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# Artificial Intelligence in Pharmacy: Applications in Drug Discovery and Clinical Decision Support Systems

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**Abstract**: Artificial intelligence (AI) transforms pharmacy by improving the speed, precision, and evidence base of pharmaceutical research and clinical practice. In drug discovery, AI assists in target identification, virtual screening, molecular docking, lead optimization, toxicity prediction, pharmacokinetic modeling, drug repurposing, and personalized drug development. In clinical decision support systems (CDSSs), AI supports diagnosis, therapy selection, drug-drug interaction alerts, medication error reduction, risk prediction, and patient-specific pharmaceutical care. The aim of this thesis is to describe the concept of AI in pharmacy and to examine its applications in drug discovery and clinical decision support systems. The thesis is based on a narrative review of scientific literature, regulatory documents, and healthcare technology reports. The study highlights that AI can reduce research time, improve decision-making, enhance patient safety, and support precision medicine; however, issues such as data quality, algorithmic bias, privacy, explainability, regulatory validation, and human oversight remain important. The conclusion of this thesis is that AI should not replace pharmacists or clinicians but should act as a decision-support tool that strengthens evidence-based pharmaceutical care. Future pharmacy practice will require pharmacists who understand digital health, data science, pharmacovigilance, ethics, and AI-assisted clinical reasoning.

**Keywords:** Artificial intelligence, pharmacy, drug discovery, clinical decision support system

## I. INTRODUCTION

Artificial intelligence is a branch of computer science concerned with developing systems that can perform tasks that normally require human intelligence. These tasks include learning from data, recognizing patterns, interpreting language, making predictions, solving problems, and recommending actions. In healthcare and pharmacy, AI is usually applied through machine learning, deep learning, natural language processing, computer vision, and rule-based expert systems. Its purpose is not merely automation but the creation of tools that can analyze large volumes of biological, chemical, clinical, and patient-level data faster than conventional manual methods. The World Health Organization has emphasized that AI technologies hold promise for diagnosis, treatment, health research, drug development, surveillance, and public health functions, while also requiring strong ethical and governance safeguards [1].

Healthcare is a data-intensive field in which decisions depend on symptoms, laboratory reports, imaging, genomics, medication history, comorbidities, and patient preferences. AI in healthcare refers to the use of algorithms that can support healthcare professionals in diagnosis, risk

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assessment, treatment selection, monitoring, documentation, workflow management, and research. It can help identify high-risk patients, predict disease progression, suggest appropriate treatment options, and reduce avoidable errors. However, WHO guidance stresses that AI for health must be built around ethics, human rights, transparency, accountability, inclusiveness, and safety.

The healthcare value of AI lies in augmenting human judgment rather than replacing it. For example, an AI system may identify that a patient is at risk of hypoglycemia after a change in antidiabetic therapy, but the clinician and pharmacist must evaluate the recommendation in the context of diet, renal function, affordability, adherence, and patient understanding. AI may also help in hospital workflows by prioritizing alerts, identifying drug interactions, analyzing adverse event reports, or summarizing medical literature. In this sense, AI becomes a bridge between biomedical knowledge and bedside care, provided that human professionals remain responsible for interpretation and final decisions.

## II. ARTIFICIAL INTELLIGENCE IN PHARMACY

### 2.1 AI in Pharmacy

Artificial intelligence in pharmacy can be defined as the use of computational systems that analyze pharmaceutical, biological, chemical, and clinical data to support decisions related to drug discovery, drug development, medicine use, patient care, and healthcare delivery. In this context, AI includes algorithms that can classify molecules, predict biological activity, screen compounds, process patient records, detect medication risks, and support therapeutic decisions. The meaning of AI in pharmacy is therefore wider than automation; it includes intelligent assistance across the medicine life cycle.

Pharmaceutical AI is multidisciplinary. It brings together computer science, statistics, medicinal chemistry, pharmacology, toxicology, clinical pharmacy, bioinformatics, regulatory science, and ethics. A pharmacy AI system may be trained on chemical structures, protein targets, adverse event reports, electronic health records, prescription claims, or medical literature. It may produce outputs such as a ranked list of candidate compounds, a toxicity risk score, a dose adjustment recommendation, or a patient-specific drug interaction warning. The value of such outputs depends on data quality, model validation, clinical relevance, and professional interpretation.

