Artificial Intelligence in Drug Discovery: Transforming the Future of Medicine

Malvika Chawla

ABSTRACT

Artificial intelligence (AI) is one of the important tools in modern drug development processes, which can work through large bodies of data and build predictive models. This aids in identifying suitable drug candidates and predicting possible interactions between drugs and specific targets as well as exploratory therapeutic areas—all of which lead to a simpler and more efficient drug development cycle at minimal cost. In this review article, we examine the state of AI in drug discovery and discuss its applications where it provides support during target identification, validation stages including the drug-designing stage, as well as clinical research. This paper also discusses challenges associated with using AI in drug discovery, such as problems with the quality and interpretability of data/models or regulatory concerns. The review also considers the future of AI-driven drug discovery, with far-reaching implications for personalized medicine, and the expansion of therapeutic repertoire in recalcitrant diseases.

Keywords: Artificial intelligence (AI) in drug discovery, Transforming the future of medicine

Former Research Scholar, Gurukula Kangri (Deemed to be University), Haridwar, Uttarakhand, India

Correspondence to: Malvika Chawla, malvika.radhe@gmail.com

Additional material is published online only. To view please visit the journal online.

Cite this as: Chawla M. Artificial Intelligence in Drug Discovery: Transforming the Future of Medicine. Premier Journal of Science 2024;1:100034

DOI: https://doi.org/10.70389/PJS.100034

Received: 1 September 2024

Revised: 11 November 2024

Accepted: 16 November 2024

Published: 21 November 2024

Ethical approval: N/a

Consent: N/a

Funding: No industry funding

Conflicts of interest: N/a

Author contribution: Malvika Chawla – Conceptualization, Writing – original draft, review and editing

Guarantor: Malvika Chawla

Provenance and peer-review: Commissioned and externally peer-reviewed

Data availability statement: N/a

Introduction

The growth of artificial intelligence (AI) in drug discovery has been exponential, driven by the need for more efficient, cost-effective, and accurate drug development processes. Over the past decade, AI has transitioned from a novel concept to a cornerstone of modern pharmaceutical research.[1] It is estimated that the expansion of AI in the drug discovery market between 2023 and 2032 will have a compound annual growth rate (CAGR) of 29.6%. It is also anticipated that the market will experience substantial growth from USD 1.9 billion (Figure 1).[2] The North American AI in the drug discovery market is estimated to hold the largest share of USD 2.08 billion by 2022 because this region saves on expenses, reduces time frames, and improves patient outcomes through AI-based platforms for drug discovery. The drug discovery and biotechnology applications continued to expand significantly in 2022, accounting for 72% of U.S. funding during the year, with Europe taking second place by market share distribution. Asia Pacific shows the highest growth rate on account of the rising incidence of chronic diseases and the presence of a well-established pharmaceutical industry. Conversely, growth is expected to be slower in the Middle East, Africa, and Latin America as a result of limited healthcare spending and fewer manufacturers entering these regions.[3]

The discovery of drugs is being revolutionized by AI as it accelerates the identification and development of new therapeutic agents, reduces costs, and improves the efficiency of clinical trials. AI greatly

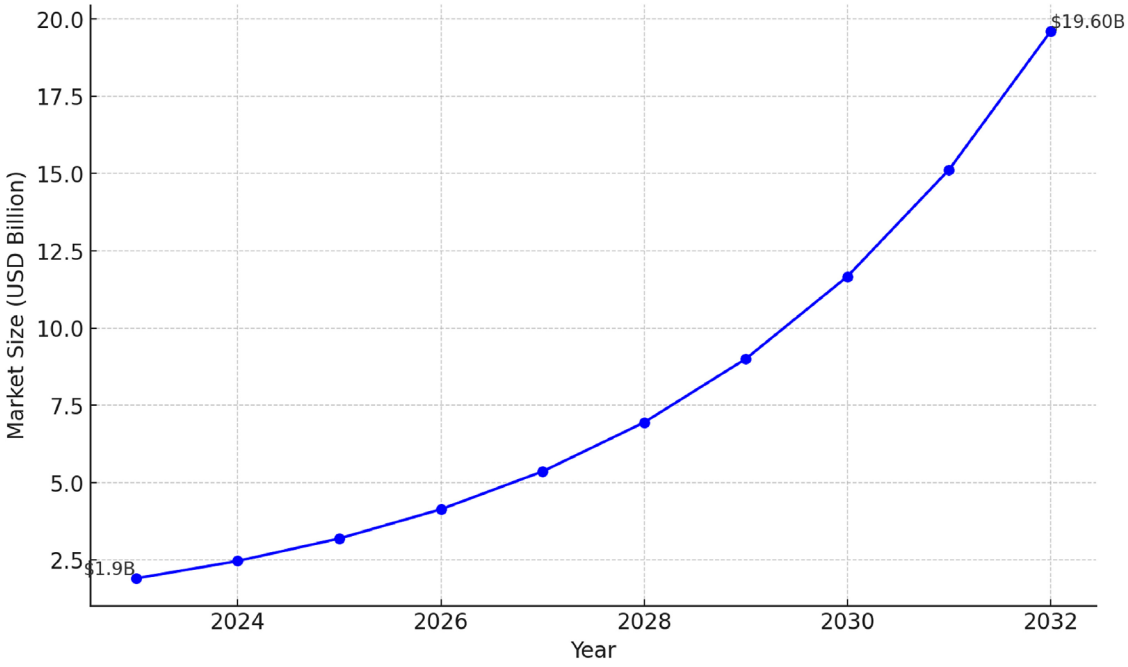

Fig 1 | Market trend showing AI in drug discovery (2023–2032)

