



Artificial Intelligence in Pharmacy – A Comprehensive Review

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ABSTRACT

AI has emerged as a transformative technology in the pharmaceutical sciences, offering unparalleled efficiency in the drug discovery, formulation development, poly pharmacology, and practice in hospital pharmacies. This review gives an overview of the gamut of AI methodologies- which include artificial neural networks, deep learning, recurrent neural networks, fuzzy logic systems, support vector machines, and generative models-and their modern applications in the fields of pharmacy. AI-driven molecular design, virtual screening, ADMET prediction, and de novo generation of drugs are superior compared with traditional experimental methodologies. In formulation science, AI is capable of superiorly predicting dissolution, optimizing polymer composition, controlling particle size, and modelling drug-release kinetics as demonstrated by different case studies. AI is increasingly integrated into clinical settings for radiological interpretation, treatment planning, medication monitoring, and managing patients. Notwithstanding the advances, challenges linger data quality limits, system interpretability, ethical issues, and poor integration into laboratory practice limit wide-scale adoption. The review provides insight into current capabilities, limitations, and future opportunities for implementing AI as a practical and reliable tool throughout pharmaceutical domains.

Keywords: Artificial Intelligence, Drug Discovery, Formulation Development, Pharmaceutical Sciences, Clinical Pharmacy.

1. INTRODUCTION

Artificial Intelligence has quickly emerged as a core technology within scientific and healthcare disciplines. Artificial Intelligence within the pharmaceutical sciences is changing how drug discovery, formulation design, and clinical pharmacy practice are conventionally conducted. A general overview of how AI algorithms are being used increasingly to solve pharmaceutical problems involves the use of artificial neural networks, deep neural networks, recurrent neural networks, fuzzy logic, and support vector machines. Multidimensional data handling, nonlinear pattern identification, and biological behaviour predictions, along with automating repetitive analysis, become feasible through AI systems, making it an indispensable element in modern pharmaceutical development.

In drug discovery, AI accelerates hit identification, molecular docking, QSAR predictions, ADMET profiling, and in silico generation of novel chemical entities. Deep Chem, REINVENT, Chomputer, and curated databases like ChEMBL and ZINC support AI-driven design pipelines.

AI-assisted modelling has a lot of advantages related to formulation science, as ANN, neuro-fuzzy systems, and hybrid AI frameworks predict dissolution profiles, optimize excipient ratios, regulate encapsulation efficiency, and improve drug-release behaviour more precisely than statistical models.

Clinical and hospital pharmacy sectors also use AI in treatment planning, monitoring patient adherence, interpreting diagnostic images for cancers, and supporting pharmacists' decisions. AI-driven radiology and computerized clinical decision systems are illustrative examples of its rising role in patient care.

Overall, the integration of AI into the pharmaceutical sciences enhances precision, productivity, and innovation. However, major gaps in interpretability, ethical challenges, and regulatory barriers continue to restrict full-scale adoption. This review will synthesize existing advances and highlight future pathways required for the integration of AI into mainstream pharmaceutical practice.



2. FUTURE SCOPE

2.1 Explainable and transparent models: AI systems should make their predictions interpretable to support their regulatory approval and clinical acceptance. There is a need for an advance in XAI approaches.

2.2 Standardized Benchmark Datasets: High quality, curated datasets on formulation predictions, toxicity modelling, and ADMET screening are required within the field to ensure that fair comparisons are made among AI models.

2.3 AI–Wet Lab Integration: In all future research, in silico predictions must be tightly linked with laboratory synthesis and biological validation to form closed-loop pipelines.

2.4 Regulatory Frameworks for AI in Pharmacy : The guidelines on the validation, safety, evaluation of bias, and deployment of AI systems are needed both in industrial and clinical settings.

2.5 Clinical AI Expansion: Large validation trials are required for the integration of AI-assisted radiology, oncology detection systems, and dosage optimization tools into the hospital pharmacy. ^[6] 6. Adoption of Next-Generation Models Transformers, LLMs, multimodal systems, and generative foundation models are highly promising for drug design, formulation modelling, and clinical decision support, far beyond what might have been possible when the article under review was written.

3. CHALLENGES IN IMPLEMENTING AI IN PHARMACY

The application of artificial intelligence in pharmacy has some notable challenges despite the benefits. First, a lack of quality and standardized health care data required for the development of artificial intelligence applications. The application of artificial intelligence in pharmacy setting requires a lot of investment for software or hardware development. Moreover, issues related to cybersecurity create a barrier for the development of artificial intelligence applications. The lack of specialists who are conversant with artificial intelligence applications in pharmacy practice creates a need for a constant flow of education. Data privacy associated with artificial intelligence applications creates a concern that should be dealt with. Moreover, a lack of clear guidelines in artificial intelligence applications creates a concern for pharmacists. The unreliability of artificial intelligence applications due to a lack of integration of pharmacy systems with artificial intelligence makes a concern for pharmacists. In addition, resistance from pharmacists who fear to lag behind due to a lack of application of artificial intelligence in pharmacy practice makes a concern.

