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# AI and digital transformation in pharmacy

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**Abstract**
Artificial Intelligence (AI) and digital technologies are reshaping the pharmaceutical industry, from drug discovery to patient care. Pharmacy is undergoing a paradigm shift where traditional processes are being replaced or enhanced with computational modeling, machine learning, and automation. This review explores the diverse applications of AI in drug discovery, clinical trials, personalized medicine, pharmacovigilance, and supply chain management. It highlights AI-powered software tools commonly used in pharmacy, discusses the challenges of implementation, and emphasizes the need for ethical frameworks. The article concludes with an outlook on the transformative potential of AI in pharmacy, while acknowledging the contributions of academic institutions, researchers, and healthcare professionals who continue to drive this evolution.

**Keywords:** Artificial Intelligence, digital technologies, drug discovery, patient care, personalized medicine, computational modeling

## Introduction
The rapid advancement of technology has brought about a profound transformation in almost every sector of society, and the field of pharmacy is no exception. Traditionally, pharmacy has been centered around drug discovery, formulation, compounding, dispensing, and patient counseling. However, in recent decades, the pharmaceutical industry and healthcare systems have grown increasingly complex, requiring innovative solutions to meet the demands of modern medicine. Rising healthcare costs, increasing chronic disease burdens, the emergence of precision medicine, and the global need for efficient healthcare delivery have driven the adoption of new digital tools. Among these, Artificial Intelligence (AI) has emerged as one of the most disruptive and promising technologies, capable of redefining how pharmacy is practiced, managed, and integrated within healthcare systems.

Artificial Intelligence encompasses a wide range of computational techniques that enable machines to learn, analyze, and make informed decisions. When applied to pharmacy, AI does not replace the role of pharmacists but rather enhances their capabilities by providing powerful tools for decision-making, data analysis, and operational efficiency. From the early stages of drug discovery to the final stages of patient-centered care, AI has introduced opportunities for increased accuracy, faster outcomes, and reduced costs. This digital transformation is reshaping both the research and clinical aspects of pharmacy.

At the level of pharmaceutical research and development, AI is expediting processes that were once time- consuming and resource-intensive. Identifying new drug molecules, predicting their interactions with biological targets, and validating potential therapies are now being achieved more efficiently with AI-powered platforms. In preclinical and clinical development, digital tools and predictive modeling help in designing safer and more effective trials, reducing both risks and expenses. Furthermore, drug repurposing finding new therapeutic applications for existing drugs has been made significantly faster with AI-driven data mining and pattern recognition approaches.

Beyond research, AI is transforming how pharmacy is practiced in healthcare systems. Hospital pharmacies, community pharmacies, and clinical settings are adopting digital solutions for dispensing automation, supply chain management, personalized medication regimens, and real-time patient monitoring. Intelligent dispensing robots, electronic prescribing systems, and AI-powered decision support tools are reducing errors while improving workflow efficiency. Digital pharmacy services, including telepharmacy and mobile health applications, are expanding access to quality care in remote and underserved regions. Another key element of digital transformation is the integration of big data, electronic health records, and wearable technologies with AI systems. These tools are enabling personalized medicine, where drug therapies can be tailored to individual genetic, lifestyle, and physiological characteristics. Such advancements are moving healthcare away from the traditional "one-size-fits-all" approach toward more precise, patient-centered treatment strategies.

In addition to direct patient care, AI and digital tools are enhancing the pharmaceutical supply chain. Real-time inventory management, predictive demand forecasting, and automated monitoring of cold-chain logistics are ensuring the availability and safety of essential medicines. These innovations are also helping to combat the growing global issue of counterfeit drugs by introducing blockchain-integrated AI systems for authentication and traceability.