improves drug discovery efficiency by optimizing different phases of the drug development process, such as target identification, lead optimization, and toxicity prediction.[4] Machine learning, deep learning (including artificial and deep neural networks), fuzzy logic, and neuro-fuzzy logic, in combination with genetic algorithms, can analyze large datasets within a short time, reducing the required timescales of drug discovery as well as related costs to run experiments for each new molecule identified. By predicting molecular properties and target interactions, these algorithms aid in selecting potential drug candidates to a great extent over the ability of predictive modeling of drug discovery studies.[5] The generation of new molecular structures and evaluation of their therapeutic efficacy have also become more effective through the application of AI methods in structure-based virtual screening and ligand-docking-based approaches.[6] The high-dimensional data exploration tasks such as antibiotic discovery and generative models designing compounds with antibacterial activity have been addressed efficiently by deep learning methods, aiding antimicrobial research.[7] Relatively same models are used for cancer drug response prediction, which gives us very accurate predictions and suggests optimal personalized treatments.[8] A major case study here is the use of AI to predict protein structures using methods such as AlphaFold, which would improve drug development much further with a great degree of precision.[9] An overview of AI in drug discovery is illustrated in Figure 2.

Moreover, utilizing AI in computer-assisted drug design (CADD) enhances the accuracy of identifying potential compounds, making the screening process more efficient and enhancing the chances of success in subsequent development phases.[10] CADD utilizes AI and big data methodologies to overcome traditional drug design limitations, improving the identification of binding sites, property prediction, and overall drug development processes.[11] These computational techniques allow for the analysis and identification of biologically active molecules, streamlining the drug discovery process and contributing to improved patient care. AI in CADD assists in the orientation of new chemical entities and screening for suitable modifications in the molecular structure that will improve the pharmacological effectiveness of lead compounds while at the same time decreasing the possibility of adverse reactions. This optimization process uses machine learning methods for predicting the structure–activity relationships on the basis of which research can be directed to the specific and probable regions. The integration of AI with CADD also facilitates drug repositioning, which is crucial for addressing complex diseases like COVID-19 and cancer, making the process faster and more cost-effective.[12] CADD approaches are also valuable in designing anticancer drugs, using *in silico* tools to develop innovative and selective small molecules for therapeutic applications.[13] Additionally, AI-driven CADD techniques are crucial in the development of targeted therapies for neurodegenerative

