidence (Chalasani et al,2023). AI adoption in pharmacy ranges from healthcare cost to safety and access to drugs.

### 1.2.1 Rising healthcare costs and economic burden of chronic diseases

Managing chronic conditions requires continuous monitoring and data interpretation. AI-powered predictive models can forecast patient deterioration and optimise pharmacotherapy, reducing hospitalisations (Topol, 2019).

### 1.2.2 Demand for personalised and precision medicine

Conventional pharmacotherapy often fails to account for genetic, environmental, and lifestyle differences among patients. AI algorithms can analyse patient- specific genomic and phenotypic data to tailor therapy, thereby enhancing therapeutic effectiveness and minimising adverse effects (Topol, 2019).

### 1.2.3 Medication safety and pharmacovigilance

Adverse drug reactions are among the leading causes of morbidity and mortality. AI models trained on pharmacogenomic and data can detect potential adverse drug reactions earlier than traditional surveillance systems (Mishra and Gupta, 2025).

### 1.2.4 Accelerating drug development

AI shortens the drug discovery timeline by identifying drug-target interactions, predicting compound toxicity, and optimising lead molecules. For instance, DeepMind’s AlphaFold has resolved protein folding problems at scale, providing a breakthrough in target identification and structure- based drug design[1] (Jumper et al,2021).

## 1.3 Applications of AI in pharmacy.

### 1.3.1 Drug Discovery and Development

Target identification and validation using Artificial Intelligence (AI) plays a transformative role in drug discovery by enabling the identification and validation of novel drug targets with increased speed, accuracy, and scalability compared to traditional experimental approaches. This is particularly powerful when combined with omics data (genomics, proteomics, metabolomics), natural language processing (NLP), and structural bioinformatics (Abubakar et al, 2024).

Omics Data Analysis and AI models: AI models can analyse large-scale omics datasets to detect dysregulated genes, proteins, or metabolic pathways that may be causally linked to disease. This process allows researchers to identify putative targets and assess their functional relevance. AI is increasingly used in emerging infectious disease drug discovery, particularly in target identification and antimicrobial research. AI enables rapid mining of genomic signatures and resistance genes across pathogens to suggest actionable targets (Bess et al,2022).

Literature Mining with natural language processing (NLP) and Transformers: Companies like BenevolentAI apply natural language processing (NLP)—particularly transformer-based models—to mine vast volumes of biomedical literature and extract relationships between genes, diseases, and drug molecules (Chakraborthy et al,2024). This reveals

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[1] Society of chemical Industry(2025) AI designed drugs in trials this year, says Google DeepMind chief : https://www.soci.org/news/2025/1/ai-designed-drugs-in-trials-this-year-says-google-deepmind-chief. (Accessed: 2 August 2025)

hidden connections that would be impractical to uncover manually. The use of transformer models, such as BERT, which are now widely employed in drug discovery platforms to parse, understand, and extract biological knowledge from unstructured text (Wolf et al, 2020). BenevolentAI, for instance, used such models to identify Baricitinib as a potential treatment for COVID-19, based on AI-predicted interactions between the drug and viral entry pathways (Richardson et al., 2020).

Structure based target validation: Beyond identifying targets, AI also contributes to target validation by assessing protein structure and druggability. Structural deep learning tools like DeeplyTough evaluate similarities between known drug-binding sites and potential new targets, supporting target prioritization. DeeplyTough, a deep learning system, can compare protein binding sites across structures to predict whether a novel protein is likely to bind existing or novel ligands, enhancing confidence in selected targets (Simonovsky and Meyers,2020).

One real-world example of AI-based target identification and repositioning is Baricitinib, originally developed for rheumatoid arthritis. BenevolentAI used its knowledge graph and literature mining tools to predict that Baricitinib could inhibit AP2-associated kinase 1 (AAK1)—a potential facilitator of SARS-CoV-2 entry—thus suggesting it as a candidate for COVID-19 treatment (Richardson et al., 2020).

Lead compound screening

Virtual screening of chemical libraries using AI significantly reduces the number of candidates for synthesis and testing. Exscientia, for example, developed an AI- generated molecule (DSP-1181) that reached clinical trials in under 12 months- a record time (Pun et al, 2023).

In Prediction of Pharmacokinetics and Toxicity, AI predicts ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) properties to filter out compounds with high failure potential early in development (Sahu et al,2022).

De novo drug design refers to the creation of entirely new molecular structures from scratch using computational tools, rather than relying on existing chemical libraries or modifying known drugs. The goal is to design novel compounds that are predicted to interact optimally with a specific biological target involved in a disease process (Ren et al, 2023).

### 1.3.2 clinical trials

Artificial intelligence has emerged as a pivotal tool in transforming the efficiency and success of clinical trials within the pharmaceutical research and development. Traditionally, clinical trials are plagued by challenges such as high costs, lengthy durations, suboptimal patient recruitment, and frequent protocol deviations, all of which contribute to the staggering failure rates of drug candidates (Harrer et al, 2019).

Generative AI, is revolutionizing the design and execution of clinical trials by enabling the development of digital twins—virtual representations of individual patients or cohorts that simulate biological behaviour and drug responses. These digital twins can be leveraged to model disease progression, predict individual treatment outcomes, and optimize trial parameters such as dosage, population stratification, and endpoint selection. This innovation significantly reduces the cost, time, and failure rates associated with traditional clinical trials (Bordukova et al,2024).

AI-driven technologies offer innovative solutions across multiple facets of the clinical trial process, beginning with trial design optimisation. By leveraging vast datasets, comprising previous trial data, electronic health records and real-world evidence. AI algorithms can simulate trial scenarios, predict protocol risks and recommend adaptive strategies to enhance study design and reduce costs (Harrer et al.,2019).

One significant advancement is in patient recruitment and retention, where AI systems analyse electronic health records, genomic data, and social determinants of health to match patients precisely to complex inclusion and exclusion criteria. Companies such as IBM Watson Health have demonstrated how AI enhances recruitment efficiency, particularly in oncology trials[2]. AI assists in selecting optimal trials sites by evaluating historical performance data, geographic trends, and investigator capabilities, thereby optimising resource allocation. During trial execution, AI supports real-time monitoring through predictive models that identify safety risks, protocol deviations, and data anomalies, enabling more effective risk-based monitoring.

Additionally, AI facilitates the development of synthetic control arms by utilising historical patient data, reducing ethical concerns associated with placebo use and decreasing trial size and durations- an approach increasingly recognised by regulatory agencies. Finally, AI's predictive analytics capabilities enable early forecasting of trial outcomes, helping sponsors make informed decisions about trial continuation or modification (Topol, 2019).

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[2] IBM.*IBM Watson for Oncology. [Internet]. [Cited 2025 July 6 ] Available from:* https://www.ibm.com/common/ssi/cgi-bin/ssialias?appname=skmwww&htmlfid=897%2FENUS5725-W51&infotype=DD&subtype=SM&mhsrc=ibmsearch_a&mhq=IBM%20WATSON%20ONcology#:~:text=IBM%20Watson%20for%20Oncology%2C%20software,Center%20physicians%20and%20other%20analysts

### 1.3.3 Personalised and Precision medicine

The evolution of healthcare toward personalised and precision medicine signifies a fundamental transformation in how diseases are diagnosed, treated and managed. Personalised medicine focuses on tailoring medical treatments to the unique genetic, environmental, and lifestyle factors of individual patients, moving beyond the conventional one-size-fits-all model (Choudhury et al,2020).

Precision medicine, a closely related concept, emphasizes the use of advanced diagnostics tools, such a genomics, proteomics, and metabolomics, to accurately classify patients into subgroups and guide targeted therapeutic interventions (Ranchon et al, 2023). The integration of artificial intelligence into these fields has been pivotal, enabling the analysis of complex, multi-dimensional datasets that would be insurmountable through traditional methods alone. AI contributes significantly by facilitating predictive analytics, biomarker discovery, treatment optimisation, and the integration of heterogenous patient data into coherent, actionable insights.

In oncology, pharmacogenomics, chronic disease management, and the treatment of rare diseases, AI- driven personalised and precision strategies have shown promise in enhancing therapeutic efficacy, reducing adverse drug reactions, and improving overall patient outcomes (Ginsburg and Phillips, 2018). However, the adoption of AI in personalised medicine is not without challenges, including data privacy concerns, algorithms biases, regulatory uncertainties, and the need for integration within existing clinical infrastructures (Schork, 2019).

Despite these obstacles, the supported by advancements in AI technologies such as explainable AI and federated learning. These developments hold the potential to foster greater trust, transparency, and adoption of AI in clinical settings. Ultimately, personalised and precision medicine, empowered by AI, represent the future of pharmacy and healthcare, offering solutions that align more closely with the unique biological and psychological realities of each patient, thereby optimising therapeutic outcomes and enhancing the quality of care (Obermeyer and Emmanuel, 2016)

### 1.3.4 AI in pharmacy operations

AI technologies have significantly reshaped pharmacy operations, offering enhanced accuracy, efficiency, and safety in various administrative and clinical tasks. One of the most notable contributions is in inventory and supply chain management, where AI systems employ predictive analytics to forecast medication demand, optimise stock levels, and prevent shortages or overstocking. These systems analyse historical data, seasonal trends, and consumption patterns, enabling pharmacies to manage resources more effectively and reduce operational costs (Allam,2025).

In addition to inventory management, AI-powered robotic dispensing systems have revolutionised medication distribution in both hospital and community pharmacy settings. These automated systems improve accuracy by minimising human error, ensure precise dispensing of medications, and enhance workflow efficiency, allowing pharmacists to devote more time to patient centred activities. AI- driven dispensing technologies also support the standardisation of medication preparation processes, contributing to overall medication safety and regulatory compliance (AL Meslamani, 2023).

Furthermore, AI applications extend to medication adherence monitoring through digital health platforms and smart devices. These tools provide reminders, track patient compliance, and notify healthcare providers about missed doses, which is particularly valuable in managing chronic disease and complex treatment regimens. Such technologies have demonstrated positive impacts on patient outcomes by fostering better adherence and reducing hospital readmissions (Chen and Asch,2017).

AI also plays a crucial role in optimising pharmacy logistics, including route planning for medication delivery and integration with electronic health records to streamline communication between healthcare providers, patients, and pharmacies. By facilitating real- time data exchange and improving operational coordination, AI enhances the overall efficiency and responsiveness of pharmacy services.

