ARTIFICIAL INTELLIGENCE FOR DRUG DISCOVERY: AN UPDATE AND FUTURE PROSPECTS

Amit M. Surjushe
Smt. Vatsalabai Naik Mahila Mahavidyalya, Pusad
amitsurjushe99@gmail.com

Abstract
Artificial Intelligence (AI) is revolutionizing traditional drug discovery and development models by seamlessly integrating data, computational power, and algorithms. This collaboration speeds up development schedules, lowers costs, and improves drug research's efficacy, precision, and success rates. When combined with machine learning (ML) and deep learning (DL), artificial intelligence (AI) has shown notable progress in a number of areas, such as small molecule drug design, target identification and validation, drug characterisation, and clinical trial speedup. While virtual screening (VS) maximizes medication candidates, artificial intelligence (AI) helps create new therapeutic compounds by forecasting their characteristics and actions through molecular generation approaches. In order to successfully combine wet and dry laboratory trials, AI-driven pharmaceutical businesses must also successfully merge biological sciences and algorithms. The potential of AI in drug discovery is still obvious in spite of these obstacles. AI-driven treatments are set for a more expansive and significant future in the pharmaceutical sector as AI technology advances and these obstacles are removed.
Keywords**:** *Artificial intelligence; Drug discovery; Drug development; Decision-making; AI-driven medicine.*

1. Introduction:

Drug discovery and development is a long, expensive, and complex process that can often take more than 10 years from molecule identification to medical drug approval and placement on the market. Each stage in the process carries a risk of failure, and most drug applicants never reach the market. This makes the process of drug innovation and development both expensive and inefficient [1,2]. In recent years, the use of artificial intelligence (AI) in this industry has increased significantly. Drug discovery requires the analysis of large databases of chemical compounds. This can be achieved rapidly using machine learning techniques [3]. These techniques have their limitations because even a little change in the molecular structure of the drug can drastically alter its effect. Drug discovery involves the analysis and comparison of the properties of different molecular structures and components. In this context, AI tools can automatically scan large datasets quickly, using a composition safety check to pick out the most effective model for a certain goal [4,5]. Several public libraries store chemical and biological data, including ChEMBL [6] and Pub Chem [7]. They contain information on millions of molecules for various disease targets. These libraries are machine-readable and are used for drug discovery models, including for drug candidate compounds targeting severe acute respiratory syndrome coronavirus [8]. AI (mostly machine learning techniques) has also been implemented to evaluate toxicity.

Current Landscape Of Drug Discover:

Traditional methods and lmitations:

Trial-and-error techniques have been a major part of drug discovery in the past, with researchers testing substances to determine whether they had the intended therapeutic effect [9]. Traditional approaches, however, are linked to long turnaround times and high failure rates. A single medicine's development can take years and a lot of money, and many therapeutic candidates fail clinical testing [10]. Furthermore, the level of knowledge necessary to completely comprehend intricate biological systems and disease causes is sometimes lacking in traditional methodologies[11].

Evolution of technology in pharmaceutical research:

Researchers can expedite the early phases of drug development by rapidly screening vast libraries of chemicals for possible therapeutic candidates using high-throughput screening techniques [12]. Researchers now have a better grasp of biological systems and disease processes thanks to developments in genomics, proteomics, and other omics technologies [13]. Because computational methods enable researchers to model molecular interactions and forecast the characteristics of possible therapeutic candidates, they have grown in significance [14].

Emergence of AI in drug discovery:

By evaluating massive datasets, forecasting molecular characteristics, and identifying possible therapeutic candidates, artificial intelligence (AI)

techniques—in particular, machine learning and deep learning—have completely changed the drug discovery process [15]. The time and expense involved in experimental screening can be decreased by using AI algorithms to virtually screen compound libraries to find compounds that have the best chance of binding to particular targets [16]. Researchers can identify the most promising candidates for additional development by using AI models to forecast the pharmacokinetic and pharmacodynamic characteristics of substances [17].