Overall, the integration of AI and digital transformation in pharmacy represents not just a technological upgrade but a paradigm shift. It is bridging the gap between research, clinical practice, and patient care, fostering innovation while improving safety and efficiency. This transformation is also reshaping the role of pharmacists, expanding their responsibilities from traditional dispensing toward becoming active contributors in clinical decision-making, precision medicine, and healthcare innovation. As the field continues to evolve, AI promises to serve as a catalyst for future breakthroughs, ultimately improving global health outcomes and redefining the practice of pharmacy for generations to come.

The transformation of pharmacy through digital technologies has been gradual but highly impactful. Traditionally, pharmacists were primarily responsible for compounding and dispensing medicines, ensuring safe use, and providing basic counseling. Over the decades, the role of pharmacists has expanded in response to the increasing complexity of therapeutics, the need for patient-centered care, and the development of advanced healthcare systems. With the growth of biotechnology, genomics, and big data, pharmacy has become highly interdisciplinary, requiring integration with information technology and computational sciences. This shift laid the groundwork for the adoption of Artificial Intelligence (AI) and other digital innovations as essential tools in modern pharmacy.

One of the most significant accelerators of digital transformation in pharmacy was the COVID-19 pandemic. The global crisis highlighted the urgent need for faster drug discovery, flexible clinical trial design, robust supply chain management, and remote healthcare delivery. During this period, AI played a critical role in identifying drug repurposing candidates for COVID-19, predicting disease spread, and supporting telepharmacy services when physical access to hospitals and pharmacies was restricted. The pandemic emphasized how digital tools can bridge gaps in traditional healthcare systems and ensure continuity of care, even during large-scale disruptions. This experience further motivated governments, regulatory authorities, and pharmaceutical companies to invest heavily in digital transformation initiatives.

Another important dimension of AI in pharmacy is its alignment with the principles of personalized and precision medicine. As healthcare moves toward individualized treatment approaches, pharmacists are now expected to integrate genetic information, biomarker data, and patient lifestyle factors into therapeutic decisions. AI-powered algorithms make it possible to analyze large datasets, identify patterns, and suggest optimized drug regimens for each patient. This not only enhances therapeutic outcomes but also reduces the risk of adverse drug reactions, which remain a significant challenge in clinical practice. The growing field of pharmacogenomics, combined with AI, is shaping a future where personalized medicine becomes the norm rather than the exception.

Ethical and regulatory considerations also play a major role in the digital transformation of pharmacy. The integration of AI raises important questions about data privacy, security, transparency of algorithms, and accountability in decision-making. Patients and healthcare providers need to trust that AI systems are safe, unbiased, and reliable. Regulatory authorities such as the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMA) are increasingly focusing on frameworks for AI-driven medical devices, digital health applications, and pharmacy tools. This ensures that innovation is balanced with safety, ethical standards, and public trust.

Globally, the adoption of AI and digital technologies in pharmacy varies across regions. Developed nations with advanced healthcare infrastructure are leading in areas such as automated dispensing, AI-supported clinical decision systems, and digital therapeutics. Meanwhile, developing countries are leveraging digital transformation to address shortages of healthcare professionals, improve access to medicines, and combat counterfeit drugs. Mobile health applications, blockchain-integrated supply chain solutions, and telepharmacy platforms are proving especially useful in resource-limited settings, ensuring that digital transformation in pharmacy is not confined to high-income countries alone.

The digital shift also has significant implications for the professional role of pharmacists. As routine tasks such as inventory management and dispensing become increasingly automated, pharmacists are freed to take on more advanced responsibilities in clinical care, research, and patient education. They are emerging as central figures in multidisciplinary healthcare teams, where their expertise is complemented by AI-powered tools that provide real- time insights. This collaborative approach fosters innovation and ensures that pharmacists remain at the forefront of improving patient outcomes.