Despite these advancements, the integration of AI into pharmacy operations presents challenges such as the need for significant upfront investment, staff training, and ensuring interoperability with existing health information systems. Addressing these barriers requires strategic planning, collaboration with technology providers, and ongoing evaluation to minimise the benefits of AI- driven solutions in pharmacy practice.[3]

### 1.4 Challenges and Limitation

Despite its potential, the widespread implementation of AI in pharmacy is constrained by several challenges:

#### 1.4.1 Data privacy and security

One of the most critical challenges in implementing AI in healthcare and pharmacy operations is ensuring robust data privacy and security. AI systems depend heavily on

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[3] Oswalt, R, Candidate, P. The Role of Artificial Intelligence in Pharmacy Practice. 2023. Available online: https://www.pharmacytimes.com/view/the-role-of-artificial-intelligence-in-pharmacy-practice (accessed on 7 may 2025).

large volumes of sensitive data, including electronic health records, genomic information, and real time patient monitoring data. Protecting this data from unauthorised access, breaches, and misuse is paramount to maintaining patient trust and complying with regulatory requirements such as the General Data Protection Regulation (GDPR) in Europe and the Health insurance portability and accountability act (HIPAA) in the United States (Yanamala and Sooryadevara,2024).

Healthcare data is particularly attractive to cybercriminals due to its high value on black markets. As AI technologies increasingly integrate with cloud computing and internet of things (IoT) devices, the number of potential vulnerabilities also grows. This necessitates the implementation of advanced cybersecurity measures, including encryption, secure access controls, and continuous monitoring for threats. However, the complexity of AI models can complicate security protocols, especially when multiple stakeholders (hospitals, pharmacies, technology vendors) shares data across interconnected systems.

Another dimension of data privacy concerns arises from the use of patient data in AI training processes. Even when datasets are anonymised, re-identification risks remain, especially when combined with other publicly available data sources. This raises ethical questions about consent, transparency, and data ownership. Patients may not fully understand how their data is being used to tarin AI models, leading to potential breaches of trust (Cohen and Mello,2019).

Moreover, cross border data sharing required for training robust AI models introduces jurisdictional complexities. Different countries impose varying legal standards on data privacy and sharing, complicating the development of globally applicable AI solutions in pharmacy. Addressing these challenges necessitates clear governance frameworks, ethical guidelines, and international cooperation to harmonise data protection standards.

Ultimately ensuring data privacy and security is fundamental not only for compliance but also for sustaining public confidence in AI- driven healthcare innovations.

### 1.4.2 Algorithmic Bias and Fairness

Another significant challenge associated with the implementation of AI in pharmacy and healthcare is the issue of algorithms bias and fairness. AI systems are inherently dependent on the quality and representativeness of the data on which they are trained. If these datasets contain historical biases, lack diversity, or are not sufficiently comprehensive, the AI models developed from them may perpetuate and even exacerbate these biases in clinical decision making. This can result in unequal treatment outcomes among different populations groups, particularly for those from minority or underserved communities (Obermeyer et al, 2019).

Algorithms bias may arise from various sources, including biased data collection, flawed data labelling processes, and the use of proxy variables that inadvertently encode social or demographic prejudices. For example, if training datasets disproportionately represent one demographic group, AI models may fail to generalise effectively across diverse patient populations, leading to inaccuracies in diagnosis, treatment recommendations or risk predictions. Such biases not only undermine the fairness and equity of healthcare delivery but also pose serious ethical and legal concerns regarding discrimination and health disparities.

Furthermore, the lack of transparency and explainability in many AI systems- often referred to as the “black box” problem- makes it challenging for healthcare professionals to understand how decisions are made, thereby complicating efforts to identify and rectify biases. Without clear insights into the decision- making processes, it becomes difficult to ensure accountability or to build trust among patients and clinicians.

Ensuring fairness in AI applications is not merely a technical challenge but a moral imperative to uphold the principles of justice, equity, and inclusivity in healthcare. As AI continues to shape the future of pharmacy and medicine, robust safeguards against bias will be crucial to realising its full potential in improving health outcomes for all patient populations.

### 1.4.3 Regulatory and Ethical Barriers

In addition to data privacy and algorithmic bias, the adoption of AI in pharmacy and healthcare is significantly hindered by regulatory and ethical barriers. Regulatory frameworks governing AI technologies are still evolving and often struggle to keep pace with the rapid advancements in AI capabilities. Current guidelines provided outline preliminary standards for AI in healthcare, yet these regulations are typically designed for static software rather than adaptive, learning systems that continuously evolve based on new data inputs.

This regulatory lag possesses substantial challenges in the validation, approval and oversight of AI tools, particularly those involved in high stakes clinical decisions. Regulators require clear evidence of safety, efficacy and reliability, which is complicated by the opaque nature of some AI algorithms and the difficulty of predicting their future behaviour as datasets change. Furthermore, the lack of standardised protocols for assessing AI performance across diverse populations and healthcare environments exacerbate these challenges.

Ethically, AI integration raises critical questions around accountability, consent, transparency, and equity. When AI-driven decisions impact patient care, it becomes essential to establish clear lines of responsibility, especially in cases where errors occur. Transparency is another concern, as healthcare professionals and patients need to understand how AI systems reach their conclusions.

Addressing these regulatory and ethical barriers requires collaboration among the policymakers, industry stakeholders, healthcare providers, and ethicists. Clear, adaptable guidelines, continuous oversight, and the development of explainable AI models are crucial to building trust and ensuring that AI innovation align with the core values of healthcare beneficence, non-maleficence. Autonomy, and justice.

### 1.4.4 Integration into Clinical Workflows

Integrating AI technologies into existing clinical workflows presents significant challenges within pharmacy and broader healthcare environments. While AI holds the potential to enhance efficiency, accuracy and patient outcomes, its successful adoption requires seamless alignment with established clinical practices, electronic health records and healthcare infrastructures. One of the primary barriers is the lack of interoperability between AI tools and existing systems, which can impede data sharing and hinder the automation of clinical processes.

Healthcare environments often operate a legacy system that are not designed to accommodate the sophisticated data inputs and outputs required by AI applications. This mismatch leads to inefficiencies, additional manual workarounds, and resistance from healthcare professionals who may perceive AI as disruptive rather than supportive. Moreover, the integration process demands significant investments in IT infrastructure, staff training, and change management to ensure that AI systems are adopted effectively and deliver their intended benefits.

Resistance from healthcare professionals is also rooted in concerns about workflow disruptions, increased workloads during the transition period, and fears of losing clinical autonomy to automated systems. Ensuring that AI tools complement rather than the replace human judgement is critical to fostering acceptance among pharmacists and clinicians.

Additionally, the lack of standardised protocols for incorporating AI outputs into clinical decision-making processes further complicate integration efforts.

### 1.4.5 Cost and Resource Limitations

Another critical barrier to the widespread adoption of AI in pharmacy and healthcare is the significant cost and resource limitations associated with its implementation. Developing, deploying and maintaining AI systems require substantial financial investments in infrastructure, including high-performance computing resources, secure data storage solutions, and sophisticated software platforms capable of handling large and complex datasets. These upfront costs can be prohibitive, particularly for smaller healthcare organisations and institutions in resource limited settings (JoyMathew et al.2020).

Beyond infrastructure, the successful integration of AI also necessitates considerable investment in human resources. Skilled professionals such as data scientists, AI engineers, and cybersecurity experts are essential to the development and maintenance of AI systems. However, there is a global shortage of such expertise, and recruiting or training these professionals adds further financial strains to healthcare organisations.

Additionally, ongoing costs related to system updates, regulatory compliance, and cybersecurity measures compound the financial burden.

Moreover, resource limitations extend beyond financial considerations. The integration of AI into clinical environments demands time and effort from healthcare staffs, who must adapt to new workflows, undergo training, and often manage transitional insufficiencies as systems are optimised. These transitional periods can temporarily increase workloads and operational complexities, reducing the perceived immediate value of AI adoption.

Financial constraints are particularly acute in low- and middle-income countries, where healthcare budgets are already stretched, and investments in cutting edge technologies may not be prioritised over basic healthcare needs. Without targeted policies, subsides, or public- private partnerships, the digital divide in AI adoption may exacerbate existing disparities in healthcare quality and access.

Addressing cost and resource barriers requires strategic planning, including phased implementation approaches, leveraging cloud-based solutions to reduce infrastructure costs, and fostering collaborations to share resources and expertise. Policymakers and healthcare leaders must also advocate for funding initiatives and incentives to support the integration of AI technologies where they can provide the greatest benefit to patient care and health system efficiency.

## Aims and Objectives

The aim of this thesis was to evaluate the role of artificial intelligence in the field of pharmacy, with a particular focus on its applications in the drug discovery, predictive analytics, and pharmacy operations. This study seeks to explore how artificial intelligence technologies are transforming traditional pharmaceutical practices, improving efficiency, and contributing to enhanced patient outcomes, while also addressing the challenges and limitations associated with their integration.

To achieve this aim, the specific objectives of the thesis are to review the current literature on the application of AI in drug discovery, development processes, and predictive analytics within the pharmaceutical sciences.

# Chapter 2

# Methodology

## 2.1 Methodology Overview

This research adopts a narrative literature review methodology to explore the role of Artificial Intelligence in pharmacy, focusing on drug discovery, predictive analytics, and pharmacy operations. A narrative review allows for in-depth, critical analysis of both established and emerging literature, facilitating the synthesis of complex information from various sources to provide a comprehensive understanding of the subject. This method is appropriate for addressing the study's objectives to evaluate current practices, challenges and future directions of Artificial Intelligence in pharmacy. This review uses publicly available documents and author-provided and supervisor guidance, prior to commencement, the study was acknowledged by the Faculty and Ethics Committee, University of Malta on 5th May 2025 (Appendix 1)

## 2.2 Literature Forage

The literature search was conducted using a structured approach to include relevant, high-quality sources. Academic and scientific databases accessed included PubMed, Scopus and Google Scholar. The search encompassed peer-reviewed journal articles, systemic reviews, clinical guidelines.

