ISSN: 2457-0400

Impact Factor: 7.675

WORLD JOURNAL OF ADVANCE HEALTHCARE RESEARCH

www.wjahr.com

Volume: 10, Issue: 7

Page N. 19-23

Year: 2026

Review Article

Coden USA: WJAMA3

ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL SCIENCES: APPLICATIONS, METHODOLOGIES, AND FUTURE TRENDS IN DRUG DISCOVERY AND HEALTHCARE

Nidhi Chauhan[1]*, Parekh Prerna Jigneshbhai[2]*, Vijay Oza[3], Siddik Ugharatdar[4], Patel Bhavani[5], Patel Brijesh[6]

Department of Pharmacy, Laxminarayan Dev College of Pharmacy, Bholav, Bharuch - 392015.

Article Received: 01 June 2026 **Article Revised:** 22 June 2026 **Article Published:** 01 July 2026

***Corresponding Author: Dr. Nidhi Chauhan**

Department of Pharmacy, Laxminarayan Dev College of Pharmacy, Bholav, Bharuch - 392015.

DOI: https://doi.org/10.5281/zenodo.21021971

How to cite this Article: Dr. Channabasawa Reddy[1], Dr. Samina Bandalagi[2]*. (2026). Artificial Intelligence In Pharmaceutical Sciences: Applications, Methodologies, And Future Trends In Drug Discovery And Healthcare. World Journal of Advance Healthcare Research, 10(7), 19–23.

ABSTRACT

Artificial intelligence (AI) has emerged as a transformative technology in pharmaceutical sciences, enabling improvements in drug discovery, clinical trials, personalized medicine, and pharmaceutical manufacturing. The integration of machine learning (ML), deep learning (DL), natural language processing (NLP), and predictive analytics has accelerated research and development (R&D) processes while reducing operational costs and improving therapeutic outcomes. Recent advances in computational pharmaceutics, digital twins, and agent-based systems have further expanded the capabilities of AI in healthcare. This review article provides a comprehensive overview of AI methodologies, applications in pharmaceutical sciences, regulatory considerations, ethical challenges, and future trends. The manuscript aims to provide a structured and publication-ready review suitable for academic journals in pharmaceutical sciences.

KEYWORDS: Artificial Intelligence, Drug Discovery, Machine Learning, Deep Learning, Personalized Medicine, Clinical Trials, Pharmaceutical Manufacturing, Computational Pharmaceutics.

1. INTRODUCTION

Artificial intelligence (AI) refers to the simulation of human intelligence in machines programmed to think, learn, and make decisions. In recent years, AI has revolutionized the pharmaceutical industry by improving efficiency, accuracy, and speed in drug discovery, diagnostics, and patient care. The pharmaceutical sector faces increasing challenges such as high research costs, long drug development timelines, regulatory complexities, and the need for personalized therapies. AI technologies provide innovative solutions to address these challenges by analyzing large datasets, predicting drug behavior, and optimizing manufacturing processes.

The global pharmaceutical industry has witnessed significant growth in the adoption of AI-based technologies. Machine learning algorithms can identify patterns in biological data, predict drug-target interactions, and support clinical decision-making. AI-driven systems are also being used to design novel drug molecules, optimize dosage regimens, and monitor patient outcomes in real time. As a result, AI has become an essential component of modern pharmaceutical research and healthcare delivery.[1–3]

