WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP
Impact Factor 8.453
Volume 14, Issue 24, 1156-1168.
Review Article
ISSN 2277–7105

INTEGRATING ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND PATIENT CARE: A NEW FRONTIER IN PHARMACEUTICAL SCIENCE

Riti Pansuriya[1], Yashvi Paghadal[2], Vishva Vyas[3], Heer Patel[4], Janki Patel*[5]

[1-4]Student, Sharda School of Pharmacy, Pethapur, Gandhinagar.

[5]Associate Professor, Sharda School of Pharmacy, Pethapur, Gandhinagar.

Article Received on 15 Nov. 2025,
Article Revised on 05 Dec. 2025,
Article Published on 16 Dec. 2025,
https://doi.org/10.5281/zenodo.17963332

***Corresponding Author**
Janki Patel
Associate Professor, Sharda School of Pharmacy, Pethapur, Gandhinagar.

How to cite this Article: Riti Pansuriya1, Yashvi Paghadal2, Vishva Vyas3, Heer Patel4, Janki Patel*5. (2025). INTEGRATING ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND PATIENT CARE: A NEW FRONTIER IN PHARMACEUTICAL SCIENCE. World Journal of Pharmaceutical Research, 14(24), 1156–1168.

ABSTRACT

Artificial intelligence (AI) is transforming pharmaceutical sciences and healthcare by accelerating drug discovery, optimizing clinical development, and enhancing patient care and safety monitoring. Through machine learning, deep learning, and generative algorithms, AI facilitates molecular modelling, structure-based drug design, and robotic drug delivery, significantly reducing timelines and costs. In clinical trials, AI improves study design, patient stratification, and data analysis, while in patient care, intelligent platforms and chatbots enhance disease management, medication adherence, and clinical decision-making. Pharmacovigilance and post-market surveillance are strengthened via automated signal detection and real-time analysis of complex datasets. Hospital operations benefit from AI-driven infection surveillance, laboratory workflow optimization, and resource management. Despite challenges including data quality, biological complexity, transparency, and regulatory oversight, AI's integration with pharmacogenomics, biomarker discovery, and digital biobanking heralds a new era of precision medicine, offering transformative potential for pharmacy practice and healthcare delivery.

KEYWORDS: Artificial Intelligence; machine learning; Pharmacogenomics; Computational Drug Discovery and Design; Chatbots; Pharmacovigilance.

1. INTRODUCTION

Artificial Intelligence (AI) is a branch of study that focuses on intelligent machine learning, mostly intelligent computer programs that produce outcomes that resemble human attention processes.[1] Drug discovery advancements have drastically altered medical practice, turning once-fatal illnesses into a type of normal therapeutic exercise. Improvements in the processes for creating and testing new medications have contributed to this medical progress. The molecular structure of a new medication typically does not mimic that of an existing medication, requiring the creation of a novel molecule.[2] With enormous potential to transform healthcare, particularly pharmacy practice, the development of such a potent and innovative technology has surfaced. AI's ability to process vast amounts of data, identify trends, and offer insight can enhance patient care, optimize medication administration, and improve healthcare delivery.[3] Predicting in vivo reactions, therapeutic pharmacokinetic characteristics, appropriate dosage, etc., is also made possible by the application of AI models. Given the significance of pharmacokinetic drug prediction, the application of in silico models makes drug research more efficient and affordable.[4] Over the years, this technology has advanced quickly in pharmacy practice, offering the benefits of time and cost savings as well as the simplification of other pharmaceutical chores. According to McKinsey Global Institute, AI technologies in the pharmaceutical industry might bring in more than $100 billion a year for the US healthcare system. AI tools are expected to have enormous potential to transform the drug supply chain, safety, medication management, and patient care, among other areas of pharmacy practice.[5]