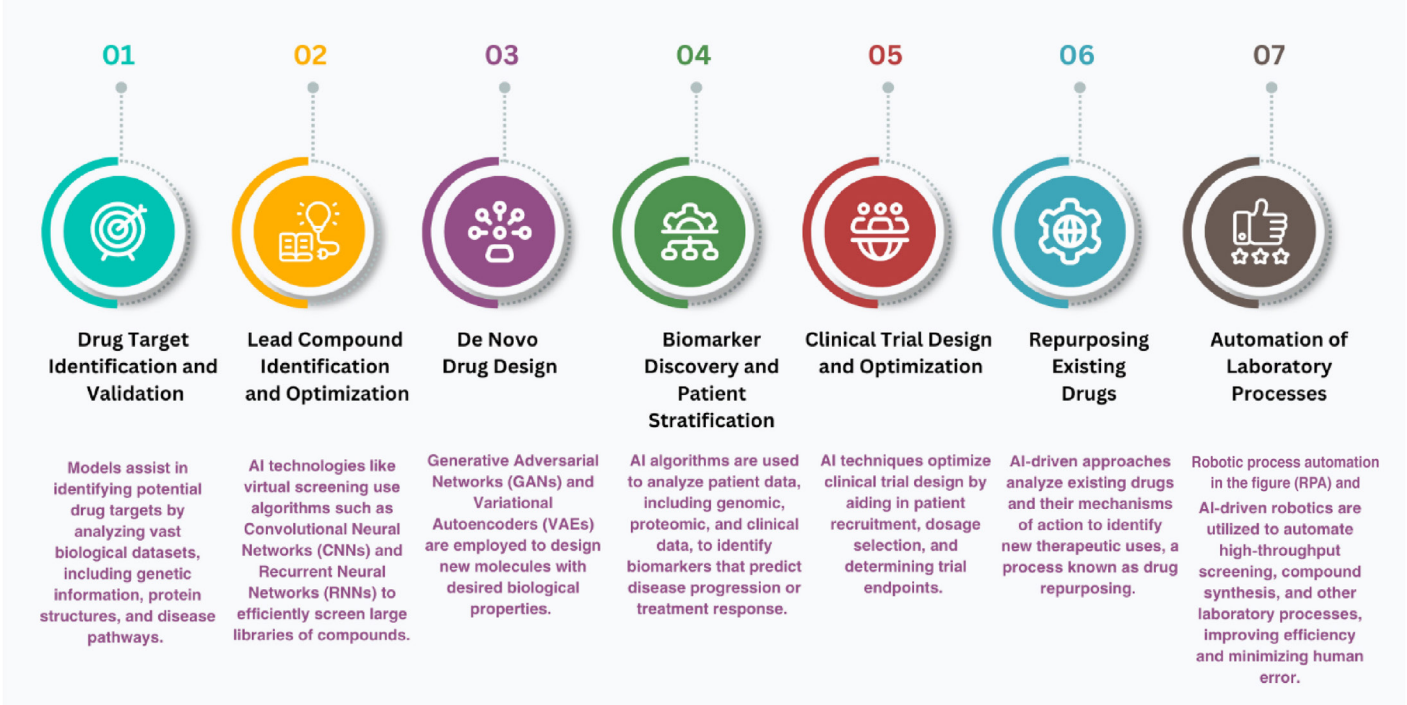

Fig 2 | Role of AI in drug discovery

DOI: https://doi.org/10.70389/PJS.100034 | Premier Journal of Science 2024;1:100034

diseases, such as Alzheimer's, where computational models help identify promising drug candidates.[14]

AI improves high-throughput virtual screening and *de novo* drug design by accurately predicting molecular interactions and biological activity better than traditional methods. By integrating *in silico* techniques and deep learning, AI systems can automate various stages of drug design, such as the identification of potential inhibitors for specific diseases, including chronic myeloid leukemia and COVID-19. These can evaluate multiple biological activities at a time and thus reduce the search for molecules in possible candidates.[15] Also, AI-virtual screening and *de novo* design tools broaden the landscape for molecular design through learning from existing data to understand relationships within molecules as well as inter-molecular interactions, thereby aiding in the better identification of drug candidates. This is evident in applications such as designing dual-target ligands for complex diseases, where AI-generated models have shown high success rates in meeting biological activity objectives.[16] AI-driven methods provide a powerful alternative to traditional drug discovery, enabling faster, more cost-effective, and precise identification of new therapeutic agents, revolutionizing the landscape of computational drug design. Numerous pharmaceutical companies have effectively utilized AI in drug discovery to create new medications for a range of illnesses, such as cancer, fibrosis, psychiatric disorders, and rare diseases, leading the way in the industry (Table 1). Many large pharmaceutical companies continuously monitor AI-driven collaborations to progress their research and development projects and identify potential partners and consultants.

AI in Target Identification and Validation

Without exception, when it comes to the development of new drugs and management of diseases, AI plays a very vital role in identifying targets in many fields. In cancer studies, AI techniques such as machine learning and deep learning assist and consider vast datasets. This also renders it easier to identify possible drugs and the likelihood of success of a research agenda.[17] Some of these AI tools are mentioned in Table 2. In the field of orphan diseases, it implements genotypes and phenotypes into the understanding of diseases at the same time. The sources of prospective targets are generated using machine learning models,

Table 1 | AI-Driven Innovations by Pharmaceutical Companies

Company	AI Platform/Technology	Key Achievements	Partnerships
Insilico Medicine	GENTRL (Generative Tensorial Reinforcement Learning)	Developed a molecule for fibrosis in 46 days	Pfizer
Exscientia	An AI platform for novel molecular design	Focus on psychiatric disorders and cancer	Sumitomo Dainippon Pharma, Celgene
Relay Therapeutics	An AI platform for protein motion targeting drugs	Lead candidate RLY-1971 in phase I for solid tumors	–
BenevolentAI	Benevolent Platform	Two targets for chronic kidney disease (CKD) and idiopathic pulmonary fibrosis (IPF)	AstraZeneca
Valo Health	Logica	A multi-program agreement for small-molecule optimization	Pioneering Medicines, Charles River Laboratories
Tempus	AI technologies for precision medicine	For advances in drug discovery and precision oncology	Pfizer, GSK, AstraZeneca
Receptor.AI	A platform focused on protein isoform selectivity	Developing technologies with high selectivity for protein variants	–