### 2.2 Types of Artificial Intelligence Used in Pharmacy

The major types of AI used in pharmacy include rule-based systems, machine learning, deep learning, natural language processing, computer vision, knowledge graphs, generative AI, and robotic automation. Rule-based systems are built on explicit instructions written by experts. They are common in drug interaction databases and traditional clinical decision support tools. Machine learning systems identify patterns in data and can improve predictions with training. Deep learning systems use multilayer neural networks and are useful for complex problems such as image analysis, protein structure prediction, and molecular generation.[14]

Natural language processing helps computers interpret written or spoken language. In pharmacy, NLP can analyze scientific literature, clinical notes, discharge summaries, drug labels, and adverse event narratives. Knowledge graphs connect drugs, genes, diseases, pathways, and clinical outcomes in a structured network. Generative AI can design new molecular structures or summarize biomedical information, but it requires strict validation because incorrect outputs may be unsafe. Robotic systems can support dispensing, inventory management, compounding, packaging, and warehouse operations. Together, these technologies create a digital foundation for modern pharmacy.

### 2.3 Machine Learning and Deep Learning in Pharmaceutical Sciences

Machine learning is a core AI approach in pharmaceutical sciences. It includes supervised learning, unsupervised learning, semi-supervised learning, reinforcement learning, and ensemble learning. Supervised learning uses labeled data to predict outcomes such as biological activity, solubility, toxicity, or patient response. Unsupervised learning identifies patterns or clusters in data, such as grouping patients with similar risk profiles. Reinforcement learning can be applied to optimization problems, including molecule generation or adaptive treatment strategies.

Deep learning uses artificial neural networks with multiple layers and can capture complex nonlinear relationships. It has been used for molecular property prediction, image-based screening, protein structure prediction, QSAR modeling, and natural language tasks. Applications of machine learning in drug discovery and development have been widely discussed in the literature, including target discovery, compound screening, lead optimization, and clinical development. The main strength of these methods is their ability to learn from high-dimensional data, while their weakness is that they may function as “black boxes” unless explainability methods are used.

### 2.4 Natural Language Processing in Pharmacy Practice

Natural language processing is important in pharmacy because much clinical and scientific information exists as text. Examples include prescription notes, discharge summaries, drug monographs, clinical guidelines, case reports, pharmacovigilance narratives, medical literature, and patient messages. NLP can extract entities such as drug names, dosages, adverse reactions, laboratory values, symptoms, and diagnoses. It can also classify documents, summarize evidence, identify safety signals, and support literature-based drug repurposing.

In clinical pharmacy, NLP may help identify undocumented medication risks from clinical notes, detect adverse drug reactions, support medication reconciliation, and improve communication between healthcare professionals. In research pharmacy, NLP may accelerate literature screening by finding papers related to drug targets, mechanisms, clinical trials, or toxicity. However, NLP systems can misinterpret abbreviations, spelling errors, context,

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negation, and patient-specific meaning. Therefore, NLP should be used as an assistive tool with pharmacist review rather than an independent clinical authority.

**2.5 Big Data and AI Integration in Pharmacy**

Big data in pharmacy refers to large, complex, and diverse datasets generated from chemical libraries, omics studies, clinical trials, electronic health records, prescriptions, claims databases, wearable devices, pharmacovigilance systems, and real-world evidence platforms. AI depends on big data because algorithms learn patterns from examples. The integration of big data and AI allows pharmacists and researchers to detect trends that may not be visible through manual review. This is useful for drug discovery, safety monitoring, patient risk stratification, and personalized medicine.

However, big data is not automatically useful. Data may be incomplete, biased, duplicated, poorly coded, or nonrepresentative. For example, an AI model trained mainly on data from one population may not perform equally well in another population. In pharmacy, this can affect dose recommendations, risk predictions, and safety alerts. Data governance, privacy protection, interoperability, and validation are therefore essential. Regulatory agencies increasingly emphasize quality, reliability, transparency, and fitness for purpose when AI is used to support drug development or regulatory decision-making.

**2.6 Benefits of AI in Pharmaceutical Sector**

AI benefits the pharmaceutical sector by improving speed, efficiency, prediction, and decision-making. In drug discovery, AI can reduce the number of compounds requiring laboratory testing by prioritizing those with desirable properties. In formulation, AI can help optimize excipient selection, release profiles, stability, and manufacturing parameters. In pharmacovigilance, AI can screen large numbers of adverse event reports and identify possible safety signals. In clinical pharmacy, AI can support medication safety and therapeutic decision-making.