## 2.3 Process of Conducting the Literature Review

### 2.3.1 Identifying Relevant Sources

The search strategy captured literature on Artificial Intelligence applications in pharmacy, drug discovery, predictive analytics, and pharmacy operations. Key searches included combinations of “artificial intelligence,” “machine learning,” “drug discovery,” “predictive analytics,” “pharmacy operations,” “pharmacogenomics,” “personalised medicine,” “pharmacy practice”, “pharmacy”, “pharmacovigilance”, “precision medicine”,

### 2.3.2 Databases Searches

Searches were performed systematically. Filter limited results to English-language publications from 2015 to 2025 to ensure inclusion of contemporary literature reflecting recent AI advancements.

## 2.4 Data Extraction and Management

Data extraction and management are essential steps in conducting a structured literature review, especially when exploring complex and interdisciplinary topics such as the role of artificial intelligence (AI) in pharmacy. In this thesis, these methods were applied systematically to collect, organise, and interpret information from various sources to ensure comprehensiveness and academic accuracy. The initial step involved identifying relevant literature from credible sources including academic journals, regulatory publications, and institutional reports. These were accessed through databases such as PubMed, Scopus, Google Scholar, and ScienceDirect, using carefully selected keywords like “artificial intelligence in pharmacy,” “AI in drug discovery,” “clinical decision support systems,” “pharmacovigilance,” and “AI ethics in healthcare.”

Once the literature pool was gathered, sources were screened for relevance based on their focus area, publication date (preferably within the last 10 years), and credibility. Studies were included if they addressed AI applications in pharmacy practice, drug development, patient safety, or ethical and operational challenges. Particular emphasis was given to research that provided real-world examples, technical implementations, or policy-related discussions.

Data extraction was conducted by summarising the critical findings and contributions of each selected study. This process involved identifying key outcomes such as AI-driven improvements in medication safety, dose prediction, or inventory management. The methodologies used in these studies were also recorded, allowing for an understanding of how conclusions were drawn and how AI tools were evaluated or validated. Information such as study type (e.g., review, trial, observational), sample size, AI model used, and domain of application was systematically noted.

Following extraction, the data were categorised and managed according to thematic areas aligned with the thesis objectives. These included: drug discovery and development, personalised medicine, pharmacy operations, ethical and regulatory issues, and predictive analytics. This categorisation facilitated comparison across studies and helped identify recurring trends, novel approaches, and gaps in the current knowledge base. Concise summaries were then created for each source to highlight key insights relevant to the research questions. This approach ensured that the literature was organised in a coherent manner, making synthesis and discussion more focused and evidence-driven.

The data extraction and management process were especially crucial given the interdisciplinary nature of artificial intelligence in pharmacy, which spans healthcare, technology, regulatory sciences, and pharmacology. By systematically identifying, verifying, and organising data, this thesis ensured that its review remained not only thorough but also dependable. This methodological rigour enabled meaningful insights into AI’s current and emerging role in pharmacy practice and drug development, while also offering a foundation for comparing global applications and limitations. Properly managed data strengthened the integrity of the literature review and increased the reliability of the study's conclusions and recommendations.

# Chapter 3

# Results

## 3.1 Overview of Results

This chapter presents the key findings from an extensive literature review investigating the implementation and impact of Artificial Intelligence across various domains within pharmacy. The systematic literature review conducted, commenced with an initial identification of 248 records from the selected electronic databases: PubMed, Scopus, and Google Scholar. Following the removal of duplicates, the titles and abstracts of 180 remaining records were screened for relevance. This process yielded 152 studies that underwent a comprehensive full-text assessment for eligibility. The application of pre-defined exclusion criteria resulted in the removal of studies for focusing on AI application in non-pharmacy healthcare fields such as radiology or surgery, and few other studies were omitted due to the lack of empirical data. 14 studies were excluded for being non- English publications or having inaccessible full text. Consequently, a total of 81 studies were deemed suitable for inclusion in the final study. The results are organised into various principal areas like Artificial intelligence in drug discovery and development, personalised and precision medicine, pharmacy practice predictive analytics for pharmacy operations and implementation challenges.

**Table 3.1: Overview of Results Sections and References**

| Main section | subsections | Number of References Cited (n) |
|---|---|---|
| 3.2 AI in Drug Discovery and Development | Target identification, drug repurposing, lead optimisation | 4 |
| 3.3 AI in personalised and precision medicine | Genomic analysis and tailored therapy,<br>Dose recommendation,<br>Adverse drug event prediction | 5 |
| 3.4 AI in pharmacy practice | Hospital pharmacy,<br>Community pharmacy,<br>Medication management and counselling,<br>Clinical decision support systems (CDSS),<br>Computerised prescriber order entry (CPOE),<br>Error reduction in dispensing | 18 |
| 3.5 AI in predictive Analytics for Pharmacy operations | Inventory management,<br>Outbreak prediction | 2 |
| 3.6 Challenges identified in AI implementation | Data privacy and regulatory compliance,<br>Cost and resource constraints,<br>Patient safety,<br>Social concerns | 7 |
| 3.7 Challenges and Limitations of AI in Drug Discovery | Data quality<br>Bias and diversity<br>Model interpretability<br>Ethical and regulatory barriers<br>Translation gaps | 7 |

### 3.2 AI in Drug Discovery and Development

AI- powered predictive models are being successfully applied across nearly all stages of drug R&D. In target discovery, algorithms are mining genomic and clinical data to flag novel disease mechanisms. For instance, BenevolentAI's NLP tools "read" the literature and databases to connect PDE10 (a phosphodiesterase) to ulcerative colitis, a link not explicitly reported before.[1] AI has also uncovered new antibiotic targets: a deep learning screen found the compound halicin, an originally an investigational human drug, to be a potent antibiotic against *E. coli* and other resistant bacteria in mice (Burkin, 2020). This demonstrates Artificial Intelligence's power to find the therapeutic uses outside conventional human-centric targets.

In high-throughout screening and lead optimisation, large machine-learning models dramatically reduce the search space. An AI model trained on ~2335 compounds screened millions of candidates to find halicin (Burkin, 2020). Exscientia's AI designed DSP-1181 by navigating chemical space, slashing development time; ~ 12 months to reach human trials vs. years typically). These AI workflows integrate predictive quantitative models (e.g. ML- based QSAR, toxicity predictors) to select viable leads. In practice, several companies report that AI- driven discovery can cut time and cost by ~25-50 percentage compared to traditional methods[4]. Another review notes that dozens of AI discovered candidates had entered trials by 2024, including Recursion's REC-2282 (HDAC inhibitor for neurofibromatosis) and BenevolentAI's BEN-8744 (PDE10 inhibitor for ulcerative colitis). These milestones indicate AI's practical impact on building new pipelines.

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[4] Chakraborty C, Bhattacharya M, Pal S, Islam MA. Generative AI in drug discovery and development: the next revolution of drug discovery and development would be directed by generative AI. *Ann Med Surg (Lond)* [Internet]. 2024 Aug 14 [cited 2025 Jan 3];86(10):6340–6343. Available from: https://journals.lww.com/annals-of-medicine-and-surgery/fulltext/2024/10000/generative_ai_in_drug_discovery_and_development_.101.aspx

For drug repurposing and development, predictive analytics leverages historical and real-world data. Recursion’s AI platform can repurpose existing oncology drugs for rare diseases; at least three such repurposed compounds reached phase II trials (Chen et al, 2018). Lantern pharma uses billions of oncology data points to triage after only ~ 3 years and less than US dollar 3.5M each. These successes are supported by data-driven biomarker identification: models predict which patient subgroups will respond, guiding more efficient clinical development. Overall, the results from the literature show the AI- driven predictive modelling can significantly accelerate earlier stages of R&D, producing viable candidates in a fraction of the usual time and with fewer resources.

Our review indicates that both biotech startups and big pharma are embracing Artificial Intelligence. Startups like BenevolentAI, Recursion, Lantern, and Exscientia are often highlighted as case studies of AI- augmented pipelines. Meanwhile, nearly all major pharmaceutical companies have initiated AI programs. Industry analysts note a rapid rise in AI partnerships. This trend reflects the widespread expectation that AI’s predictive analytics will boost productivity across R&D.

AI models have demonstrated remarkable success in identifying novel drug targets by analysing complex biological and genomic data. A significant breakthrough was achieved by DeepMind’s AlphaFold Model, which reduced the time required to predict protein structures from years to mere days. This leap in speed and accuracy enables a deeper understanding of disease mechanisms and facilitates the design of targeted therapeutics (Jumper et al, 2021).

Similarly, Insilico Medicine utilised AI to identify a novel target for idiopathic pulmonary fibrosis, completing the process from discovery to preclinical candidate selection in just 18 months. This represents a major advancement compared to the traditional multi-year timeline, highlighting how AI accelerates early-stage drug discovery efficiently and cost effectively (Kamya et al, 2024).

### 3.2.1 Clinical Trail Optimisation

AI is also transforming the clinical trial landscape. It predicts patient recruitment challenges, identifies optimal study populations, and aids in the design of adaptive trial protocols. AI tools can analyse historical data and health records to anticipate enrolment delays and optimise inclusion/exclusion criteria, which improves retention rates and overall trial efficiency.

By leveraging predictive analytics and real-world evidence, AI contributes to more agile, precise and cost-effective clinical development strategies. These tools are particularly valuable in streamlining operations and enhancing outcomes in both early and late-phase trials.

## 3.3 AI in Personalised and Precision Medicine

Artificial Intelligence (AI) has transformed the landscape of personalised and precision medicine by enabling individualised treatment strategies based on a patient’s genetic makeup, medical history, and real-world data. Two key areas where AI has shown significant impact are genomic analysis for therapy selection and adverse drug event prediction.

### 3.3.1 Genomic Analysis and Tailored Therapy Recommendations

AI integrates genomic, transcriptomic, and proteomic data to recommend personalised therapeutic regimens. One of the landmark examples is IBM Watson for oncology, which uses natural language processing and machine learning to match genetic profiles with evidence-based cancer treatment guidelines. The platform helps oncologists develop tailored treatment plans by analysing thousands of tailored clinical papers, patient records, and drug databases in seconds. This capability exemplifies the potential of AI in real-time clinical decision support for personalised cancer therapy (Topol, 2019)

By processing large-scale genomic datasets, AI can stratify patients into subpopulations based on their likelihood of responding to specific treatments. This ensures optimised efficacy, minimises trial-and-error prescribing, and reduces the incidence of adverse effects. In disease such as breast cancer, colorectal cancer, and rare genetic disorders, AI-based platforms are being used to propose more targeted and effective treatment regimens, reducing healthcare costs and improving patient outcomes (Aronson and Rehm, 2015).