In summary, the digital transformation of pharmacy, powered by AI, represents a convergence of technological innovation, evolving healthcare needs, and global challenges. It is not merely an upgrade to existing systems but a redefinition of how medicines are discovered, developed, delivered, and optimized for patients. By combining traditional pharmacy knowledge with digital intelligence, the profession is entering a new era where efficiency, precision, and accessibility are prioritized. The introduction of AI into every stage of pharmacy practice ensures that the future of healthcare will be more personalized, responsive, and resilient. Pharmacy has historically relied on rigorous experimentation, manual data collection, and evidence-based medicine to ensure safe and effective use of drugs. However, the increasing complexity of diseases, rising demand for personalized treatment, and the explosion of biomedical data have pushed pharmacy into the era of digital transformation [1]. Artificial Intelligence (AI), big data analytics, cloud computing, and the Internet of Things (IoT) are playing pivotal roles in modernizing pharmacy practice and pharmaceutical research [2].

AI is broadly defined as the ability of computer systems to perform tasks that normally require human intelligence, such as pattern recognition, problem-solving, and decision-making [3]. In pharmacy, AI is being applied to various domains including drug discovery, dosage optimization, pharmacovigilance, clinical decision support, and supply chain management [4].

Digital transformation refers to the integration of these intelligent technologies into all aspects of pharmacy, resulting in improved efficiency, accuracy, and patient outcomes [5]. Unlike digitalization (which simply converts data from analog to digital form), digital transformation involves a complete rethinking of workflows and value chains within pharmaceutical sciences [6].

The significance of this transformation is profound. For instance, AI-enabled drug discovery platforms can screen millions of compounds within hours, compared to years of manual experimentation [7]. In hospitals, AI-driven clinical decision support systems assist pharmacists in ensuring accurate drug therapy, reducing medication errors, and enhancing patient safety [8]. In the supply chain, blockchain integrated with AI ensures real-time tracking of drugs, preventing counterfeit medicines from reaching patients [9].

This review provides a detailed analysis of how AI and digital transformation are revolutionizing the pharmaceutical sector, with special emphasis on AI software tools, implementation challenges, and future perspectives.

## AI in Drug Discovery and Development

Drug discovery is traditionally a time-consuming and expensive process, often taking 10-15 years and costing billions of dollars before a single drug reaches the market [10]. AI has emerged as a game-changer by accelerating the identification of drug targets, screening compounds, and predicting drug-drug interactions. Top pharmaceutical companies are collaborating with AI vendors and leveraging AI technology in their manufacturing processes for research and development and overall drug discovery. Reports show nearly 62 percent of healthcare organizations are thinking of investing in AI shortly, and 72 percent of companies believe AI will be crucial to how they do business in the future. To get a better sense of the future of AI in the sector, *Pharma News Intelligence* [47] dives into current AI use cases, the best uses for the technology, and the future of AI and machine learning. The McKinsey Global Institute estimates that AI and machine learning in the pharmaceutical industry could generate nearly $100B annually across the US healthcare system. According to researchers, the use of these technologies improves decision-making, optimizes innovation, improves the efficiency of research/clinical trials, and creates beneficial new tools for physicians, consumers, insurers, and regulators. Top pharmaceutical companies, including Roche, Pfizer, Merck, AstraZeneca, GSK, Sanofi, AbbVie, Bristol-Myers Squibb, and Johnson & Johnson have already collaborated with or acquired AI technologies. In 2018, the Massachusetts Institute of Technology (MIT) partnered with Novartis and Pfizer to transform the process of drug design and manufacturing with its Machine Learning for Pharmaceutical Discovery and Synthesis Consortium [47].

Research works are carried out daily to find new active principles for the currently incurable diseases and conditions; increase the safety profile of already existing drugs; combat drug resistance and minimize therapeutic failure. Hence, there is an increase in the size and variety of biomedical data sets involved in drug design and discovery. This factor and many more contributed to the advancement of AI in the pharmaceutical industry. Today, some companies offer software with much relevance in drug design and data processing, as well as in predicting treatment outcomes.

