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ENHANCING DRUG DISCOVERY AND RESEARCH THROUGH ARTIFICIAL INTELLIGENCE
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წამლის აღმოჩენისა და კვლევის პროცესების გაუმჯობესება ხელოვნური ინტელექტის დახმარებით
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რეზიუმე

ხელოვნური ინტელექტი (AI) სულ უფრო აქტიურად მკვიდრდება ფარმაცევტულ მეცნიერებაში და ახალ შესაძლებლობებს ქმნის წამლის კვლევისა და შექმნის სფეროში. ამ ტექნოლოგიის საშუალებით შესაძლებელი ხდება დიდი მოცულობის სამეცნიერო მონაცემების ანალიზი ძალიან მოკლე დროში, რაც ამცირებს კვლევის ხანგრძლივობას და ხარჯებს. AI ეხმარება მეცნიერებს უფრო სწრაფად აღმოაჩინონ სამკურნალო სამიზნეები, შეაფასონ ქიმიური ნაერთების პოტენციური მოქმედება და შეარჩიონ უსაფრთხო და ეფექტური მოლეკულები წამლის განვითარების საწყის ეტაპზე. მიუხედავად მრავალი უპირატესობისა, AI-ის გამოყენება წამლის კვლევაში აჩენს გარკვეულ გამოწვევებს, განსაკუთრებით ეთიკისა და მონაცემთა დაცვის კუთხით.

ნაშრომი განიხილავს, თუ როგორ ცვლის ხელოვნური ინტელექტი წამლის შექმნის ტრადიციულ პროცესს და როგორ შეიძლება ის გამოყენებულ იქნეს ეფექტიანად, უსაფრთხოდ და გონივრულად ფარმაცევტულ პრაქტიკაში.

Introduction. Artificial intelligence (AI) has emerged as a groundbreaking technology across various industries, with particularly transformative potential in healthcare. In drug discovery and pharmacy practice, AI is poised to revolutionize processes and optimize operations. The continuous evolution of AI, driven by advances in machine learning and data science, has contributed to innovative solutions for the complex challenges facing the pharmaceutical sector. The integration of AI into pharmacy practice goes beyond traditional roles, fundamentally reshaping processes such as clinical decision-making, personalized medicine, pharmaceutical manufacturing, and operations management. While the potential of AI to enhance efficiency, accuracy, and innovation is evident, its implementation faces significant challenges that must be addressed to fully realize its benefits. [1,2]

Research Aim. The primary objective of this study is to explore the role of artificial intelligence (AI) within the pharmaceutical field, with a specific focus on its application in drug research and development. This paper aims to highlight how contemporary pharmaceutical science employs AI technologies for various purposes, including the identification of therapeutic targets, molecular design optimization, strategic planning of clinical trials, and the development of personalized treatment approaches. Additionally, the study seeks to identify the opportunities and challenges that arise from the integration of AI systems into pharmaceutical practice.

Methodology. This research adopts a literature review approach, relying on a comprehensive analysis of existing academic and institutional publications. The reviewed sources include peer-reviewed journal articles, systematic reviews, and reports from international organizations.

Results. This paper investigates the growing influence of Artificial Intelligence (AI) on the pharmaceutical industry, with a primary focus on its significant role in drug discovery, development, and improving pharmacy practices. AI is revolutionizing several aspects of the pharmaceutical field, from optimizing medication adherence and enhancing patient education to increasing operational efficiency in

pharmacy settings. This study emphasizes the ways in which AI can bridge existing gaps in knowledge and suggests actionable strategies for incorporating AI technologies into pharmaceutical care, aiming to balance technology-driven solutions with a patient-centered approach for the future of healthcare.