2. DRUG DISCOVERY AND DEVELOPMENT

2.1 Search strategy

Several databases, including PubMed, Scopus, Web of Science, IEEE Xplore, and Google Scholar, were thoroughly searched. We concentrated on a variety of study types, including case studies, clinical trials, research articles, review articles, and meta-analyses. Our search terms included (“Artificial intelligence” OR “AI”) AND (“Drug discovery” OR “Drug development”) AND (“Machine learning” OR “Deep learning” OR “Neural networks”) AND (“Pharmaceuticals” OR “Medications” OR “Compounds”), (“Computational chemistry” OR “Cheminformatics”) AND (“Drug design” OR “Molecular modelling”), and (“Data mining” OR “Big data analytics” AND (Pharmacology” OR “Therapeutics). Using this approach, we were able to compile pertinent literature on the use of AI in computational chemistry, molecular modelling, data mining, and pharmacological analysis, among other phases of drug discovery and development.[6] Boolean operators (AND/OR) were used in these strings to link keywords for more accurate data set selections. In order to reflect current trends and viewpoints, the database search primarily focused on recently released papers using filters (year of publication and language). Every publication that was chosen was written in English.[7]

2.2 Molecular descriptors and structure representations

The transfer of molecules into computer-readable format while retaining their inherent physicochemical properties is a crucial aspect of AI-based drug discovery and analysis, given the increasing development of natural products. Different kinds of descriptors have been proposed to represent pharmaceuticals; based on their dimensionality, these descriptors can be divided into four groups (figure 1). A number of open-source toolkits, including Open Babel and Chemmani, have been developed to calculate molecular descriptors and structure representations to speed up the drug development process.[8]

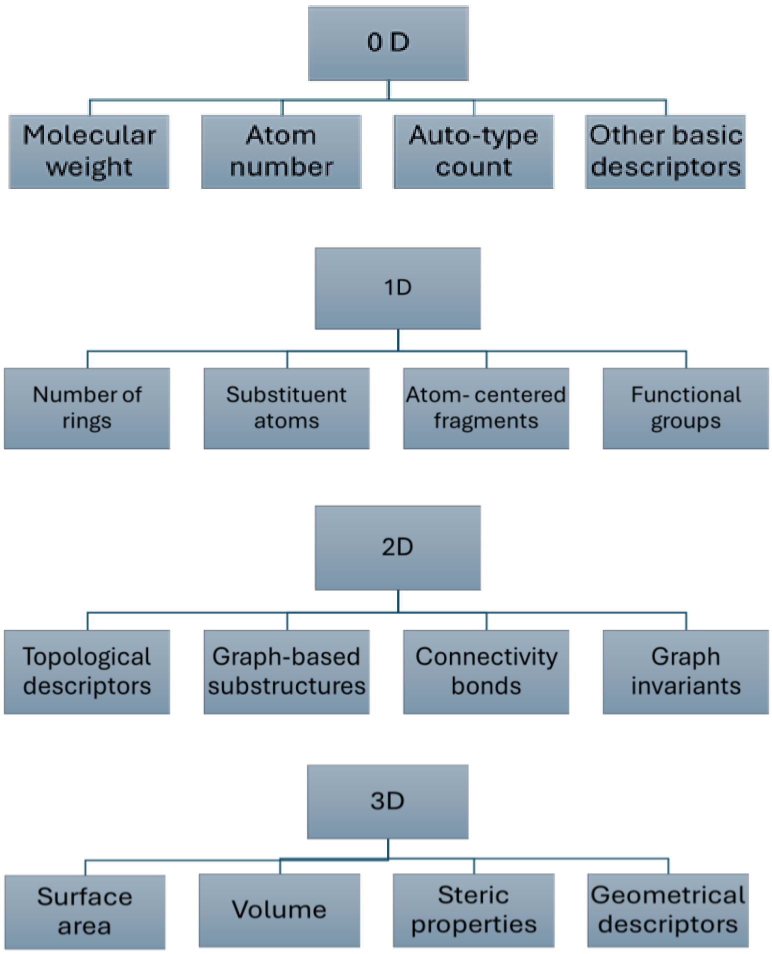

Figure 1: Summary of molecular and structural representation schemes.