### 3.3.2 Dose Recommendation

Artificial Intelligence (AI) has shown significant promise in optimising dose recommendations, particularly in clinical pharmacology and oncology, by personalising treatment regimens based on individual patient profiles and therapeutic responses.

According to Johnson et al (2023). AI-driven dose recommendations systems are capable of integrating diverse patient data such as demographics, genetic markers, organ function, and pharmacokinetics to offer real-time, individualised dosing guidance. These systems can outperform traditional population-based dosing algorithms by continuously learning from patient outcomes and adjusting doses accordingly. The study highlighted Artificial Intelligence platforms, when trained on high quality datasets, significantly reduce inter-patient variability and the risk of adverse drug reactions, especially for narrow therapeutic index drugs.

A notable advancement in AI-based dose personalisation was demonstrated in the PRECISE CURATE.AI trial, conducted by Blasiak et al. (2022). This prospective feasibility study evaluated an AI platform designed to dynamically tailor chemotherapy dosing for oncology patients based on their daily treatment response. The CURATE AI system used minimal patient-specific data to create a unique response profile and modulated chemotherapy doses accordingly. Results from the trial showed improved treatment tolerance and maintained therapeutic efficacy, highlighting Artificial Intelligence's potential to optimise dose intensity while minimising toxicity.

Furthermore, AI-based dose recommendations are particularly beneficial in complex cases where static dosing protocols are inadequate. AI models can account for nonlinear relationships and hidden variables that may influence drug metabolism, enabling more precise titration (Johnson et al, 2023). These findings underscore the capacity of Artificial Intelligence to support precision dosing in both acute and chronic care settings, enhancing medication safety and therapeutic outcomes.

AI applications in dose recommendation are transforming pharmacotherapy by enabling precision medicine. These systems not only facilitate real-time, adaptive dose adjustments but also hold the potential to improve clinical outcomes, reduce adverse events, and support clinician decision-making in complex treatment scenarios.

### 3.3.3 Adverse Drug Event Prediction and Drug-Drug Interactions

Another key application of AI in personalised medicine is the prediction and prevention of adverse drug reactions (ADRs). Machine learning models trained on electronic health records (EHRs), pharmacovigilance databases, and clinical trial reports can detect complex drug-drug interactions (DDIs) that are often missed by human clinicians.

Machine learning algorithms can identify hidden patterns in drug interaction profiles and flag high risk combinations. This improves prescribing safety in patients with polypharmacy or co-morbid conditions. These predictive tools also support dosing individualisation, especially in vulnerable populations such as the elderly or those with impaired hepatic or renal function. (Hammann et al, 2010)

Overall, the integration of AI into personalised medicine enhances precision, safety, and efficiency across patient care. It paves the way for a data-driven, patient-centered healthcare system that can adapt to each individual's unique biology and circumstances.

### 3.4 AI in Pharmacy Practice

Artificial Intelligence has also made transformative contributions to pharmacy practice particularly in the areas of medication management and error reduction.

The integration of artificial intelligence (AI) into hospital pharmacy settings has significantly transformed clinical workflows, enhanced medication safety, and optimized therapeutic outcomes. Recent evidence suggests that AI technologies are playing an increasingly pivotal role in improving efficiency, reducing errors, and supporting clinical decision-making within hospital pharmacy environments. Al Meslamani (2023) provides a comprehensive overview of AI applications across hospital and community pharmacy settings, highlighting its contributions to drug inventory management, automated dispensing, and real-time clinical support. In hospital pharmacies, AI-powered systems are increasingly used to assist pharmacists with identifying potential drug interactions, optimizing dosing regimens, and flagging high-risk prescriptions. These systems not only enhance patient safety but also reduce pharmacist workload by automating time-consuming processes.

One notable application in oncology is IBM Watson for Oncology, which has demonstrated high concordance with expert clinical decisions. A study by Zhou et al (2019), in China reported that Watson's treatment recommendations for cancer patients matched clinical practice in over 90% of breast cancer cases, indicating its value as a decision-support tool in complex treatment planning. This system aids hospital pharmacists and oncologists in selecting evidence-based regimens, particularly in resource-limited or high-volume hospital settings.

Medication safety is another critical area where AI demonstrates measurable impact. Naeem and Coronato (2022) described an AI-empowered infrastructure that integrates smart home and hospital systems to minimize medication errors. Their model monitors medication adherence and administration timing, which is particularly valuable for patients transitioning between inpatient and outpatient care — a common point of medication-related errors.

Additionally, predictive analytics models in hospital settings are used to assess patient risk and prevent adverse outcomes. Poplin et al. (2018) showed that deep learning algorithms applied to retinal images can predict cardiovascular risk factors with accuracy comparable to traditional diagnostic methods. Such predictive capabilities, when integrated into hospital electronic health record

(EHR) systems, allow pharmacists to proactively manage pharmacotherapy for high-risk patients.

Furthermore, Huang et al. (2019) introduced CASTER, an AI tool designed to predict drug-drug interactions using chemical substructure representations. This model significantly enhances the accuracy of drug interaction alerts and supports pharmacists in making more informed decisions, especially in complex polypharmacy cases often seen in hospitals.

In terms of infrastructure and data security, Powles and Hodson (2017) raised important considerations in the use of AI within large hospital systems, particularly concerning data governance and algorithm transparency. Their discussion of Google DeepMind’s partnership with UK hospitals underscored both the immense potential and ethical responsibilities associated with AI implementation in healthcare.

Finally, Simpson and Qasim (2025) emphasized the need for hospital pharmacies to invest in AI infrastructure as part of broader healthcare innovation. They argue that AI-driven pharmacy operations — including stock prediction, electronic prescribing checks, and real-time analytics — are essential to meet modern healthcare demands, especially amid increasing patient volumes and chronic disease burdens.

In summary, AI adoption in hospital pharmacy is yielding substantial benefits, including improved clinical decision support, enhanced medication safety, predictive patient monitoring, and operational efficiency. However, successful integration requires attention to algorithm transparency, data privacy, and the ongoing training of clinical pharmacists to collaborate with AI systems effectively.

The integration of artificial intelligence (AI) into community pharmacy settings has expanded the scope of pharmaceutical care, particularly in patient engagement, disease surveillance, and operational optimization. Community pharmacies serve as a crucial link between the healthcare system and the public, and AI has the potential to significantly augment their role by enabling faster decision-making, personalised services, and public health interventions.

One of the primary applications of AI in community pharmacy is improving medication counselling and adherence support. Al Meslamani (2023) notes that AI-powered chatbots and virtual assistants have been deployed in several community pharmacy settings to assist patients with medication instructions, dose reminders, and minor health queries. These tools enable pharmacists to dedicate more time to complex clinical tasks while still ensuring patients receive necessary support. Additionally, AI platforms are being used to identify patients at risk of non-adherence through behavioural pattern recognition and to initiate targeted interventions.

Raza et al. (2022) further highlight AI’s role in streamlining inventory management in community pharmacies. By analysing historical dispensing data, AI algorithms can predict stock requirements more accurately, reducing waste and ensuring consistent medication availability. This predictive capability is particularly important during health crises, such as pandemics or seasonal outbreaks, where demand can fluctuate unpredictably.

AI also contributes to public health through disease surveillance in the community setting. Community pharmacies, being accessible healthcare points, can participate in early disease detection efforts. Bohr and Memarzadeh (2020) describe how AI algorithms can integrate data from over-the-counter sales, symptom reporting, and wearable devices to flag emerging health trends. This can enable pharmacies to act as first-line detectors for outbreaks such as influenza or COVID-19.

A practical example of AI's public health potential in pharmacy settings is illustrated by Venkatramanan et al. (2021), who demonstrated that machine-learned mobility and prescription data could be used to forecast influenza activity with high accuracy. Community pharmacies equipped with such AI tools could prepare in advance for surges in medication demand and improve resource allocation to vulnerable populations.

Furthermore, AI supports personalised customer experiences in community pharmacies. By analysing purchase history, preferences, and health data (where consent is provided), AI tools can recommend over-the-counter products, wellness supplements, or health screening services tailored to individual patients. This aligns with the increasing trend toward personalised medicine in retail health environments.

However, while AI presents significant advantages in community pharmacy, its adoption remains limited due to infrastructure variability, data integration challenges, and a lack of digital literacy among some pharmacy staff. Despite these challenges, the initial results from pilot programs suggest that with proper implementation, AI can transform community pharmacies into intelligent health hubs that extend beyond dispensing to offer proactive, data-driven care.

In summary, AI applications in community pharmacy include automated patient counselling, inventory optimisation, outbreak prediction, and personalised service delivery. These advances enhance the efficiency, accessibility, and preventative role of community pharmacies, reinforcing their importance within a modern, AI-enhanced healthcare ecosystem.

### 3.4.1 Medication Management and Patient Practice

AI- driven chatbots are increasingly being used to support pharmacists in providing medication information and counselling. For instance, Sensely, an AI-powered virtual assistant, interacts with patients using speech recognition and natural language processing to offer medication guidance, adherence reminders, and symptom triage. This technology improves accessibility to pharmaceutical care and reduces the burden on human pharmacists (Garcia-cardenas et al,2020). These systems are particularly valuable in community and outpatient settings, where pharmacists face high patient volumes. By automating routine inquiries and providing consistent, accurate, and evidence-based responses, AI chatbots ensure timely, patient-centered care, enhancing medication adherence and health literacy. Moreover, AI systems allow for 24/7 availability, providing patients with ongoing support even outside of normal pharmacy hours. This enhances the continuity of care and builds trust in pharmaceutical services. Furthermore, AI tools can be programmed to deliver multilingual support, enabling equitable access to medication information across diverse populations.

### 3.4.2 Clinical decision support system (CDSS)

The integration of Artificial Intelligence (AI) in pharmacy has significantly advanced clinical decision support system (CDSS) leading to improved medication safety, optimised therapeutic choices, and enhanced patient outcomes. AI- powered Clinical Decision Support System tools assist pharmacists and healthcare professionals in making informed decision by analysing vast datasets, predicting potential risks, and recommending personalised treatment options.

Artificial Intelligence enhanced Clinical Decision Support System (CDSS) provide real-time, evidence based clinical recommendations by synthesising patient data such as medical history, laboratory results, and pharmacogenomic information (Sutton et al, 2020). These systems reduce human errors, especially in complex decision-making scenarios, and enhance the consistency of care delivery. Thus AI-CDSS has the potential to decrease adverse events, improve diagnostic accuracy, and increase compliance with clinical guidelines.