Another benefit is cost reduction. Drug development is expensive, and many candidates fail because of lack of efficacy, toxicity, poor pharmacokinetics, or manufacturing challenges. AI cannot eliminate these risks, but it can help identify them earlier. Reviews of drug discovery AI describe its potential in virtual screening, de novo design, drug repurposing, and ADMET prediction.[4,18] In hospitals and community pharmacies, AI can reduce repetitive workload, improve prescription screening, and support better patient counseling by providing relevant information quickly.

**2.7 Challenges of AI Implementation in Pharmacy**

The challenges of AI implementation in pharmacy include data quality, limited transparency, algorithmic bias, lack of clinical validation, privacy concerns, regulatory uncertainty, cost of infrastructure, and resistance from professionals. A model may show high accuracy in development data but perform poorly in real-world practice. This can happen when patient

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populations differ, when data coding changes, or when workflows do not match the assumptions of the model. Therefore, AI tools must be locally validated and continuously monitored.

Another major challenge is overdependence on AI outputs. If pharmacists and clinicians accept AI recommendations without critical review, errors may occur. On the other hand, if systems generate too many irrelevant alerts, alert fatigue may lead users to ignore important warnings. AHRQ/NCBI evidence indicates that CDSSs can reduce medication errors and adverse drug events, but high override rates, alert fatigue, and unintended consequences remain important concerns.[11] The successful implementation of AI in pharmacy therefore requires human oversight, training, explainability, governance, and ongoing quality improvement.

## III. AI IN CLINICAL DECISION SUPPORT SYSTEMS

A clinical decision support system is a health information tool that provides clinicians, pharmacists, nurses, or patients with knowledge-based assistance at the point of care. CDSSs may generate alerts, reminders, recommendations, order sets, diagnostic suggestions, dose calculators, or monitoring prompts. In pharmacy, CDSSs are commonly used for drug allergies, drug-drug interactions, drug-disease interactions, dose adjustment, duplicate therapy, contraindications, therapeutic monitoring, and medication reconciliation [11].

### 3.1 Role of AI in Clinical Decision-Making

AI supports clinical decision-making by processing large amounts of patient-specific and evidence-based information. It can calculate risk scores, predict disease progression, identify probable diagnoses, recommend therapy options, and highlight safety concerns. In pharmaceutical care, AI can support decisions related to medicine selection, dosing, monitoring, adherence, adverse reactions, and patient counseling. It can also help pharmacists prioritize high-risk prescriptions or patients requiring intervention.

The role of AI is supportive, not authoritative. Healthcare decisions involve values, preferences, affordability, clinical context, and professional accountability. For example, an AI system may recommend a particular anticoagulant based on stroke risk, but the pharmacist and physician must consider bleeding risk, renal function, cost, adherence, drug interactions, pregnancy status, and patient preference. AI improves the availability of information, while human professionals determine its appropriate application.

### 3.2 AI-Based Diagnosis and Treatment Recommendation

AI-based diagnostic tools can analyze symptoms, laboratory values, imaging, clinical notes, and patient history to suggest possible diagnoses or risk categories. In pharmacy, diagnostic AI is relevant because medicine use depends on accurate diagnosis and disease severity. For example, diabetes, hypertension, infections, asthma, cardiovascular disease, and renal impairment require therapy decisions that depend on patient-specific data. AI may assist by identifying abnormal patterns and supporting earlier recognition of disease complications.

Treatment recommendation systems can suggest evidence-based therapies, dose ranges, monitoring plans, or guideline-concordant care pathways. However, these systems must be aligned with current clinical guidelines and local formularies. They must also consider contraindications, allergies, interactions, organ function, and patient factors. The pharmacist's role is to verify whether the recommendation is pharmacologically appropriate and clinically safe. This is especially important because AI systems may provide outputs that appear confident but are incomplete, outdated, or unsuitable for a specific patient.

### 3.3 AI in Drug-Drug Interaction Detection

Drug-drug interactions occur when one drug affects the pharmacokinetics, pharmacodynamics, efficacy, or toxicity of another drug. Traditional DDI alerts are common in prescribing and dispensing systems, but they often generate too many warnings, including clinically insignificant interactions. This can cause alert fatigue. AI can improve DDI detection by prioritizing interactions according to patient-specific risk, interaction severity, dose, duration, route, laboratory values, comorbidities, and history.

AI may also identify potential new interactions by analyzing pharmacovigilance reports, electronic health records, biomedical literature, and molecular mechanisms. Medication alert optimization is an active area of research because irrelevant alerts are frequently overridden.8 The goal is not to increase the number of alerts but to improve their clinical value. Pharmacists are central to this process because they understand mechanisms such as CYP enzyme inhibition, protein binding, additive toxicity, QT prolongation, and therapeutic duplication.

