








Artificial intelligence in drug discovery and pharmaceutical care: a narrative review

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ABSTRACT



Artificial intelligence (AI) is quickly changing the field of pharmacy and pharmaceutical sciences by making healthcare and drug-related processes more efficient, more accurate, and faster. With the help of AI technologies like machine learning and deep learning, the deep analysis of voluminous biological, chemical, and clinical data is possible, and this facilitates enhanced decision-making in drug discovery and development. AI is also used to aid drug discovery in the identification of targets as well as molecular design, virtual screening, and repurposing of drugs, which saves a lot of time and expense. AI has been used to enhance drug development via predictions of pharmacokinetics and toxicity as well as clinical trials optimization. In the pharmaceutical industry, AI can be used to optimize the processes, to monitor the quality and to predictive maintain the machinery to maintain the quality and efficiency of the products and the process. The usage of AI in pharmaceutical care is also important to assist the clinic in clinical decision systems, medication therapy management, prediction of adverse drug reaction, and personalized medicine. Moreover, it enhances medication safety and patient compliance because of its incorporation into both hospital and community pharmacy. Nonetheless, AI can transform the future of pharmacy practice and healthcare delivery despite the difficulties of data privacy and bias in the algorithm, as it has a great potential.

Keywords: Artificial Intelligence; Pharmacy Practice; Drug Discovery; Drug Development; Machine Learning; Deep Learning; Pharmacokinetics; Clinical Decision Support Systems; Virtual Screening; Precision Medicine; Healthcare Innovation.

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INTRODUCTION

Artificial Intelligence (AI), a field of computer science, is a concept that allows computers to do what is otherwise considered as a task that humans need intelligence to accomplish, including perception, reasoning, learning, and problem-solving. Over the past few years, AI has been drawing a lot of attention due to its transformative nature in healthcare and pharmaceutical sciences. The combination of modern computational methods with extensive biological and clinical data can help AI enhance the decision-making process and increase the efficiency of various drug development and patient care steps. The recent research published between 2018-2025 suggests a solid amount of evidence regarding the increased significance of AI in pharmacy and pharmaceutical research. The pharmaceutical industries have been demonstrated to benefit greatly by AI-based technologies in terms of reduced time and cost of developing drugs and overall increase in the returns to investment [1]. In drug discovery, AI algorithms can effectively and efficiently analyse large amounts of biological, chemical, and pharmacological data to arrive at potential drug candidates. These are also

computational models that can determine drug efficacy and safety profiles and thus enhance accuracy of drug screening in early stages and reduce chances of failures in the late stages [2]. The requirement of AI in the contemporary drug development is becoming more urgent due to the fact that conventional drug discovery processes are usually lengthy, costly, and suffer high attrition. The AI technologies have found applications in the drug development pipeline by accelerating different stages in the process, aiding in the identification of new therapeutic targets, and decreasing the use of the animal-based testing. In addition, AI can be used to create personalized medicine, which combines patient-specific genetic and clinical data to maximize therapeutic effects [3]. Besides the development of drugs, AI is also significant in enhancing the services provided to the patient and pharmaceutical development. Clinical decision support systems based on AIs can process data about patients, their health history, and laboratory data to help medical professionals make well-informed treatment choices. These systems assist in detecting possible drug-drug interactions, prescribing the right number of drugs to the patient, and increasing the medication adherence in patients [4]. Altogether, the literature reviewed reveals a consistent focus on the fact that AI can transform the pharmacy practice, enhance healthcare delivery, and result in safer and more efficient therapeutic results.

Overview of Artificial Intelligence

Artificial Intelligence (AI) can be defined as the use of computer science methods to create a machine and systems capable of accomplishing any tasks usually performed by human intellect, including learning, reasoning, and decision-making. AI has become one of the most effective technologies used in the healthcare and pharmaceutical sciences in recent years. It allows computers to process data in large volumes and extract patterns and assist in complex clinical and research choices. According [5] AI can be described as the science and engineering of intelligent machines. Likewise, [6] identified AI as a technology that could simulate the human cognitive processes, including learning and problem-solving, by working on massive amounts of health-related information, such as medical imaging, electronic health records, diagnostic data, and drug development knowledge. These abilities will enable AI to aid disease diagnosis, clinical decision-making, drug discovery, and individualized treatment approach development. The scientific evidence of AI technology involvement in healthcare is vast as pointed out [7] Artificial intelligence technology is actively employed to analyse the complex data in healthcare to enhance the efficiency and quality of the medical services. Earlier works like [5,6] have been used extensively in the literature, and this is why they were important in the definition of AI and how it can be applied in medicine. In AI, two significant subfields