2.3 Robotic Drug Delivery Systems

Innovative robotic drug delivery systems are being developed to improve the efficiency, safety, and patient experience in drug administration. These systems often incorporate advanced technologies such as artificial intelligence, machine learning, and automation to optimize treatment outcomes. The development of innovative robotic drug delivery systems (**figure 2**) promises to revolutionize the way medications are administered to patients, offering more precise and personalized treatments.[9]

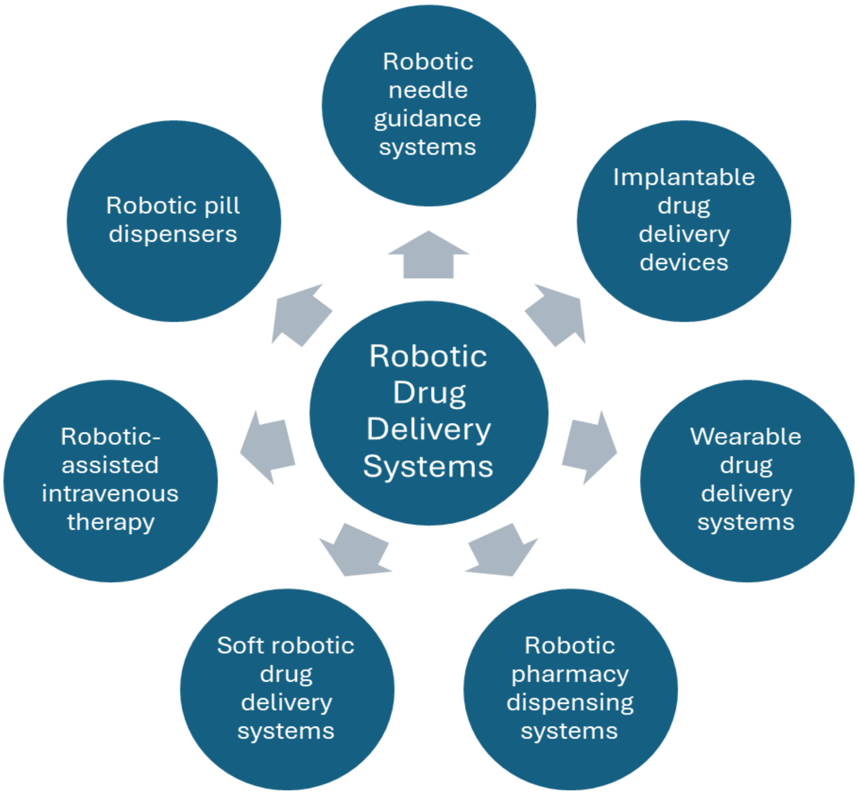

Figure 2: Applications of innovative robotic drug delivery systems in medicine.

2.4 Clinical Trials

Clinical trials currently face a number of difficulties, including a heavy administrative load, problems recruiting and retaining participants, laborious data entry, and insufficient representation that restricts trial generalizability. Generative AI expands this capability by utilizing clinical data to produce new material, such as writing and graphics, whereas nongenerative AI can combine complicated inputs from clinical data to forecast patient outcomes or patients' likelihood to benefit from a particular medication. Prediction performance can be further enhanced by using generative AI to generate artificial data sets for simulations. By quickly creating preliminary trial protocol drafts and informed consent forms, generative AI can support research.[10]