GNS healthcare [48] uses AI machine software known as Reverse Engineering and Forward Simulation (REFS). REFS determines the cause-and-effect relationships between various types of data, that are unforeseen ordinarily by direct data evaluation. GNS claims that REFS can transfer millions of data points ranging from clinical to genetics, laboratory, imaging, drug, consumer, geographic, pharmacy, mobile, proteomic, and so on. In drug design, a company known as Atomwise developed the first deep learning neural network for structure-based drug design and discovery that they called AtomNet [49]. AtomNet makes use of a statistical approach to extract information from millions of experimental affinity measurements and thousands of protein structures to predict the binding properties of small molecules with proteins. By presenting 3-dimensional images of the protein and ligand pair showing channels for carbon, oxygen, nitrogen, and other types of atoms, Atom Net technology enables the pharmaceutical chemists to perform core processes of drug discovery and design like hit discovery, lead optimization, and prediction of toxicity with high precision and accuracy in weeks as against years.

### Target Identification & Validation

AI algorithms analyze genomic, proteomic, and clinical data to identify disease-related targets. For example, DeepMind's AlphaFold has revolutionized protein structure prediction, enabling researchers to model 3D protein conformations essential for drug binding [11].

- **Virtual Screening & Lead Optimization**

Machine learning models can screen millions of chemical compounds against a target protein in silico. Platforms like Atomwise (AtomNet) use deep learning to predict binding affinities of molecules with high accuracy [12].

- **Drug creation**

The development or creation of pharmaceuticals takes more than a decade and consumes billions of rupees. "Atomwise[46], an AI technology that uses supercomputers, is useful to find out the therapies from the database of molecular structure. It hurled a virtual search program for safe and effective therapy for the Ebola virus with the existing drugs. The technology identified two drugs that caused Ebola infection. This analysis was completed within one day compared to months to years with manual analysis. A Biopharma company in Boston developed big data for the management of patients. It reserves data to find the reasons why some patients survive diseases. They used patients' biological data and AI technology to find out the difference between healthy and disease-friendly atmospheric conditions. It helps in the discovery and design of drugs, healthcare, and problem-solving applications.

- **Drug Repurposing:**

AI identifies new therapeutic uses for existing drugs by analyzing biomedical databases. During the COVID- 19 pandemic, AI-driven platforms suggested candidates such as remdesivir and baricitinib for repurposing [13]. Drug repurposing (also called drug repositioning) is the strategy of identifying new therapeutic uses for existing drugs. This approach is highly valuable because it reduces the cost, time, and risk associated with de novo drug discovery. Traditional drug development may take 10-15 years and cost over $2 billion, whereas repurposing allows faster clinical translation since safety, toxicity, and pharmacokinetics are already known. Artificial Intelligence (AI) has revolutionized this area by analyzing vast biomedical datasets, predicting new drug-disease associations, and enabling efficient hypothesis generation.

**1. AI Techniques Used in Drug Repurposing**

**a. Machine Learning & Deep Learning Models**

Algorithms such as Random Forest, Support Vector Machines (SVM), and Neural Networks are trained on large- scale drug and disease datasets to predict new indications [32]. Deep learning models like Graph Neural Networks (GNNs**)** capture structural and functional relationships between drugs and targets [33].

**b. Natural Language Processing (NLP)**

AI systems like IBM Watson for Drug Discovery mine scientific literature, patents, and clinical trial databases to identify hidden links between drugs and diseases [34]. NLP helps extract drug-target-disease associations from unstructured biomedical text.

**c. Network-Based Approaches**

AI builds drug-target interaction (DTI) networks, integrating proteomics, transcriptomics, and metabolomics data [35]. Network pharmacology identifies potential repositioning candidates by analyzing molecular pathways and disease-gene associations.

**d. Knowledge Graphs**

AI-powered knowledge graphs connect drugs, targets, side effects, and diseases.Tools like DrugBank, Open Targets, and Hetionet are used for AI-driven drug repurposing [36].

