

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY: RESHAPING THE FUTURE OF THERAPEUTICS

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Abstract

Traditional drug discovery methods involve target identification, hit to lead optimization, preclinical and clinical trials that are often time consuming, expensive with high failure rates. Artificial intelligence (AI) has emerged as an innovative and transformative force in drug discovery addressing the limitations encountered in drug research. Integration of computations methods such as Machine learning (ML), Deep learning (DL) and Reinforcement learning (RL) enables efficient analysis of vast chemical and biological data sets significantly accelerating the growth of drug development. AI plays a critical role in virtual screening, target identification, drug design, physicochemical assessment, ADMET studies, pharmacodynamics and drug repurposing strategies. In clinical trials, AI enhances patient selection, trial design, outcome prediction and therapeutic intervention. Despite these advancements, challenges such as data set quality, model interpretability, computational demands and ethical concerns remains significant concerns. Nevertheless, ongoing innovations in technology and biopharmaceutics, the hybrid computational and experimental methods are helping to overcome these limitations. Overall, AI is reshaping drug discovery into a faster, more accurate, cost effective process with a potential to revolutionize in the field of therapeutics with a better health care outcome.

Key words: Artificial intelligence, Drug discovery, Therapeutics, Pharmaceutical industry, Clinical trials.

Introduction

Drug discovery is the process of identifying a new drug molecule for the treatment of disease which requires an interdisciplinary collaboration between biology and pharmacology to transform into an effective therapy (Mehran et al., 2026). Traditional approach in drug discovery comprise of identification of the biological targets responsible for disease occurrence, screening of compounds to find the lead molecules, safety evaluations and clinical trials. The conventional drug discovery is a systematic approach involving multiple aspects in drug discovery from finding a target to making it available in the market. With lengthy time lines, late stage failures, poor pharmacokinetic and toxicity predictions

costing billions of dollars to bring a single drug in to the market, emphasizing the need

for better predictive and computation approaches (Mullard, 2014). In modern era, Artificial intelligence, a data driven process reshaping the drug discovery in a faster and more efficient way, influencing the therapeutics by improving the efficacy, reducing adverse effects, rational optimization, cost effective, multi target drug design strategies and personalized medicine (Chen et al., 2023).

The Role of Artificial Intelligence in Drug Discovery

Artificial intelligence term coined by John McCarthy in 1956 is a revolutionary concept, enables researchers to analyze vast

datasets through identifying the molecular patterns, detailing the complex tasks and enhancing the efficacy of drugs (Mak and Pichika, 2018). Large data base available in public domains such as ChEMBL and PubChem act as a fuel in AI models. The core concepts of renowned Pharma companies such as Bayer, Pfizer and Roche integrating these AI based predictive modelling concepts in drug innovation through collaborations with Technology firms (Mak & Pichika 2019). Several AI techniques contribute to address the challenges in drug discovery. Machine learning (ML) algorithms such as supervised, unsupervised, deep learning navigate the complex biological data sets to identify potential drug targets. (Vemula et al., 2023). Supervised learning is used for prediction tasks such as classifying compounds, to train the models for target-drug interactions, analyze bio-chemical properties, while unsupervised learning helps identify patterns and clusters in complex chemical data. These approaches allow efficient exploration of chemical space and improve prediction accuracy. Machine learning typically involves transforming chemical structures into numerical depictions like SMILES strings, enables prediction of biological activity and toxicity. Deep learning (DL) manage large data sets and complex molecular structures, Natural language processing extracts information from scientific literature and Graph neural networks analyse molecular structures with high accuracy. Reinforcement learning further enhances drug discovery by generating novel molecular structures tailored to specific therapeutic targets (Dara et al., 2022; Vemula et al., 2023).

