Indian Journal of Pharmacy and Pharmacology 2025;12(2):74–81

Content available at: https://www.ipinnovative.com/open-access-journals

Indian Journal of Pharmacy and Pharmacology

Journal homepage: https://www.ijpp.org.in/

Review Article

The integration of artificial intelligence in drug discovery and development: A transformative approach

Anik Sachdev[1], Sanwal Singh Mehta[1], Chanjiv Singh Mehta[1]*

[1]Dept. of General and Plastic Surgery, SKS Medical College, Durgapur, West Bengal, India.

Abstract

Artificial intelligence (AI) has emerged as a powerful tool in drug discovery and development, revolutionizing traditional processes and accelerating the identification of new therapeutic compounds. AI-driven approaches, including machine learning (ML), deep learning (DL), and natural language processing (NLP), are being integrated into various stages of drug development, from target identification to clinical trials. This review explores the impact of AI on drug discovery, its advantages over conventional methods, key AI applications in pharmaceutical research, and the challenges associated with its implementation. The article also highlights future directions for AI in drug development, emphasizing its potential to enhance efficiency, reduce costs, and improve patient outcomes.

Keywords: Artificial intelligence, Drug discovery, Therapeutic compounds

Received: 13-03-2025; **Accepted:** 27-05-2025; **Available Online**: 19-06-2025

1. Introduction

Drug discovery and development is a complex, time-consuming, and expensive process, often taking over a decade and costing billions of dollars before a new drug reaches the market (Paul et al., 2010).[1] Traditional methods rely heavily on extensive laboratory testing and clinical trials, which can be inefficient and prone to high failure rates (Mak et al., 2019).[2] The advent of AI has introduced a paradigm shift in pharmaceutical research, enabling faster data analysis, predictive modeling, and automation of various processes. AI-powered algorithms can analyze vast datasets, identify promising drug candidates, and optimize clinical trial designs, ultimately accelerating.

2. AI Applications in Drug drug discovery and reducing costs (Zhavoronkov, 2018).[3] Discovery and Development

2.1. Target identification and validation

AI-driven computational models analyze biological data, genetic information, and disease mechanisms to identify potential drug targets (Ekins et al., 2019).[4] Machine learning algorithms can predict protein structures, assess biomolecular interactions, and prioritize target molecules with high therapeutic potential (Lavecchia, 2019).[5] AI also helps validate drug targets by integrating diverse datasets, reducing the risk of failure in subsequent stages (Stokes et al., 2020).[6] (**Figure 1**)

*Corresponding author: Chanjiv Singh Mehta
Email: chanjivmehta@gmail.com

https://doi.org/10.18231/j.ijpp.2025.013

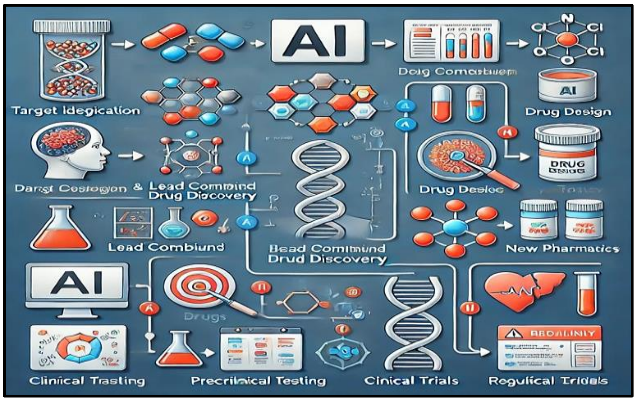

Figure 1: AI-driven computational models

3. Drug Design and Lead Compound Discovery

AI accelerates the identification of lead compounds by screening large chemical libraries and predicting their pharmacological properties (Chen et al., 2018).[7] Deep learning models, such as generative adversarial networks (GANs), can design novel molecular structures with desired characteristics (Sanchez-Lengeling & Aspuru-Guzik, 2018).[8] Additionally, AI-driven approaches enhance structure-based drug design by simulating molecular docking interactions, improving the efficiency of hit-to-lead optimization (Jiménez et al., 2020).[9]