The growing adoption of AI- driven Clinical Decision Support System (CDSS) in pharmacy practice, particularly in medication therapy management. Tools equipped with machine learning algorithms can flag high-risk prescriptions, detect drug-drug interactions, and alert pharmacists about contraindications[5]. These functions are especially valuable in outpatient and hospital pharmacy settings, where patient complexity and medication overload are high. Moreover, Clinical Decision Support System platforms contribute to time savings and reduce cognitive burden by automating repetitive clinical assessments.

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[5] Sangave NA, Cheung C, Berkley E. Artificial Intelligence Applications in Education and Pharmacy Practice. *Pharmacy Times* [Internet]. 2022 . [cited 2025 Mar 3]. Available from: https://www.pharmacytimes.com/view/artificial-intelligence-applications-in-education-and-pharmacy-practice

Chalasani et al, (2023) reinforced these findings through a systematic literature review, stating that Clinical Decision Support System (CDSS) applications powered by Artificial Intelligence help bridge the gap between clinical data and therapeutic decisions. Their review has demonstrated that AI-CDSS enhances patient specific medication recommendations and supports precision pharmacotherapy. Furthermore, the use of Artificial Intelligence reduces prescription errors and supports clinical auditing by maintaining comprehensive records of decision pathways and rationale.

Overall, the implementation of Artificial Intelligence in Clinical Decision Support System represents a significant advancement in pharmacy practice. By enabling proactive identification of therapy-related problems, reducing errors, and supporting individualised patient care, these systems serve as a cornerstone of clinical pharmacy transformation in the digital error.

### 3.4.3 Computerised Prescriber Order Entry

Computerised Prescriber Order Entry systems represent one of the earliest and most impactful applications of Artificial Intelligence and digital technology in medication management. By allowing healthcare professionals to electronically enter medication management. By allowing healthcare professionals to electronically enter medication orders, Computerised Prescribe Order Entry systems minimise transcriptional errors, improve documentational quality, and support safer prescribing practices.

A landmark study by Lesar et al. (1997) identified that a significant proportion of prescribing errors originated from manual order entry processes, including illegible handwriting, ambiguous abbreviations, and dosing inaccuracies. Their findings underscored the necessity for electronic systems that could provide decision support and error checking during the prescribing phase. Computerised Prescriber Order Entry systems directly address these vulnerabilities by embedding AI-driven alerts, standardised order sets, and automated dose checks into the workflow.

Further, supporting these benefits, Jungreithmayr et al, (2021) conducted a before and after study assessing the implementation of Computerised Prescriber Order Entry across 20 medication documentation criteria. The results demonstrated substantial improvements in the completeness and accuracy of medication orders post-implementation. Specifically, there was enhanced adherence to prescribing protocols, reduced omission of critical information such as dosing frequencies and routes, and improved legibility and standardisation. Their findings affirm that Computerised Prescriber Order Entry systems not only reduce human error but also streamline documentation practices critical for continuity of care.

Moreover, a report at Birgham and Women's Hospital highlighted that when integrated with clinical decision support, Computerised Prescriber Order Entry systems significantly enhance medication safety. The system automatically cross-checks for drug-allergy interactions, contraindications, duplication, and inappropriate dosing. The study also emphasised the importance of designing user-friendly interfaces and customising alerts to avoid alert fatigue, a known challenge in digital prescribing platforms[6].

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[6] Schiff GD, Wright A, Bates DW, Salazar A, Amato MG, et al. Computerized Prescriber Order Entry Medication Safety (CPOEMS): uncovering and learning from issues and errors [Internet]. Brigham and Women's Hospital, Harvard Medical School, Partners HealthCare; supported by U.S. FDA; [published ca. 2015] [Accessed on 6 Jan 2025] Available from: https://www.fda.gov/files/drugs/published/Computerized-Prescriber-Order-Entry-Medication-Safety.pdf.

Overall, the integration of Artificial Intelligence into Computerised Prescriber Order Entry systems has redefined the medication prescribing process in pharmacy practice. By improving data integrity, reducing prescription-related errors, and enhancing patient safety, these systems contribute to more reliable and efficient pharmaceutical care. As Artificial Intelligence capabilities continue to evolve, Computerised Prescriber Order Entry is expected to serve as a foundation for more sophisticated, context aware prescribing systems that adapt to individual patient characteristics and real-time clinical data.

### 3.4.4 Error Reduction in Dispensing

AI technologies also being employed to reduce medication errors in pharmacy operations. AI assisted dispensing systems reduced errors by 45 percentage compared to traditional manual processes. These systems use barcode scanning, image recognition, and machine learning algorithms to validate prescriptions, verify dosages, and detect discrepancies before the medication reaches the patient. (Graafsma et al,2024)

In addition to automated dispensing cabinets, AI is integrated with electronic prescribing systems and inventory management platforms to enhance medication safety. By cross-verifying prescriptions with patient records, allergies, and contraindications, AI minimises transcription errors and enhances clinical decision making. In high throughput hospital environments, AI-powered automation significantly alleviates pharmacist's workload and allows reallocation of resources to clinical services, such as medication therapy management and patient education.

## 3.5 AI in Predictive Analytics for Pharmacy Operations

AI- powered predictive analytics is playing a pivotal role in optimising pharmacy operations by enabling data-driven forecasting and proactive decision making. Two major application areas include inventory management and disease outbreak prediction.

### 3.5.1 Inventory Management and Demand Forecasting

AI algorithms can analyse historical sales data, seasonal trends, prescription patterns, population demographics, and external variables (such as public health alerts, socioeconomic factors, and weather changes) to accurately forecast medication demand. Pharmacies that adopted AI- based inventory management systems experienced a 20-percentage reduction in overstock levels, leading to decreased wastage and improved cost efficiency. (chen and see,2020)

By minimising both overstock and stockouts, AI helps pharmacy managers make informed procurement decisions, adjust reorder thresholds, and automate supply chain coordination. Predictive tools can detect spikes in demand for critical medications, such as antipyretics or antibiotics during flu seasons, enabling pre-emptive restocking. Furthermore, AI systems can continuously learn and refine their forecasts based on evolving trends and anomalies, improving reliability over time. Integrating AI with enterprise resource planning and pharmacy management systems facilitates real time decision making, ensuring seamless inventory flow from supplier to dispensary.

These capabilities not only enhance operational efficiency but also contribute to improved patient satisfaction, as medications are more likely to be in stock when needed. For resource-constrained healthcare settings, optimised inventory planning supported by AI can reduce operational costs while maintaining essential medicine availability.

### 3.5.2 Outbreak Prediction and Public Readiness

AI Models have also demonstrated exceptional capability in early outbreak detection and epidemic surveillance. For instance, BlueDot, a Canadian AI platform, detected and flagged the emergence of COVID-19 several days before the World Health Organisation issued its official alert. It achieved this by processing a wide range of data sources like news reports, airline ticketing records, digital surveillance logs, and global health bulletins, in multiple languages using natural language processing and machine learning algorithms. (Rajkomar et al,2019)

Pharmacies equipped with access to such outbreak prediction tools can proactively adjust stock levels, prioritise inventory for high demand medications such as antivirals, vaccines, or respiratory support drugs, and support infection control efforts. These AI tools also facilitate collaboration with public health authorities, allowing pharmacy professionals to contribute meaningfully to broader outbreak containment strategies.

In addition, predictive modelling can help identify geographical hotspots and vulnerable populations, enabling targeted intervention strategies and equitable resource distribution. Pharmacies in these areas can deploy mobile health services, increase staffing, or extend hours to manage surges in healthcare demand. Ultimately, AI-powered outbreak prediction empowers pharmacy operations with strategic foresight, transforming them into active contributors to emergency preparedness and public health response.

## 3.6 Challenges Identified in AI Implementation

Despite the broad promise of AI in pharmacy, multiple challenges hinder its seamless implementation. These include data privacy concerns and financial barriers.

### 3.6.1 Data Privacy and Regulatory Compliance

A critical challenge to AI adoption in healthcare, including pharmacy, is maintaining data privacy and regulatory compliance. 60-percentage of studies reviewed cited General Data Protection Regulation (GDPR) and Health Insurance Portability and Accountability Act (HIPAA) compliance as significant barriers. (mudroch,2021)

AI systems often require access to extensive patient level data to achieve accuracy in prediction and personalisation. However, the sensitivity of healthcare data means organisations must ensure strict compliance with legal frameworks governing data protection. Healthcare providers and pharmacy institutions face difficulties in balancing innovation with stringent data governance. Ensuring that datasets are anonymised and securely stored is technically complex and resource intensive. Inadequate compliance could lead to reputational damage, legal repercussions, and erosion of patient trust.

The rapid expansion of big data in healthcare, coupled with the involvement of major technology companies, has created a tension between innovation and patient privacy. Artificial Intelligence systems frequently depend on access to sensitive patient information, including electronic health records (EHRs), genetic profiles, and behavioural data. While this information is crucial for algorithmic learning and precision medicine, it also significantly increase the risk of data breaches and misuse if robust protections are not in place (Cohen and Mello, 2019)

The study also highlights that many of the current legal safeguards such as Health Insurance Portability and Accountability Act (HIPAA) in the United States are not fully equipped to handle the complex data-sharing ecosystems created by Artificial Intelligence. These regulations were not designed to address the ways in which tech companies interact with health data, particularly when data is de-identified or shared across platforms, consequently, patients often remain unaware of how their data is being used, and consent frameworks may fall short in capturing the dynamic nature of AI-driven analytics.

Moreover, Artificial Intelligence systems pose challenges to traditional data security practices. Unlike, conventional databases, AI platforms often involve continuous data exchange across multiple nodes, increasing the vulnerability to cyberattacks. According to Cohen and Mello (2019), this risk is magnified when third party vendors are involved in the development and deployment of AI models, creating additional layers of liability and accountability concerns.

Healthcare professionals and institutions require clearer policy guidelines and standardised protocols to facilitate compliant AI deployment. Investment in robust encryption technologies, audit trails, federated learning methods (that train models without sharing data), and continuous staff training in data ethics are imperative steps toward overcoming this challenge.

