INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

Review Article

Review on Artificial Intelligence in Drug Discovery

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ARTICLE INFO

Published: 30 July 2026
Keywords:
AI techniques in drug discovery, target identification, machine learning.
DOI:
10.5281/zenodo.21713032

ABSTRACT

By increasing the speed, precision, and effectiveness of pharmaceutical research, artificial intelligence (AI) is revolutionizing the field of drug design and discovery. Conventional drug discovery is a drawn-out, costly, and intricate process that frequently necessitates years of study and substantial financial outlay. In order to overcome these obstacles, artificial intelligence (AI) methods such as machine learning (ML), deep learning (DL), natural language processing (NLP), reinforcement learning (RL), and quantum computing (QC) have become effective tools. Rapid target identification, virtual screening, de novo drug design, lead optimization, toxicity prediction, drug repurposing, and enhanced clinical trial management are all made possible by these technologies. AI-driven methods enable precision medicine through individualized treatment plans, improve prediction accuracy, lower development costs, and speed up drug discovery. Despite its enormous promise, there are still issues including poor data quality, interpretability of the model, ethical dilemmas, and regulatory obstacles. All things considered, AI is a game-changing technology that is changing pharmaceutical research and hastening the creation of safer and more potent treatments for a variety of illnesses

INTRODUCTION

The impact of AI extends into many domains, including healthcare, finance, and transportation, where it powers applications ranging from personalized recommendations to automated diagnostics. As the demand for AI-driven solutions grows, the evolution of these techniques continues to advance, promising a future in which AI could play an increasingly central role in addressing complex global challenges and enhancing human capabilities AI has an impact on a wide range of industries, including healthcare, banking, and transportation, where it powers anything from automated diagnosis to tailored suggestions. The development of these methods keeps progressing as the need for AI-driven solutions increases, suggesting a future in which

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

AI may become more and more important in solving difficult global problems and improving human potential. By providing cutting-edge techniques that speed up the identification and development of new pharmaceuticals and drastically cut down on the time and expenses involved with conventional processes, artificial intelligence (AI) is transforming the field of drug design and discovery. It frequently takes years of research and billions of dollars to bring a single medicine from conception to market due to the inherent complexity and resource-intensive nature of drug discovery. [1-3]

However, by speeding up important phases of drug research, such as target identification, drug interaction prediction, and molecular structure optimization, AI has transformative potential. Additionally, scientists can select the drugs most likely to succeed in clinical trials by using deep learning algorithms to unravel complicated correlations within molecular data. Precision medicine, de novo drug discovery, and virtual screening have all benefited from recent developments in AI integration. Virtual screening reduces the number of compounds that require physical testing by using AI to predict molecular interactions with target proteins. AI creates completely new molecular structures with desirable features in de novo drug design, allowing researchers to concentrate on the most promising candidates right away. [4-6]

AI has emerged as a key technology in several fields, enabling systems to carry out activities that have historically required human intelligence. A variety of approaches, each suited to certain applications and difficulties, are among the fundamental AI strategies propelling this revolution. [7-8]

AI TECHNIQUES IN DRUG DISCOVERY:

Drug discovery has historically been a drawn-out, complicated, and expensive process that frequently takes more than 10 years and billions of dollars to bring a new medication to market. Artificial Intelligence (AI) has become a potent tool in contemporary pharmaceutical research due to the proliferation of biomedical data and the increasing need for quicker and more effective medication discovery. From target selection and molecule design to preclinical testing and clinical trial optimization, AI approaches are transforming every phase of the drug discovery process. Machine Learning (ML), Deep Learning (DL), Natural Language Processing (NLP), Reinforcement Learning (RL), and Quantum Computing (QC) are some of the most influential AI methods. Massive dataset analysis, pattern identification, and predictive modelling are made possible by these techniques, which would be impossible or extremely time-consuming employing traditional approaches. Ai techniques given below.