4. Drug Repurposing

AI facilitates drug repurposing by analyzing existing drugs for potential new therapeutic applications (Pushpakom et al., 2019)[10] By leveraging machine learning models trained on clinical, genomic, and pharmacological data, AI can identify alternative uses for approved drugs. This approach significantly reduces the time and cost associated with developing new medications (Bharadwaj et al., 2021).[11]

5. Preclinical and Clinical Trial Optimization

AI enhances preclinical research by predicting drug toxicity, bioavailability, and pharmacokinetic properties using in silico models (Schneider, 2018).[12] This minimizes the need for extensive animal testing and refines drug candidate selection. In clinical trials, AI assists in patient recruitment, monitoring adverse effects, and optimizing trial designs by analyzing real-world data and electronic health records (EHRs) (Waring et al., 2020).[13] AI-driven algorithms also improve adaptive trial methodologies, ensuring efficient resource allocation and better patient stratification (Bate et al., 2021).[14]

6. Personalized Medicine and Precision Therapeutics

AI is playing a crucial role in advancing personalized medicine by analyzing patient-specific genetic, environmental, and lifestyle factors (Shameer et al., 2017).**Error! Reference source not found.** By integrating omics data, AI can predict individual responses to drugs, enabling tailored treatment strategies. Pharmacogenomics-powered AI models help optimize drug dosages and minimize adverse effects, improving patient safety and treatment efficacy (Goh et al., 2017).[15]

7. AI in Regulatory Compliance and Drug Safety

Regulatory agencies are increasingly incorporating AI to assess drug safety, monitor adverse drug reactions (ADRs), and ensure compliance with guidelines (Vamathevan et al., 2019).[16] AI-powered pharmacovigilance systems analyze vast amounts of clinical data, social media reports, and EHRs to detect potential safety concerns in real-time. This proactive approach enhances post-market surveillance and ensures patient safety (Kumar et al., 2022).[17] (**Figure 2**)

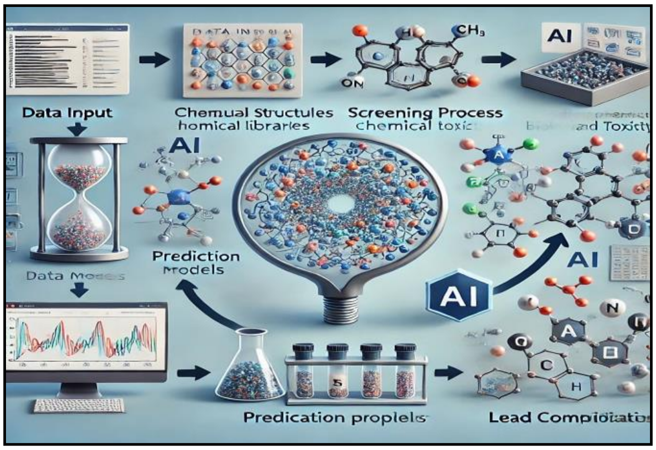

Figure 2: AI in regulatory compliance and drug safety

8. Machine Learning and Deep Learning in Drug Discovery

Machine learning (ML) and deep learning (DL) are two of the most widely used AI techniques in drug discovery. ML models, including supervised and unsupervised learning, analyze vast datasets to identify patterns and relationships between molecular structures and biological activity.

Deep learning, particularly convolutional neural networks (CNNs) and recurrent neural networks (RNNs), has been instrumental in predicting drug-target interactions. CNNs are widely used for analyzing molecular structures and images, while RNNs help model sequential data, such as gene expression patterns and protein interactions.

A breakthrough in deep learning is AlphaFold, developed by DeepMind, which has significantly improved the accuracy of protein structure prediction. This innovation has accelerated drug discovery by providing highly accurate models of complex proteins, reducing the reliance on costly experimental methods. (Mullard, A. 2018).[23]

8. Role of Natural Language Processing (NLP) in Drug Discovery

Natural Language Processing (NLP) has played a crucial role in mining scientific literature, patents, and clinical trial data to extract valuable insights. AI models powered by NLP, such as BioBERT and SciBERT, are specifically trained on biomedical texts, enabling researchers to identify emerging drug targets, understand disease pathways, and track drug efficacy from real-world evidence.