Table 2 | AI-Integrated Tools Used in Target Identification and Validation

Tools	Description	References
BioMap	The method integrates AI algorithms for enhancing leads and identifying targets, along with real-time data analytics and predictive modeling, to accelerate drug development.	[26]
deepDTnet	Identifies new targets and repurposing drugs	[27]
GENTRL	Discovers potent inhibitors of discoidin domain receptor 1 (DDR1)	[28]
KDeep	Predicts protein–ligand absolute binding affinity using 3D-convolutional neural networks	[29]
KG-DTI	A deep learning approach using knowledge graphs for predicting drug–target interactions and repositioning drugs for Alzheimer's disease.	[30]
LibINVENT	A tool for ***de novo*** drug design	[31]
PIGNet	A deep learning model informed by physics for predicting drug–target interactions in a generalized manner	[32]
Reinvent	A tool for ***de novo*** drug design	[33]
RELATION	A complex generative model for creating new drugs based on structure	[34]

and the targets generated are checked to confirm the effectiveness of the models.[18] In the same manner, AI-based solutions help prioritize novel cancer therapeutic targets that should balance the levels of novelty, confidence, and commercial practicability in order to enhance the drug discovery processes and the consequences.[19]

AI has also been used in the search and confirmation of new drug targets in diseases, such as endometriosis and glioblastoma. For example, the AI process helped determine ENDO01 and ENDO02 as therapeutic targets for endometriosis following *in vitro* and *in vivo* validation.[20] In glioblastoma studies, technology such as PandaOmics has been useful in finding drug target dualism that could be useful in addressing aging, as well as glioblastoma multiforme.[21] In addition, pharmacophore comparison using only AI and reverse ligand-protein docking have been found useful in establishing the protein targets for herbal ingredients, hence providing a glimpse of the mode of action of these ingredients.[22]

With the help of an AI-powered tool, researchers created inhibitors for the BMX protein implicated in cancer and immune diseases.[23] For the 13-thioesterase (TE) domain of the polyketide synthase, which is essential for mycobacteria survival, Reinvent 4, pKCSM, KDeep, and SwissADME have been employed.[24] The identification of potential drugs and natural compounds for liposarcoma (LPS) treatment was done through *in silico* analysis with Kantify's Zeptomics, in which 10,000 drugs and natural compounds were analyzed.[25] Using this strategy, it was possible to identify seven compounds that effectively inhibited LPS cell viability, with an IC50 value between 1 μM and the nanomolar (nM) scale. The compounds typically exist in the concentrations of 5 μM to nM scales.

AI in Drug Design

Different stages of drug discovery have been improved by AI in drug design, as shown in Figure 3. Big data analysis, predicting molecular interactions and lead optimization using various AI procedures, can be used by researchers. Applications of DeepChem and Chemistry 42 are common in drug design to help make processes more efficient and results in biomedical chemistry better. These tools enable the enhanced creation of small molecules to have a high computed binding propensity to particular targets to make drug discovery more rapid and efficient.[35] Moreover, the AI application is also involved in the analysis of high-content screening data, synthesis, and molecular design to help in discovering regions of chemical space.[36] Broudy et al. have endeavored to find inhibitors for Casitas B-lymphoma proto-oncogene-b (Cbl-b) by using a generative AI tool known as the REINVENT design engine in parallel with medicinal chemistry in addition to structure-based engineering techniques.[37] The decision to introduce multiple rounds of *in silico* structure-based drug design into the design–make–test–analyze cycle significantly changed the "design"