MACHINE LEARNING (ML):

Because machine learning (ML) algorithms can assess complicated and high-dimensional biological data, they have become an essential tool in current drug discovery. In order to find patterns and forecast future data, machine learning algorithms learn on preexisting datasets. Support vector machines (SVMs) and random forests are two examples of supervised learning approaches that are frequently used to predict pharmacokinetic parameters, toxicity profiles, and drug-target interactions (ADMET). For instance, ML models can forecast a compound's probability of binding to a specific protein, allowing for virtual screening of enormous chemical libraries without the need for expensive trials. Compounds with similar properties can be grouped together or new chemical scaffolds can be found using

unsupervised learning techniques like clustering. Although less popular, reinforcement learning is becoming more popular for chemical synthesis pathway optimization. The combination of ML with high-throughput screening and omics data accelerates target selection and validation, allowing researchers to choose the most promising drug candidates early in the development pipeline . Despite their achievements, machine learning models need large, high-quality datasets and are susceptible to biases or overfitting, which calls for meticulous model validation and interpretability efforts. All things considered, machine learning improves the effectiveness and accuracy of drug research, cutting expenses and time while raising success rates. [9]

DEEP LEARNING (DL):

A subfield of machine learning called deep learning (DL) uses multi-layered neural networks to identify intricate, non-linear correlations in data. DL techniques have transformed the analysis of biological structures and molecular data in drug discovery. When it comes to accurately predicting binding affinities and drug-target interactions, Convolutional Neural Networks (CNNs) are particularly good at interpreting spatial data, such as 3D chemical structures and protein-ligand binding sites. In order to find patterns that conventional models might overlook, Recurrent Neural Networks (RNNs) and their variations examine sequential data, such as chemical sequences (SMILES) or protein sequences. Graph Neural Networks (GNNs), which naturally depict molecules as graphs and allow for the direct modeling of atom connectivity and chemical connections, have had a particularly significant impact in more recent times. DL models have also helped AlphaFold achieve extraordinary accuracy in protein structure prediction, which speeds up target characterization. Despite these developments, the use of DL models may be restricted due to their high computing resource and big labeled dataset requirements. However, these difficulties are being lessened more and more via transfer learning and data augmentation methods. Thus, deep learning plays a critical role in the digital transformation of pharmaceutical research by improving the accuracy and speed of virtual screening, molecular property prediction, and de novo drug discovery. [10]

NATURAL LANGUAGE PROCESSING (NLP):

Techniques for Natural Language Processing (NLP) are becoming more and more crucial for deriving valuable insights from enormous volumes of unstructured biomedical literature, patents, and clinical trial reports. Manual curation is impracticable due to the exponential development of scientific publications; NLP automates information extraction, allowing for the quick identification of pertinent chemical entities, biological targets, and experimental results. While connection extraction models find interactions and pathways and provide structured data for further analysis, named entity recognition (NER) algorithms can identify drug names, genes, and diseases. NLP also makes it easier to create knowledge graphs, which link different data sources to reveal potential biomarkers or new drug repurposing prospects. Transformer-based models like BERT and its biomedical adaptations (BioBERT, SciBERT), which show greater comprehension of domain-specific linguistic nuances, are used in recent developments. Additionally, NLP facilitates the creation of clinical trial protocols and summarizes research findings, which expedites the decision-making process in medication development. While handling contradicting data and deciphering scientific terminology continue to be challenges,

NLP's accuracy and usefulness are being improved by continuous advancements in model architectures and training datasets. All things considered, NLP accelerates research creativity, bridges information gaps, and unlocks the latent knowledge contained in textual data to empower drug discovery.[11]

REINFORCEMENT LEARNING:

An AI method called reinforcement learning (RL) teaches an agent how to make choices by interacting with its surroundings in order to maximize cumulative rewards over time. In contrast to supervised learning, reinforcement learning (RL) learns optimal techniques by trial and error under the guidance of feedback signals (rewards or penalties). RL has become a potent technique in drug development for optimizing intricate, multi-step procedures including pharmacological property optimization, synthesis planning, and molecular design. By characterizing chemical synthesis or molecular modification as sequential decision-making processes, RL frameworks facilitate the creation of novel compounds. Iteratively altering molecular structures, the agent is rewarded according to factors such as drug-likeness, binding affinity, toxicity, or synthetic accessibility. RL models outperform conventional rule-based or heuristic methods by using this dynamic exploration to find novel molecules that simultaneously satisfy several requirements. Furthermore, by adding domain-specific reward functions, RL can be integrated with generative models, like Variational Autoencoders or Generative Adversarial Networks, to further direct molecule production toward desired attributes. In addition to molecular design, RL is used in synthetic route optimization, where the agent learns effective chemical reaction paths to produce target compounds at a lower cost and in less time in the laboratory. Nonetheless, there are still difficulties in creating suitable reward functions that strike a compromise between conflicting goals and guaranteeing adequate chemical space exploration without reaching local optima. Pipelines due to its capacity to learn from consecutities. [12-13]

QUANTUM COMPUNTING (QC):

By utilizing quantum mechanical phenomena like superposition and entanglement to carry out some computations tenfold faster than conventional computers, quantum computing (QC) offers a paradigm change in processing capacity. Because molecular interactions are intrinsically quantum and chemical simulations are difficult for classical computers to accurately model, QC has great potential in drug discovery. Quantum algorithms allow for precise simulation of molecular electronic structures and protein folding, which are essential for comprehending drug-target interactions at an atomic level. This capacity could speed up lead optimization and cut down on expensive experimental repeats by significantly increasing the accuracy of predicting binding affinities, reaction routes, and physicochemical attributes. The magnitude and complexity of issues that can be successfully solved are limited by the fact that current quantum technology is still in the noisy intermediate-scale quantum (NISQ) period. Nonetheless, small-molecule simulations and optimization issues related to drug discovery are already being investigated using hybrid quantum-classical algorithms as the Quantum Approximate Optimization Algorithm (QAOA) and Variational Quantum Eigensolver (VQE). Businesses and academic teams are looking into QC to improve protein design, molecular docking simulations, and even combinatorial optimization of chemical libraries. Even though quantum computing technology is still in its infancy, its potential to transform drug development by providing

unmatched simulation accuracy and resolving challenging computational issues has spurred substantial investment and research efforts globally. QC is anticipated to become a crucial element in the pharmacological AI toolset as quantum hardware develops. [14-15]

AI IN DRRUG DESIGN AND DRUG DISCOVERY

TARGET IDENTIFICATION:

In order to direct the creation of novel treatments, target identification is a crucial stage in the drug discovery process. Potential biological targets are frequently proteins or genes linked to certain diseases. AI models have become indispensable in this procedure due to their sophisticated analytical skills. They can find patterns and connections that conventional techniques would overlook by analyzing large biological and chemical datasets, such as proteomics, metabolomics, and genomes. AI can expedite the discovery of viable therapeutic targets by sorting through large and complicated information, perhaps leading to more accurate and effective drug development. For instance, deep learning methods may aid in the prediction of protein–protein interactions that are crucial to disease pathways, while machine learning models can analyze genomic data to find genetic markers and mutations associated with particular diseases. Researchers can obtain important insights from scientific publications, patents, and clinical trial data by using natural language processing (NLP) in AI systems, which offers a comprehensive method for target identification. Precision medicine is progressing quickly thanks to this combination of computational techniques and biological sciences, which also has great potential for novel and focused drug discovery strategies. To find possible biological targets, the AI models analyze massive datasets like proteomics and genomes. [16]

DRUG DESIGN AND LEAD IDENTIFICATION:

Once a viable biological target has been found, the drug design and lead identification process becomes much more efficient. AI currently plays a crucial part in this phase, especially through virtual screening, which makes it possible to quickly analyze enormous compound libraries in order to choose those that have the best chance of interacting with the target. Advanced AI techniques, such deep learning models taught to predict drug-target interactions based on structural traits, are increasingly being added to traditional virtual screening methods to improve accuracy and efficiency. Generative AI models have brought a new method to medication design in addition to screening already-existing molecules. New, drug-like compounds can be created from start using methods like reinforcement learningal gorithms and Generative Adversarial Networks (GANs). This method offers creative solutions for creating leads with a high chance of success in clinical testing, significantly broadening the chemical area investigated in drug development. AI's influence on lead identification and drug design has revolutionary potential, enabling the development of targeted treatments more quickly and effectively than with conventional techniques. The potential of AI to transform healthcare and meet unmet clinical requirements is highlighted by this paradigm shift in drug discovery. [17]