are especially important in health care applications two are Machine Learning (ML) and Deep Learning (DL). Machine learning is concerned with building algorithms which allow computers to learn through data and make predictions or decisions without them being explicitly programmed. A more advanced form of machine learning, called deep learning, involves artificial neural networks that mimic the form and behaviour of the human brain to process advanced patterns and big data sets. According [8] the fields of cardiology, radiology, and neurology are some of the medical specialties that are increasingly using AI as a subfield. Their power to process sophisticated clinical information has resulted in an increased number of applications in disease detection, medical image interpretation, and predictive analytics. Consequently, AI, specifically, machine learning and deep learning, have become indispensable elements of the contemporary healthcare innovation and pharmaceutical research.

Role of AI in Drug Discovery

The concept of the artificial intelligence (AI) has emerged as a revolutionary technology used in all of the principal steps of drug discovery to enhance the efficiency, accuracy, and speed of creating new therapeutic agents. Over the past years, expert research has revealed that AI technologies can be used to support various phases of the drug discovery process, such as target identification, molecular design, virtual screening, and drug repurposing. Through its combination of computational algorithms and high biological and chemical-data, AI can help the researcher detect some potential drug candidates much faster than possible under standard experimental procedures. Target identification is one of the most significant AI in drug discovery applications in which computational models are used to analyze genomic and proteomic data to draw potential biological targets related to diseases. Complex AI applications like the protein structure prediction application AlphaFold have transformed protein structure and functions knowledge. Identification of potential drug targets has been greatly enhanced through this technology by predicting the correct structure of proteins that are needed in the design of effective therapeutic molecules [9]. AI is also important in drug design and molecular generation. Genetic algorithms like Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs) can be used to create new chemical designs that have specific pharmacological properties. Such AI-based models allow ab initio design of molecules, that is, some completely novel compounds can be designed computationally without necessarily using chemical libraries [10]. A second significant application is virtual screening, in which machine learning models and quantitative structure-activity relationship

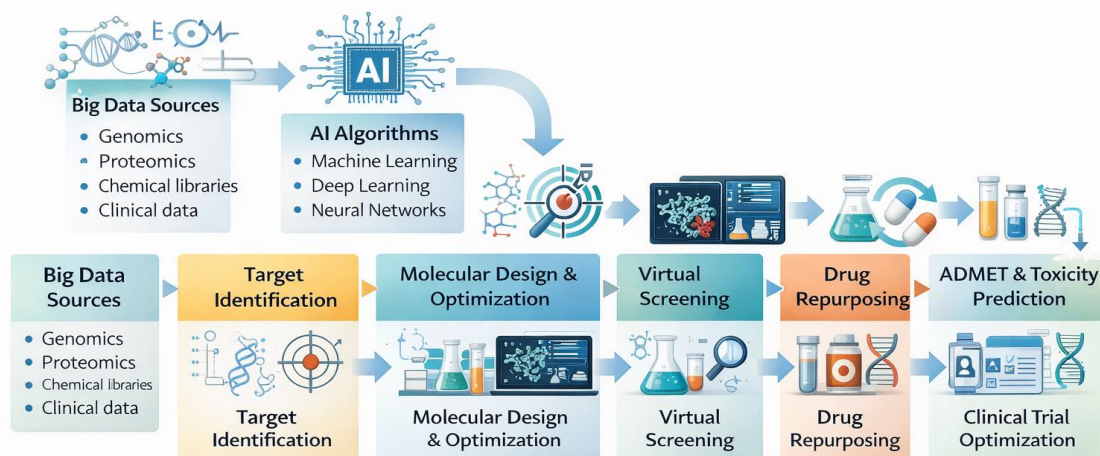


Figure 1: Artificial intelligence-driven drug discovery workflow. AI integrates large biological and chemical datasets to facilitate target identification, molecular design, virtual screening, drug repurposing, ADMET prediction, and clinical trial optimization, ultimately accelerating the development of safe and effective therapeutics.