### 3.6.2 Cost and Resource Constraints

High costs remain a significant barrier to the implementation of Artificial Intelligence, particularly in small or independently owned pharmacies. As noted, Artificial intelligence implementation costs frequently exceed the budgetary capabilities of smaller healthcare facilities. (Alsudairy et al, 2025)

Artificial Intelligence systems require substantial initial investment in digital infrastructure, including hardware upgrades, cloud storage, cybersecurity frameworks, and software licencing. Beyond installation, ongoing expenses include system maintenance, algorithm updates, staff retraining, and performance validation. These expenses are manageable for large hospitals or pharmacy chains but can be prohibitive for rural or resource limited settings.

Furthermore, there is a lack of uniform funding pathways or reimbursements models for Artificial Intelligence based solutions in pharmacy. This uncertainty makes it difficult for smaller institutions to justify long-term investment. Many organisations are hesitant to divert limited resources from immediate patient care needs to high-tech innovations with uncertain returns.

The disparity in digital readiness across pharmacies may result in inequitable access to Artificial Intelligence, exacerbating healthcare inequalities. While urban centres may benefit from state-of-the-art technologies, smaller facilities risk falling behind unless supported through government grants, public-private collaborations, or shared access Artificial intelligence platforms.

Policy interventions that promote affordability and offer financial incentives for Artificial Intelligence adoption especially among the small and mid-sized providers are crucial to overcoming cost related challenges. Additionally, scalable cloud-based AI services and open-source tools can help democratize access to Artificial Intelligence innovation across the healthcare spectrum.

### 3.6.3 Patient safety

The integration of Artificial Intelligence into clinical settings is not without challenges that may also introduce new risks if not properly manged. AI technologies particularly in clinical decision support systems (CDSS) can reduce human error by standardising treatment recommendations and enhancing the detection of abnormal patterns in patient data. However, the Artificial Intelligence systems are only as reliable as the data and design behind them. If trained on biased or incomplete datasets, Artificial Intelligence may produce inaccurate recommendations, potentially jeopardising patient outcomes. The concept of “distributional shift” where Artificial Intelligence performs well on training data but poorly in real-world, diverse patient populations is a key risk factor that can undermine patient safety (Aung et al, 2021). This is particularly concerning in underrepresented groups or rare disease scenarios where data may be sparse.

On one hand, Artificial Intelligence tools such as predictive analytics and early warning systems have shown promise in minimising diagnostic errors and improving clinical workflow efficiency. On the other hand, the danger of automation bias, where healthcare professionals may over rely on Artificial Intelligence outputs without sufficient clinical validation. The risk is heightened when AI tools are deployed without adequate transparency or interpretability, commonly referred to as black box problem (Ali et al, 2023).

Moreover, as AI systems evolve, there is an inherent need for continuous monitoring and recalibration to account for new medical evidence, updated guidelines, and shifting population health trends. A lack of ongoing validation can lead to outdated or unsafe recommendations being made to clinicians, particularly in high-risk or time-sensitive situations.

### 3.6.4 Social Concerns

The integration of Artificial Intelligence (AI) into pharmacy and broader healthcare systems has raised a range of social concerns that extend beyond technical and clinical challenges. These concerns encompass public trust, health equity, workforce disruption, and the readiness of society to accept Artificial Intelligence as a legitimate actor in clinical decision-making.

Public scepticism toward Artificial Intelligence in healthcare is one of the leading barriers to its adoption. Many patients and healthcare workers express unease about the perceived dehumanisation of care and the delegation of medical decisions to machines. The fear of being treated as data points rather than individuals contributes to reduced trust in AI-enabled services (Sun and Medaglia, 2019). This hesitancy can slow the acceptance of AI-driven pharmacy applications, even when those systems demonstrate clinical benefit.

Low awareness and utilisation of technology-based interventions among the healthcare professionals across the European Union, particularly in the management of substance use disorders. The broader issue of digital readiness and varying levels of digital literacy, which would hinder equitable Artificial intelligence adoption across healthcare systems (Quaglio et al,2019). If pharmacists and healthcare workers are not adequately trained or informed about the value, limitations, and functioning of Artificial Intelligence, it may lead to underutilisation, improper application, or over-reliance on AI tools, ultimately affecting patient outcomes and staff confidence.

Furthermore, Artificial Intelligence may exacerbate existing social inequalities if implementation is not carefully managed. For instance, AI algorithms trained on skewed or non-representative datasets risk reinforcing systemic biases, resulting in unequal healthcare access, especially for minority or socioeconomically disadvantaged populations. There is also around algorithmic discrimination in medication access, pricing, and treatment prioritisation that reflect societal biases embedded in historical data[7].

In addition, the potential displacement or deskilling of healthcare professionals, including pharmacists, raises societal and labour-related concerns. While Artificial Intelligence is often presented as an aid rather than a replacement, the fear of automation displacing human roles contributes to resistance within the profession. Ethical concerns are compounded by the absence of clear guidelines on the roles and responsibilities of AI systems versus human clinicians, especially when it comes to accountability in clinical errors.

### 3.7 Challenges and Limitation of Using AI in Drug Discovery

While Artificial Intelligence (AI) has shown transformative potential in drug discovery, several significant challenges and limitations persist, impacting its reliability, scalability, and integration into existing pharmaceutical research frameworks.

One of the primary challenges lies in data availability and quality. As highlighted by Vamathevan et al. (2019), AI models depend heavily on large volumes of high-quality, annotated data to make accurate predictions about drug efficacy, toxicity, and molecular interactions. However, real-world pharmaceutical datasets are often heterogeneous, sparse, and siloed, making it difficult to train robust,

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[7] *European Parliament Directorate-General for Parliamentary Research Services, Lekadir K., Quaglio G., Tselioudis Garmendia, et al. Artificial intelligence in healthcare – Applications, risks, and ethical and societal impacts. European Parliament. 2022. [Accessed on: 8 Apr 2025] available from:https://data.europa.eu/doi/10.2861/568473*

generalizable models. This is particularly problematic in early-stage discovery, where failed experiments and negative results are rarely published or shared.

Data bias and lack of diversity also present major concerns. According to Tsuji et al (2021), biased training data can skew AI models toward producing misleading results that may not generalize across populations or disease types. For instance, drug-target interaction models may fail to identify promising candidates for rare or complex diseases like Alzheimer's if insufficient or unbalanced data is used. This limits the inclusivity and fairness of AI-driven drug discovery platforms.

Another limitation is the interpretability of AI models. As noted by Gómez-Bombarelli et al. (2018) and Arrieta et al. (2020), many deep learning models function as "black boxes," providing predictions without transparent reasoning. This lack of explainability creates scepticism among researchers and regulators, hindering the adoption of AI-generated drug candidates in preclinical and clinical settings. Minh et al. (2022) emphasize that explainable AI (XAI) is essential for fostering trust, validating hypotheses, and enabling human experts to interpret and act on AI recommendations meaningfully.

Ethical and regulatory considerations also form a critical barrier. Basu et al. (2020) discuss the current ethical vacuum surrounding AI in drug discovery, particularly in the context of accountability, patient consent, and algorithmic bias. Questions remain regarding who is responsible for errors made by AI in the drug development pipeline and how ethical safeguards can be embedded into AI tools. Additionally, Chin et al (2023) highlights inherent trade-offs in algorithmic fairness, where optimizing a model for one fairness metric may compromise another. This tension is especially problematic in drug development, where a balance must be struck between model performance and equitable access to treatments.

Lastly, integration of AI outputs into traditional pharmaceutical workflows remains limited. Vamathevan et al. (2019) point out that despite advances in AI-based molecule generation and virtual screening, experimental validation remains time-consuming and costly. Many AI-generated compounds fail to translate into clinically viable drugs due to issues like poor bioavailability or unexpected toxicity during in vivo testing.

In summary, while AI holds great promise in accelerating drug discovery, current limitations include poor data quality, lack of transparency, ethical uncertainty, and translational gaps. Addressing these challenges through improved data governance, regulatory frameworks, and explainable AI development is essential for the responsible and effective deployment of AI in pharmaceutical innovation.

# Chapter 4

# Discussions

Artificial intelligence has emerged as a transformative force across pharmacy sectors, demonstrating potential in drug discovery, personalised medicine, pharmacy operations, and patient care. However, alongside these advancements are multifaceted challenges spanning ethics, technology, regulation, workforce readiness, patient safety, and social dynamics. This chapter critically analyses these findings in the context of real-world implementation.

### 4.1 Advancements in Pharmacy Through AI

Artificial Intelligence technologies have notably accelerated target identification and drug discovery. For example, DeepMind's AlphaFold model reduced protein structure prediction time from years to days. (Jumper et al,2021), while Insilico Medicine identified a novel fibrosis target within just 18 months. These case studies highlight the speed and precision Artificial Intelligence brings to molecular biology and pharmacology[8].

In personalised medicine, platforms like IBM Watson for oncology integrate patient genomic data with clinical literature to recommend tailored cancer therapies (Topol,2019). Artificial intelligence also plays a vital role in predicting adverse drug reactions, with machine learning models flagging drug-drug interactions missed by traditional methods (Hammann et al,2010). These advancements enhance treatment efficacy, safety, and patient satisfaction.

Pharmacy practice has also seen improvement with Artificial Intelligence integration. Chatbots such as Sensely assist in patient counselling, providing 24/7 multilingual

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[8] Insilico Medicine launches trial for AI-discovered drug.,2021,Outsourcing-Pharma.*; Available from:* [*https://www.outsourcing-pharma.com/Article/2021/12/15/Insilico-Medicine-launches-trial-for-AI-discovered-drug*](https://www.outsourcing-pharma.com/Article/2021/12/15/Insilico-Medicine-launches-trial-for-AI-discovered-drug) . [accessed on: 7 May 2025]

support and improving medication adherence (Garcia-Cardenas et al,2020). Meanwhile, AI-assisted dispensing systems have reduced medication errors by 45% (Graafsma et al,2024), boosting safety and pharmacist productivity.

AI- driven predictive analytics enhances pharmacy operations, notably inventory management and outbreak response. Algorithms reduce overstock by up to 20% (chen et al, 2020) and platforms like BlueDot successfully flagged COVID -19 risks before WHO alerts (Rajkomar et al,2019). These capabilities demonstrate Artificial Intelligence's value in operational planning and public health readiness.

