A Brief Review on Artificial Intelligence in Drug Discovery

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Abstract: Artificial intelligence (AI) has revolutionized drug discovery and development by accelerating timelines, reducing costs, and increasing success rates. AI leverages machine learning (ML), deep learning (DL), and natural language processing (NLP) to analyze vast datasets, enabling the rapid identification of drug targets, prediction of compound efficacy, and optimization of drug design. It accelerates lead discovery by predicting pharmacokinetics, toxicity, and potential side effects while also refining clinical trial designs through improved patient recruitment and data analysis. 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.

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) Discovering a drug is a complex and expensive endeavor, with a high rate of failure. Developing a new drug typically costs over $2.5 billion on average and can take more than a decade to complete [1]. Additionally, only a small fraction of drug candidates that enter clinical trials ultimately receive regulatory approval [2]. Despite the efforts, only

2.01% of drug development projects ultimately result in a successful marketable drug [3]. These challenges highlight the urgent need for innovative approaches to accelerate and improve the success rates of drug discovery [2]

Traditional methods rely heavily on extensive laboratory testing and clinical trials, which can be inefficient and prone to high failure rates (Make et al., 2019). The advent of AI has introduced a paradigm shift in pharmaceutical research, enabling faster data analysis, predictive modelling, and automation of various processes. AI-powered algorithms can analyse vast datasets, identify promising drug candidates, and optimize clinical trial [3].

AI also has a more general role in the management and analysis of big data [3]. Big data is a recent paradigm describing the acquisition of extremely large datasets and their coupling with sophisticated analytics enabling new knowledge or insights into these data. In the pharmaceutical industry, traditional data storage methods are thus becoming obsolete as the amount of data increases. Big data provides a huge opportunity for more in-depth research as a result of data min-ing in this industry, and may augment pharmaceutical manufacturing, using a three-step data management process following acquisition in-volving the following steps: extraction and collation of big chunk of scattered and heterogeneous data; data configuration to ensure uniformformatting; and finally data analysis using various analytical platformsto yield a final output, the interpretation of which may inform decisions on which compounds or medicines to develop or which processes to use to maximise efficiency AI-enabled technology is actively being adopted to tackle minor[3]

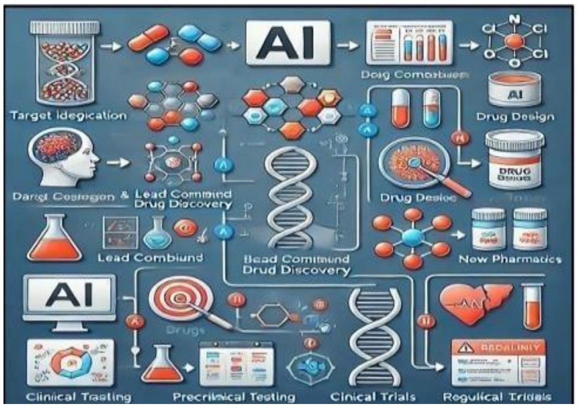


Figure 1: AI-driven computational models

1. AI in drug discovery

AI-driven computational models analyze biological data, genetic information, and disease mechanisms to identify potential drug targets (Ekins et al., 2019).[1] Machine learning algorithms can predict protein structures, assess biomolecular interactions, and prioritize target molecules with high therapeutic potential (Lavecchia, 2019). AI also helps validate drug targets by integrating diverse datasets, reducing.[1]

2. Future Directions and Innovations.

Deep learning is advanced machine learning that could be applied in the field of drug discovery. It is a neural network that can extract information from public databases and create scientific conclusions based on them. Deep learning is applicable to reduce the costs of the clinical trials by predicting their outcome before they start. Another promising application of AI in the field of drug discovery is drug repurposing. Finding new applications for already existing drugs reduces the time and cost of their development Another new trend in the field of drug discovery and development is AI application in nanotechnologies, especially nanocarriers. AI is also crucial in smart drug release systems that deliver the medicine when it is needed [3]

3. Fundamentals of Artificial Intelligence

Artificial intelligence (AI) accounts for several calculation technologies and simulates cognitive functions in the human mind. Machine learning (ML), deep learning (DL), and natural language processing (NLP) are three different types of AI devices. The ability to process and analyze raw data separates AI systems like machine learning, natural language processing, and deep learning. Some AI techniques, such as predictive modeling and data analysis, can process vast quantities of data before planning an appropriate approach. A definition of AI is offered by one individual. Artificial intelligence is an algorithm or device involving computational intelligence with a capacity to execute complex functions. [4]