## IV. BENEFITS AND LIMITATIONS OF AI IN PHARMACY

### 4.1 Benefits of AI in Pharmacy Practice

The benefits of AI in pharmacy practice include faster information processing, improved medication safety, better risk prediction, support for personalized therapy, and reduction of repetitive workload. Pharmacists frequently manage large volumes of prescriptions, laboratory results, drug information, patient histories, and safety alerts. AI can organize this information and identify patients or prescriptions that need attention. This allows pharmacists to spend more time on clinical judgment and patient counseling.

In community pharmacy, AI can support inventory management, adherence monitoring, patient reminders, prescription screening, and drug information services. In hospital pharmacy, it can support antimicrobial stewardship, renal dosing, anticoagulation monitoring, chemotherapy verification, and high-alert medicine safety. In industrial pharmacy, AI can support research, formulation, manufacturing, quality control, and regulatory documentation. These benefits show that AI has relevance across the entire pharmaceutical sector.

### 4.2 Improvement in Accuracy and Efficiency

AI improves efficiency by analyzing large datasets rapidly and consistently. In drug discovery, it can screen millions of compounds computationally before laboratory testing. In clinical pharmacy, it can review medication orders for risks faster than manual checking alone. This does not mean AI is always more accurate than humans; rather, it can reduce the time needed to identify possible problems and support more systematic review.

Accuracy depends on data quality, algorithm design, validation, and appropriate use. If an AI tool is trained on unreliable or biased data, its outputs may be inaccurate. Therefore, improvement in accuracy should be measured in real-world settings and compared with standard practice. CDSS evidence suggests that improved and targeted decision support can reduce medication errors and adverse drug events, but unintended consequences must also be assessed. The most effective approach is a combination of AI assistance and pharmacist review.

### 4.3 Reduction in Time and Cost of Drug Development

Drug development is costly because many candidates fail during preclinical or clinical stages. AI can reduce time and cost by prioritizing promising targets, predicting compound properties, identifying toxicity risks, optimizing trial design, and supporting drug repurposing. By reducing the number of low-quality candidates entering laboratory and clinical testing, AI may improve resource utilization. FDA engagement with AI for drug development reflects the increasing regulatory importance of these tools [2, 3].

However, AI does not remove the need for experimental studies, animal data where required, clinical trials, quality assurance, and regulatory review. The cost-saving potential depends on whether AI predictions are reliable and integrated into decision-making. If AI outputs are unvalidated, they may create false confidence or direct resources toward unsuitable candidates. Therefore, reduction in cost must be balanced with scientific rigor.

### 4.4 Better Patient Safety and Treatment Outcomes

Patient safety is one of the strongest reasons to use AI in pharmacy. Medication-related problems are common in healthcare, especially among patients with polypharmacy, chronic disease, renal impairment, liver disease, pregnancy, pediatric age, elderly age, or complex therapies. AI-enabled CDSSs can help detect risks early and provide actionable recommendations. They can also support monitoring by identifying abnormal laboratory trends or high-risk medication combinations.

Better treatment outcomes may occur when AI supports appropriate drug selection, dose adjustment, adherence interventions, and follow-up monitoring. For example, an AI system may identify patients likely to discontinue therapy and prompt counseling. Another system may support antimicrobial stewardship by suggesting appropriate spectrum, dose, and duration. Nevertheless, patient outcomes depend on implementation, workflow, acceptance, and clinical response. AI alerts alone do not improve outcomes unless healthcare professionals act appropriately.

## V. FUTURE PROSPECTS OF AI IN PHARMACY

### 5.1 Future Trends in AI-Based Drug Discovery

The future of AI-based drug discovery will likely involve multimodal models that combine chemical structures, protein structures, omics data, imaging, literature, and clinical data. Generative models may design molecules with desired properties, while graph neural networks and transformers may improve molecular representation. Structure prediction tools such as

AlphaFold and AlphaFold 3 have already changed expectations in structural biology and may support target analysis and ligand interaction studies [6, 7].

Future drug discovery platforms may integrate AI with automated synthesis, robotic laboratories, high-throughput screening, and real-time feedback loops. This could create self-improving research systems in which AI designs compounds, robots synthesize and test them, and the results are fed back into the model. Nevertheless, future success will depend on validation, reproducibility, transparency, and collaboration between computational scientists, medicinal chemists, pharmacologists, pharmacists, and clinicians.