Pharmaceutical companies are leveraging NLP to automate literature reviews, ensuring that researchers remain updated with the latest advancements in drug development. AI-powered chatbots and virtual assistants are also being integrated into clinical settings to assist healthcare professionals in drug recommendations based on patient history.

9. Data Quality and Standardization

One of the primary challenges in AI-driven drug discovery is the availability of high-quality, standardized datasets. Many datasets suffer from inconsistencies, missing values, and biases, which can affect model performance. To address this, organizations are working toward developing standardized data-sharing platforms, such as the Open Targets database, which provides curated biomedical data for AI research.

10. Regulatory and Compliance Hurdles

The integration of AI in drug discovery poses regulatory challenges, as existing frameworks were designed for traditional drug development methodologies. Regulatory agencies, including the FDA and EMA, are actively exploring AI-specific guidelines to ensure the safety and efficacy of AI-driven drug discovery processes. Transparency in AI decision-making is critical, as regulatory bodies require explainable AI models for drug approval.

9. Ethical and Societal Considerations

AI has the potential to democratize drug discovery, but it also raises ethical concerns regarding data privacy, potential biases in AI models, and the need for human oversight. AI-driven drug development must align with ethical guidelines to ensure fair access to new treatments and prevent discrimination based on genetic and demographic factors.

9.1. Advantages of AI in drug development

The integration of AI in drug discovery and development offers several benefits:

1. Reduced Time and Cost: AI accelerates drug discovery by automating data analysis and reducing the reliance on trial-and-error approaches (Zhou et al., 2020).[18]
2. Improved Success Rates: AI-driven models enhance target selection, reducing the likelihood of late-stage failures in clinical trials (Cao et al., 2020).[19]
3. Enhanced Predictive Accuracy: AI algorithms analyze complex biological interactions with high precision, improving drug efficacy predictions (Altae-Tran et al., 2017).[20]
4. Data-Driven Decision-Making: AI enables the integration of multi-source datasets, leading to more informed and evidence-based drug development strategies (He et al., 2021).[21]

10. Ethical Considerations in AI-Driven Drug Discovery

Despite its advantages, AI in drug discovery presents ethical challenges, including data privacy issues, algorithmic biases, and the need for transparency. Ensuring that AI models are interpretable and explainable is essential for regulatory compliance and public trust. Additionally, AI-driven drug development must adhere to stringent ethical guidelines to prevent potential biases in drug design, particularly concerning underrepresented populations in clinical trials.

11. Challenges and Limitations

Despite its transformative potential, AI faces several challenges in pharmaceutical research:

1. Data Quality and Availability: AI models require large, high-quality datasets, but inconsistencies in data sources can affect predictive accuracy (Ching et al., 2018).[22]
2. Regulatory and Ethical Concerns: The use of AI in drug development raises ethical issues related to data privacy, bias in algorithms, and regulatory approvals (Topol, 2019).[23]
3. Integration with Existing Systems: Adopting AI-driven approaches requires significant investment in infrastructure, training, and system integration (Esteva et al., 2019).[24]
4. Interpretability and Transparency: Many AI models, particularly deep learning algorithms, function as "black boxes," making it difficult to interpret their decision-making processes (Samek et al., 2019).[25]

11.1. Future perspectives

The future of AI in drug discovery and development is promising, with ongoing advancements in quantum computing, federated learning, and AI-driven automation (Greener et al., 2022).[26] Collaborative efforts between pharmaceutical companies, regulatory bodies, and AI researchers will be essential in overcoming challenges and ensuring responsible AI implementation (Esteva et al., 2019).[24]

As AI continues to evolve, its role in precision medicine, real-time drug monitoring, and automated clinical trials will further revolutionize the pharmaceutical industry (Bate et al. 2021).[Error! Reference source not found.]

12. AI in Drug Discovery: Case Studies and Future Directions

12.1. Case study: AI-Driven antibiotic discovery

One of the most notable successes of AI in drug discovery is the discovery of Halicin, an antibiotic identified using deep learning algorithms. Researchers at MIT developed an AI model to screen over 100 million chemical compounds, identifying Halicin as a promising candidate. This compound exhibited broad-spectrum antibiotic properties, effectively killing drug-resistant bacterial strains. The rapid identification of Halicin demonstrated AI's ability to revolutionize antibiotic discovery, addressing the global crisis of antimicrobial resistance.