(QSAR) models are applied to high numbers, or even millions of, chemical compounds in a short time. It is a process that is used to identify the molecules with the highest potential of interacting well with a biological target, thus saving a lot of laboratory experimentation and consequently, making this process much less costly in terms of research [11]. Moreover, AI has also been useful in drug repurposing, which is the process through which drugs can be repurposed to be used in a new therapeutic application. The AI systems will also be able to identify previously unknown interactions between drugs and diseases by examining biomedical data, clinical records, and molecular interactions. This method has a potential to hasten the treatment development through the use of drugs that have already been approved and have known safety profiles [9]. Although these are the benefits, there are still some issues with the use of AI in drug discovery. Such problems as the absence or insufficient quality of datasets, the absence of transparency and interpretability of complex AI models, and the possibility of algorithmic bias may influence the reliability of predictions. The necessity to overcome these obstacles is aimed at achieving maximum benefits of AI in pharmaceutical research and drug development [11]. The integration of artificial intelligence across the drug discovery pipeline, including target identification, molecular design, virtual screening, drug repurposing, and toxicity prediction, significantly accelerates the development of novel therapeutic agents. The overall AI-driven drug discovery workflow is illustrated in **Figure 1**.

AI in Drug Development: Artificial Intelligence (AI) has demonstrated a lot of potential during different phases of drug development, especially in the field of pharmacokinetics and pharmacodynamics (PK/PD) prediction, toxicity analysis, and clinical trial optimization. The most recent investigations can be found in the period of 2022-2025 noting the rising

usage of AI methods in these spheres. AI can aid in making better predictions of drug behavior, conducting a better safety assessment, and making clinical trials more efficient through one potential application, pharmacokinetics and pharmacodynamics prediction, where machine learning models are trained on biological and chemical data to make predictions about drug behavior in the human body. AI is able to approximate drug absorption, distribution, metabolism and excretion (ADME) parameters and forecast therapeutic efficacy. In the review [12], it is emphasized that AI-based models can enhance PK/PD analysis by detecting trends in the intricate pharmacological data, and help researchers optimize drug dosing and treatment options. The use of AI in the process of the development of a drug is also noted to improve toxicity prediction and safety assessment. Conventional toxicity tests are lengthy and mostly heavily depend on animal tests. Predictive models developed using AI can be used to assess the chemical structures and biological data to predict the possible toxic effects prior to clinical testing. Investigations [13,14] indicate that AI has a higher ability to detect possible toxicological risks and adverse drug reaction. On the same note, simultaneously [15] reported that AI technologies can forecast such significant drug development parameters as ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) that allows researchers to evaluate the safety and pharmacokinetic profiles of drugs at an early stage. Patient data, genetic data and clinical records can be analyzed using AI technologies to enhance the design and efficiency of trials. As it is stated in [16,17], AI aids in the discovery of pertinent biomarkers, the selection of proper drug doses, and stratification of patient groups to improve the results of clinical trials. Moreover, [18] reported that AI has the potential to support the recruitment of patients and allow new models of trial, including synthetic control arms and digital twins, which can simulate

the behavior of patients and eliminate the necessity of maintaining large control groups. However, the existing body of literature has its limitations. The majority of the sources that are available are review articles, which present an overview of the existing research but do not include the detailed experimental information. Consequently, the exact quantitative results, including the sizes of effects, half-participants, or the direct comparison of AI-based techniques with conventional ones, can be frequently not reported. However, the similarities in the findings of various reviews also suggest that AI can significantly improve pharmacokinetic modeling, toxic system forecasting, and clinical trial design in the development of contemporary medicines.