### 5.2 AI and Robotic Pharmacy Systems

Robotic pharmacy systems are already used in some hospitals and large pharmacy networks for dispensing, packaging, inventory management, and medication distribution. When combined with AI, robotic systems can predict stock requirements, reduce dispensing errors, optimize storage, monitor expiry dates, and support workflow efficiency. In sterile compounding and unit-dose dispensing, automation may improve accuracy and reduce contamination risks.

AI and robotics may also support community pharmacy services through automated refill reminders, adherence packaging, patient triage, and virtual counseling support. However, pharmacy robotics must be carefully supervised because medication errors can occur if barcoding, loading, labeling, or software settings are incorrect. The human pharmacist remains responsible for verifying therapy appropriateness, patient counseling, and clinical decision-making. Robots can support technical tasks, but professional judgment remains central.

### 5.3 AI in Precision Medicine

Precision medicine is expected to be one of the most important future applications of AI in pharmacy. As genetic testing, biomarker analysis, wearable devices, and electronic health records become more common, AI can integrate these data to guide individualized drug therapy. This may improve response rates, reduce adverse reactions, and support earlier intervention. Pharmacists will be needed to interpret pharmacogenomic results and translate them into practical medication recommendations.

Future precision pharmacy may include AI-based dose calculators, genotype-guided prescribing, real-time therapeutic drug monitoring, and personalized adherence interventions. For example, a patient’s genetic profile, renal function, drug levels, and side effect history could be combined to adjust therapy. However, precision medicine raises privacy and equity issues. Access to genetic testing and AI-supported care should not be limited to privileged populations. Ethical governance is necessary to ensure fair benefits.

### 5.4 AI in Community and Hospital Pharmacy

In community pharmacy, AI may support prescription verification, refill prediction, medication adherence, patient education, chronic disease screening, and identification of patients needing referral. Chatbot-assisted services may answer basic medicine-related questions, but they must be supervised and should not replace professional counseling. Community pharmacists may

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use AI to identify high-risk patients, improve medication therapy management, and provide preventive health services.

In hospital pharmacy, AI may support antimicrobial stewardship, critical care dosing, chemotherapy review, renal dose adjustment, anticoagulation, parenteral nutrition, medication reconciliation, formulary decisions, and pharmacovigilance. AI can also help prioritize pharmacist workload by identifying patients most likely to benefit from intervention. The future hospital pharmacist may work closely with informatics teams to refine alert rules, evaluate model performance, and improve patient safety systems.

### 5.5 Integration of AI with Digital Health Records

Integration with digital health records is essential for AI to be clinically useful. A CDSS can only generate meaningful recommendations if it has access to accurate medication lists, allergies, laboratory values, diagnoses, demographics, and clinical notes. Interoperability allows data to move between hospitals, pharmacies, laboratories, and public health systems. Without integration, AI outputs may be incomplete or unsafe.

Future AI systems may automatically summarize patient histories, detect gaps in therapy, identify abnormal trends, and suggest monitoring plans. However, integration must be accompanied by governance. EHR data may be messy, outdated, or duplicated. AI systems must therefore handle uncertainty and allow human verification. Pharmacists can help ensure medication lists are accurate, drug information is current, and alerts are clinically relevant.

### 5.6 Future Role of Pharmacists in AI-Driven Healthcare

The future role of pharmacists in AI-driven healthcare will expand rather than disappear. Pharmacists will be needed as medication experts, clinical decision-makers, patient educators, data interpreters, safety monitors, and ethical guardians. They may participate in AI system design by defining clinical requirements, evaluating drug knowledge bases, reviewing alert logic, and measuring outcomes. They may also lead medication safety programs supported by AI analytics.

Pharmacy education should therefore include digital health, data literacy, AI basics, pharmacogenomics, evidence appraisal, ethics, and informatics. Pharmacists who understand both medicines and AI will be able to bridge the gap between technology and patient care. The future of pharmacy will depend on combining computational intelligence with human compassion, professional judgment, and accountability.

## VI. CONCLUSION

Artificial intelligence is becoming an important component of modern pharmacy. It offers opportunities to accelerate drug discovery, improve clinical decision support, reduce medication errors, strengthen personalized medicine, and enhance pharmaceutical care. AI can process complex data faster than humans and provide useful recommendations, but it cannot replace human judgment, empathy, ethical responsibility, or professional accountability.

The conclusion of this thesis is that AI should be integrated into pharmacy as a scientifically validated, ethically governed, and professionally supervised tool. Pharmacists must develop digital competence and participate actively in AI-supported healthcare systems. The most successful future model will be a collaborative one in which AI provides data-driven support and pharmacists provide clinical interpretation, communication, and patient-centered care.

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