Applications Of Ai In Drug Discovery

Biomarker discovery and validation:

The development of biomarkers improves the drug discovery process in the age of molecular medicine. The process of finding biomarkers necessitates the collection of numerous samples and their uniform, in-depth analysis. Validation guarantees that the marker's sensitivity and specificity are appropriate as well as that it is repeatable and dependable. In this step, AI could be used. Biomarkers aid in the identification and validation of therapeutic targets in the context of drug development by serving as an outcome measure in clinical trials. As a result, each patient would receive the appropriate treatment depending on the biomarkers that were analyzed[18].

High-throughput screening and data analysis:

One method for finding possible molecules to be included in additional investigation is high-throughput screening. To determine which of the molecules found in the preceding stage are most relevant to the desired health issue, they are screened. The stability and interactions of molecules are also part of the process [19]. Numerous techniques are used, such as the analysis of variance, decision trees, neural networks, and multiple linear regression [20,21].

Predictive modeling for drug design:

The process of designing drugs is crucial. It comprises the excipients (the additional substances) and the shape (such as a tablet or solution). At this point, AI is also used. The blend bulk and tapped density, flowability, angle of repose, appearance, friability, resistance to crushing, and tablet disintegration time are among the factors that are examined.

Challenges And Ethical Considerations:

Data quality and bias in AI models:

Accurate forecasts and decision-making depend on the quality and dependability of the data used to train AI models. Results may be faulty as a result of biases, errors, and incompleteness in the data [22]. Biased predictions or choices may result from AI models that inherit biases from the training data. This is especially troubling in the medical field, where racial, sexual, or socioeconomic biases can affect patient outcomes [23]. For ethical AI applications in drug development, methods for detecting and reducing biases in AI models must be developed, along with training datasets that are representative and diverse [24].

Interpretability and transparency:

Since their fundamental mechanisms are difficult for humans to understand, many AI models—especially deep learning models—are frequently referred to as "black boxes." This lack of openness erodes confidence in AI systems and raises questions about decision-making processes [25]. The demand for interpretable AI models—where domain experts and regulatory bodies can comprehend the logic behind predictions or recommendations—is rising [26]. Maintaining ethical norms in drug development requires the establishment of procedures to guarantee accountability for AI-driven decisions, including openness regarding model training and validation [27].

Regulatory and ethical implications:

Regulations established by organizations like the European Medicines Agency and the Food and Drug Administration must be followed by AI applications in drug research. Because AI technologies are unique, it can be difficult to ensure compliance with rules created for conventional drug development methods [28]. Regulatory approval of AI-generated medication candidates or therapy suggestions requires proof of their safety and effectiveness. To reduce patient hazards, strong validation and testing protocols are required [29]. It is crucial to safeguard private patient information and sensitive medical data used in AI applications. Maintaining trust and ethical standards requires adherence to data protection laws, such as the Health Insurance Portability and Accountability Act and the General Data Protection Regulation [30].

Future Directions And Innovations:

Advancements in AI technologies:

Drug discovery may benefit from the use of deep learning, a sophisticated form of machine learning. This neural network is capable of gathering data from open sources and using it to generate scientific findings. By forecasting the results of clinical studies before they begin, deep learning can

help lower their costs [31]. Drug repurposing is another exciting way that AI is being used in drug discovery. Drug development takes less time and money when new uses are found for already-approved medications. The use of AI in nanotechnologies, particularly nanocarriers, is another recent advance in the realm of drug discovery and development. In intelligent drug release systems that administer medication as required, artificial intelligence plays a critical role.

Collaborative approaches and industry trends:
Application of AI in the field of drug discovery requires a multidisciplinary approach by default. Collaboration between researchers, clinical experts, engineers, and data managers is crucial. Thus, multidisciplinary education is required to meet the new demands of pharmaceutical trends[33].