AI in Pharmaceutical Manufacturing: The Artificial Intelligence (AI) and machine learning (ML) technologies are becoming more and more disruptive, as they enhance the manufacturing process of the pharmaceutical industry, making the manufacturing process more efficient, more quality-focused, and predictive of maintenance. Over the last several years, various works have shown that AI-powered solutions can greatly enhance the manufacturing process, as they are able to examine a great amount of operational data and give real-time guidance to make decisions. The technologies enable the pharmaceutical industries to streamline their production processes, ensure a steady product quality, and minimize disruptions in the operations. Process optimization is one of the largest areas of AI application in the pharmaceutical production. Complex manufacturing data can be analyzed using AI and ML algorithms and patterns that can assist in optimizing production parameters can be identified. Multivariate data analysis, artificial neural networks, and reinforcement learning are AI-ML tools that are indispensable in the design and monitoring of biopharmaceutical manufacturing processes (according [19]). Such high-level analytical tools allow manufacturers to have more efficient production systems and the quality of products can be controlled at the same time, which is also applied to process analytical technology (PAT) systems, controlled in real time. According to research [20], the PAT systems provided by AI can dynamically optimize production parameters in the manufacturing process and guarantee increased process efficiency and uniformity in the products. Moreover, the technologies like EdgeAI enable identifying faults very quickly and performing an automated control of pharmaceutical formulations, which increases the credibility of the manufacturing processes [21] The other field where AI can be highly effective is the quality control. The conventional quality assurance tests in pharmaceutical production may be resourceful and time-consuming. The AI systems are able to process the production information, identify the variances and make sure that the high-quality standards are followed during

the manufacturing process. The researchers [22] and other scholars have demonstrated that AI-monitored systems enhance quality testing processes and assist in ensuring high regulatory standards throughout the production of pharmaceutical products. The increase of AI usage in the predictive maintenance of pharmaceutical manufacturing plants as well. Implementation of the AI in connection with the Internet of Things (IoT) technologies gives the manufacturers an opportunity to monitor the equipment performance and identify possible failures in advance. As it is claimed in [23], AI-IoT integration can promote real-time control over the most important parameters in the manufacturing process and minimize the unplanned downtime of equipment. This proactive form of prediction will guarantee a smoother production process and reduce the cost of upkeep. Moreover, the recent studies emphasize some other advantages of integrating AI in the pharmaceutical production. Research [24] cited that AI-based technologies have the ability to increase the pace of technological advancement, enhance the stability of the processes, and minimize the frequency of the products defects in the production. Altogether, the increasing number of papers points to the fact that AI and machine learning are becoming vital in ensuring the modernization of pharmaceutical production through various means of efficiency, quality assurance, and reliability of operations.

Role of AI in Pharmaceutical Care: Pharmaceutical care is becoming more and more improved by the use of Artificial Intelligence (AI) through better clinical decision-making, pharmaceutical management, enhanced monitoring of drug safety, and personalized treatment plans. Recent findings suggest that AI technologies can process the high volumes of clinical and patient data and assist healthcare professionals to make more correct and timely therapeutic decisions. The creation of Clinical Decision Support Systems (CDSS) can be considered one of the most significant AI applications in pharmaceutical care. These systems will help healthcare professionals when making decisions on the right drugs and detect possible issues with drugs. As stated in [25], computer-assisted programs that are powered by AI like drug-drug interaction checkers and smart CDSS platforms can greatly improve clinical decision-making and assist in the prevention of medication errors. Likewise, it was also reported that AI-based CDSS is used to analyze patient records, laboratory information, and medication histories to guide effective and safe medication-related decisions. AI is also relevant in Medication Therapy Management (MTM). Through the analysis of patient-centered data, including disease states, medication history, and laboratory data, AI systems can be useful to pharmacists and clinicians in streamlining medication regimens. It has been shown that AI models can be helpful in

supporting MTM services by suggesting the right dosage of drugs and monitoring drug reactions and safety, which further enhances the effectiveness of treatment and patient compliance [26]. Another crucial aspect of AI use is the prediction of adverse drug reaction (ADR) and safety surveillance. Predictive analytics using AI have the potential to analyze large datasets of pharmacovigilance and clinical records to identify possible adverse drug events. It is possible to say [27] that AI technologies can recognize the trends that are connected with the adverse drug events and prevent the medication-related harm. Moreover, [28] stated that AI algorithms may forecast possible toxicity and adverse drug reactions in drug development and as well as in clinical practice. AI is also making a significant contribution to the development of personalized or precision medicine. Combining genetic data, clinical data, and patient-specific features, AI systems may facilitate the creation of custom treatment plans [29] underscored the fact that AI technologies can be used to create personalized treatment plans that are informed by genetic profiles and disease features. Likewise, highlighted that AI-based tools are significant to further the development of precision medicine because they allow the desire to obtain customized treatment patterns enhancing therapeutic experiences. Nevertheless, there are still some obstacles in the implementation of AI in pharmaceutical care. The challenges of data privacy concerns, bias in algorithms, and the incorporation of AI technologies with current healthcare operations are some of the issues likely to restrain the proliferation of AI technologies. It has been mentioned that close ethical supervision and regulatory measures would be necessary to promote the safe and responsible application of AI in healthcare and pharmacy practice.