4. Integration Of Ai Into Mainstream Drug Discovery

The use of AI in mainstream drug research signifies a watershed moment set to transform the pharmaceutical business. Adoption strategies and industry readiness are critical components of this transformation, which need strong frameworks for AI adoption and organizational readiness AI can play a role in a range of research and development activities within the discovery-to-market pipeline. While the hurdles of drug development are well documented, this section aims to provide readers with an understanding of a few potential application areas in which AI could be employed to support inefficiencies in terms of research and process. AI can make it much easier to search for potential drug targets. [4]There are a number of subfields focused on optimizing virtual screening and compound design, based on the myriad of chemical compounds to which a given protein target may be able to bind It's already possible to point to specific case studies where AI engines have been employed successfully within pharmaceutical development to deliver new molecules to clinical trials or to market in a faster time than traditional approaches..(5)

5. Challenges and Future Directions

Drug discovery and development is a complex, lengthy, and expensive process, requiring the nurturing and integration of a multitude of scientific disciplines. In this review, we have presented multiple areas in which, in recent years, AI and machine learning in particular have impacted the progression of drug discovery and development and helped in accelerating the progression of novel drugs to the clinic. These areas span from early pre-clinical drug discovery stages such as virtual screening, QSAR, and de novo drug design, to large-scale phenotypic drugs in complex biological contexts. [7]

6.Challenges and limitations.

Despite the promising advancements and successful applications of AI in ophthalmologic drug discovery, several challenges and limitations remain that require acknowledgment and resolution. First and foremost, the quality and quantity of data available for AI models significantly influence their performance and reliability.In the realm of ophthalmology, highquality, diverse, and annotated datasets, especially from clinical settings, are often scarce or fragmented. This limitation can lead to biases in AI models, reducing their generalizability and accuracy when applied to broader, more diverse populations. Furthermore, the computational resources required for AI research are substantial. The processing of large datasets and the training of sophisticated models necessitate advanced hardware and significant computational power, which can be a barrier for institutions with limited resources. This technological and financial barrier may lead to disparities in research advancements and the adoption of AI technologies across different regions and institutions. Moreover, AI is set to play a crucial role in overcoming the challenges associated with the clinical trial phase of drug development. [7]

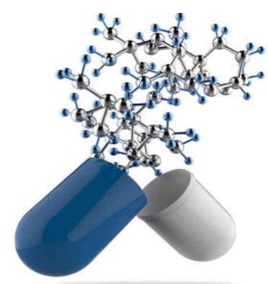
7. AI in Clinical Trial Design

Clinical trials are directed toward establishing the safety and efficacy of a drug product in humans for a particular disease condition and require 6–7 years along with a substantial financial investment. However, only one out of ten molecules entering these trials gain successful clearance, which is a massive loss for the industry These failures can result from inappropriate patient selection, short-age of technical requirements, and poor infrastructure. However,with the vast digital medical data available, these failures can be reduced with the implementation of AI The enrolment of patients takes one-third of the clinical trial.[10]

8. Drug Design

After the identification of a suitable target, AI algorithms can be applied in drug design by predicting the molecular structures and properties of potential drug candidates. By analyzing a vast biological dataset, machine learning models can identify druggable targets and design molecules with the ability to interact with the targets possessing the desired pharmacological properties. In silico Medicine is a biotechnological company that has developed a novel drug candidate for idiopathic pulmonary fibrosis in just 18 months using an in-house AI algorithm after screening billions of molecules and identifying promising candidate that moved on into preclinical trials[11].

Figure 2: AI-driven computational models



9. AI In Drug Formulation

Pharmaceutical sciences have seen various formulations, for example solid dispersions, extrudates, pellets, nanoparticles, and liposomes, arise in addition to standard dosage forms. The name "formulation techniques" is given to these techniques because they empower the development of formulations or incorporate functionality into common dosage forms such as tablets. AI applications in formulation techniques are even more worthwhile to investigate in order to create next-generation drug products with desired efficacy and health outcomes because these methods can successfully address a variety of API issues, such as low solubility, stability, bioavailability, and production capability [12]

10.Drug Repurposing:

One notable application of AI in drug development involves the analysis of extensive biomedical data to identify approved drugs that exhibit therapeutic potential for different diseases. Through this process of repurposing, AI expedites the drug discovery process and contributes to cos reduction. [13]AI facilitates drug repurposing by analyzing existing drugs for potential new therapeutic applications (Pushpakom et al.,2019)[1]By leveraging machine learning models trained on clinical, genomic, and pharmacological data, AI can identify alternative uses for approved drugs. [13]

11.AI In Diagnosis And Targeted Genomic Treatments

There are several applications of AI in hospital-based health care systems [19, 20] in organizing dosage forms for individualized patients and selecting suitable or available administration routes or treatment policies. [16]Maintaining of medical records: Maintenance of the medical records of patients is a complicated task. The collection, storage normalizing, and tracing of data are made easy by implementing the AI system. Google Deep Mind health project (developed by Google) assists to excavate the medical records in a short period. Hence, this project is a useful one for better and faster health care. The Moor fields Eye hospital NHS is assisted by this project for the improvement of eye treatment. [16]

12. AI-powered drug delivery optimization: Modern and mRNA vaccines

Background: Modern, a biotechnology company known for its ability to produce a COVID-19 mRNA vaccine, has lever-aged AI and ML to optimize the delivery of mRNA-based therapies. The delivery of mRNA, a delicate and unstable molecule, requires sophisticated delivery systems to ensure that it reaches target cells effectively Case Study: Modern used AI and ML to optimize lipid nanoparticles that deliver mRNA into cells. [20]

13. AI Ethics and Governance in Drug Discovery

AIgovernance 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. (Zamorano, A 2028)[1]

14. 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.[1]

15.Machine learning in drug discovery

The use of machine learning is increasing in various avenues of the pharmaceutical industry, including drug discovery, enabling improve-ments in the industry as a whole. The achievements of machine learning are demonstrated by the expanding number of companies in which ML is key to their business structure. [3]

CONCLUSION

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-centred. Schneider, G. (2018)(Page 1) AI is reshaping the landscape of drug discovery and development, providing significant improvements in efficiency, cost reduction, and speed. From early target identification to clinical trial optimization, AI offers numerous benefits that can overcome the traditional bottlenecks of drug development. While AI has already demonstrated success in various stages of the drug pipeline, its broader adoption faces challenges related to data quality, integration of biological knowledge, and regulatory approval. Moving forward, interdisciplinary collaboration between AI experts, biologists, and regulatory bodies will be essential to fully harness the transformative power of AI and ensure its seamless incorporation into the pharmaceutical industry[4]

REFERENCES

[1] Anik Sachdev, Sanwal Singh Mehta1, Chanjiv Singh Mehta1, The integration of artificial intelligence in drug discovery and development: A Transformative approach Dept. of General and Plastic Surgery, SKS Medical College, Durgapur, West Bengal, India, Indian Journal of Pharmacy and Pharmacology 2025.

[2] Shashi Kant, Deepika Saheli Roy, Artificial intelligence in drug discovery and development transforming challenges into opportunities, Pharmaceutical Sciences, February 2025

[3] Veer Patel, Manan Shah, Artificial intelligence and machine learning in drug discovery and development., Ahmedabad International School, Ahmedabad, Gujarat, India 2 Department of Chemical Engineering, School of Technology, Pandit Dindayal Energy University, Gandhinagar, Gujarat, India Intelligent Medicine.2024

[4] Namukasa Mulgrew F. The Impact of AI on Drug Discovery and Development Faculty of Medicine Kampala International University Uganda, EURASIAN EXPERIMENT JOURNAL OF PUBLIC HEALTH (EEJPH)September 2024 https://www.eejournals.org2024.

[5] Maria Kokudeva, Mincho Vichev, Emilia Naseva, Dimitrina Georgieva Miteva, Tsvetelina Velikova, Artificial intelligence as a tool in drug discovery and development Maria Kokudeva, Department of Pharmacology and Toxicology, Faculty of Pharmacy, Medical University of Sofia, Sofia 1000, BulgariaWorld Journal of W J E M Experimental Medicine WJEM https://www.wjgnet.com,years2024.

[6] Siddharth Gandhi1 and Michael Balas2, Artificial intelligence for ophthalmic drug Discovery and development: Publish ,2024.

[7] Amal Abdulrahim Abdullah Althubiti,*Artificial Intelligence in Drug Discovery And, American Journal of Biomedical Science & Research, November 16 2023.