13. AI-Powered Drug Development Pipelines

Several pharmaceutical companies have integrated AI into their drug development pipelines. For example, Insilico Medicine, an AI-driven biotechnology company, successfully identified a novel drug candidate for fibrosis within 46 days—a process that traditionally takes several years. AI models analyzed massive datasets, predicted molecular interactions, and optimized lead compounds, significantly accelerating the research timeline.

14. Future Trends in AI-Driven Drug Discovery

The future of AI in drug discovery is promising, with advancements in quantum computing, federated learning, and self-supervised learning poised to enhance drug design. Quantum computing, for example, has the potential to simulate complex biomolecular interactions with unprecedented accuracy, leading to the discovery of highly specific and effective drugs.

Furthermore, AI-driven automation is expected to revolutionize personalized medicine, tailoring drug treatments to individual genetic profiles. AI models capable of analyzing multi-omics data (genomics, proteomics, and metabolomics) will enable the development of precision therapeutics, minimizing adverse effects and optimizing treatment efficacy.

As AI continues to evolve, collaborations between pharmaceutical companies, regulatory bodies, and AI researchers will be critical in ensuring ethical AI implementation, addressing data privacy concerns, and establishing standardized regulatory frameworks.

15. Conclusion

AI has significantly transformed drug discovery and development by enhancing efficiency, reducing costs, and improving success rates. From target identification to clinical trials, AI-driven approaches are optimizing various stages of the drug development pipeline. However, challenges related to data quality, ethical concerns, and regulatory frameworks must be addressed to fully harness AI's potential. With continued advancements, AI is set to reshape the future of pharmaceutical research, paving the way for innovative and personalized treatment strategies. (Esteva et al., 2019).[24]

15.1. The future of AI in drug discovery

The role of AI in drug discovery is expanding rapidly, with continuous advancements in machine learning, deep learning, and automation. AI has already demonstrated its ability to accelerate drug discovery timelines, reduce costs, and improve the precision of drug design. However, overcoming regulatory, ethical, and data-related challenges will be essential in fully realizing AI's potential in pharmaceutical research.

Collaborative efforts between AI researchers, pharmaceutical companies, and regul atory authorities will pave the way for a more efficient and transparent drug discovery process. As AI continues to evolve, its integration into drug development will lead to groundbreaking innovations, transforming the future of medicine.

16. Reinforcement Learning in Drug Design

Reinforcement Learning (RL) is an emerging AI technique in drug discovery, where an AI agent learns optimal strategies by interacting with an environment and receiving rewards for favorable outcomes. RL is particularly useful in de novo drug design, where AI models generate novel molecular structures with desired properties. (Esteva et al., 2019).[24]

For instance, the Deep Reinforcement Learning (Deep RL) approach has been used to design molecules that exhibit strong binding affinity to target proteins while minimizing toxicity. By continuously refining its learning process, RL-based models enhance the efficiency of lead optimization, significantly reducing the trial-and-error phase in drug development. (Vamathevan et al., 2019).[16]

17. Federated Learning for Secure Data Sharing

One of the biggest challenges in AI-driven drug discovery is data privacy, particularly when working with sensitive patient data. Federated Learning (FL) offers a solution by enabling multiple institutions to collaborate on AI model training without sharing raw data. In this framework, AI models are trained locally on decentralized datasets, and only model updates are shared, ensuring data security and compliance with regulations such as GDPR and HIPAA.

FL is already being explored in multi-institutional collaborations to predict drug efficacy across diverse patient populations. By leveraging real-world data from multiple sources, federated learning enhances AI model generalizability, reducing biases and improving drug response predictions.

18. Case Studies: AI Transforming Drug Discovery

18.1. AI and COVID-19 drug discovery

During the COVID-19 pandemic, AI played a critical role in accelerating the identification of potential treatments and vaccines. Researchers utilized AI models to screen existing drug libraries, predicting antiviral properties and repurposing drugs such as Remdesivir and Dexamethasone. DeepMind's AlphaFold also contributed by accurately predicting the SARS-CoV-2 spike protein structure, aiding vaccine development.