Conclusion:
This review demonstrated how incorporating AI can transform the process of finding and developing new drugs. AI is able to anticipate pharmacokinetics and toxicity, optimize lead compounds, and speed up target identification through the use of machine learning algorithms, deep learning approaches, and data analytics. This review showed the necessity of strong validation and ethical concerns in AI-driven drug development by recognizing the inherent difficulties, such as a lack of resources and model interpretability on a broader scale. However, the future shows that in order to overcome these obstacles and fully utilize AI to spur innovation and enhance patient outcomes in medical research, industry stakeholders and the research community must work together.

References:

1. Hughes, J. P., Rees, S., Kalindjian, S. B., & Philpott, K. L. (2011). Principles of early drug discovery. *British Journal of Pharmacology, 162*(6), 1239–1249.
2. Bohr, H. (2020). Drug discovery and molecular modeling using artificial intelligence. In *AI in Health* (pp. 61–83).
3. Ekins, S., Puhl, A. C., Zorn, K. M., Lane, T. R., Russo, D. P., Klein, J. J., Hickey, A. J., & Clark, A. M. (2019). Exploiting machine learning for end-to-end drug discovery and development. *Nature Materials, 18*(5), 435–441.
4. Zhang, L., Tan, J., Han, D., & Zhu, H. (2017). From machine learning to deep learning: Progress in machine intelligence for rational drug discovery. *Drug Discovery Today, 22*(11), 1680–1685.
5. Lavecchia, A. (2019). Deep learning in drug discovery: Opportunities, challenges and future prospects. *Drug Discovery Today, 24*(10), 2017–2032.
6. Gaulton, A., Bellis, L. J., Bento, A. P., Chambers, J., Davies, M., Hersey, A., Light, Y., McGlinchey, S., Michalovich, D., Al-Lazikani, B., & Overington, J. P. (2012). ChEMBL: A large-scale bioactivity database for drug discovery. *Nucleic Acids Research, 40*(D1), D1100–D1107.
7. Kim, S. (2021). Exploring chemical information in PubChem. *Current Protocols, 1*(5), e217.
8. Ashraf, F. B., Akter, S., Mumu, S. H., Islam, M. U., & Uddin, J. (2023). Bio-activity prediction of drug candidate compounds targeting SARS-CoV-2 using machine learning approaches. *PLoS ONE, 18*(6), e0288053.
9. Korinek, M., Hsieh, P. S., Chen, Y. L., Hsieh, P. W., Chang, S. H., Wu, Y. H., & Hwang, T. L. (2021). Randialic acid B and tomentosolic acid block formyl peptide receptor 1 in human neutrophils and attenuate psoriasis-like inflammation in vivo. *Biochemical Pharmacology, 190*, 114596.
10. Tingaud-Sequeira, A., Carnevali, O., & Cerdà, J. (2011). Cathepsin B differential expression and enzyme processing and activity during *Fundulus heteroclitus* embryogenesis. *Comparative Biochemistry and Physiology Part A: Molecular & Integrative Physiology, 158*(2), 221–228.
11. Wingender, E. (2008). The TRANSFAC project as an example of framework technology that supports the analysis of genomic regulation. *Briefings in Bioinformatics, 9*(4), 326–332.
12. Baig, M. H., Ahmad, K., Rabbani, G., Danishuddin, M., & Choi, I. (2018). Computer-aided drug design and its application to the development of potential drugs for neurodegenerative disorders. *Current Neuropharmacology, 16*(6), 740–748.
13. Dana, D., Gadhiya, S. V., St Surin, L. G., Li, D., Naaz, F., Ali, Q., Paka, L., Yamin, M. A., Narayan, M., Goldberg, I. D., & Narayan, P. (2018). Deep learning in drug discovery and medicine: Scratching the surface. *Molecules, 23*(9), 2384.
14. Urban, G., Bache, K. M., Phan, D., Sobrino, A., Shmakov, A. K., Hachey, S. J., Hughes, C., & Baldi, P. (2020). Deep learning for drug discovery and cancer research: Automated

analysis of vascularization images. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, *17*(6), 2136–2145.