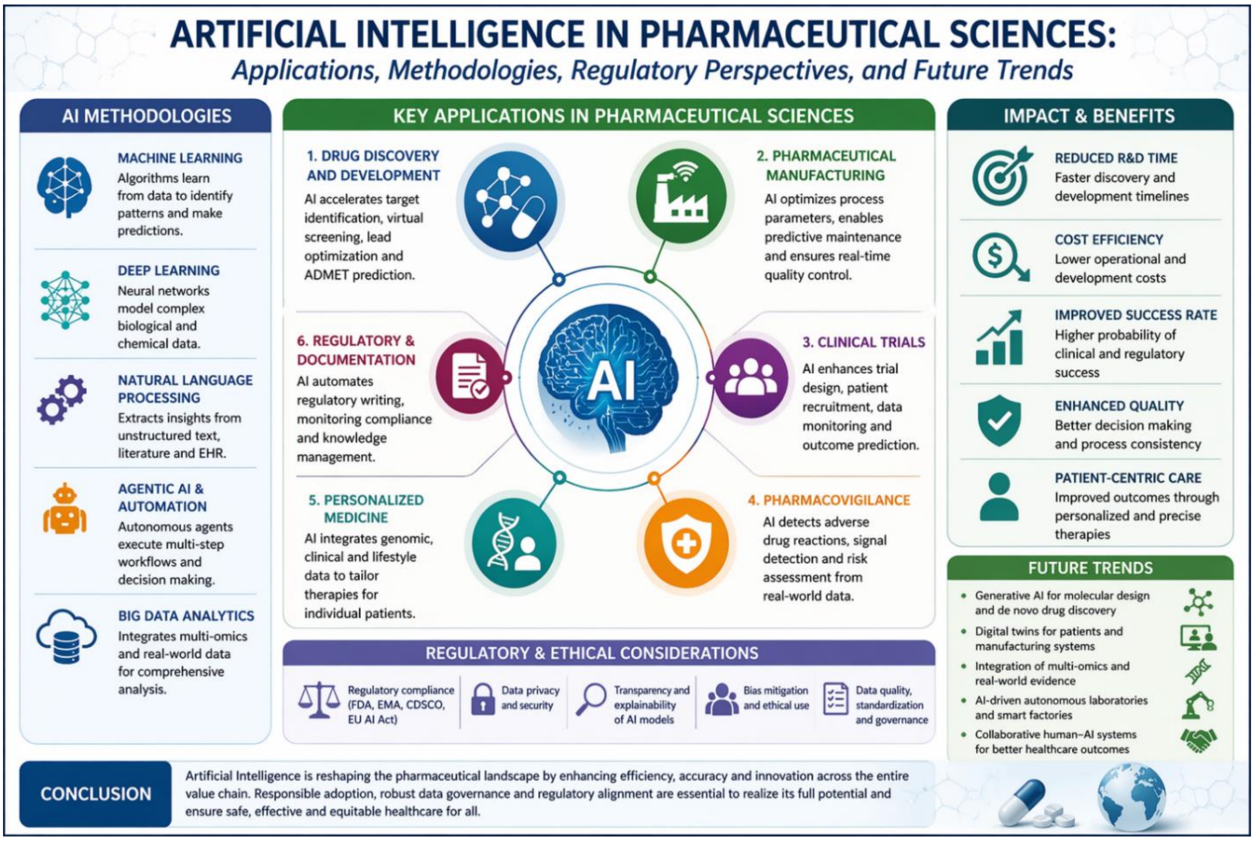

Fig. 1: Artificial Intelligence in Pharmaceutical Sciences.

2. Core Methodologies in Artificial Intelligence

2.1 Machine Learning (ML)

Machine learning is a subset of AI that enables computers to learn from data without explicit programming. ML algorithms analyze historical datasets to identify trends, make predictions, and support decision-making processes. Common ML techniques used in pharmaceutical sciences include supervised learning, unsupervised learning, and reinforcement learning. These techniques are widely applied in drug discovery, disease diagnosis, and patient monitoring.[4,5]

2.2 Deep Learning (DL)

Deep learning is an advanced form of machine learning that uses artificial neural networks with multiple layers to process complex data. DL models can analyze large volumes of biomedical data, including genomic sequences, medical images, and electronic health records. These models have demonstrated high accuracy in disease detection, drug toxicity prediction, and protein structure analysis.[6–8]

2.3 Natural Language Processing (NLP)

Natural language processing enables computers to understand and interpret human language. In pharmaceutical research, NLP is used to analyze scientific literature, extract clinical data, and automate regulatory documentation. NLP tools can process large volumes of medical records to identify relevant information and support clinical decision-making.[9]

2.4 Computer Vision

Computer vision involves the use of AI algorithms to interpret visual information from images and videos. In pharmaceutical manufacturing, computer vision systems are used for quality control, defect detection, and packaging inspection. These systems improve product quality and reduce human errors in manufacturing processes.[10]

2.5 Predictive Analytics

Predictive analytics uses statistical models and machine learning techniques to forecast future outcomes based on historical data. In healthcare, predictive analytics helps identify patients at risk of disease, predict treatment responses, and optimize clinical trial design.[11]

3. Applications of Artificial Intelligence in Pharmaceutical Sciences

3.1 Drug Discovery and Development

Drug discovery is a complex and time-consuming process that involves identifying potential drug candidates, evaluating their safety, and conducting clinical trials. AI technologies have significantly accelerated drug discovery by analyzing large datasets, predicting drug-target interactions, and optimizing molecular structures.

