WJPMR, 2026, 12(7), 416-418

Review Article

Impact Factor: 7.533

WORLD JOURNAL OF PHARMACEUTICAL AND MEDICAL RESEARCH

www.wjpmr.com

ISSN (O): 2455-3301

ISSN (P): 3051-2557

Coden USA: WJPMBB

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY: A REVIEW

Prof. Shital K. Datir[1*], Kapil G. Jagtap[1], Aaditi S. Unavane[2], Madhuri K. Jore[3], Diksha V. Gangurde[4], Prema K. Tevar[5], Dhanashree D. Shinde[6]

[1*]Department of Pharmaceutics, NGSPM'S College of Pharmacy, Anjaneri, Trimbakeshwar, Nashik, Mharashtra, India
[1,2,3,4,5,6]B Pharmacy Student at NGSPM'S College of Pharmacy, Anjaneri, Trimbakeshwar, Nashik, Mharashtra, India.

***Corresponding Author: Prof. Shital K. Datir**

Department of Pharmaceutics, NGSPM'S College of Pharmacy, Anjaneri, Trimbakeshwar, Nashik, Mharashtra, India. **DOI:** https://doi.org/10.5281/zenodo.21154918

How to cite this Article: Prof. Shital K. Datir[1*], Kapil G. Jagtap[1], Aaditi S. Unavane[2], Madhuri K. Jore[3], Diksha V. Gangurde[4], Prema K. Tevar[5], Dhanashree D. Shinde[6] (2026). Artificial Intelligence In Drug Discovery: A Review. World Journal of Pharmaceutical and Medical Research, 12(7), 416–418.

Article Received on 05/06/2026 **Article Revised on 25/06/2026** **Article Published on 01/07/2026**

ABSTRACT

Artificial Intelligence (AI) has emerged as a transformative technology in pharmaceutical research and drug discovery. Traditional drug discovery is a lengthy, expensive, and complex process that often requires more than 10 years and billions of dollars to bring a new drug to market. AI techniques, including machine learning (ML), deep learning (DL), natural language processing (NLP), and neural networks, have significantly accelerated various stages of drug discovery. AI assists in target identification, lead optimization, virtual screening, drug repurposing, toxicity prediction, and clinical trial design. By analyzing large datasets rapidly and accurately, AI reduces research costs, shortens development timelines, and improves success rates. This review discusses the role of AI in modern drug discovery, its applications, advantages, limitations, and future prospects in pharmaceutical sciences.

KEYWORDS: Artificial Intelligence, Drug Discovery, Machine Learning, Deep Learning, Virtual Screening, Drug Developmen.

INTRODUCTION

Drug discovery is a complex, expensive, and time-consuming process that typically requires several years and substantial financial investment to bring a new therapeutic agent to market.[1,2] The high failure rate during drug development has encouraged researchers to explore advanced computational approaches for improving efficiency and success rates.[2]

Artificial Intelligence (AI) refers to the simulation of human intelligence by computer systems capable of learning, reasoning, and decision-making.[3] Recent advances in machine learning, deep learning, and big data analytics have transformed pharmaceutical research by enabling rapid analysis of large biological and chemical datasets.[4,5]

AI has emerged as a powerful tool for target identification, lead optimization, virtual screening, toxicity prediction, and clinical trial design, significantly accelerating drug discovery processes.[6]

History of AI in Drug Discovery

The application of computational methods in drug discovery began with computer-aided drug design approaches during the late twentieth century.[7] The development of machine learning algorithms and availability of large biological datasets further expanded the role of AI in pharmaceutical sciences.[8]

Deep learning and neural network technologies have recently enabled the prediction of molecular properties and biological activities with unprecedented accuracy.[9]

Types of Artificial Intelligence

✓ **Machine Learning (ML)**

Machine learning utilizes algorithms that learn patterns from historical data to make predictions regarding drug activity, toxicity, and pharmacokinetic behavior.[10]

✓ **Deep Learning (DL)**

Deep learning employs multilayer neural networks capable of processing large and complex datasets,

making it highly valuable in molecular modeling and drug design.[11]

✓ **Natural Language Processing (NLP)**
NLP enables extraction of valuable information from scientific literature, patents, clinical reports, and biomedical databases.[12]

Applications of AI in Drug Discovery

✓ **Target Identification**
AI can analyze genomic, proteomic, and transcriptomic data to identify disease-associated therapeutic targets more efficiently than conventional methods.[13]

✓ **Target Validation**
Machine learning algorithms assist in validating biological targets and predicting their therapeutic relevance.[13]

✓ **Virtual Screening**
AI-powered virtual screening rapidly evaluates millions of compounds to identify promising drug candidates, reducing both cost and development time.[14]

✓ **Lead Identification and Optimization**
Deep learning models predict molecular properties and optimize lead compounds for improved efficacy, safety, and pharmacokinetic performance.[14,15]

✓ **Drug Repurposing**
AI facilitates identification of new therapeutic applications for existing drugs by analyzing biological pathways and clinical datasets.[16]