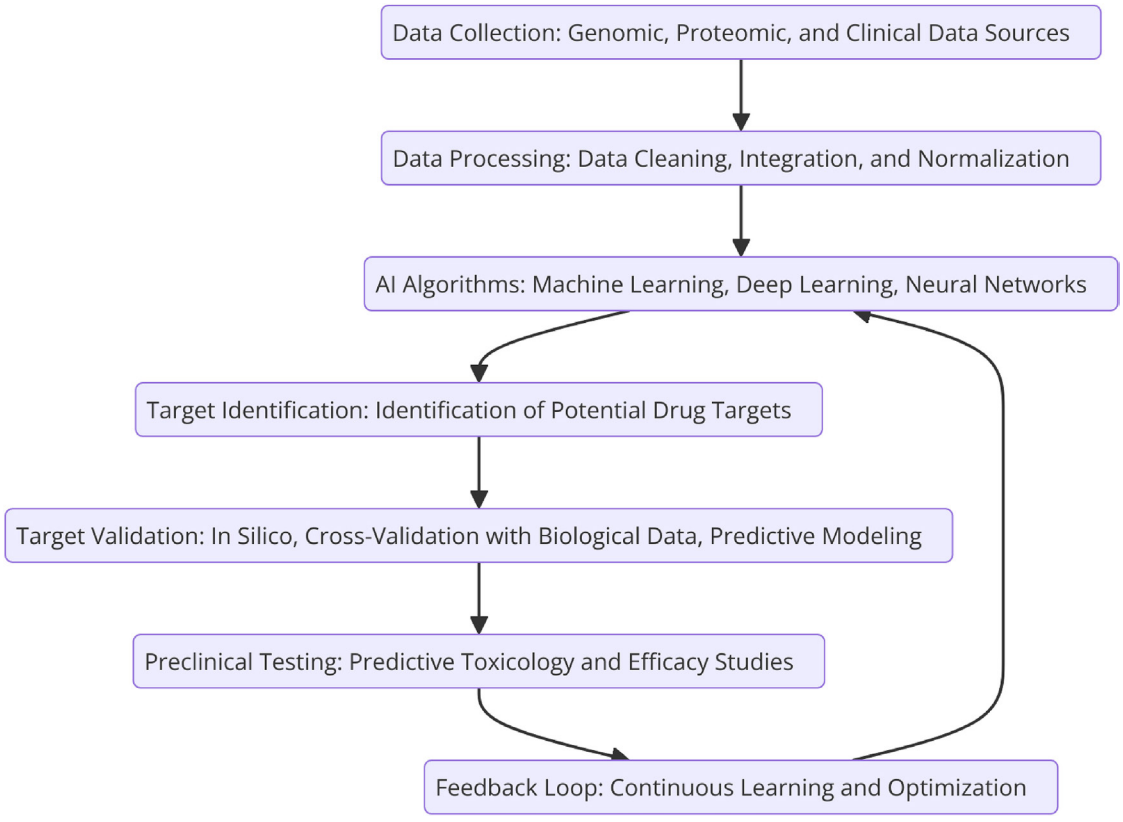

Fig 3 | Different stages of the AI-integrated drug discovery process

DOI: https://doi.org/10.70389/PJS.100034 | Premier Journal of Science 2024;1:100034

phase. Shirani and Hashemianzadeh employed an ANI-1x neural network model to predict the potential energy surface of the antiparkinsonian drug levodopa (L-3,4-dihydroxyphenylalanine).[38] Importantly, this model was able to do all calculations in a short time, making it a potential instrument for computationally efficient and effective drug design.

AI in Clinical Studies

The quantitative systems pharmacology (QSP) approach is extensively utilized in drug discovery and development to address critical questions, such as elucidating therapeutic mechanisms of action, patient stratification, and mechanistic insights into disease progression. Using a QSP model to generate virtual patients, it was demonstrated that nonsteroidal mineralocorticoid receptor antagonists (MRAs), such as finerenone and apararenone, present a lower hyperkalemia risk compared to the steroidal MRA eplerenone.[39] Prospective simulations using QSP models offer a valuable tool for prioritizing drug candidates in clinical development and validating mechanism-based pharmacological concepts before large-scale clinical trials. Williamson et al. have presented the possibility of AI in advancing recruitment strategies specifically in the context of the many trials that are currently being conducted in the advanced stage of age-related macular degeneration with geographic atrophy.[40] In a similar vein, a group of researchers proposed that by using an AI model, high-risk patients can be first flagged to significantly decrease the number of patients needed or the time required to achieve the clinical trial end points.[41]

Recent Trends in the Applications of AI in Drug Discovery

Multi-Omics Integration

Using Omics, where the aim is to develop a hypothesis for discovery biology, is the best way to come up with targets for drug development. In this method, researchers collect data from significantly different biomolecular levels, such as DNA, RNA, proteins, metabolites, and epigenetic modifications, to substantiate systems biology approaches and define how living organisms work and interact.[42] Many of the new methods that were developed and implemented in the last few years involve the use of data and have been employed to address the complexity of multi-omics in oncology, particularly with regard to patient profiling, biomarker discovery, and drug repositioning for personalized medicine.[43] According to the research, *Mycobacterium tuberculosis* omics technologies might be helpful in the early stages of creating rational antimicrobial drugs for tuberculosis.[44]

Robotics and Automation in Drug Synthesis

Self-optimized synthesis processes can benefit from the applications of AI. Software that relies on algorithms could quickly analyze and enhance inadequate responses using a learning model based on previous reactions found in the literature. The robotic arm that is linked can be programmed to execute the best response automatically. For instance, the iChemFoundry platform, created at the ZJU-Hangzhou Global Scientific and Technological Innovation Center, is an intelligent automated platform for high-throughput chemical synthesis that will change the traditional disciplines' mindset, encourage disruptive technique innovation, redefine chemical synthesis speed, and revolutionize material manufacturing methods.[45]

Enhanced Predictive Modeling

Recent enhancements in the ability to model AI have been seen to increase the reliability of predictions whenever in harmony with clinical investigation, a key factor in the applicability of AI in personalized medicines.[46] Machine learning has become important in bettering predictive modeling through fast analysis of large chemical libraries while arriving at higher hit prediction and better assessment of molecular frameworks. This leads to improved evaluations of the safety and effectiveness of drugs, thus speeding up the drug discovery process.[47] Additionally, AI methods, which encompass both machine learning and deep learning, play a substantial role in improving predictive models and enhancing the efficiency of the drug discovery process.[48] The merging of AI and big data boosts predictive modeling abilities, leading to advancements and accuracy in the drug discovery process. This combination has had a significant effect in areas such as cardiovascular pharmacology, where the use of predictive modeling and the integration of big data are changing drug development processes and patient care.[49] AI's transformative power is demonstrated in the field of retro drug design, where it aids in developing new small-molecule drugs with specific properties, making the discovery of therapeutic agents more efficient.[50]