15. Lim, J., Ryu, S., Park, K., Choe, Y. J., Ham, J., & Kim, W. Y. (2019). Predicting drug–target interaction using a novel graph neural network with 3D structure-embedded graph representation. *Journal of Chemical Information and Modeling*, *59*(9), 3981–3988.
16. Chen, Z., Liu, X., Hogan, W., Shenkman, E., & Bian, J. (2021). Applications of artificial intelligence in drug development using real-world data. *Drug Discovery Today*, *26*(5), 1256–1264.
17. Lavecchia, A., & Di Giovanni, C. (2013). Virtual screening strategies in drug discovery: A critical review. *Current Medicinal Chemistry*, *20*(23), 2839–2860.
18. Sivakumar, B., & Kaliappan, I. (2023). Lead drug discovery from imidazolinone derivatives with Aurora kinase inhibitors. *Pharmaceutical Chemistry Journal*, *70*(11), 1529–1540.
19. Malo, N., Hanley, J. A., Cerquozzi, S., Pelletier, J., & Nadon, R. (2006). Statistical practice in high-throughput screening data analysis. *Nature Biotechnology*, *24*(2), 167–175.
20. Dara, S., Dhamercherla, S., Jadav, S. S., Babu, C. M., & Ahsan, M. J. (2022). Machine learning in drug discovery: A review. *Artificial Intelligence Review*, *55*(3), 1947–1999.
21. Shockley, K. R., Gupta, S., Harris, S. F., Lahiri, S. N., & Peddada, S. D. (2019). Quality control of quantitative high throughput screening data. *Frontiers in Genetics*, *10*, 387.
22. Behei, N., Tryhubchak, O., & Pryymak, B. (2022). Development of amlodipine and enalapril combined tablets based on quality by design and artificial neural network for confirming qualitative composition. *Pharmaceutical Chemistry Journal*, *69*(9), 779–789.
23. Kraus, V. B. (2018). Biomarkers as drug development tools: Discovery, validation, qualification and use. *Nature Reviews Rheumatology*, *14*(6), 354–362.
24. Pu, L., Naderi, M., Liu, T., Wu, H. C., Mukhopadhyay, S., & Brylinski, M. (2019). eToxPred: A machine learning-based approach to estimate the toxicity of drug candidates. *BMC Pharmacology and Toxicology*, *20*(1), 2.
25. Mak, K. K., & Pichika, M. R. (2019). Artificial intelligence in drug development: Present status and future prospects. *Drug Discovery Today*, *24*(3), 773–780.
26. Harrer, S., Shah, P., Antony, B., & Hu, J. (2019). Artificial intelligence for clinical trial design. *Trends in Pharmacological Sciences*, *40*(8), 577–591.
27. Hutson, M. (2024). How AI is being used to accelerate clinical trials. *Nature*, *627*(8017 Suppl.), S2–S5.
28. Johnson, K. B., Wei, W. Q., Weeraratne, D., Frisse, M. E., Misulis, K., Rhee, K., Zhao, J., & Snowdon, J. L. (2021). Precision medicine, AI, and the future of personalized health care. *Clinical and Translational Science*, *14*(1), 86–93.
29. Schork, N. J. (2019). Artificial intelligence and personalized medicine. In *Cancer Treatment and Research* (Vol. 178, pp. 265–283).
30. Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Ferran, E., Lee, G., Li, B., Madabhushi, A., Shah, P., Spitzer, M., & Zhao, S. (2019). Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery*, *18*(6), 463–477.
31. Walters, W. P., Barzilay, R., & Jaakkola, T. S. (2020). Applications of deep learning in molecule generation and molecular property prediction. *Accounts of Chemical Research*, *53*(2), 263–270.
32. Rifaioglu, A. S., Atas, H., Martin, M. J., Cetin-Atalay, R., Atalay, V., & Doğan, T. (2019). Recent applications of deep learning and machine intelligence on in silico drug discovery: Methods, tools and databases. *Briefings in Bioinformatics*, *20*(5), 1878–1912.
33. Mohs, R. C., & Greig, N. H. (2017). Drug discovery and development: Role of basic biological research. *Alzheimer's & Dementia: Translational Research & Clinical Interventions*, *3*(4), 651–657.