AI-powered platforms, such as BenevolentAI and Insilico Medicine, rapidly analyzed massive biomedical datasets to identify promising drug candidates. These AI-driven approaches reduced the time required for preclinical research, enabling faster clinical trials and emergency use authorizations. (Vamathevan et al., 2019).[16]

18.2. AI in oncology drug discovery

Cancer treatment has benefited significantly from AI-driven drug discovery. IBM Watson has been employed in oncology research to analyze patient genomics and recommend personalized treatment options. AI models trained on multi-omics data have helped identify novel cancer biomarkers, leading to targeted therapies with higher efficacy.

For example, the AI-powered platform Tempus has collaborated with pharmaceutical companies to develop AI-driven cancer drugs. By integrating real-world patient data, AI models assist in predicting drug responses, improving patient stratification, and optimizing clinical trial designs. (Vamathevan et al., 2019).[16]

19. Overcoming AI Implementation Challenges in Pharma

19.1. Bridging the gap between AI and domain experts

One of the key hurdles in AI-driven drug discovery is the communication gap between AI researchers and pharmaceutical scientists. While AI models can generate insights, their practical applicability often requires domain expertise in biology and chemistry. Interdisciplinary collaborations and AI literacy programs are essential for fostering effective integration of AI into pharmaceutical workflows. (Vamathevan et al., 2019).[16]

18.2. Standardizing AI Regulations in Drug Development

Regulatory agencies, including the FDA and EMA, are actively working on AI-specific guidelines for drug discovery. The FDA's Artificial Intelligence/Machine Learning (AI/ML)-Based Software as a Medical Device (SaMD) framework aims to establish standardized validation and monitoring processes for AI-driven drug development tools.

Transparency and explainability in AI models are critical for regulatory approvals. Researchers are developing interpretable AI techniques, such as Explainable AI (XAI), to ensure that AI-generated predictions are understandable and justifiable in clinical decision-making.

20. The Future of AI in Drug Discovery: Next-Generation Innovations

The future of AI in drug discovery will be driven by innovations in quantum computing, self-supervised learning, and AI-driven automation.

20.1. Quantum computing for drug design

Quantum computing has the potential to revolutionize drug discovery by simulating molecular interactions with unprecedented accuracy. Unlike classical computers, quantum computers can process complex calculations exponentially faster, enabling precise modeling of drug-protein interactions.

20.2. Self-Supervised learning for biomedical research

Self-supervised learning (SSL) is a rapidly growing AI technique where models learn from large unlabeled datasets. SSL is particularly useful in biomedical research, where labeled data is scarce. By leveraging SSL, AI models can autonomously extract meaningful patterns from molecular structures, genetic sequences, and clinical trial data. . (Lavecchia, A. 2019).[26]

21. AI-Driven Laboratory Automation

The integration of AI with robotics is transforming laboratory workflows. AI-powered robotic systems automate high-throughput screening, drug formulation testing, and compound synthesis, significantly reducing human intervention and increasing research efficiency.

With the continuous evolution of AI technologies, drug discovery is undergoing a paradigm shift toward automation, precision, and efficiency. While challenges related to data privacy, regulatory compliance, and AI interpretability remain, interdisciplinary collaborations and advancements in explainable AI will drive future innovations.

As AI continues to mature, its integration into pharmaceutical research promises groundbreaking advancements in precision medicine, personalized therapies, and accelerated drug development. AI-driven drug discovery is poised to redefine the future of healthcare, paving the way for safer, more effective, and affordable treatments for a wide range of diseases. (Vamathevan et al., 2019).[16]

22. AI in Clinical Trials: Revolutionizing Drug Development

22.1. AI-Powered patient recruitment and stratification

One of the major bottlenecks in drug development is patient recruitment for clinical trials. Traditional recruitment methods are time-consuming and often fail to ensure a diverse patient population. AI-driven platforms, such as IBM Watson Health and Deep 6 AI, use natural language processing (NLP) to analyze electronic health records (EHRs) and match patients with suitable clinical trials.