4. ETHICAL AND PRIVACY CONCERNS

Ethical and privacy issues are some of the challenges associated with implementing artificial intelligence (AI) technology within pharmacy. This is due to the fact that AI works with high volumes of patient data, posing a threat of breach of privacy and confidentiality of such sensitive data. Patient consent and confidentiality and clarity associated with data collection, processing, and use within artificial intelligence technology are not well defined. Other ethical concerns within pharmacy due to AI technology include bias within algorithms used to create AI models, which not only provide unfair outcomes but also generate inaccurate clinical decisions. Lack of clarity and explanation associated with decision-making within AI technology makes it difficult for pharmacists to justify and rely on decisions generated through such technology. Furthermore, there is lack of clarity associated with liability within AI technology that leads to medication error.

5. TECHNICAL LIMITATIONS

Technical limitations stand in the way of the adoption of AI in pharmacy practice. The majority of AI systems face significant challenges regarding their interoperability and integration with the presently applied pharmacy information systems, electronic health records, and hospital software due to poor interoperability and the lack of standardization. AI models perform well only if high-quality and enough data are provided. Single errors either in data input or algorithm training may lead to incorrect predictions and recommendations. Many AI models serve as "black-box" systems, showing limited transparency and explain ability, which makes it difficult for the pharmacist to understand how decisions are generated. Besides, technical issues like system failures, software bugs, and regular updates and validation further limit reliability. All these limitations require continuous monitoring, technical support, and human supervision to ensure safe and effective application of AI in pharmacy settings.

6. APPLICATIONS OF AI IN PHARMACY

Artificial intelligence (AI) is becoming more important in pharmacy. It offers applications that improve patient care, drug development, and the efficiency of healthcare systems. AI supports personalized medicine by analysing patient data to create tailored treatment plans, as shown by IBM Watson for Oncology. It helps manage medical records by allowing quick access and organization



of patient information. Tools like Google DeepMind Health Project improve clinical workflows. In diagnostics, AI helps interpret imaging data like X-rays, CT scans, ECGs, and ECHOs. This increases accuracy and reduces repetitive tasks, as seen in IBM Medical Sieve. AI also supports medication adherence and patient care through virtual assistants and apps like Molly and AiCure. In genomics, systems such as Deep Genomics and Human Longevity identify genetic mutations and guide targeted therapies. Moreover, AI speeds up drug discovery and development by predicting molecular interactions and efficiently screening potential drug candidates, demonstrated by Atomwise. Additionally, AI improves healthcare systems by analyzing large data sets to enhance clinical decisions, manage pharmacy workflows, and lower hospitalizations. This showcases its potential to transform modern pharmacy practice.

7. CONCLUSION

Artificial intelligence has become an essential driver of innovation across pharmaceutical fields. Evidence from the reviewed article proves that AI significantly enhances the efficiency of drug discovery through deep learning, neural networks, and generative models with the capability to create new chemical entities with the most accurate prediction of their properties. Formulation science will be aided too by AI tools, which outperform traditional statistical techniques in predicting dissolution, particle size, polymer ratios, and kinetics of drug release. In hospital and clinical pharmacy, AI-driven systems enhance diagnostic precision, optimize treatment planning, and reinforce patient monitoring.

Despite these developments, general application of AI is still being hindered by data quality issues, deep-learning system transparency, limited integration with experimental validation, and newly emerging ethical and regulatory challenges. In order for the full realization of AI, interdisciplinary collaboration among computational scientists, pharmacists, clinicians, and regulatory bodies will be necessary. As such challenges are overcome, AI stands ready to assume a central and indispensable role within the pharmaceutical enterprise.

8. REFERENCES

1. Topol EJ. High-performance medicine: the convergence of human and artificial intelligence. *Nat Med.* 2019;25(1):44–56.
2. Davenport T, Kalakota R. The potential for artificial intelligence in healthcare. *Future Healthc J.* 2019;6(2):94–98.
3. Chen J, Li K, Zhang Z, Li K, Yu PS. A survey on applications of artificial intelligence in pharmacy. *Comput Methods Programs Biomed.* 2022; 213:106538.
4. Jimenez-Morales A, Gomez A, Martinez M. Artificial intelligence in clinical pharmacy practice: current applications and future perspectives. *J Clin Pharm Ther.* 2021;46(6):1463–1473.
5. Vyas M, Thakur S, Riyaz B, Bansal KK. Artificial intelligence in pharmaceutical sciences: opportunities and challenges. *Pharmaceutics.* 2023;15(2):415.
6. Amisha, Malik P, Pathania M, Rathaur VK. Overview of artificial intelligence in medicine. *J Family Med Prim Care.* 2019;8(7):2328–2331.

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