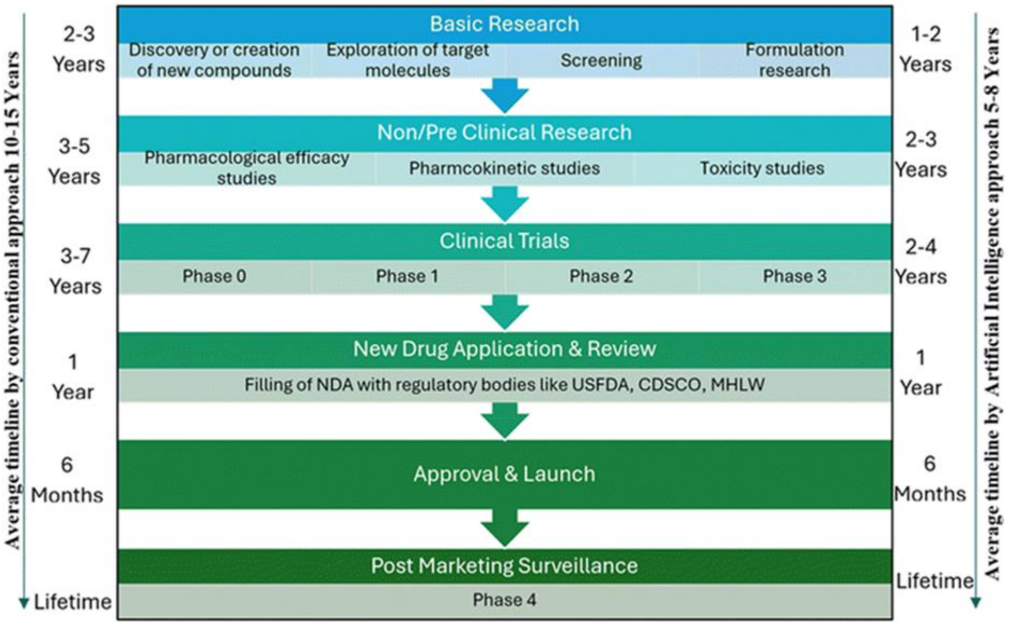

Figure 3: Comparative representation of how AI can impact drug discovery and approval processes in terms of timelines for different key steps.

3. AI ASSISTED PATIENT CARE

3.1 Disease management

The prediction of breast cancer recurrence is also aided by the development of various AI approaches. Instead of doctors, in-home AI systems might manage patients with swallowing issues and insulin irregularities. AI can optimize treatment for patients with common, but complex diseases that are attributed to multiple factors (e.g., genetic, environmental, or behavioural) like cardiovascular diseases are more likely to benefit from more precise treatments because of the AI algorithms based on big data. However, on a broader scale, AI-assisted hospital management systems may also help reduce the financial and temporal expenses related to logistics.[12]

3.1 Tools for patient support to enhance medication adherence

Many nations now Favor electronic prescribing systems, which help to improve medication management's accuracy and efficiency as well as remove issues with prescription accessibility and reading.[13] While digital technology has already addressed issues like readability, the increasing number of pharmaceuticals on the market, and drug interaction alerts, other issues still call for more intelligent solutions, such as the requirement for individualized care and instructions tailored to patients' reading levels. Electronic systems relate to other organizational tools, such pharmaceutical information systems and electronic health records, to address these issues. Reduced healthcare expenditures, fewer prescription errors, better pharmaceutical results, more patient safety, and improved clinical decision-making are some of the advantages.[14]

3.2 Chatbots

The potential of chatbots to summarize data and offer health advice about screening, diagnosis, treatment, and illness prevention has been examined in studies on chatbot health advice (CHAS).[14] Chatbots using artificial intelligence (AI) are being investigated as possible remedies to these problems, providing accessible and prompt assistance. Consequently, the features and efficacy of AI chatbots created especially for medical professionals must be methodically assessed.[15]

4. PHARMACOVIGILANCE

To ensure drug safety and monitor adverse drug reactions (ADRs), pharmacovigilance is essential. Artificial intelligence (AI) increases productivity and accuracy in handling increasingly complicated data through automation and advanced analytics, while traditional approaches are slow and inconsistent.[16]

Finding possible causal links between a medication and an adverse occurrence that needs more research is known as signal detection. Adverse event reports that were submitted to pharmacovigilance databases were previously manually examined by regulatory bodies. Because it relied on people to complete the work, this procedure was slow, and mistakes were frequently made.[17]

Signal detection has been transformed by AI. Our ability to identify signals has significantly improved thanks to artificial intelligence. It finds hidden patterns in enormous volumes of data using machine learning algorithms.[17]

5. MARKETING SURVEILLANCE

Artificial intelligence (AI) greatly enhances post-market monitoring by increasing the ability to track, evaluate, and react to information about the efficacy and safety of products after they are put on the market.[18]

AI is redefining post-market surveillance by changing how we keep an eye on the efficacy and safety of products in the real world. By utilizing proactive monitoring, predictive analytics, and comprehensive data integration, AI improves public health protection. This gives stakeholders the ability to guarantee that goods live up to their promises while reducing risks to patients and customers.[18]