Personalized Medicine

It is advantageous to integrate AI within the approach of personalized medicine because of the complexity of diseases, such as cancer and genetic disorders, where standard therapies are nonproductive.[51,52] Personalized medicine is a process in which drug treatments are developed for a particular person by taking into consideration the genetic profile, biomarkers, and other characteristics of the client. AI enhances this process through the optimization of drug development, patient eligibility, dose regimes, and biomarker discovery through the use of modeling algorithms.[46] Moreover, the involvement of AI also has a part in customizable medicine, such as employing patient-derived models, including the organoids of a tumor, for swift drug screening. These models are individualized treatment options, particularly for patients who have undergone all the conventional clinical approaches.[53]

Challenges of AI in Drug Discovery

While there have been significant advancements, several research areas still lack adequate information. A significant barrier to the development of AI in drug discovery is that many pharmaceutical datasets are

proprietary and, therefore, not publicly available to allow researchers a suitable volume of training data with which they can validate their models. Not only that, the data is often unreliable or incomplete and may suffer from sampling issues—it might be biased (not a true representation of society)—and records can exist in different units across sites and could fail complete standardization between sources.

Sophisticated biological systems can be difficult for AI to adequately model, frequently leading to oversimplifications in the predictions. Moreover, such models may not be able to capture the inherent dynamical behavior of bio-networks where interactions could evolve in complex manners depending on different factors other than time (such as condition variation and disease). An additional challenge for AI in drug discovery is regulation. Government agencies such as the US Food and Drug Administration (FDA) need a great deal of proof and have very strict rules around validation, which even AI-created drugs must follow. The validation of AI models and their predictions is a moving target but a far more nuanced process, which may delay regulatory approval for the discovery of new drugs by AI.

Yet another challenge is the integration of AI with existing drug discovery pipelines. Traditional processes for drug discovery are well defined and go through a lot of phases, starting from target identification to clinical trials. The integration of AI into this process will mean drastic changes in workflows, collaborative work between AI experts and domain scientists, and resistance to change in organizations. The development and deployment of AI models in drug discovery come at extremely high costs. Other components that could be costly are high-performance computing, domain-specific software, and access to large datasets. In addition, updates for training the model with new data may also escalate the cost further. Moreover, AI might lead to an affinity of models to a compound type, target, or patient population, causing biased results in drug development.

Conclusion

The integration of AI into the course of drug discovery is drastically changing the future of medicine. AI is advancing at a fast pace, enriching the processes of personalized medicine, making a large number of data analyses fast, assessing the potential of drugs, and enhancing treatment plans. This technology is helping to speed up the process of coming up with new medications and delivering treatment that is more personalized by considering the genes of an individual and even the molecular composition of the body. As discussed above, the rising application of AI in the field of drug discovery is expected to revolutionize health care in terms of predictiveness, preventiveness, and personalization in the near future. There is a good chance that AI's role in medicine's future will enable better cures, superior patient outcomes, and the likelihood of conquering complex diseases more efficiently than at present.