AI-based platforms can screen thousands of chemical compounds in a short period, reducing the time required for drug development. Machine learning algorithms can predict pharmacokinetic and pharmacodynamic properties, enabling researchers to identify promising drug candidates early in the development process.[12–14]

3.2 Clinical Trials and Patient Recruitment

Clinical trials are essential for evaluating the safety and efficacy of new drugs. However, patient recruitment and data management remain major challenges in clinical research. AI systems can analyze electronic health records to identify eligible patients, monitor trial progress, and detect adverse events.

AI-driven tools improve patient enrollment rates and reduce the time required to complete clinical trials. These technologies also enhance data accuracy and ensure compliance with regulatory requirements.[15–17]

3.3 Personalized Medicine

Personalized medicine involves tailoring medical treatments to individual patients based on their genetic profiles, lifestyle, and medical history. AI algorithms analyze genomic data to identify biomarkers associated with specific diseases and predict treatment responses.

Personalized medicine improves treatment outcomes and reduces the risk of adverse drug reactions. AI-powered decision support systems enable healthcare professionals to select the most effective therapies for individual patients.[18–20]

3.4 Pharmaceutical Manufacturing and Quality Control

Pharmaceutical manufacturing processes require strict quality control to ensure product safety and efficacy. AI technologies are used to monitor production processes, detect defects, and optimize manufacturing parameters.

Predictive maintenance systems analyze equipment performance data to identify potential failures before they occur. This approach reduces downtime, improves efficiency, and ensures consistent product quality.[21,22]

3.5 Drug Repurposing

Drug repurposing involves identifying new therapeutic uses for existing drugs. AI algorithms can analyze biological data to discover potential drug-disease relationships. This approach reduces development costs and accelerates the availability of new treatments for patients.[23]

4. Role of Artificial Intelligence in Healthcare and Diagnostics

AI technologies have significantly improved disease diagnosis and patient care. Machine learning models can analyze medical images to detect abnormalities such as tumors, fractures, and infections. These models provide accurate and timely diagnoses, enabling healthcare professionals to initiate appropriate treatments.

AI-powered wearable devices and remote monitoring systems allow continuous tracking of patient health parameters, including heart rate, blood pressure, and glucose levels. These technologies support preventive healthcare and reduce hospital admissions.[24–26]

5. Ethical and Regulatory Considerations

5.1 Data Privacy and Security

The use of AI in healthcare involves the collection and analysis of sensitive patient data. Ensuring data privacy and security is essential to maintain patient trust and comply with regulatory requirements. Healthcare organizations must implement robust cybersecurity measures to protect patient information.[27]

5.2 Bias and Transparency

AI algorithms may produce biased results if trained on incomplete or unrepresentative datasets. Researchers must ensure that training data are diverse and representative of different populations. Transparent algorithms improve trust and accountability in AI systems.[28]

5.3 Regulatory Frameworks

Regulatory agencies such as the Food and Drug Administration (FDA) and the European Medicines Agency (EMA) have developed guidelines for the use of AI in healthcare. These guidelines ensure the safety, effectiveness, and reliability of AI-based medical devices and pharmaceutical products.[29]

6. Challenges in Implementing Artificial Intelligence

Despite its advantages, the implementation of AI in pharmaceutical sciences faces several challenges:

1. **High Implementation Costs:** Developing and maintaining AI systems requires significant financial investment.
2. **Limited Data Availability:** Access to high-quality datasets is essential for training accurate AI models.
3. **Technical Expertise:** Skilled professionals are required to design, implement, and manage AI systems.
4. **Regulatory Compliance:** Compliance with regulatory standards can be complex and time-consuming.