**2. Applications and Case Studies**

Sildenafil (Viagra®): Originally developed for angina, repurposed for erectile dysfunction and later pulmonary hypertension, supported by computational screening [37].

Thalidomide: Repurposed from an anti-nausea drug to a treatment for multiple myeloma and leprosy reactions [38].

Remdesivir: Initially investigated for Ebola virus, repurposed for COVID-19 treatment using AI-driven screening of antiviral libraries [39].

Baricitinib: Identified by BenevolentAI as a potential COVID-19 therapy by predicting its inhibitory effects on viral entry [40].

Metformin: Studied for anti-cancer and anti-aging effects beyond its original use in diabetes, with AI models validating new mechanisms [41].

- **Preclinical Development**

AI models predict toxicity, solubility, and pharmacokinetics of compounds, reducing reliance on animal studies [14]. Preclinical development is a critical stage of the drug pipeline where potential drug candidates are evaluated for safety, toxicity, pharmacokinetics (PK), and pharmacodynamics (PD) before human trials. This stage is time-consuming, resource-intensive, and involves extensive *in vitro* and *in vivo* testing. AI is transforming preclinical research by simulating experiments, predicting outcomes, and reducing reliance on animal testing.

**1. Toxicity Prediction and Safety Assessment**

AI models such as DeepTox, ProTox-II, and ADMET Predictor use machine learning to predict mutagenicity, hepatotoxicity, cardiotoxicity, and genotoxicity of drug molecules [20, 21]. AI can replace early animal studies with in silico toxicity screening, lowering cost and ethical concerns [22].Natural language processing (NLP) allows mining of published toxicology data to identify adverse effects and molecular patterns.

- **ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) Modeling**

  Predicting ADMET properties is essential to reduce late-stage drug failures.Tools like pkCSM, SwissADME, QikProp, and GastroPlus provide accurate simulations of solubility, permeability, metabolic stability, and excretion pathways [23].AI-enhanced physiologically based pharmacokinetic (PBPK) modeling predicts human PK from preclinical data.

- ***In Vitro* and *In Vivo* Experiment Optimization**

  AI-powered robotics automate high-throughput screening (HTS) assays, testing thousands of compounds rapidly [24].Computer vision and deep learning improve histopathological analysis by detecting subtle morphological changes in tissues [25].Virtual animals or digital twins simulate disease states and treatment responses, reducing animal use [26].

- **Drug-Target Interaction and Mechanistic Studies**

  Preclinical studies focus on understanding mechanisms of action. AI software like DeepChem, ChemProp, and BindingDB predictors analyze molecular docking and receptor-ligand interactions [27].Systems biology approaches integrate multi-omics data (genomics, transcriptomics, proteomics, metabolomics) for better mechanistic insights.

- **Biomarker Discovery**

  AI enables discovery of predictive biomarkers for efficacy and safety using omics datasets.Tools like Ingenuity Pathway Analysis (IPA), TensorFlow-based neural networks, and Bioconductor packages are applied for biomarker identification [28].This reduces risk in clinical translation by identifying patient populations likely to benefit.

- **Case Studies and Applications**

  Insilico Medicine reported an AI-designed anti-fibrotic compound entering preclinical testing in <18 months, compared to 4-6 years in traditional methods [29].

  IBM Watson Toxicology demonstrated the ability to predict chemical toxicity pathways in preclinical models [30]. GastroPlus and Simcyp Simulator are widely used for PBPK modeling in regulatory submissions [31].

**AI in Clinical Trials**

Artificial intelligence (AI) is revolutionizing clinical trials by improving design, recruitment, monitoring, and analysis. Traditional clinical trials are costly, lengthy, and often face challenges such as slow patient enrollment, protocol deviations, and high failure rates. AI, combined with big data, electronic health records (EHRs), and wearable technologies, addresses these challenges, making trials faster, more efficient, and cost-effective.Clinical trials are one of the most resource-intensive stages in drug development, often facing challenges like patient recruitment, protocol adherence, and data variability. AI tools have proven to be highly effective in this domain [15].