References

1 Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. Drug Discov Today. 2021;26(1):80–93.
2 Artificial Intelligence in Drug Discovery Market Size Report, 2032. Global Market Insights. Available from: https://www.gminsights.com/industry-analysis/ai-in-drug-discovery-market (2024, accessed 26 August 2024).
3 Artificial Intelligence (AI) In Drug Discovery Market Report by 2030. Fortune Business Insights. Available from: https://www.fortunebusinessinsights.com/artificial-intelligence-in-drug-discovery-market-105354 (2024, accessed 26 August 2024).
4 Gholap AD, Uddin MJ, Faiyazuddin M, Omri A, Gowri S, Khalid M. Advances in artificial intelligence for drug delivery and development: a comprehensive review. Comput Biol Med. 2024;178:108702.
5 Khaire S, Bhaladhare P. A comprehensive review on machine learning and deep learning methods in drug discovery. Int J Recent Innov Trends Comput Commun. 2022;10:1–8.
6 Muller C, Rabal O, Diaz Gonzalez C. Artificial intelligence, machine learning, and deep learning in real-life drug design cases. Methods Mol Biol. 2022;2390:383–407.
7 Cesaro A, Bagheri M, Torres M, Wan F, de la Fuente-Nunez C. Deep learning tools to accelerate antibiotic discovery. Expert Opin Drug Discov. 2023;18(11):1245–57.
8 Singh DP, Kaushik B. A systematic literature review for the prediction of anticancer drug response using various machine-learning and deep-learning techniques. Chem Biol Drug Des. 2023;101(1):175–94.
9 Nussinov R, Zhang M, Liu Y, Jang H. AlphaFold, artificial intelligence (AI), and allostery. J Phys Chem B. 2022;126(34):6372–83.
10 Satpathy R. Artificial intelligence techniques in the classification and screening of compounds in computer-aided drug design (CADD) process. In: Artificial Intelligence and Machine Learning in Drug Design and Development. Wiley, pp. 473–97.
11 Lee JW, Maria-Solano MA, Vu TNL, Yoon S, Choi S. Big data and artificial intelligence (AI) methodologies for computer-aided drug design (CADD). Biochem Soc Trans. 2022;50(1):241–52.
12 Rawat S, Subramaniam K, Subramanian SK, Subbarayan S, Dhanabalan S, Chidambaram SKM, et al. Drug repositioning using computer-aided drug design (CADD). Curr Pharm Biotechnol. 2024;25(3):301–12.
13 Del Carmen Quintal Bojórquez N, Campos MRS. Traditional and novel computer-aided drug design (CADD) approaches in the anticancer drug discovery process. Curr Cancer Drug Targets. 2023;23(5):333–45.
14 Niu Y, Lin P. Advances of computer-aided drug design (CADD) in the development of anti-Alzheimer's-disease drugs. Drug Discov Today. 2023;28(8):103665.
15 Floresta G, Zagni C, Patamia V, Rescifina A. How can artificial intelligence be utilized for de novo drug design against COVID-19 (SARS-CoV-2)?. Expert Opin Drug Discov. 2023;18(10):1061–4.
16 Perron Q, Mirguet O, Tajmouati H, Skiredj A, Rojas A, Gohier A, et al. Deep generative models for ligand-based de novo design applied to multi-parametric optimization. J Comput Chem. 2022;43(10):692–703.
17 Sharma V, Singh A, Chauhan S, Sharma PK, Chaudhary S, Sharma A, et al. Role of artificial intelligence in drug discovery and target identification in cancer. Curr Drug Deliv. 2024;21(6):870–86.
18 Suresh T, Kaliappan S, Ali HM, Vijay Kumar B AI-driven drug discovery and therapeutic target identification for rare genetic diseases. In: 2024 International Conference on Advancements in Smart, Secure and Intelligent Computing (ASSIC). IEEE. 2024. pp. 1–6.
19 Long X, Steurer B, Wong CW, Kozlova E, Naumov V, Pun FW et al. AI-enabled cancer target prioritization with optimal profiles balancing novelty, confidence and commercial tractability. Futur Med AI. 2. Epub ahead of print March 2024. DOI: 10.2217/fmai-2023-0019.
20 Wang CC, Pun FW, Liu BHM, Lin Y, Ren F, Zhavoronkov A. #296 : identification and validation of two novel therapeutic targets for endometriosis with artificial intelligence (AI). Fertil Reprod. 2023;5:645.
21 Olsen A, Harpaz Z, Ren C, Shneyderman A, Veviorskiy A, Dralkina M, et al. Identification of dual-purpose therapeutic targets implicated