[8] Kanagala Anusha1*, Konduru Sai Mala Jasmitha1, Korapu Sattibabu2, Gowtham Reddy INTEGRATING OF ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT: A COMPARATIVE STUDY1Koneru Lakshmaiah Business School, KLEF, Guntur, India. PharmacophoreJun 2023.

[9] Alberto Ocana1,2*, Atanasio Pandiella3, Cristian Privat4, Iván Bravo5, Miguel LuengoOroz6, Eitan Amir7And Balazs Gyorffy8,9,10Integrating artificial intelligence in drug Discovery and early drug development: A transformative Biomarker Research,2025.

[10] Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia and Rakesh K. Tekade, Artificial intelligence in drug Discovery and development National Institute of Pharmaceutical Education and Research-Ahmedabad (NIPER-A), An Institute of National Importance, Government of India, Department of Pharmaceuticals, Ministry of Chemicals and Fertilizers, Palaj, Opp. Air Force Station, Gandhinagar, 382355, Gujarat, India KEYNOTE REVIE January 2021.

[11] Dolores R. Serrano 1,2*, Francis C. Luciano 1, Brayan J. Anaya 1, Baris Ongoren 1, Aytug Kara 1, Gracia Molina 1, Bianca I. Ramirez 1, Sergio A. Sánchez-Guirales 1, Jesus A. Simon 1, August 2024.

[12] Kazi Asraf Ali1*, SK Mohin1, Puja Mondal1, Susmita Goswami1, Soumya Ghosh1 and Sabyasachi Choudhuri1Influence of artificial intelligence in modern pharmaceutical formulation and drug development Future Journal of Pharmaceutical Sciences2024.

[13] Dr. Chinmoyee Deori1, Dr. Leena Hujuri2, Dr Gayatri Sarma3, Dr. Tonushyam Sonowa

Artificial Intelligence (AI): It's Role in Drug Discovery and Novel Drug Delivery International Journal of Science and Research 2022.

[14] Francis-Dominic Makong Ekpan1* | Merit Oluchi Ori2 | Humphrey SamSamuel3 | Odii Peter Egwuatu4The Synergy of AI and Drug Delivery: A Revolution in Healthcare1Department of BioTechnology

[15] Muhammad Ahmer Raza1,2; Shireen Aziz3,4; Misbah Noreen2,5; Amna Saeed6,7; Irfan Anjum8,9; Mudassar Ahmed2,5; Shahid Masood Raza2,4,1Artificial Intelligence (AI) in Pharmacy: An Overview of Innovations,

[16] Sudipta Das1,*, Rimi Dey1, Amit Kumar Nayak2Artificial Intelligence in Pharmacy Department of Pharmaceutics, Netaji Subhas Chandra Bose Institute of Pharmacy, Nadia, West Bengal, INDIA. 2Department of Pharmaceutics, Seemanta Institute of Pharmaceutical Sciences, Mayurbhanj, Odisha, INDIAIndian Journal of Pharmaceutical Education and Research 2020.

[17] Yunan Luo ,1,2 Jian Peng,1 and Jianzhu Ma 3Next Decade's AI-Based Drug Development Features TightIntegration of Data and ComputationDepartment of Computer Science, University of Illinois at Urbana-Champaign, Urbana, IL 61801,

[18] Goutam Kumar Jena1*, Ch Niranjan Patra1, Sruti Jammula1, Rabinarayan Rana2, and Shibani Chand2, Artificial Intelligence and Machine Learning Implemented Drug Delivery Systems: A Paradigm Shift in the Pharmaceutical Industry Department of Pharmaceutics, September 2024

[19] Sara Gerke1, Timo Minssen2 and Glenn Cohen3Ethical and legal challenges of artificial intelligence-driven healthcare The Petrie-Flom Center for Health Law Policy, Biotechnology, and Bioethics at Harvard Law School,

[20] Rohan Kumar Ochani1, Ameema Asad1, Farah Yasmin1, COVID-19 pandemic: from origins To outcomes. A comprehensive Review of viral pathogenesis, clinical Manifestations, diagnostic evaluation, And

[21] Lalitkumar K. Vora 1* Amol D. Gholap 2, Keshava Jetha 3,4, Raghu Raj Singh Thakur Hetvi K. Solanki 5 and Vivek P. Chavda 3* Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. School of Pharmacy,