**Patient Recruitment**

Natural Language Processing (NLP) algorithms can scan electronic health records (EHRs) to match eligible patients with trial criteria. For example, IBM Watson for Clinical Trial Matching increases recruitment efficiency [16].

a) **Eligibility Screening:** Machine learning (ML) scans EHRs, genomic data, and imaging to identify eligible participants faster than manual screening [58].
b) **Precision Recruitment:** AI predicts which patients are most likely to adhere to treatment and follow trial protocols.
c) **Diversity Enhancement:** Algorithms ensure demographic diversity in recruitment, reducing biases and improving generalizability of results.
d) **Retention Monitoring:** Chatbots, mobile apps, and AI-based reminders improve patient adherence and engagement during trials.

- **Trial Design & Monitoring**

Predictive analytics assist in identifying optimal trial designs, minimizing dropout rates, and reducing costs [17]. Clinical trials are the most resource-intensive phase of drug development, often taking 6-8 years and consuming nearly 40% of the total drug development cost. Despite this, over 80% of trials fail due to poor patient recruitment, inadequate trial design, or inefficiencies in monitoring [42]. Artificial Intelligence (AI) is transforming trial design, execution, and monitoring by making the process faster, cost-effective, and more patient centric.

a) **Real-time Data Capture**
AI-powered wearables and IoT devices enable remote monitoring of patient vitals, ensuring real-time trial data collection [18].
b) **Adaptive Trials**

Machine learning enables “adaptive trial designs,” where protocols evolve dynamically based on ongoing patient responses [19].

**Types of Adaptive Trial Designs Enhanced by AI**

1. **Response-Adaptive Randomization (RAR)**
   In traditional randomized controlled trials (RCTs), patients are randomly assigned in fixed ratios (e.g., 1:1). With AI-powered RAR, the probability of assigning patients to a treatment arm increases if that arm shows superior efficacy during interim analysis [50]. This minimizes patient exposure to inferior treatments.
   Example: Oncology trials often use RAR to prioritize promising therapies.
2. **Sample Size Re-Estimation (SSR)**
   AI models predict the optimal sample size required during the trial based on emerging variability and effect sizes [51]. Prevents underpowered or overpowered studies, saving time and resources.
3. **Adaptive Dose-Finding**
   Reinforcement learning algorithms adjust dosing schedules based on real-time safety and efficacy data [52]. Especially useful in oncology and rare disease trials where dosing windows are narrow.
4. **Seamless Phase II/III Designs**
   AI facilitates merging of Phase II (exploratory) and Phase III (confirmatory) into a single continuous trial, reducing development timelines by years [53]. Machine learning analyzes early-phase data to predict late-phase outcomes and dynamically adjust trial endpoints.
5. **Platform and Basket Trials**
   AI enables multi-arm, multi-stage (MAMS) trials, such as basket trials (multiple diseases, same biomarker) and umbrella trials (one disease, multiple drugs) [54].

**Examples**

SPY 2 Trial in breast cancer uses adaptive platform design.

Recovery Trial during COVID-19 tested multiple therapies simultaneously using adaptive designs.

**AI in Pharmacovigilance and Safety Monitoring**

Drug safety is a critical component of pharmacy practice. Traditional pharmacovigilance systems rely on manual reporting of adverse drug reactions (ADRs), which can be incomplete or delayed [20].

- **Signal Detection**
  AI-based algorithms detect patterns in post-marketing surveillance data, identifying ADR signals earlier than conventional methods [21].
- **Spontaneous Reporting Systems**
  Tools like MedEffect and VigiBase integrate AI for global monitoring of ADRs [22].
- **Social Media Mining**
  AI scrapes patient-reported outcomes from platforms like Twitter and patient forums to identify unreported ADRs [23].
- **Regulatory Compliance**
  Pharmaceutical companies use AI to comply with pharmacovigilance reporting requirements set by agencies like the FDA and EMA [24].