in aging and glioblastoma multiforme using PandaOmics – an AI-enabled biological target discovery platform. Aging (Albany NY). 2023;15(8):2863–76.
22 Zhang H, Pan J, Wu X, Zuo AR, Wei Y, Ji ZL. Large-scale target identification of herbal medicine using a reverse docking approach. ACS Omega. 2019;4(6):9710–9.
23 Elsanhoury R, Alasmari A, Parupathi P, Jumaa M, Al-Fayoumi S, Kumar A, et al. AI & experimental-based discovery and preclinical IND-enabling studies of selective BMX inhibitors for development of cancer therapeutics. Int J Pharm. 2023;645:123384.
24 Chikhale RV, Choudhary R, Malhotra J, Eldesoky GE, Mangal P, Patil PC. Identification of novel hit molecules targeting M. tuberculosis polyketide synthase 13 by combining generative AI and physics-based methods. Comput Biol Med. 2024;176:108573.
25 Subramanian N, Maignan N, Tieo G, Ravinder R, Martin S, Jeitany M, et al. 103P Using AI to break new ground in oncological drug discovery: rapid identification of novel targets and polypharmacological compounds for effective liposarcoma treatment. ESMO Open. 2024;9:102492.
26 Sampene AK, Nyirenda F. Evaluating the effect of artificial intelligence on pharmaceutical product and drug discovery in China. Futur J Pharm Sci. 2024;10:58.
27 Zeng X, Zhu S, Lu W, Liu Z, Huang J, Zhou Y, et al. Target identification among known drugs by deep learning from heterogeneous networks. Chem Sci. 2020;11(7):1775–97.
28 Zhavoronkov A, Ivanenkov YA, Aliper A, Veselov MS, Aladinskiy VA, Aladinskaya AV, et al. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nat Biotechnol. 2019;37(9):1038–40.
29 Jiménez J, Škalič M, Martínez-Rosell G, De Fabritiis G. KDEEP: protein-ligand absolute binding affinity prediction via 3D-convolutional neural networks. J Chem Inf Model. 2018;58(2):287–96.
30 Wang S, Du Z, Ding M, Rodriguez-Paton A, Song T KG-DTI: a knowledge graph based deep learning method for drug-target interaction predictions and Alzheimer's disease drug repositions. Appl Intell. 2022;52 846–57.
31 Fialková V, Zhao J, Papadopoulos K, Engkvist O, Bjerrum EJ, Kogej T, et al. LibINVENT: reaction-based generative scaffold decoration for in silico library design. J Chem Inf Model. 2022;62(9):2046–63.
32 Moon S, Zhung W, Yang S, Lim J, Kim WY. PIGNet: a physics-informed deep learning model toward generalized drug-target interaction predictions. Chem Sci. 2022;13(13):3661–73.
33 Blaschke T, Arús-Pous J, Chen H, Margreitter C, Tyrchan C, Engkvist O, et al. REINVENT 2.0: an AI tool for de novo drug design. J Chem Inf Model. 2020;60(12):5918–22.
34 Wang M, Hsieh CY, Wang J, Wang D, Weng G, Shen C, et al. RELATION: a deep generative model for structure-based de novo drug design. J Med Chem. 2022;65(13):9478–92.
35 Shirolkar A, Kethar J, Appavu R. The process of AI-aided drug design. J Student Res. 12. Epub ahead of print 30 November 2023. DOI: 10.47611/jsrhs.v12i4.5630.
36 Walters WP, Barzilay R. Critical assessment of AI in drug discovery. Expert Opin Drug Discov. 2021;16(9):937–47.
37 Quinn TR, Giblin KA, Thomson C, Boerth JA, Bommakanti G, Braybrooke E, et al. Accelerated discovery of carbamate Cbl-b inhibitors using generative AI models and structure-based drug design. J Med Chem. 2024;67(16):14210–33.
38 Shirani H, Hashemianzadeh SM. Quantum-level machine learning calculations of Levodopa. Comput Biol Chem. 2024;112:108146.
39 Saito R, Nakada T. Insights into drug development with quantitative systems pharmacology: a prospective case study of uncovering hyperkalemia risk in diabetic nephropathy with virtual clinical trials. Drug Metab Pharmacokinet. 2024;56:101019.
40 Williamson DJ, Struyven RR, Antaki F, Chia MA, Wagner SK, Jhingan M, et al. Artificial intelligence to facilitate clinical trial recruitment in age-related macular degeneration. Ophthalmol Sci. 2024;4(6):100566.
41 Chen A, Montesano G, Lu R, Lee CS, Crabb DP, Lee AY. Visual field endpoints for neuroprotective trials: a case for AI-driven patient enrichment. Am J Ophthalmol. 2022;243:118–24.
42 Zielinski JM, Luke JJ, Guglietta S, Krieg C. High throughput multi-omics approaches for clinical trial evaluation and drug discovery. Front Immunol. 2021;12:590742.
43 Nicora G, Vitali F, Dagliati A, Geifman N, Bellazzi R. Integrated multi-omics analyses in oncology: a review of machine learning methods and tools. Front Oncol. 2020;10:1030.
44 Goff A, Cantillon D, Muraro Wildner L, Waddell J. Multi-omics technologies applied to tuberculosis drug discovery. Appl Sci. 2020;10:4629.
45 Lu J-M, Pan J-Z, Mo Y-M, Fang Q. Automated intelligent platforms for high-throughput chemical synthesis. Artif Intell Chem. 2024;2:100057.
46 Paliwal A, Jain S, Kumar S, Wal P, Khandai M, Khandige PS, et al. Predictive modelling in pharmacokinetics: from in-silico simulations to personalized medicine. Expert Opin Drug Metab Toxicol. 2024;20(4):181–95.
47 Husnain A, Rasool S, Saeed A. Revolutionizing pharmaceutical research: harnessing machine learning for a paradigm shift in drug discovery. Int J Multidiscip Sci Arts. 2023;2:149–57.
48 Nwosu SN. Revolutionizing drug discovery: the impact of artificial intelligence on efficiency and accuracy. J Adv Med Pharm Sci. 2024;26:56–63.
49 Alex H. SmartBeats: riding the wave of AI innovation in cardiovascular pharmacology. Int J Multidiscip Res; 6. Epub ahead of print 28 January 2024. DOI: 10.36948/ijfmr.2024.v06i01.12587.
50 Wang Y, Michael S, Yang SM, Huang R, Cruz-Gutierrez K, Zhang Y, et al. Retro drug design: from target properties to molecular structures. J Chem Inf Model. 2022;62(11):2659–69.
51 Chinnaiyan K, Mugundhan SL, Narayanasamy D. Revolutionizing healthcare and drug discovery: the impact of artificial intelligence on pharmaceutical development. Curr Drug Ther. 19. Epub ahead of print 19 July 2024. DOI: 10.2174/0115748855313948240711043701.
52 Zahra MA, Al-Taher A, Alquhaidan M, Hussain T, Ismail I, Raya I, et al. The synergy of artificial intelligence and personalized medicine for the enhanced diagnosis, treatment, and prevention of disease. Drug Metab Pers Ther. 2024;39:47–58.
53 Pauli C, Hopkins BD, Prandi D, Shaw R, Fedrizzi T, Sboner A, et al. Personalized *in vitro* and *in vivo* cancer models to guide precision medicine. Cancer Discov. 2017;7(5):462–77.