### 4.2 Ethical Barriers

Ethical concerns remain a formidable barrier to AI adoption. Central issues include patient privacy, consent, trust, and conflicts of interest. The need for large datasets in Artificial Intelligence development raises tension between innovation and patient confidentiality. General Data Protection regulation and Health Insurance Portability and Accountability (HIPAA) demand informed consent and transparency, yet studies show these conditions are often inadequately met (Mudroch, 2021).

Patients must understand who has access who has access to their data, how it is stored, and its intended use. Several studies recommend revisiting existing definitions of data privacy and ownership in light of Artificial Intelligence's data-intensive nature. Furthermore, commercial involvement in Artificial Intelligence raises trust issues, particularly when developers lack transparency regarding algorithm design, a phenomenon often referred to as the "black box" (Lester et al,2025). Kelly et al. (2019) emphasized that transparency and patient education are essential, especially as Artificial Intelligence systems become more deeply integrated into decision-making processes.

Sakamoto et al. (2020) also noted that the opaque nature of Artificial Intelligence algorithms- the “black box” problem – compromises trust and impedes validation and clinical oversight.

Data ownership and consent were highlighted in Ten studies, with He et al. (as sited in Reddy et al, 2020) recommending a redefinition of confidentiality and privacy norms in light of Artificial Intelligence’s broad data use. Reddy et al, 2020 further stress the importance of comprehensive governance frameworks to guide the secure use, sharing, and storage of data.Trust in Artificial Intelligence tools is another ethical concern. Chen et al. (2018) reported that clinicians often lack confidence in Artificial Intelligence systems due to insufficient training, lack of robust prospective trials, and commercial interests that may prioritise profit over patient safety.

Moreover, Artificial Intelligence may struggle with nuanced or complex cases involving multisystem diseases, further reducing clinician confidence in its utility (Ahmed et al,2023). The inability of developers to explain hoe decisions are made creates barriers to integration within clinical practice and damages the physician-patient relationship.

Conflicts of interest present additional ethical challenges. Brady et al. (2020) highlighted concerns among radiologists who may have commercial ties to the AI tools they use. This dual role user and developer raises serious questions about impartiality and ethical conduct. They recommend managing these conflicts similarly to how conflicts in drug development are regulated.

A final yet evolving concept is algorithmic fairness. McCradden et al. (2020) discuss the attempt to build models that actively detect and correct bias across gender, race, or other social factors. while encouraging, these methods are not foolproof, and ethical dilemmas will continue to arise, particularly as Artificial Intelligence is applied across diverse patient populations.

In summary, ethical barriers including privacy concerns, lack of transparency, data governance gaps, trust deficits, and commercial conflicts must be addressed systematically. Policies that enforce transparency, explainability, and accountability must accompany Artificial Intelligence deployment, and ethical training should be integrated into pharmacy curricula for Artificial Intelligence enhanced decision-making.

### 4.3 Technical Barriers

Technological limitations remain a significant obstacle to the widespread implementation of Artificial Intelligence in pharmacy and broader healthcare settings. Among the most cited barriers are data quality and availability, lack of interoperability, limited transparency of Artificial Intelligence systems, challenges in validation, and infrastructural inadequacies.

Firstly, the performance of Artificial Intelligence systems is intrinsically linked to the quality and quantity of data used to train them. The low-quality datasets, or those lacking inn diversity, impair algorithmic learning and reduce generalizability, leading to biased or inaccurate outputs (Ben-Israel et al.,2020). Artificial Intelligence systems may overfit on small datasets or fail to recognise confounding variables such as ethnicity, age, and comorbidities. (Singh et al,2020).

Despite the proliferation of Artificial Intelligence applications during the COVID-19 pandemic, many failed to reach clinical relevance due to poor dataset representativeness and inconsistencies in data labelling (Chen and see, 2020). This reinforces the idea that high-performing models in laboratory settings do not always translate effectively to real-world environments.

Interoperability remains another key technological hurdle. Healthcare systems often use siloed and non-standardised data formats, making it difficult for Artificial Intelligence tools to access and analyse data across platforms. The absence of sharable clinical guidelines and standards restricts Artificial Intelligence's ability to integrate smoothly into clinical workflows (Ahmed et al,2023). Even when the interoperability exists. The usability of Artificial Intelligence systems many not align with current clinical processes, leading resistance from healthcare workers.

Furthermore, the black box nature of many Artificial Intelligence models prevents users from understanding how decisions are made. This lack of interpretability hampers trust and limits clinical adoption (Poon and Sung, 2021). Without the ability to explain outputs, professionals may be hesitant to act on Artificial Intelligence generated recommendations, especially when the accountability is not clearly defined.

Validation and real-world testing of Artificial Intelligence applications are still limited. The most neuroimaging-based Artificial Intelligence tools lack rigorous clinical validation, calling into question their reliability and reproducibility. Additionally, Sing et al (2020), emphasise the need for large-scale, multi-centre trials that reflect the heterogeneity of real-world patient populations.

Finally, the infrastructural demands of Artificial Intelligence such as computing power, data storage, and cybersecurity measures pose logistical and financial barriers, particularly for smaller or under-resourced institutions. The need for consistent internet connectivity, cloud-based platforms, and dedicated IT teams can make Artificial Intelligence deployment unfeasible in many healthcare settings (Kelly et al,2019).

In conclusion, while AI holds tremendous promise for pharmacy and healthcare, technological barriers related to data, interoperability, system usability, transparency, and infrastructure must be overcome. Collaborative efforts involving pharmacists, technologists, and policymakers are essential to bridge these gaps and create systems that are both effective and scalable.

### 4.4 Implications for pharmacists and their practice

The integration of artificial intelligence (AI) into pharmacy practice holds profound implications for pharmacists' roles, responsibilities, and professional identity. As AI systems become increasingly embedded in drug discovery, clinical decision support, inventory management, and patient engagement, pharmacists must adapt to a rapidly evolving healthcare landscape. This transition requires not only technical upskilling but also a redefinition of traditional pharmacist functions to align with AI-augmented healthcare delivery (Raza et al, 2022)

One of the most significant implications is the shift from task-oriented to cognitive and clinical responsibilities. With AI taking over repetitive and operational tasks such as stock forecasting, drug interaction alerts, and even preliminary patient triage, pharmacists are now positioned to focus more on advanced clinical decision-making and direct patient care. This allows pharmacists to play a greater role in personalised medicine, using AI-generated insights to recommend tailored therapies based on genetic, lifestyle, and comorbidity data. However, this shift necessitates a deeper understanding of data analytics and interpretation skills, highlighting the need for curriculum reform in pharmacy education and ongoing professional development.

AI also challenges traditional notions of pharmaceutical judgment and autonomy. Clinical decision support systems (CDSS) and computerised physician order entry (CPOE) tools can influence pharmacists' clinical choices by presenting algorithm-based recommendations. While this can improve consistency and safety, there is a risk that pharmacists may become over-reliant on AI tools, potentially leading to automation bias. Thus, pharmacists must learn to balance AI input with their own clinical reasoning, maintaining professional accountability and critical thinking.

In addition, pharmacists must navigate ethical, legal, and regulatory considerations associated with AI tools. Questions around data privacy, algorithm transparency, and patient consent require pharmacists to understand the digital and legal frameworks within which AI operates. As custodians of sensitive patient information and frontline healthcare providers, pharmacists must advocate for ethical AI use and ensure that patients are informed participants in AI-supported care.

Workforce implications are also notable. As AI adoption increases, job roles within pharmacy practice are likely to evolve, with new specialisations emerging in areas such as pharmacoinformatic, digital therapeutics, and AI governance. While some fear that automation may displace pharmacy roles, current evidence suggests that AI will act as a complement rather than a replacement, allowing pharmacists to expand their services into new domains such as public health analytics, medication adherence monitoring, and remote patient support.

Furthermore, AI may enhance pharmacists' ability to contribute to multidisciplinary teams, as their familiarity with both clinical and technological aspects of medication management become increasingly valuable. Pharmacists can act as intermediaries between data scientists, healthcare providers, and patients, ensuring that AI applications are safe, practical, and patient-centred.

Finally, the successful integration of AI into pharmacy practice depends on institutional support, policy alignment, and digital infrastructure. Pharmacists will need access to AI-enabled systems, appropriate training, and interdisciplinary collaboration to fully realise the benefits of AI in their day-to-day work.

### 4.5 Future Directions of Artificial Intelligence in Pharmacy

As artificial intelligence (AI) continues to revolutionize pharmacy practice, drug discovery, and healthcare delivery, it is imperative to consider its future trajectory. The coming years will likely see significant advancements in both the technical performance and regulatory oversight of AI, with far-reaching implications for pharmacists, clinicians, and patients alike.

One of the primary areas of growth lies in the transparency and standardization of AI reporting models. Despite promising results from AI applications, reproducibility and interpretability remain major challenges. Turlip et al. (2025) emphasize the importance of transparent AI model development, calling for consistent reporting frameworks that enable clinicians and stakeholders to assess the quality and validity of prediction tools. This need is further addressed by initiatives such as the TRIPOD-AI and PROBAST-AI protocols (Collins et al., 2021), which aim to improve the reporting of AI-based diagnostic and prognostic models. These guidelines will enhance trust and usability, ensuring AI applications are both scientifically sound and clinically interpretable.

Building on this, the TRIPOD+AI statement (Collins et al., 2024) introduces updated standards for reporting AI-based prediction models using machine learning or regression. As more AI tools are integrated into clinical decision-making and pharmacy operations, adherence to these guidelines will be essential to mitigate bias, validate algorithms, and ensure accountability. This move toward standardization reflects the broader push for responsible AI, where transparency, fairness, and explainability are prioritized alongside performance.

Looking ahead, integration of AI into clinical education and training will also be crucial. As Alowais et al. (2023) suggest, embedding AI competencies into medical and pharmacy curricula will prepare future healthcare professionals to critically assess and collaborate with AI tools. Pharmacists, in particular, will need to acquire fluency in data analytics, algorithm evaluation, and digital health ethics to remain effective in AI-augmented environments.

The application of AI in drug discovery and clinical trials will continue to expand, particularly in areas such as target identification, virtual screening, and trial optimization. Malheiro et al,2025 predict that AI will increasingly support adaptive trial designs and biomarker discovery, reduce development timelines and improve treatment outcomes. As pharmaceutical companies adopt AI for real-time monitoring and trial recruitment, regulatory bodies must adapt their frameworks to accommodate these innovations without compromising patient safety or data integrity.