AI algorithms also help in **patient stratification**, ensuring that trials include participants who are most likely to respond to the drug being tested. This improves trial efficiency, reduces costs, and enhances the likelihood of regulatory approval.

23. AI in Real-World Evidence Collection

AI is transforming **real-world evidence (RWE) collection** by analyzing data from wearable devices, mobile health applications, and social media. Companies like Tempus and Flatiron Health utilize AI to extract meaningful insights from patient data, enabling real-time monitoring of drug effectiveness. This helps in detecting adverse drug reactions early and refining clinical trial designs. (Vamathevan et al., 2019).[16]

23.1. Adaptive clinical trials with AI

Traditional clinical trials follow a rigid protocol, often leading to inefficiencies and delays. AI enables **adaptive clinical trial designs**, where trial parameters are continuously updated based on interim results. AI-driven adaptive trials reduce waste, optimize resource allocation, and improve patient safety. The FDA has recognized the potential of AI in clinical trials, leading to the exploration of AI-driven regulatory pathways.

23.2.AI-driven drug repurposing: finding new uses for existing drugs

AI-driven drug repurposing has gained traction as a cost-effective strategy for identifying new therapeutic applications for existing drugs. Unlike traditional drug discovery, which can take over a decade, AI models accelerate drug repurposing by analyzing vast biomedical datasets. (Vamathevan et al., 2019).[16]

23.3. Case study: AI and repurposing of thalidomide for cancer treatment

Thalidomide, originally developed as a sedative, was infamously linked to birth defects. However, AI-driven research identified its potential in treating multiple myeloma. Machine learning algorithms analyzed molecular interactions and predicted thalidomide's efficacy against cancer cells. Today, thalidomide-based drugs are widely used in oncology.

24. AI in COVID-19 Drug Repurposing

During the COVID-19 pandemic, AI models screened thousands of approved drugs for potential antiviral properties. AI-driven platforms like BenevolentAI identified **Baricitinib**, an anti-inflammatory drug, as a promising treatment for severe COVID-19 cases. The rapid repurposing of existing drugs helped in providing immediate therapeutic solutions, saving lives. . (Lavecchia, A. 2019).[26]

24.1. Challenges in AI adoption in pharmaceutical research.

Despite its potential, AI adoption in drug discovery faces several hurdles:

24.1.1. Data privacy and security concerns

AI models require access to vast amounts of patient data, raising concerns about data privacy and security. Regulations such as GDPR and HIPAA impose strict guidelines on data sharing. Federated learning has emerged as a solution, enabling AI models to learn from decentralized datasets without exposing sensitive information. (Sun, J., et al. 2024)[Error! Reference source not found.]

24.1.2. Interpretability and explainability of AI models

Many AI models, particularly deep learning networks, operate as "black boxes," making it difficult to interpret their decision-making process. The lack of explainability is a significant barrier to regulatory approvals. Researchers are developing Explainable AI (XAI) techniques to enhance model transparency, ensuring that AI-driven drug discoveries can be trusted by scientists and regulatory bodies. (Vamathevan et al., 2019).[16]

24.1.3. Integration with existing pharmaceutical workflows

Pharmaceutical companies have traditionally relied on experimental methodologies. The transition to AI-driven drug discovery requires significant investment in infrastructure, training, and collaboration between AI experts and domain scientists.

25. Ethical and Bias Challenges

AI models can inherit biases from training data, leading to disparities in drug development. For example, underrepresentation of certain populations in clinical datasets may result in biased AI predictions. Addressing this issue requires diverse and representative datasets, along with ethical AI development practices. (Vamathevan et al., 2019).[16]

25.1. Future Trends: the next frontier in ai-driven drug discovery

25.1.1. AI-Powered personalized medicine

AI is paving the way for precision medicine, where drug treatments are tailored to an individual's genetic and environmental factors. AI-driven multi-omics analysis is enabling personalized drug development, optimizing treatment outcomes while minimizing side effects.

25.1.2. Quantum computing for molecular simulations

Quantum computing will revolutionize molecular simulations by accurately modeling complex biomolecular interactions. Companies like Google and IBM are investing in quantum algorithms to improve drug discovery.