Applications of AI in Hospital and Community Pharmacy:

The concept of Artificial Intelligence (AI) is gradually becoming part of the hospital and community pharmacy practice, where it offers considerable clinical and operational advantages. The use of AI-driven technologies is related to automated dispensing systems, smarter prescription analysis, and better patient counseling service. Through the examination of big data of medication and patient records, AI has assisted the pharmacists in minimizing medication errors, treating patients more effectively, and enhancing overall patient outcomes. In hospitals, AI has shown significant progress in medication safety and workflow efficiency in pharmacists. It has been noted [30] that AI-based pharmacy systems have also decreased prescription distribution error by up to 75% and detection of adverse medication reaction by an average of 65 percent. These may aid pharmacists by automatically scrutinizing drug prescriptions, diagnosing possible drug-drug interactions, and verifying drug orders before they are dispensed, thus

lowering the likelihood of medication-related errors. AI is also largely applicable to community pharmacy practice, especially in enhancing prescription adherence and patient compliance. Studies [31] found that AI pharmacy systems increased medication compliance rates by 40 percent and decreased the number of pharmacy prescription refills by 55 percent in patients. Also, AI-based pharmacy services have already proven to be effective as the number of medication errors and patient compliance increased by about 15 and 10 percent respectively due to the implementation of AI technologies in community pharmacies. The AI can be able to analyse the prescriptions, check medication orders, and identify possible drug-drug interactions before the medication is dispensed. Research [26] which described the advantages of AI-based tools in enhancing prescription analysis and medication safety also indicated that 19 studies reviewed represented quantitative studies that found that the most prevalent AI application in clinical pharmacy services was medication order review (9 studies) and health product dispensing (4 studies). These results indicate that AI technologies are finding more and more applications in assisting daily pharmacy activities and clinical decision making. AI-based systems are also useful in helping to conduct personalized patient counseling and monitoring medication adherence. Pharmacists can use smart digital platforms and mobile technologies to monitor the use of medications and prescribe them automatically as well as guide them through personalized counseling, depending on patient health data. As explained in [26] the technologies will enhance patient engagement and enhancing better therapeutic results. In general, AI implementation in hospital and community pharmacy environments is revolutionizing pharmaceutical care by increasing medication safety, workflow efficiency and treatment adherence in patients. Such developments demonstrate AI increasing significance in contemporary pharmacy practice.

Advantages of AI in Pharmacy: In the field of pharmacy, artificial intelligence (AI) greatly improves patient outcomes, accuracy, efficiency, and cost-effectiveness. The beneficial impact of AI technologies in pharmaceutical research, drug development, and clinical pharmacy practice has been repeatedly observed, according to recent articles published between 2022 and 2025. The improved accuracy of clinical decision-making and medication management is one of AI's main advantages. Compared to traditional ways of assessing large amounts of patient data, electronic health records and pharmacological data, AI systems are capable of analyzing them to determine possible interactions between drugs and drug problems and identifying them more accurately. Associating with [26], AI assists pharmacists to identify potential drug-to-drug interactions and drug mistakes based on the