Additionally, there is increasing interest in the development of regulatory sandboxes and real-world evidence (RWE) frameworks that allow AI tools to be tested in controlled but realistic environments before widespread deployment. According to Secinaro et al. (2021), such strategies will be vital in bridging the gap between experimental AI models and clinical utility, ensuring a smoother pathway to implementation.

Another important direction is the use of federated learning and privacy-preserving AI architectures, which allow models to learn from decentralized datasets without compromising patient confidentiality. As data privacy remains a critical barrier to AI adoption, these innovations could enable more inclusive, secure, and compliant data use—particularly in highly regulated domains like pharmacy.

Ultimately, the future of AI in pharmacy is not solely dependent on technological advancement, but also on ethical governance, interdisciplinary collaboration, and societal readiness. The shift toward AI-enhanced pharmacy practice must be accompanied by robust oversight mechanisms, standardized validation protocols, and continuous stakeholder engagement to ensure that these tools are effective, equitable, and aligned with public values.

### 4.6 Limitations of the Research Study

Despite providing valuable insights into the applications, opportunities, and challenges of Artificial Intelligence (AI) in pharmacy, this study is not without limitations. First, the research is based on a narrative literature review, which relies on secondary data sources. Consequently, the findings are dependent on the quality, scope, and accuracy of previously published studies rather than original empirical evidence. This approach may inadvertently introduce publication bias, as studies with positive results are more likely to be published than those reporting negative or inconclusive outcomes.

Second, the review was limited to articles available in English and indexed in commonly used academic databases. This restriction might have excluded relevant studies published in other languages or in grey literature (e.g., conference proceedings, industry reports, unpublished data), potentially narrowing the comprehensiveness of the analysis.

Third, given the rapid pace of AI innovation, the findings of this review may quickly become outdated. New algorithms, regulatory frameworks, and healthcare policies are continuously emerging, which may shift both the opportunities and challenges highlighted in this research. Additionally, the heterogeneity of study designs and populations across the reviewed literature limits the generalizability of findings to specific pharmacy contexts such as hospital, community, or clinical research settings.

### 4.7 Proposals for Future Studies

Future research should seek to overcome these limitations by adopting more rigorous and comprehensive methodologies. Systematic reviews and meta-analyses are recommended to provide stronger evidence on the effectiveness of AI tools across different pharmacy domains, including drug discovery, personalized medicine, hospital operations, and community pharmacy. Additionally, mixed-methods studies combining quantitative outcomes (e.g., error reduction rates, cost-effectiveness) with qualitative insights (e.g., pharmacist and patient experiences) would provide a more holistic understanding of AI integration.

Further investigations should also prioritize longitudinal studies to evaluate the sustainability of AI implementation over time, especially in resource-limited healthcare systems. Clinical trials assessing AI-driven interventions in real-world pharmacy settings are particularly necessary to establish safety, efficacy, and cost-effectiveness.

Another important area for future research is the ethical and regulatory dimensions of AI adoption. Studies exploring governance frameworks, patient consent mechanisms, and strategies for ensuring algorithmic transparency and fairness are crucial to build public and professional trust. Additionally, exploring workforce readiness—such as training programs for pharmacists to interact effectively with AI systems—remains a critical direction for ensuring smooth integration.

Finally, more comparative international studies are needed to examine how AI adoption differs across healthcare systems, economies, and regulatory environments. Such research would help identify best practices and adaptable models for AI integration in pharmacy worldwide.

### 4.8 Conclusion

Artificial Intelligence (AI) is transforming the landscape of pharmacy by reshaping how drugs are discovered, developed, prescribed, and monitored. This thesis explored the multifaceted applications of AI in pharmacy, with a particular emphasis on drug discovery and development, predictive analytics, pharmacy operations, and personalized medicine. Through a comprehensive literature review and critical analysis, this research has demonstrated that AI holds significant promise in accelerating pharmaceutical innovation, enhancing treatment precision, and improving overall healthcare delivery.

AI-enabled platforms such as DeepMind's AlphaFold and Insilico Medicine have already showcased remarkable breakthroughs in target identification and novel molecule prediction, significantly reducing the time and cost associated with traditional drug discovery processes. Clinical decision support systems (CDSS), computerized prescriber order entry (CPOE), and dose recommendation tools exemplify AI's ability to optimize clinical workflow, reduce medication errors, and personalize therapy based on patient-specific data. These advancements directly address the long-standing inefficiencies in pharmacotherapy and healthcare delivery.

Furthermore, AI-driven predictive analytics are revolutionizing inventory management, demand forecasting, and outbreak surveillance, thereby streamlining pharmacy operations and supporting proactive public health responses. In community and hospital pharmacy settings, AI is also enhancing medication counselling, adherence monitoring, and adverse drug reaction prediction—strengthening the pharmacist's role in patient-centered care.

However, the integration of AI into pharmacy is not without significant challenges. Ethical barriers such as data privacy, lack of transparency, trust deficits, and conflicts of interest persist. Technological limitations, including data quality, model interpretability, and algorithmic bias, hinder the full realization of AI's potential. Moreover, regulatory uncertainty and the high costs of implementation pose additional barriers, particularly in resource-constrained settings.

Despite these limitations, the future of AI in pharmacy remains promising. The development of standardized reporting frameworks like TRIPOD-AI, PROBAST-AI, and explainable AI (XAI) models, alongside increased investment in digital health education, will be crucial in overcoming current barriers. As AI continues to mature, its successful implementation will depend on ethical governance, multidisciplinary collaboration, transparency, and a strong alignment with patient needs and healthcare values.

In conclusion, AI has the potential to revolutionize pharmacy practice and pharmaceutical science. It is not merely a tool for efficiency, but a transformative force capable of driving precision medicine, enhancing patient safety, and enabling more equitable access to care. For pharmacists, embracing AI will mean expanding their role as data-literate healthcare professionals, capable of leveraging intelligent technologies to deliver safer, more effective, and patient-tailored therapies. The integration of AI must be approached with responsibility and foresight, ensuring that innovation complements, rather than compromises, the core principles of pharmaceutical care.

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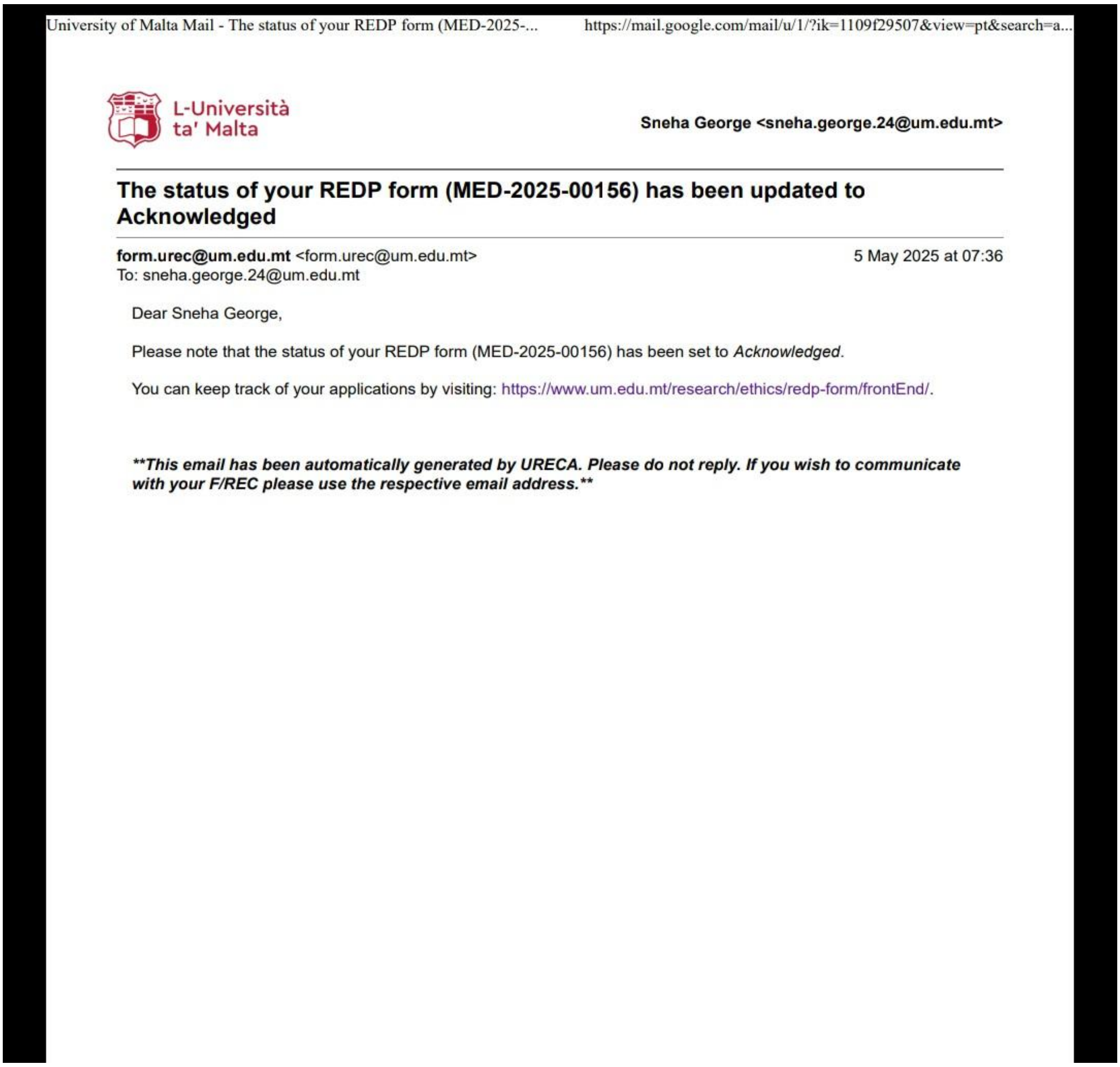
# Appendix 1

## Acknowledgement of Study by Faculty Research and Ethics Committee



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**Sneha George <sneha.george.24@um.edu.mt>**

**The status of your REDP form (MED-2025-00156) has been updated to Acknowledged**

**form.urec@um.edu.mt** <form.urec@um.edu.mt> 5 May 2025 at 07:36
To: sneha.george.24@um.edu.mt

Dear Sneha George,

Please note that the status of your REDP form (MED-2025-00156) has been set to *Acknowledged*.

You can keep track of your applications by visiting: https://www.um.edu.mt/research/ethics/redp-form/frontEnd/.

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