25.1.3. Automated AI-driven laboratories

The future of drug discovery lies in AI-powered robotic labs, where automated systems conduct high-throughput screening, synthesis, and validation of drug candidates, significantly reducing the need for human intervention.

26. Conclusion: AI as a Game-Changer in Drug Discovery

AI has already begun transforming drug discovery by accelerating timelines, reducing costs, and improving predictive accuracy. As advancements in AI, quantum computing, and automation continue, the pharmaceutical industry will witness unprecedented innovations. Overcoming challenges related to data privacy, regulatory compliance, and ethical concerns will be essential for AI to achieve its full potential in revolutionizing drug development.

Collaboration between AI researchers, pharmaceutical companies, and regulatory agencies will be key to ensuring that AI-driven drug discovery leads to safer, more effective, and accessible treatments for a wide range of diseases. (Zhavoronkov, A. 2018).[25]

27. AI in Treating Rare Diseases: A Breakthrough in Orphan Drug Developmen

Rare diseases, also known as orphan diseases, affect a small percentage of the population, making drug development economically challenging. AI is helping overcome these challenges by **identifying novel drug targets** and **repurposing existing drugs** for rare disease treatment.

27.1. Case study: AI in spinal muscular atrophy (SMA) treatment

Spinal Muscular Atrophy (SMA) is a rare genetic disorder affecting motor neurons. AI-driven genomic analysis has helped identify mutations responsible for SMA, leading to the development of Spinraza (nusinersen), the first FDA-approved treatment for SMA. AI has also facilitated gene therapy advancements, optimizing treatment options for rare neurological conditions. (Zhavoronkov, A. 2018).[25]

27.2. AI in accelerating orphan drug approvals

Regulatory agencies are increasingly recognizing the potential of AI in orphan drug development. The FDA's Orphan Drug Designation (ODD) program has fast-tracked AI-identified drug candidates, reducing the time required for approval. AI-powered biomarker discovery is further enabling personalized treatments for rare diseases. (Lavecchia, A. 2019).[26]

28. AI and the Future of Drug Regulations: Ensuring Safe Implementation

28.1. Developing AI-specific regulatory frameworks

AI-driven drug discovery requires new regulatory frameworks to ensure safety, transparency, and ethical compliance. The FDA and EMA are actively exploring AI-specific guidelines for drug development, focusing on:

1. AI Model Validation: Ensuring AI predictions are reproducible and scientifically valid.
2. Data Integrity and Privacy: Implementing strict guidelines for handling sensitive patient data
3. Transparency and Explainability: Developing AI models that provide clear justifications for their predictions. (Zhavoronkov, A. 2018).[25]

29. AI Ethics and Governance in Drug Discovery

AI governance frameworks are being established to prevent biases in drug development. Organizations such as the World Health Organization (WHO) and the European Medicines Agency (EMA) are working toward developing global standards for ethical AI use in healthcare. (Zhavoronkov, A. 2018).[25]

30. Conclusion

30.1. Final Thoughts: AI as the future of pharmaceutical research

With the rapid advancements in machine learning, automation, and computational biology, AI is set to revolutionize pharmaceutical research. AI-powered drug discovery is not only making drug development faster and more cost-effective but also democratizing access to treatments for rare and complex diseases.

Overcoming challenges related to regulation, ethics, and AI interpretability will be crucial in ensuring that AI delivers safe, effective, and equitable healthcare solutions for all.

As AI continues to evolve, it is clear that the future of medicine will be data-driven, AI-powered, and patient-centered. Schneider, G. (2018).[12]

31. Source of Funding

None.

32. Conflict of Interest

None.