analysis of intricate datasets of patients. Likewise, [33] found that AI algorithms can discover patterns and correlations in biomedical data that the human scientists might not have otherwise been able to identify, thus enhancing diagnostic accuracy and therapeutic decision-making. The other important outcome of AI in pharmacy is accelerated drug discovery and development. The conventional drug development systems tend to be time consuming and involve a lot of experimentation. The AI technologies help speed up this process as they can quickly analyse biological, chemical, and even clinical data and outline possible areas of therapeutic action and promising drug candidates. Research conducted by [33] revealed that AI could contribute greatly to the time saved in different drug development. Moreover, [3] mentioned that AI-based systems are capable of accelerating the drug discovery process via the detection of disease-related targets in large amounts of data. Moreover, [34] pointed out that AI-based models have the capability of expediting the process of discovering lead compounds by making precise predictions in terms of pharmacokinetics and molecular screening. AI can be useful in reducing costs in pharmaceutical research and in drug development. AI can greatly reduce the costs of research and development by automating data analysis, optimizing the design of experiments, and reducing the workload of large laboratory experiments. The reduction in time taken to develop the medicines through AI is a reduction in the costs of the entire research as stated in [35]. Moreover, Usman et al. (2025) have also remarked that AI technologies could facilitate the research process and minimize the necessity to use expensive testing on animals, which would also contribute to cost-effectiveness in pharmaceutical development. The study found that AI-based personalized treatment plans would enhance patient adherence and treatment response. [3] reports that AI application on actual patient data, such as genetic data, clinical conditions, and treatment response, has the potential to enhance treatment outcomes and medication adherence. Moreover, [33] noted that AI technologies can be effectively used to monitor the adverse drug reactions in real-time in a clinical trial, which can enhance the safety and quality of care delivered to patients and pharmaceutical studies. In sum, the increasing number of studies indicate that AI can be of great use in various areas of pharmacy practice and pharmaceutical research. AI is currently a crucial component of the promotion of contemporary healthcare and pharmaceutical science by refining precision, accelerating medications development, decreasing expenses, and increasing patient outcomes.

Future Perspectives of AI in Pharmacy: It is believed that Artificial Intelligence (AI) will greatly change the future of pharmacy by making personalized medicine possible through the

combination of big data, genomics, and sophisticated computational technologies. Recent research papers published in 2023-2025 show consistent opinions on how AI can be used to facilitate personalized medicine and enhance therapeutic results and reduce adverse outcomes. As [36] explains, AI when used together with machine learning technologies can be utilized to analyze complex genomic and clinical data and help in the creation of personalized medicines. These technologies can enable researchers to determine disease-specific biomarkers and to design drug therapies based on the specific characteristics of patients. In a similar vein, [37] also said AI algorithms can be used to analyze large volumes of patient data to identify possible drug-to-drug interactions and offer personalized treatment choices. Moreover, [38] highlighted that the professional role of pharmacists could be changed because AI technologies could offer highly personalized healthcare services due to their ability to aid in a more accurate diagnosis and a more specific set of therapeutic interventions. Pharmacists have traditionally been in charge of dispensing medications, but the implementation of AI into healthcare systems is altering their roles by assigning them clinical decision-making and patient-centered roles. Similarly, [39] proposed that the pharmacy practice in the future will be characterized by the close collaboration between humans and intelligent machines, with pharmacists having to acquire the skills in both the medical sciences and digital technologies. The AI technologies will be able to help the pharmacists analyze patient data and optimize the medication therapy, as well as detect any possible issues with medications. Moreover, [41] has indicated that AI can assist pharmacists in delivering single patient guidance, drug adherence observation and workflow streamline in the healthcare environment, though the accessible body of literature is mainly review-based and offers scanty quantitative information on the actual effect of genomic integration in medical facilities. However, the accumulating evidence is that AI will be instrumental in changing the pharmacy practice through personalized healthcare and increasing the clinical skills of a pharmacist.

AI-Assisted Drug Repurposing and Computational Pharmacology:

Artificial intelligence has also demonstrated significant potential in computational pharmacology and drug repurposing strategies. AI-based molecular docking and virtual screening approaches enable researchers to rapidly evaluate drug-target interactions and identify alternative therapeutic applications for existing drugs. For instance, computational studies involving molecular docking and pharmacokinetic prediction tools have been used to identify potential therapeutic candidates against infectious diseases. A recent in-silico investigation demonstrated the potential repurposing of Omadacycline against *Orientia tsutsugamushi* by targeting deubiquitylase

(OtDUB), where strong binding affinity and favorable pharmacokinetic profiles were observed, suggesting a promising alternative therapeutic strategy for scrub typhus management [42]. Such AI-supported computational approaches significantly reduce the time and cost associated with early drug discovery.