6. AI IN HOSPITAL

With models for surgical site infections and urinary tract infections often obtaining area-under-the-curve (AUC) ratings surpassing 0.80, suggesting good reliability, AI models showed high predictive accuracy for the detection, surveillance, and prevention of numerous HAIs. While both machine learning and deep learning techniques perform well, comparative data indicates that certain deep learning models may provide marginal benefits in complicated data situations. When combined with EHRs, sophisticated algorithms like random forests, decision trees, and neural networks greatly increased detection rates, allowing for rapid treatments and real-time monitoring. Non-real-time AI models using past EHR data shown significant scalability in resource-constrained environments, enabling wider adoption in infection detection and management.[19]

Maturity models can be applied in the healthcare industry to handle the complexity and wide range of requirements of healthcare systems. The public health system is under pressure because to poor workforce segregation, rising prices, and constrained healthcare budgets. The COVID-19 pandemic's effects on hospitals have demonstrated the differences in healthcare providers' readiness and the degree of quality management maturity needed to offer safe, efficient, patient-centred, timely, and equitable patient care. Aligning a quality improvement intervention with the unique requirements and features of the targeted health system is crucial to its efficacy.[20]

With its cutting-edge approaches to management, surveillance, and prevention, artificial intelligence is a game-changing weapon in the battle against hospital-acquired infections. The healthcare industry must prioritize strict validation requirements, thorough data quality reporting, and the use of interpretability tools to boost clinician confidence if it is to reach its full potential.[19]

7. APPLICATIONS

7.1 One Building confidence between patients and healthcare providers is facilitated by open communication regarding laboratory procedures, any delays, or problems with test results. Misunderstandings are decreased and expectations are managed with clear and honest communication. Numerous tactics have been put forth to help healthcare organizations build patient confidence.[21]

7.2 All team members will be competent in communicating the importance of laboratory tests if training and seminars on effective communication techniques are held for medical professionals and laboratory personnel. Interactive sessions and role-playing can improve learning.[21]

7.3 Particularly in remote or underdeveloped areas, telemedicine systems can help clinicians and laboratory professional's consult.[21]

7.4 By examining past data and seeing trends, AI can forecast how a disease will develop and how well a therapy would work. The long-term benefits of laboratory testing in treating chronic illnesses and enhancing patient outcomes can be illustrated using predictive analytics.[21]

8. CHALLENGES

1. Data Quality and Standardization

Diverse and high-quality datasets are necessary for AI systems to operate at their best. AI's capacity to produce precise insights and forecasts may be hampered by the absence of standardized data formats and the requirement for thorough data curation.[22]

2. Safety and Efficacy Concerns

Ensuring the safety and effectiveness of AI technologies in clinical trials is one of the biggest regulatory hurdles. Without adequate validation, AI-driven decision-making systems may provide dangers such as improper patient classification, misdiagnosis, and faulty medical recommendations.[23] Trial outcomes could be jeopardized, for example, if an AI system intended to select trial participants based on particular biomarkers unintentionally excludes eligible patients or includes ineligible ones. The need for strict preclinical and clinical validation procedures designed especially for AI technologies is highlighted by these safety issues.[22]

The "black box" issue, which refers to the lack of transparency in many AI systems, further complicates regulatory agencies' evaluation of these systems. An AI system's incapacity to properly explain how it arrives at its findings erodes confidence and raises moral questions regarding responsibility when mistakes are made.[22]

3. Health care challenges

Artificial Intelligence (AI) is revolutionizing the healthcare industry by providing previously unheard-of gains in patient care efficiency, tailored treatment, and diagnostic accuracy.[24]

However, in order to guarantee safe, moral, and efficient use, it is crucial to address AI's limitations and difficulties as it becomes more integrated into healthcare workflows. This chapter explores the various applications of AI in healthcare, stressing that it is a tool to support human decision-making and enhance patient outcomes rather than a substitute for human experts.[24]

The possibility of AI-driven mistakes, which, if left unchecked, could have a negative impact on patient outcomes, as well as the difficulties posed by the variety and calibre of medical data required to train AI models, are important issues. In order to avoid biases and guarantee dependability, we examine the necessity of strong data governance, with a focus on representative, high-quality datasets. The use of AI in healthcare also depends on ethical and legal considerations, such as protecting patient privacy, data security, informed permission, and strict validation requirements.[24]