   Addressing these challenges requires collaboration among researchers, healthcare providers, and regulatory authorities.[30–32]

7. Future Trends in Artificial Intelligence in Pharmaceutical Sciences

The future of AI in pharmaceutical sciences is promising, with several emerging trends expected to shape the industry:

7.1 Digital Twins in Healthcare

Digital twins are virtual models of patients or biological systems used to simulate disease progression and treatment outcomes. These models enable personalized treatment planning and improve clinical decision-making.

7.2 AI-Driven Drug Design

Advanced AI algorithms can design new drug molecules with specific therapeutic properties. These technologies are expected to reduce drug development timelines and improve success rates.

7.3 Integration with Internet of Medical Things (IoMT)

The integration of AI with IoMT devices enables real-time monitoring of patient health and supports remote healthcare services.

7.4 Automation in Pharmaceutical Manufacturing

Automation technologies powered by AI will improve production efficiency, reduce human errors, and enhance product quality.[33–35]

8. Summary Tables

Table 1: AI Tools and Platforms in 2026.

Tool/Platform	Primary Method	Function	Impact
AlphaFold-3	Deep Learning	Protein/Ligand interaction	Faster structure prediction
Boltz-2	Generative Models	Binding prediction	High-accuracy virtual screening
LIMS-Agents	Agentic AI	Workflow automation	Reduced manual labor in labs
Digital Twins	Predictive Modeling	Clinical trial controls	Reduced placebo arms

9. CONCLUSION

Artificial intelligence (AI) has emerged as a transformative technology in pharmaceutical sciences, significantly influencing drug discovery, clinical trials, personalized medicine, diagnostics, and pharmaceutical manufacturing. The integration of machine learning, deep learning, and predictive analytics has enabled faster identification of drug candidates, improved accuracy in disease diagnosis, and enhanced efficiency in healthcare delivery systems. AI-driven technologies have reduced development timelines, minimized operational costs, and improved patient outcomes by supporting evidence-based decision-making.

Despite these advancements, the successful implementation of AI in pharmaceutical sciences requires careful consideration of ethical, regulatory, and technical challenges. Issues such as data privacy, algorithm transparency, interoperability of healthcare systems, and the need for skilled professionals remain significant barriers. Regulatory agencies continue to develop guidelines to ensure the safety, reliability, and quality of AI-based healthcare technologies.

In conclusion, artificial intelligence is expected to remain a cornerstone of innovation in pharmaceutical sciences, enabling precision medicine, automated drug discovery, and intelligent healthcare systems. Continued collaboration among researchers, healthcare professionals, industry stakeholders, and regulatory authorities will be essential to fully realize the potential of AI in improving global healthcare outcomes.

Author Contributions

All authors contributed significantly to the conception, design, literature review, data interpretation, and preparation of the manuscript. All authors participated in drafting and revising the article critically for important intellectual content and approved the final version of the manuscript for publication.

ACKNOWLEDGEMENT

The authors express their sincere gratitude to the management and faculty of Laxminarayan Dev College of Pharmacy for providing the necessary facilities, guidance, and support to complete this review work successfully.

Funding

This research received no external funding. The work was carried out using the institutional facilities available at Laxminarayan Dev College of Pharmacy.

Conflict of Interest

The authors declare that there is no conflict of interest regarding the publication of this manuscript.

Ethical Approval

Not applicable. This article is a review based on previously published literature and does not involve any studies with human participants or animals.

10. REFERENCES

1. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. *Drug Discovery Today*, 2019; 24(3): 773–780.
2. Jiang F, Jiang Y, Zhi H, et al. Artificial intelligence in healthcare: past, present and future. *Stroke and Vascular Neurology*, 2017; 2(4): 230–243.
3. Topol EJ. High-performance medicine: the convergence of human and artificial intelligence. *Nature Medicine*, 2019; 25(1): 44–56.
4. Agatonovic-Kustrin S, Beresford R. Basic concepts of artificial neural network modeling. *Journal of Pharmaceutical and Biomedical Analysis*, 2000; 22(5): 717–727.
5. Vamathevan J, Clark D, Czodrowski P, et al. Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery*, 2019; 18(6): 463–477.