Throughout this analysis, real-life examples and case studies are used to demonstrate how AI is already improving pharmacy practices. These case studies highlight the tangible benefits of AI, such as better medication management, personalized patient care, and more streamlined operations within pharmacies. The research also delves into the challenges faced by healthcare professionals when adopting AI, including technological limitations, data privacy concerns, and the necessity for specialized training. The study provides practical recommendations for overcoming these obstacles, focusing on how AI can be efficiently integrated to improve both patient outcomes and pharmacy services. In addition, the scope of the research extends to the increasing influence of AI in drug discovery, showcasing its role in the development of new drugs and therapeutic methods [3].

As depicted in the figure below, the integration of artificial intelligence is fundamentally transforming the pharmaceutical development pipeline, enhancing efficiency and precision across all stages—from drug discovery through to post-marketing surveillance. The subsequent analysis delineates how these advancements correspond to the visual elements presented in the figure [4].

1. Discovery & Development	2. Pre-Clinical Research	3. Manufacturing	4. Supply Chain Management	5. Post-Market Surveillance
•AI facilitates the identification of promising drug candidates by analyzing datasets of chemical compounds and predicting their therapeutic efficacy, supports the repurposing of existing drugs for new clinical applications.	•AI simulates biological processes to predict experimental outcomes, thereby reducing dependence on animal models. Furthermore, it enables rapid analysis of pre-clinical data for safety and toxicity, accelerating the progression to clinical trials	•AI systems monitor and optimize production workflows to ensure consistent drug quality. Additionally, predictive maintenance tools forecast equipment servicing needs, thereby minimizing downtime in manufacturing operations.	•Through demand forecasting and inventory optimization, AI helps prevent shortages and overstock scenarios. It also enhances logistics by streamlining delivery routes and mitigating real-time supply chain disruptions.	•AI assists in detecting adverse drug reactions by analyzing patient data and clinical reports. It also monitors social media and other digital platforms to identify emerging safety concerns in real-time.

In recent years, AI's involvement in drug discovery has grown significantly, as pharmaceutical companies increasingly collaborate with AI technology providers. Companies such as Roche, Pfizer, Merck, and AstraZeneca are investing heavily in AI-driven R&D processes. These partnerships are accelerating the drug discovery process by utilizing machine learning algorithms to identify promising drug candidates, improve drug designs, and even forecast potential side effects before clinical trials take place. According to reports, nearly 62% of healthcare organizations are considering or planning to invest in AI technologies, with 72% of pharmaceutical companies recognizing the critical role AI will play in shaping the future of their operations. These trends highlight the growing appreciation of AI's potential to reduce costs, enhance decision-making, and improve research results.

For instance, a partnership between the Massachusetts Institute of Technology (MIT), Novartis, and Pfizer, launched in 2018, explores how AI and machine learning can be applied to drug design and manufacturing processes. This collaboration is accelerating drug development by utilizing AI to improve

both drug creation and synthesis. Such initiatives demonstrate how AI can not only speed up drug discovery but also make the entire development process more cost-effective and efficient.

The core aim of pharmaceutical research is to identify novel active pharmaceutical ingredients (APIs) capable of treating previously incurable diseases. AI plays a crucial role in analyzing vast and intricate datasets, which include clinical, genetic, laboratory, and mobile health data, in order to identify new therapeutic compounds. As biomedical data collections grow in size and diversity, AI's ability to process these data sets allows researchers to identify promising drug candidates, design optimized clinical trials, and more accurately predict the outcomes of treatments. For example, companies like GNS Healthcare and Atomwise are utilizing AI to revolutionize drug design. GNS Healthcare employs its platform, Reverse Engineering and Forward Simulation (REFS), which analyzes large datasets to uncover cause-and-effect relationships, predicting the efficacy of drugs by integrating various data forms. Atomwise, known for developing AtomNet, the first deep learning neural network for drug discovery, uses AI to predict the properties of compounds and their potential therapeutic effects, enhancing the accuracy and speed of identifying viable drug candidates [5,6].