LEAD OPTIMIZATION:

In order to optimize the biological activity, pharmacokinetics, and safety profiles of chemical compounds known as leads, lead optimization is a critical stage in the drug development process. Optimization efforts concentrate on increasing a lead compound's potency, selectivity, and stability while reducing toxicity and unfavorable side effects after it has encouraging biological activity

in vitro or in vivo. Under the direction of structural-activity relationship (SAR) research, the approach usually entails methodical modifications to the lead's molecular structure. By offering insights into the interactions between the drug candidate and its target protein, advances in computational methods like molecular docking and quantitative structure-activity relationship (QSAR) modeling have greatly improved lead optimization. [18]

DRUG REPURPOSING:

Finding new applications for already-approved medications is referred to as "drug repurposing," sometimes called "drug repositioning." Due of its potential to shorten the time and expense involved in medication development, this strategy has attracted a lot of interest lately. Drug repurposing is investigating the therapeutic effects of medications that have already been approved for other conditions, as contrast to traditional drug discovery, which begins with the identification of a new molecular target. Repurposed medications can avoid early-stage preclinical and clinical testing, resulting in quicker clinical deployment, making this technique especially useful in solving unmet medical needs. Furthermore, repurposing might provide treatments for uncommon or neglected illnesses for which conventional drug discovery pipelines would not be as effective because of a lack of commercial rewards.By examining enormous databases of current medications and illness models, recent developments in computational techniques, such as network pharmacology and AI-driven algorithms, have improved the detection of repurposing potential. Repurposing drugs has the potential to improve patient outcomes in a wide range of therapeutic areas as well as to respond quickly to new health emergencies like the COVID-19 pandemic. [19]

CLINICAL TRIAL AND PATIENT STRATIFICATION:

Before new medications are put on the market, clinical studies are crucial for assessing their efficacy and safety. But performing clinical studies is a difficult, expensive, and time-consuming process. The capacity to find and enlist the appropriate patient population is crucial to the success of these trials. Patients have historically been chosen using broad eligibility criteria, which may not always accurately reflect the diversity of illnesses and how each patient reacts to a particular course of treatment. Because of this, a lot of trials encounter difficulties like sluggish enrollment, large dropout rates, and inadequate proof of efficacy across a variety of patient categories. Particularly in the domain of patient stratification, recent developments in AI have demonstrated tremendous potential for revolutionizing the clinical trial process. Large datasets, such as genetic data, demographics, medical histories, and response data from prior trials, can be analyzed by AI-driven models to determine which patient populations are most likely to benefit from a new medication. By enabling a more accurate selection of trial participants, these predictive models optimize trial design and raise the likelihood of success.

AI can help stratify patients into discrete subgroups, each of which may react differently to the medication under test, by finding biomarkers that correlate with treatment response. In order to enhance patient recruitment and result prediction, AI technologies can also aid in the study of real-world evidence (RWE), integrating data from electronic health records (EHRs) and other non-clinical settings. By reducing the requirement for sizable, diverse trial cohorts, the application of AI can help shorten trial duration and lower expenses. Particularly in personalized medicine techniques,

where the objective is to customize therapy to each patient rather than using a one-size-fits-all approach, it can speed up the identification of beneficial treatments. In the end, AI-driven patient stratification is opening the door to more effective, focused, and fruitful clinical trials. [20-21]