6. LeCun Y, Bengio Y, Hinton G. Deep learning. *Nature*, 2015; 521(7553): 436–444.
7. Zhavoronkov A, Ivanenkov YA, Aliper A, et al. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. *Nature Biotechnology*, 2019; 37(9): 1038–1040.
8. Bender A, Cortés-Ciriano I. Artificial intelligence in drug discovery: what is realistic, what are illusions? *Nature Reviews Drug Discovery*, 2021; 20(5): 353–354.
9. Wang Y, Wang L, Rastegar-Mojarad M, et al. Clinical information extraction applications: a literature review. *Journal of Biomedical Informatics*, 2018; 77: 34–49.
10. Kakani V, Nguyen VH, Kumar BP, et al. A critical review on computer vision and artificial intelligence in industry. *Journal of Agricultural and Food Research*, 2020; 2: 100033.
11. Deo RC. Machine learning in medicine. *Circulation*, 2015; 132(20): 1920–1930.
12. Mullard A. The drug discovery companies using AI. *Nature*, 2022; 602(7896): 19–20.
13. Paul D, Sanap G, Shenoy S, et al. Artificial intelligence in drug discovery and development. *Drug Discovery Today*, 2021; 26(1): 80–93.
14. Schneider G. Automating drug discovery. *Nature Reviews Drug Discovery*, 2018; 17(2): 97–113.
15. Harrer S, Shah P, Antony B, et al. Artificial intelligence for clinical trial design. *Trends in Pharmacological Sciences*, 2019; 40(8): 577–591.
16. Weng C, Szolovits P. Predictive modeling for clinical trial recruitment. *Journal of Biomedical Informatics*, 2017; 68: 1–8.
17. Chen H, Yang B, Pei H, et al. Data mining in healthcare. *Artificial Intelligence in Medicine*, 2016; 66: 1–14.
18. Ashley EA. The precision medicine initiative: a new national effort. *Nature*, 2016; 529(7584): 507–509.
19. Collins FS, Varmus H. A new initiative on precision medicine. *New England Journal of Medicine*, 2015; 372(9): 793–795.
20. Relling MV, Evans WE. Pharmacogenomics in clinical practice. *Nature*, 2015; 526(7573): 343–350.
21. Lee J, Bagheri B, Kao HA. A cyber-physical systems architecture for predictive manufacturing. *International Journal of Production Research*, 2018; 56(1–2): 1–18.
22. Qin SJ. Process analytics in pharmaceutical manufacturing. *Journal of Process Control*, 2014; 24(8): 1177–1186.
23. Pushpakom S, Iorio F, Eyers PA, et al. Drug repurposing: progress, challenges and recommendations. *Nature Reviews Drug Discovery*, 2019; 18(1): 41–58.
24. Esteva A, Kuprel B, Novoa RA, et al. Dermatologist-level classification of skin cancer with deep neural networks. *Nature*, 2017; 542(7639): 115–118.
25. Rajkomar A, Oren E, Chen K, et al. Scalable and accurate deep learning for healthcare. *NPJ Digital Medicine*, 2018; 1(1): 18.
26. Topol EJ. The patient will see you now: The future of medicine is in your hands. New York: Basic Books, 2015.
27. Roff HM. Advancing human security through artificial intelligence. London: Chatham House, 2017.
28. Obermeyer Z, Powers B, Vogeli C, et al. Dissecting racial bias in an algorithm used to manage population health. *Science*, 2019; 366(6464): 447–453.
29. U.S. Food and Drug Administration. Artificial Intelligence/Machine Learning regulatory framework for medical devices, 2023.
30. Davenport T, Kalakota R. The potential for artificial intelligence in healthcare. *Future Healthcare Journal*, 2019; 6(2): 94–98.
31. Yu KH, Beam AL, Kohane IS. Artificial intelligence in healthcare. *Nature Biomedical Engineering*, 2018; 2(10): 719–731.
32. Shortliffe EH, Sepulveda MJ. Clinical decision support in the era of artificial intelligence. *Journal of the American Medical Association*, 2018; 320(21): 2199–2200.
33. Bruynseels K, Santoni de Sio F, van den Hoven J. Digital twins in health care. *Nature Medicine*, 2018; 24(8): 1211–1214.
34. Mesko B. The role of artificial intelligence in precision medicine. *Journal of Medical Internet Research*, 2017; 19(11): e376.
35. Patel VL, Shortliffe EH, Stefanelli M, et al. The coming of age of artificial intelligence in medicine. *Journal of Biomedical Informatics*, 2009; 42(5): 760–763.