AI-Driven Target Identification and Drug Design

Identifying the correct biological target is a crucial step in drug discovery. AI enhances this process by integrating genomics and biological data. Genomics-based approaches use gene expression data and genome-wide studies to identify disease-related targets. Network-based methods

analyze protein interactions to determine key pathways involved in disease progression. AI also enables accurate prediction of protein structures, helping identify binding sites and facilitating structure-based drug design. These advancements significantly improve target validation and drug development success rates. Revolution of AI in drug design enabled to screen millions of compounds in minimal amount of time using AI based molecular docking, Pharmacophore modelling and Deep reinforcement learning techniques successfully designed targeting receptors involved in metabolic and inflammatory diseases (Udegbe, 2024). AI intertwines with the data science, uses algorithms to analyse and visualize complex data sets. Drug-likeness is evaluated using Lipinski's Rule of Five, ensuring optimal pharmacokinetic properties. A major advantage with AI in drug discovery is its ability to predict ADMET with Tools such as DeepTox and Molecule Net helps to reduce the drug failure in the early stages and ensure to proceed with the most promising candidates. AI models also predict potential toxic effects such as hepatotoxicity and cardiotoxicity at early stages (Mayr et al., 2016). This early prediction reduces late-stage failures and helps prioritize the most promising drug candidates for further development.

AI driven drug discovery work flow begins with preparation of chemical structure and optimization using tools like AVOGADRO and Open Babel. Physicochemical properties are analyzed using swissADME and pkCSM platforms. Target prediction tools like SwissTarget Prediction identify potential biological targets by analyzing genomic and proteomic data. Molecular Docking using AutoDock Vina or PyRx evaluates binding interactions, followed by molecular dynamics simulations to study stability using GROMACS. Further Pharmacokinetic and Pharmacodynamic modeling are performed using tools like PK-Sim, R or Python and integrated using MoBi or nlmixr2, toxicity prediction using **ProTox-II** ensures safety, Clinical trials and followed

by drug approval. AI-driven approaches increase early-stage success rates, more efficient decision-making and a higher likelihood of developing effective drugs.

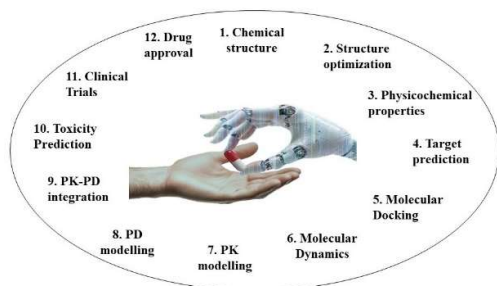


Fig. 1. Artificial Intelligence (AI) driven drug discovery work flow

AI in Clinical Trials

Clinical trials rely up on patient selection. AI enhance the trial efficiency by selecting suitable participants through analysing their electronic health records, biomarkers and genetic data. The process is further enhanced through wearable devices, remote monitoring, real-time data acquisition and better patient engagement (Khan et al., 2024). AI also paving way to personalized therapy for chronic hepatitis B condition (Cascini et al., 2022) and within 18 months' development of drug for idiopathic pulmonary fibrosis (Serrano et al., 2024) enhances the therapeutic efficiency, reducing the cost and increasing the success percentage. Ethical concerns are another aspect which requires accountability and transparency. AI contribute to 3R's especially replacement of animal studies to certain extent in Behavioural research, drug screening and Toxicity testing enabling transparency and enhancing the ethical standards.

Challenges and Limitations

AI is reshaping the therapeutics and its need is inevitable especially in pharmaceutical and healthcare sector. Nevertheless, it has limitations, for instance AI is based on evaluating data quality but biased data sets lead to unreliable predictions, regulatory concerns, ethical considerations and further need for evaluation in the laboratory using animal models are major concerns. Many AI systems also lack interpretability, making it

difficult to understand how decisions are made (Wiens et al., 2019). Additionally, computational methods such as molecular docking may not always accurately reflect real biological interactions, especially when protein flexibility and solvent effects are not fully considered (Pantsar & Poso, 2018). Even advanced tools like AlphaFold may fail to capture dynamic protein conformations, limiting their applicability in certain scenarios (Bowman, 2024).