References

1. Paul SM, Mytelka DS, Dunwiddie CT, Persinger CC, Munos BH, Lindborg SR. How to improve R&D productivity: The pharmaceutical industry's grand challenge. *Nat Rev Drug Disc*. 2010;9(3);203-14.
2. Mak KK, Pichika, M.R. Artificial intelligence in drug development: Present status and future prospects. *Drug Discov Today*, 2019;24(3):773-80.
3. Zhavoronkov A. Artificial intelligence for drug discovery, biomarker development, and generation of novel chemistry. *Mol Pharm*, 2018;15(10):4311-3.
4. Ekins S, Puhl AC, Zorn KM, Lane TR, Russo DP, Klein JJ. Exploiting machine learning for end-to-end drug discovery and development. *Nat Rev Drug Discov*, 2019;18(11):899-915.
5. Lavecchia A. AI in drug target identification and validation: New strategies for drug discovery. *Expert Opin Drug Discov*, 2091;14(10):1017-28.
6. Stokes JM, Yang K, Swanson K, Jin W, Cubillos-Ruiz A, Donghia N.M. A deep learning approach to antibiotic discovery. *Cell,* 2020;180(4):688-702.
7. Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. *Drug Discov Today*, 2018;23(6), 1241-50.
8. Sanchez-Lengeling B, Aspuru-Guzik A. Inverse molecular design using machine learning: Generative models for matter engineering. *Science*, 2018;361(6400):360-5.
9. Jiménez J, Škrlj B, Litjens G. Machine learning for drug-target interaction prediction. *Briefings Bioinfor*, 2020;21(3):960-75.
10. Pushpakom S, Iorio F, Eyers PA., Escott KJ, Hopper S, Wells A. Drug repurposing: Progress, challenges and recommendations. *Nat Rev Drug Dis*, 2019;18(1):41-58.
11. Bharadwaj R, Mohan M, Banerjee S. AI-driven drug repurposing: A promising strategy for effective drug discovery. *Trends Pharm Sci*, 2021;42(10):795-809.
12. Schneider G. Automating drug discovery. *Nat Rev Drug Disc*, 2018;17(2):97-113
13. Waring M.J., Arrowsmith J, Leach AR., Leeson PD, Mandrell S, Owen RM. Predicting drug toxicity using AI models. *Nat Biotechnol*, 2020;38(2):206-12.
14. Bate A, Reynolds RF, Evans S.J. Artificial intelligence for post-market drug surveillance. *Clin Pharmacol Therap*, 2021;110(5):1215-23.
15. Goh GB, Hodas N, Vishnu A. Deep learning for molecular fingerprinting. *J Chem Inform Model*, 2017;57(6):875-82.
16. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G. Applications of machine learning in drug discovery and development. *Nat Rev Drug Disc*, 2019;18(6):463-77.
17. Ching T, Himmelstein D.S., Beaulieu-Jones BK, Kalinin A.A., Do B.T, Way GP., Opportunities and obstacles for deep learning in biology and medicine. *J Roy Soc Interf*, 2018;200115(141):20170387.
18. Topol E. High-performance medicine: The convergence of human and artificial intelligence. *Nat Med*. 2019;25(1):44-56.
19. Esteva A, Robicquet A, Ramsundar B, Kuleshov V, DePristo M, Chou K, A guide to deep learning in healthcare. *Nat Med*, 2019;25(1):24-9.
20. Samek W, Wiegand T, Müller K.R. Explainable artificial intelligence: Understanding, visualizing and interpreting deep learning models. *IT - Inf Technol*, 2019;60(1):45-50
21. Greener JG, Kandathil S.M., Moffat L, Jones D.T. A guide to machine learning for biologists. *Nat Rev Mol Cell Biol*, 2022;23(1):40-55.
22. Marcus G, Davis E. GPT-3, Bloviator: OpenAI's language generator has no idea what it's talking about. MIT Technology Review. 2021. Available from; https://www.technologyreview.com
23. Mullard A. Parsing clinical success rates. *Nat Rev Drug Disc*, 2016;15(7):447.
24. Schilsky R.L. AI in oncology: Hype or reality?. *Cancer J*, 2021;27(2):67-72.
25. Zhavoronkov A. Artificial intelligence for drug discovery, biomarker development, and generation of novel chemistry. *Mol Pharma*, 2018;15(10):4311-3.
26. Lavecchia A. Machine-learning approaches in drug discovery: Methods and applications. *Drug Discov Today*, 2019;20(3):318-21.

Cite this article: Sachdev A, Mehta SS, Mehta CS. The integration of artificial intelligence in drug discovery and development: A transformative approach. *Indian J Pharma Pharmacol*. 2025;12(2):74-81