AI-driven pharmacovigilance reduces the risks associated with new therapies and enhances patient safety across populations.

**AI in Personalized Medicine and Pharmacy Practice**

Artificial Intelligence (AI) is significantly transforming personalized medicine and pharmacy practice by enabling precision-based therapies, improving patient care, and optimizing medication management. Personalized medicine focuses on tailoring treatments to individual patients based on genomic, phenotypic, behavioral, and environmental data. Pharmacy practice benefits from AI through improved clinical decision support, medication adherence, inventory management, and patient counseling. Personalized medicine aims to tailor treatments according to an individual's genetic profile, lifestyle, and environment. AI provides the analytical power required to process large datasets for this purpose [25].

- **Pharmacogenomics**
  AI integrates genetic data to predict drug metabolism and optimize dosing. For instance, PharmGKB database uses AI-driven algorithms to guide pharmacogenomic decisions [26].
- **Decision Support Systems (DSS)**
  AI-enabled DSS in hospitals help pharmacists detect drug interactions, contraindications, and suggest optimal dosing [27].
- **Smart Prescription Systems**
  Platforms like MediSafe use AI to improve medication adherence by sending reminders and monitoring usage patterns [28].
- **Oncology Applications**
  AI predicts tumor mutations and guides targeted therapies, significantly improving cancer treatment outcomes [29].

Thus, AI is enabling precision medicine and improving patient outcomes by ensuring safe, effective, and individualized therapies.

### AI in Supply Chain and Hospital Pharmacy Automation

Artificial Intelligence (AI) is increasingly integrated into the pharmaceutical supply chain and hospital pharmacy systems to enhance efficiency, reduce errors, improve patient safety, and optimize resource utilization. Given the complexity of drug distribution and hospital operations, AI offers predictive, real-time, and automated solutions that ensure continuous availability of essential medicines and streamlined pharmacy services. Efficient supply chain management is crucial in preventing drug shortages, counterfeit drugs, and inefficiencies in hospital pharmacies. AI and blockchain are transforming these areas [30].

- **Drug Tracking & Counterfeit Prevention**
  Blockchain combined with AI ensures end-to-end traceability of pharmaceuticals, reducing counterfeit circulation [31].
- **Inventory Optimization**
  AI predicts drug demand using consumption patterns and epidemiological data, ensuring optimal stock levels in hospitals [32]
- **Robotic Dispensing Systems**
  AI-driven robots in hospital pharmacies automate drug dispensing, packaging, and labeling, reducing human errors [33].
- **Logistics & Distribution**
  Machine learning models optimize distribution routes, minimizing delays in delivering critical medications [34].
  This digital transformation improves operational efficiency and ensures uninterrupted access to essential medicines.

### AI Software and Digital Tools in Pharmacy

Numerous AI-powered platforms and digital solutions are being applied in various pharmacy domains, from drug discovery to hospital automation. Below is a detailed list of widely used tools and their applications.