Future Prospects

The future of drug discovery lies in the integration of AI with emergent technologies such as quantum computing, multi-omics data analysis, and digital biomarkers. These innovations will help formulate more precise and personalized treatments customized to individual patients. AI is also expected to advance drug repurposing and polypharmacology, identifying new therapeutic uses for existing drugs and targeting multiple pathways simultaneously (Han et al., 2023). Continued progress will depend on improved data quality, transparent AI models, and strong collaboration between computational scientists and experimental researchers (Paul et al., 2021). Interdisciplinary collaboration, open data sharing, and methodological advancements will be essential to fully capture the benefits of AI in pharmaceutical research.

Conclusion

Artificial Intelligence is restructuring drug discovery by transforming it into a predictive, well-organized, and data-driven process. From target identification, drug design to clinical trials and safety assessment, AI improves every stage of the workflow while drastically cutting down cost, time, and failure rates. Despite the challenges and limitations, the ongoing developments in AI and initiatives such as interdisciplinary collaborations are anticipated to propel pharmaceutical Research and Development, leading to superior healthcare outcomes globally. Future of AI is promising and

expected to grow exponentially creating that demand integration of professional and myriad of opportunities not only in health care technical skills. but also in manufacturing and other sectors

References:

- Bowman, G. R. (2024). AlphaFold and Protein Folding: Not Dead Yet! The Frontier Is Conformational Ensembles. *Annual Review of Biomedical Data Science*, 7(1), 51–57.
- Cascini, F., Beccia, F., Causio, F. A., Melnyk, A., Zaino, A., Ricciardi, W. (2022). Scoping Review of the Current Landscape of AI- Based Applications in Clinical Trials. *Frontiers in Public Health*, 10, 949377.
- Chen, W., Liu, X., Zhang, S., Chen, S. (2023). Artificial Intelligence for Drug Discovery: Resources, Methods, and Applications. *Molecular Therapy - Nucleic Acids*, 31, 691–702.
- 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.
- Han, R., Yoon, H., Kim, G., Lee, H., Lee, Y. (2023). Revolutionizing Medicinal Chemistry: The Application of Artificial Intelligence (AI) in Early Drug Discovery. *Pharmaceutics*, 16(9), 1259.
- Khan, M. K., Raza, M., Shahbaz, M., et al. (2024). The Recent Advances in the Approach of Artificial Intelligence (AI) Towards Drug Discovery. *Frontiers in Chemistry*, 12, 1408740.
- Mak, K.-K., Pichika, M. R. (2019). Artificial Intelligence in Drug Development: Present Status and Future Prospects. *Drug Discovery Today*, 24(3), 773–780.
- Mayr, A., Klambauer, G., Unterthiner, T., Hochreiter, S. (2016). DeepTox: Toxicity Prediction Using Deep Learning. *Frontiers in Environmental Science*, 3, 80.
- Mullard, A. (2014). New drugs cost US\$2.6 billion to develop. *Nature Reviews Drug Discovery*, 13(12), 877.
- Pantsar, T., Poso, A. (2018). Binding Affinity via Docking: Fact and Fiction. *Molecules*, 23(8), 1899.
- Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., Tekade, R. K. (2021). Artificial Intelligence in Drug Discovery and Development. *Drug Discovery Today*, 26(1), 80–93.
- Serrano, D. R., Luciano, F. C., Anaya, B. J., Ongoren, B., Kara, A., Molina, G., Ramirez, B. I., Sánchez-Guirales, S. A., Simon, J. A., Tomietto, G., Rapti, C. (2024). Artificial intelligence (AI) applications in drug discovery and drug delivery: revolutionizing personalized medicine. *Pharmaceutics*, 16(10), 1328.
- Udegbe, F. C., Ebulue, O. R., Ebulue, C. C., Ekesiobi, C. S. (2024). Machine Learning in Drug Discovery: A Critical Review of Applications and Challenges. *Computer Science & IT Research Journal* 5(4), 892–902.
- Wiens, J., Saria, S., Sendak, M., et al. (2019). Do No Harm: A Roadmap for Responsible Machine Learning for Health Care. *Nature Medicine*, 25(9), 1337–1340.
- Wu, Z., Ramsundar, B., Feinberg, E. N., et al. (2018). Moleculenet: A Benchmark for Molecular Machine Learning. *Chemical Science*, 9(2), 513–530.

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