4. Biological Complexity

AI methods might have trouble effectively capturing this complexity, which would restrict their ability to forecast safety and efficacy. A solid ground truth and access to pertinent data are essential for developing trustworthy AI models. For instance, Cannabis sativa presents difficulties for specialists in phytochemistry, synthetic chemistry, pharmacology, and artificial intelligence due to its pharmacologically complicated phytoconstituents. It is difficult to establish a definitive ground truth, which emphasizes how difficult it is to classify medications with distinct pharmacological effects and mechanisms of action. The constantly changing knowledge of human biology exacerbates this problem. Machine learning models will become more accurate and predictive as biological research advances.[25]

9. FUTURE SCOPE OF AI

9.1 Pharmacogenomic

The real era of precision pharmacotherapy will be ushered in by the fusion of pharmacogenomics, the study of the connection between genes and medication response, and artificial intelligence. Big Data can determine the appropriate medications and dose by identifying the unique characteristics of each patient based on genetic variations. AI, for example, can assist in the tailoring of cancer therapy interventions by scanning tumour profiles, identifying genetic characteristics of patients' cancer, and predicting the efficacy of certain chemotherapy.[26]

9.2 Disease Diagnosis and Prediction

Deep learning is also significantly advancing the diagnosis and prognosis of diseases, allowing for the earlier and more precise identification of a variety of ailments. DL algorithms can find small patterns in medical pictures, EHRs, and other clinical data that human clinicians might overlook, improving diagnosis precision and enabling more individualized treatment, Plans.[27]

9.3 Artificial Intelligence in Medical Research

The field of scientific study in healthcare could be transformed by future machine learning platforms. The capacity of AI-ML to quickly collect and analyse large data sets and find intricate patterns and correlations is one of its most significant effects. This will outperform current data discovery techniques, especially in subspecialties like population health, medical imaging, and genomics. In the field of genomics, AI-ML systems can analyse genetic read data to identify possible illness biomarkers, an important task for precision medicine and targeted treatment development. In addition to expanding molecular biomarker discoveries beyond genomics to encompass transcriptomics and epigenomics, AI-ML has found new biomarkers in radiomics and path omics.[28]

AI-related research must advance past proof-of-concept in order to successfully integrate AI into medical systems. Since most studies do not compare their interventions to human comparators or current standards of care, it is still difficult to predict how AI will be used into current systems. Other issues with AI include whether doctors and medical personnel would find it challenging to interact with AI-based products and whether inadequate technology literacy will lead to mistakes. In addition to evaluating costs, practicality, and integration, future research must include prospective controlled trials to ascertain genuine superiority.[29]

REFERENCE

1. Raza, Muhammad Ahmer, et al. "Artificial intelligence (AI) in pharmacy: an overview of innovations." innovations in pharmacy, 2022; 13.2: 10-24926.

2. Farghali, Hassan, Nikolina Kutinová Canová, and Mahak Arora. "The potential applications of artificial intelligence in drug discovery and development." Physiological Research, 2021; 70(4): S715.
3. Rammal, Dania Saad, Muaed Alomar, and Subish Palaian. "AI-Driven pharmacy practice: Unleashing the revolutionary potential in medication management, pharmacy workflow, and patient care." Pharmacy Practice, 2024; 22.2: 1-11.
4. Das, Sudipta, Rimi Dey, and Amit Kumar Nayak. "Artificial intelligence in pharmacy." Indian J Pharm Educ Res., 2021; 55.2: 304-318.
5. Jarab, Anan S., Shrouq R. Abu Heshmeh, and Ahmad Z. Al Meslamani. "Artificial intelligence (AI) in pharmacy: an overview of innovations." Journal of Medical Economics, 2023; 26.1: 1261-1265.
6. Kokudeva, Maria, et al. "Artificial intelligence as a tool in drug discovery and development." World Journal of Experimental Medicine, 2024; 14.3: 96042.
7. Ferreira, Fábio JN, and Agnaldo S. Carneiro. "AI-Driven Drug Discovery: A Comprehensive Review." ACS omega, 2025.
8. Chen, Wei, et al. "Artificial intelligence for drug discovery: Resources, methods, and applications." Molecular therapy Nucleic acids, 2023; 31: 691-702.
9. Stasevych, Maryna, and Viktor Zvarych. "Innovative robotic technologies and artificial intelligence in pharmacy and medicine: paving the way for the future of health care—a review." Big data and cognitive computing, 2023; 7.3: 147.
10. Foote, Henry P., et al. "Embracing Generative Artificial Intelligence in Clinical Research and Beyond: Opportunities, Challenges, and Solutions." JACC: Advances, 2025; 4.3: 101593.
11. Saini, Jaskaran Preet Singh, Ankita Thakur, and Deepak Yadav. "AI driven Innovations in Pharmaceuticals: Optimizing Drug Discovery and Industry Operations." RSC Pharmaceutics, 2025.
12. Shen, Jiayi, et al. "Artificial intelligence versus clinicians in disease diagnosis: systematic review." JMIR medical informatics, 2019; 7.3: e10010.
13. Reis, Zilma Silveira Nogueira, et al. "Artificial intelligence-based tools for patient support to enhance medication adherence: a focused review." Frontiers in Digital Health, 2025; 7: 1523070.
14. Huo, Bright, et al. "Large language models for chatbot health advice studies: a systematic review." JAMA Network Open, 2025; 8.2: e2457879-e2457879.