Beyond drug discovery, AI plays an expanding role in optimizing clinical trials, pharmacovigilance, and post-market surveillance. AI systems are increasingly used to streamline participant recruitment by analyzing electronic health record data, identifying eligible candidates more quickly and accurately. Furthermore, AI's capacity to predict drug safety and efficacy early on helps optimize trial designs, reducing the risk of failure and lowering costs associated with late-stage clinical trials. The AI market in drug discovery was valued at approximately $1.5 billion in 2023, with projections suggesting a compound annual growth rate (CAGR) of 29.7%, potentially reaching $11.8 billion by 2030. This growth underscores the economic value AI technologies bring to transforming the drug discovery landscape.

AI's role extends to both the preclinical and clinical phases of drug development. In preclinical stages, AI is used to predict the toxicity and safety of new drugs, which minimizes reliance on animal testing and offers faster and more reliable testing results. In clinical trials, AI's predictive capabilities help optimize trial designs, anticipate adverse effects, and facilitate patient recruitment. AI algorithms can predict the likelihood of a drug succeeding in trials, enabling pharmaceutical companies to focus on the most promising compounds while eliminating those with low chances of success. AI-driven systems also monitor and optimize drug manufacturing, ensuring that production processes comply with regulatory standards while enhancing efficiency and reducing costs.

In pharmacy practice, AI is driving progress in medication management and personalized healthcare. AI tools are assisting pharmacists in managing complex medication regimens by analyzing large volumes of patient data, including medical histories, lab results, and current prescriptions, to provide personalized recommendations. These systems help optimize medication dosages, predict adverse drug reactions, suggest alternative treatment plans tailored to individual patient needs. By offering pharmacists data-driven insights, AI enhances clinical decision-making and improves patient outcomes [7].

However, certain aspects of AI's potential in pharmacy practice remain underdeveloped, particularly in the areas of medication adherence and patient education. Medication adherence is essential for achieving optimal health outcomes, but research on using AI to improve adherence is still limited. AI's role in educating patients about proper medication usage—an essential factor for enhancing patient compliance—also remains underexplored. Incorporating AI into these areas of pharmacy practice could improve patient engagement, reduce medication errors, and contribute to more personalized care. While AI's integration into these aspects is still in its early stages, further research is necessary to fully realize its potential.

Challenges such as data privacy concerns, the need for pharmacist training, and technological limitations are obstacles that must be addressed to fully leverage AI in pharmacy practice. Specifically, the use of AI in clinical decision-making raises important issues regarding patient privacy and data security, which need to be carefully managed to maintain trust in AI technologies. Additionally, AI tools must be integrated into pharmacists' workflows in a way that enhances their decision-making without overwhelming them with excessive data [8].

In conclusion, AI is transforming the pharmaceutical industry by improving drug discovery, optimizing clinical trials, and revolutionizing pharmacy practices. The increased adoption of AI technologies by major pharmaceutical companies reflects the growing recognition of AI's ability to reduce costs, accelerate drug development, and enhance patient care. As technology progresses, its integration into the pharmaceutical sector will undoubtedly continue to drive the next wave of healthcare innovations, benefiting patients, healthcare providers, and the broader pharmaceutical industry alike.

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SUMMARY

Artificial intelligence (AI) is increasingly becoming a key component in pharmaceutical science, offering new avenues for drug research and development. By analyzing vast volumes of scientific data within a short time, AI reduces both the duration and cost of traditional drug discovery processes. It assists researchers in identifying therapeutic targets more efficiently, evaluating the potential effects of chemical compounds, and selecting the safest and most promising molecules in early development stages. Despite these benefits, integrating AI into drug research brings forth challenges, particularly related to data privacy, transparency, and ethical responsibility.

This paper explores how artificial intelligence is reshaping the traditional drug development landscape and emphasizes the importance of applying these technologies responsibly and ethically in pharmaceutical innovation.

Keywords: Artificial Intelligence, Drug Discovery, Drug Development, Medicines, Research