| AI Tool/ Software | Domainof Application | Key Features | References |
|---|---|---|---|
| AlphaFold (DeepMind) | Drug discovery, protein structure prediction | Predicts 3D protein folding structures with high accuracy | [35] |
| Atomwise (AtomNet) | Virtual drug screening | Deep learning-based prediction of ligand-protein interactions | [36] |
| Schrödinger Suite | Molecular modeling, drug design | Physics-based simulations, AI for binding affinity prediction | [37] |
| BenevolentAI | Drug discovery | Integrates biomedical data to identify novel targets | [38] |
| Exscientia | AI-driven drug design | Automated molecule generation and lead optimization | [39] |
| IBM Watson Health | Clinical trials, decision support | NLP for trial matching, clinical decision assistance | [40] |
| BioSymetrics Augusta | Clinical data analysis | AI-powered patient data harmonization for research | [41] |
| MedAware | Prescription error prevention | Machine learning for drug safety alerts in prescriptions | [42] |
| PharmGKB | Pharmacogenomics | AI-assisted gene-drug interaction database | [43] |
| MediSafe | Medication adherence | AI-based patient reminders and adherence tracking | [44] |
| Corti | Emergency response | Real-time AI for triaging emergency calls | [45] |
| SOPHiA GENETICS | Genomics & precision medicine | AI-based genomic analysis for oncology & rare diseases | [46] |
| Deep Genomics | RNA therapeutics | AI for predicting RNA mutations and drug design | [47] |
| GNS Healthcare | Personalized medicine | Causal AI models for treatment outcome prediction | [48] |
| Insilico Medicine | Generative AI for drugs | Deep learning models for small molecule discovery | [49] |
| Ayasdi | Clinical analytics | AI for identifying hidden patterns in patient data | [50] |
| MedEffect & VigiBase | Pharmacovigilance | AI-driven ADR signal detection | [51] |
| SAP Integrated Business Planning (IBP) | Supply chain optimization | AI-powered forecasting for pharmaceutical logistics | [52] |
| Talyst AutoPharm | Hospital pharmacy automation | Robotics and AI for drug dispensing and inventory | [53] |
| Omnicell XR2 | Automated medication dispensing | Robotic pharmacy automation with AI optimization | [54] |

**Challenges, Limitations, and Ethical Issues in AI and Digital Transformation in Pharmacy**

While AI and digital transformation hold significant promise for pharmacy, several barriers hinder widespread adoption.

- **Data Privacy and Security -** AI models require massive amounts of patient data, raising concerns over HIPAA/GDPR compliance and the risk of breaches [56].
- **Bias in AI Algorithms -** Machine learning models may inherit bias from training datasets, leading to disparities in drug recommendations and trial enrollment [57].
- **High Implementation Cost** - Setting up AI infrastructure (cloud servers, licenses, trained staff) can be financially challenging, especially for small-scale hospitals and developing nations [58].
- **Regulatory and Legal Issues** - AI-based drug recommendations raise questions regarding accountability in case of medical errors [59].
- **Interpretability ("Black Box" Problem)** - Many AI models, especially deep learning, provide predictions without clear explanations, making clinical validation difficult [60].
- **Workforce Adaptation** - Pharmacists and healthcare professionals require reskilling to integrate AI tools into clinical and research workflows [61].
- **Ethical Concerns** - Patient autonomy, informed consent, and decision-making transparency remain crucial issues in AI-driven healthcare [62].

Thus, although AI promises great efficiency, its responsible use requires strict ethical frameworks, regulations, and continuous human oversight.

**Summary**

Artificial Intelligence (AI) and digital transformation are redefining the role of pharmacy across drug discovery, clinical trials, pharmacovigilance, hospital automation, and personalized medicine. Numerous AI platforms such as AlphaFold, Atomwise, IBM Watson Health, MedAware, Omnicell XR2, and Insilico Medicine are already transforming practice and research. Despite these advancements, challenges including data security, high costs, algorithmic bias, and ethical issues need to be addressed.

AI is not intended to replace pharmacists but to augment decision-making, reduce errors, accelerate research, and enhance patient safety. Digital transformation, when combined with human expertise, ensures that pharmacy continues to evolve in line with the needs of modern healthcare.

**Conclusion**

AI and digital technologies represent a paradigm shift in pharmacy, promising improved efficiency, safety, and personalized care. By integrating advanced computational tools into daily practice, pharmacy professionals can transform drug discovery pipelines, optimize clinical decision-making, and strengthen pharmacovigilance systems.

The future of pharmacy lies in collaboration between AI systems, pharmacists, and regulatory bodies. Investments in training, infrastructure, and ethical frameworks will ensure AI adoption benefits both patients and healthcare providers. Ultimately, AI and digital transformation in pharmacy symbolize not just technological advancement but a commitment to better, safer, and faster healthcare delivery.

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