15. Baek G, Cha C, Han JH. AI Chatbots for Psychological Health for Health Professionals: Scoping Review. JMIR Hum Factors, Mar. 19, 2025; 12: e67682. doi: 10.2196/67682. PMID: 40106346; PMCID: PMC11939020.
16. Algarvio, Rogério Caixinha, et al. "Artificial intelligence in pharmacovigilance: a narrative review and practical experience with an expert-defined Bayesian network tool." International Journal of Clinical Pharmacy, 2025; 1-13.
17. Patil, Harshal G., and Vinit S. Khairnar. "Impact of AI on Pharmacovigilance: A Systematic Review." International Journal of Research in Pharmacy and Allied Science, 2025; 4.5: 26-35.
18. Khinvasara, Tushar, Nikolaos Tzenios, and Abhishek Shanker. "Post-market surveillance of medical devices using AI." Journal of Complementary and Alternative Medical Research, 2024; 25.7: 108-122.
19. El Arab, Rabie Adel, et al. "Artificial intelligence in hospital infection prevention: an integrative review." Frontiers in Public Health, 2025; 13: 1547450.
20. Aiwerioghene, Erhauyi Meshach, Janice Lewis, and David Rea. "Maturity models for hospital management: a literature review." International Journal of Healthcare Management, 2025; 18.4: 902-915.
21. Pillay, Tahir S. "Increasing the impact and value of laboratory medicine through effective and AI-assisted communication." EJIFCC, 2025; 36(1): 12.
22. Allam, Hesham. "Prescribing the future: The role of artificial intelligence in pharmacy." Information, 2025; 16.2: 131.
23. Lee, A.; Purcell, R.; Steele, S.J. Advancing an agile regulatory ecosystem to respond to the rapid development of innovative technologies. Clin. Transl. Sci., 2022; 15: 1332–1339.
24. Van Booven, Derek, Chen Cheng-Bang, and Manoharan Meenakshy. "Limitations of artificial intelligence in healthcare." Artificial intelligence in urologic malignancies. Academic Press, 2025; 231-246.
25. Gangwal, Amit, and Antonio Lavecchia. "Artificial intelligence in natural product drug discovery: current applications and future perspectives." Journal of medicinal chemistry, 2025; 68.4: 3948-3969.
26. Alanazi, Asma Nazal Jaloud, et al. "The use of artificial intelligence in clinical pharmacy: current applications and future prospects: a review article." International Journal of Medicine in Developing Countries, 2025; 8.12: 3827-3827.

27. Mulani, Altaf Osman, et al. "Transforming Drug Therapy with Deep Learning: The Future of Personalized Medicine." Drug Research, 2025; 75.08: 326-333.
28. Hanna, Matthew G., et al. "Future of artificial intelligence (AI)-machine learning (ML) trends in pathology and medicine." Modern Pathology, 2025; 100705.
29. Kirubarajan, Abirami, et al. "Artificial intelligence in emergency medicine: a scoping review." JACEP Open, 2020; 1.6: 1691-1702.