✓ **ADMET Prediction**
Machine learning algorithms predict absorption, distribution, metabolism, excretion, and toxicity profiles during early drug development stages.[15]

✓ **Clinical Trial Optimization**
AI improves patient recruitment, trial monitoring, and outcome prediction, thereby increasing clinical trial success rates.[17]

✓ **Precision Medicine**
AI supports personalized treatment approaches by integrating genetic, molecular, and clinical information from individual patients.[17]

Advantages of AI in Drug Discovery

- ✓ Reduces drug discovery timelines.[18]
- ✓ Decreases research and development costs.[18]
- ✓ Improves prediction accuracy.[11]
- ✓ Accelerates lead identification.[14]
- ✓ Enhances drug repurposing opportunities.[16]
- ✓ Supports personalized medicine.[17]
- ✓ Facilitates rapid analysis of large datasets.[10]

Limitations and Challenges

- ✓ Despite its advantages, AI faces challenges including limited data quality, algorithm bias, model interpretability issues, regulatory concerns, and privacy considerations.[19]
- ✓ Additionally, successful implementation requires multidisciplinary expertise in pharmaceutical sciences, biology, computer science, and data analytics.[19]

Future Perspectives
Future developments are expected to focus on generative AI, autonomous laboratories, digital twins, and AI-assisted personalized therapeutics.[20] Integration of AI with genomics, proteomics, and real-world clinical data may revolutionize drug discovery and precision medicine in the coming years.[20]

CONCLUSION
Artificial Intelligence has transformed drug discovery by accelerating target identification, virtual screening, lead optimization, drug repurposing, and clinical development.[1,6] Although challenges remain regarding data quality, regulatory acceptance, and model transparency, AI has the potential to significantly reduce the cost and time associated with traditional drug development while improving therapeutic outcomes.[18,20]

REFERENCES

1. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G, et al. Applications of machine learning in drug discovery and development. Nature Reviews Drug Discovery, 2019; 18(6): 463–477.
2. Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. Drug Discovery Today, 2021; 26(1): 80–93.
3. Topol EJ. High-performance medicine: the convergence of human and artificial intelligence. Nature Medicine, 2019; 25(1): 44–56.
4. Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug Discovery Today, 2018; 23(6): 1241–1250.
5. Ekins S, Puhl AC, Zorn KM, Lane TR, Russo DP, Klein JJ, et al. Exploiting machine learning for end-to-end drug discovery and development. Nature Materials, 2019; 18(5): 435–441.
6. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Development Research, 2019; 80(7): 849–860.
7. Fleming N. How artificial intelligence is changing drug discovery. Nature, 2018; 557: S55–S57.
8. Chan HS, Shan H, Dahoun T, Vogel H, Yuan S. Advancing drug discovery via artificial intelligence. Trends in Pharmacological Sciences, 2019; 40(8): 592–604.
9. Schneider P, Walters WP, Plowright AT, Sieroka N, Listgarten J, Goodnow RA Jr, et al. Rethinking drug

design in the artificial intelligence era. Nature Reviews Drug Discovery, 2020; 19(5): 353–364.
10. Bender A, Cortés-Ciriano I. Artificial intelligence in drug discovery: what is realistic and what are the challenges? Drug Discovery Today, 2021; 26(2): 511–524.
11. Stokes JM, Yang K, Swanson K, Jin W, Cubillos-Ruiz A, Donghia NM, et al. A deep learning approach to antibiotic discovery. Cell, 2020; 180(4): 688–702.
12. Hessler G, Baringhaus KH. Artificial intelligence in drug design. Molecules, 2018; 23(10): 2520.
13. Zhavoronkov A, Aliper A, Zhebrak A, Zagribelnyy B, Terentiev V, Bezrukov DS, et al. Potential of artificial intelligence for drug discovery and development. Molecular Pharmaceutics, 2020; 17(1): 1–11.
14. Walters WP, Murcko MA. Assessing the impact of generative AI on medicinal chemistry. Nature Biotechnology, 2020; 38(2): 143–145.
15. Gupta R, Srivastava D, Sahu M, Tiwari S, Ambasta RK, Kumar P. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. Molecular Diversity, 2021; 25: 1315–1360.
16. Pushpakom S, Iorio F, Eyers PA, Escott KJ, Hopper S, Wells A, et al. Drug repurposing: progress, challenges and recommendations. Nature Reviews Drug Discovery, 2019; 18(1): 41–58.
17. Schork NJ. Artificial intelligence and personalized medicine. Current Opinion in Genetics & Development, 2019; 58–59: 11–16.
18. Van Norman GA. Drugs, devices, and artificial intelligence: opportunities and challenges. JACC: Basic to Translational Science, 2020; 5(4): 378–389.
19. Batool M, Ahmad B, Choi S. A structure-based drug discovery paradigm using artificial intelligence. Molecules, 2023; 28(3): 1126.
20. Walters WP, Barzilay R. Critical assessment of AI in drug discovery. Expert Opinion on Drug Discovery, 2021; 16(9): 937–947.