AI and Immunotherapy-Driven Precision Medicine: Artificial intelligence is also playing an emerging role in the advancement of modern immunotherapeutic approaches. Machine learning algorithms are increasingly used to analyse complex genomic and immunological datasets to identify suitable targets for advanced therapies such as CAR-T cell therapy. CAR-T therapy has revolutionized the management of hematological malignancies, particularly pediatric acute lymphoblastic leukemia (ALL). Recent reviews highlight that AI-assisted analysis of genomic and clinical data may support the identification of novel CAR targets, predict treatment response, and optimize therapy design, thereby improving safety and efficacy outcomes in pediatric oncology [43].

AI Applications in Genetic and Rare Disease Research: Rare genetic disorders represent an area where AI-based technologies can significantly improve diagnosis and therapeutic development. The integration of genomic data analysis with machine learning algorithms enables early identification of disease-causing mutations and the discovery of potential therapeutic strategies. Recent comprehensive reviews on skeletal dysplasias, including achondroplasia, emphasize the importance of advanced computational tools in understanding molecular mechanisms, improving diagnostic accuracy, and supporting targeted therapeutic research for rare genetic diseases [44].

AI in Natural Product Drug Discovery and Novel Drug Delivery Systems: Natural products continue to serve as important sources of bioactive compounds for drug discovery. Artificial intelligence tools can accelerate the screening of phytochemicals, optimize molecular structures, and design innovative drug delivery systems for improved therapeutic efficacy. Studies focusing on anti-inflammatory agents derived from natural products have highlighted the development of novel drug delivery systems to enhance drug stability, bioavailability, and targeted therapeutic action [45]. AI-driven formulation design and predictive modeling can further improve the development of such advanced pharmaceutical delivery systems.

AI-Guided Pharmacological Screening of Bioactive Compounds: Artificial intelligence techniques are also useful in the pharmacological evaluation of bioactive compounds derived from medicinal plants. Computational modeling and predictive analytics can help identify potential antioxidant and anti-inflammatory agents by analysing chemical structures and biological activity

data. Experimental studies on plant extracts such as *Flacourtia jangomas* have demonstrated significant antioxidant and anti-inflammatory activities, highlighting the importance of integrating computational tools with experimental pharmacology to accelerate the discovery of novel therapeutic compounds [46].

AI and Global Health Surveillance: Artificial intelligence can also play a critical role in monitoring emerging and re-emerging infectious diseases. AI-based epidemiological models and predictive analytics can analyse large datasets from clinical reports, surveillance systems, and environmental factors to predict disease outbreaks and guide public health responses. Reviews focusing on emerging viral diseases highlight the importance of advanced data analytics and computational tools in understanding disease epidemiology and developing effective prevention strategies [47].

CONCLUSION

Artificial Intelligence (AI) is rapidly emerging as a transformative technology in the pharmacy and pharmaceutical sciences. The integration of AI into drug discovery, drug development, pharmaceutical manufacturing, and pharmaceutical care has significantly improved the efficiency, accuracy, and speed of healthcare processes. AI-based computational models enable researchers to analyze large biological and clinical datasets, identify potential drug candidates, predict pharmacokinetic and toxicity profiles, and optimize clinical trial designs. In pharmaceutical manufacturing, AI enhances process optimization, quality control, and predictive maintenance, ensuring consistent product quality and operational efficiency. Furthermore, AI-driven technologies support pharmacists through clinical decision support systems, medication therapy management, and adverse drug reaction prediction, thereby improving patient safety and treatment outcomes. The application of AI in hospital and community pharmacy settings also contributes to reduced medication errors and better patient adherence. Although challenges such as data privacy, algorithm bias, and limited quantitative evidence remain, the growing body of research indicates that AI will play a crucial role in advancing personalized medicine and transforming the future role of pharmacists in healthcare.

Author Contributions

All authors contributed equally in this research work.

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Conflict of Interest

The authors declare that there are no conflicts of interest related to this work.

Ethical Approval

Ethical approval was not required for this study, as it is a systematic review based exclusively on previously published data.

Informed Consent

Informed consent was not applicable, as no individual patient data were collected or analyzed in this study.

Data Availability Statement

All data analyzed in this study are included in the published articles identified through the systematic review and are available within the manuscript and its supplementary materials.

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