TOXICITY PREDICTION

Because adverse drug reactions (ADRs) can result in expensive failures, delays in clinical trials, or even the removal of pharmaceuticals from the market, toxicity prediction is a crucial challenge in drug development. Early in the drug development process, AI and machine learning (ML) models have become indispensable tools for forecasting the toxicity of chemical compounds, providing a way to evaluate safety prior to the start of clinical trials. Analyzing chemical compounds to forecast their possible toxicity is one of the most significant applications of AI. Molecular structural patterns that correlate to toxicological effects can be found using methods like support vector machines (SVM) and deep learning. Biological interactions and methods of action, such as protein binding, metabolic processes, and receptor interactions, are also taken into account by AI models. Forecasting these interactions can help determine which biological systems a substance may impact and how it would behave in the human body. AI is used by a number of toxicity prediction programs, including Tox21 and DEREK Nexus, to forecast results based on established biological pathways. Numerous research have demonstrated the potential of AI, which has significantly improved the effectiveness and accuracy of drug development. In large drug screening databases like ChEMBL and PubChem, AI-driven virtual screening methods, such as deep neural networks (DNNs) and graph convolutional networks (GCNs), have achieved 80–90% accuracy in distinguishing between active and inactive chemicals. Additionally, compared to traditional techniques like AutoDock and Glide, AI-assisted docking technologies like Deep Dock and GNINA have shown Pearson correlation coefficients (r) ranging from 0.75 to 0.85 with experimental binding affinities. AI-driven drug design has successfully found at least 15 novel compounds that have advanced to clinical trials, and the use of AI in hit discovery has produced a 40–60% increase in success rates compared to traditional high-throughput for COVID-19 treatment is an example of how artificial intelligence has accelerated medicine repurposing, reducing the time from 5-7 years to just 1-3 years. Additionally, AI has reduced drug development costs by 20–30%, saving up to $300 million per drug. It has also shortened the time it takes to find new drugs from four to six years to one to two years. At least five AI-generated medications have entered clinical trials as a result of AI-driven de novo drug discovery, with experimental validation success rates of roughly 60%, far above the 20–30% success rates of traditional approaches. Furthermore, DeepTox and ADMETlab, two AI models for ADMET prediction, have shown an accuracy of 80–95% in predicting toxicity, solubility, and bioavailability, highlighting their superiority over conventional QSAR models. These results demonstrate AI's growing dependability and effectiveness in medication design and discovery, highlighting its revolutionary impact on the pharmaceutical industry. [22-24]

FUTURE DIRECTIONS

With a clear emphasis on exploratory case studies and model prototypes, the literature on generative AI in pharmaceutical drug discovery is still in its infancy. As the field develops, a number of research gaps emerge that need to be filled in order

to properly utilize AI's purported promise in pharmaceutical innovation.

First, a dearth of research in the preclinical and particularly the clinical domains is shown by the disproportionate concentration of studies in the discovery phase. Later stages of drug discovery involve more biological and regulatory complexity, which generative AI has not yet adequately addressed, reflecting the uneven maturity of evidence across phases. Early drug discovery benefits from the high degree of computational control and the availability of large molecular datasets.

The lack of methodological consistency between studies is another significant gap. Comparability between studies is hampered by the fact that many papers use proprietary datasets or describe internally generated generative models with poor reproducibility. It is challenging to assess the relative strengths, generalizability, or limitations of generative architectures—like GENTRL, Dr. VAE, and Deep VCT—across various phases of drug development due to the lack of comparative benchmarking. Future studies should prioritize open datasets, honest reporting, and the use of established performance indicators that enable methodical model comparisons in order to progress the field.

Similar restrictions have been reported in related clinical domains outside of pharmaceutical research and development. A recent analysis of artificial intelligence in diagnostic imaging, clinical decision support, pathology, surgery, and drug discovery reveals enduring issues such data bias, limited explainability, retroactive validation, and ambiguous regulatory pathways. Additionally, validation procedures need to be improved. Nowadays, a lot of research uses in silico benchmarks or retrospective datasets to evaluate the usefulness of AI-generated output. Although these methods provide first insights, they do not take the place of experimental validation, which is still necessary to determine biological plausibility and translational potential. To verify the dependability and practical effects of generative techniques, prospective research that incorporate AI outputs into real experimental designs—like virtual trial simulations or predictive toxicity models—are required to close the gap between biological translation and in-silico performance, such effort is necessary.

Lastly, adopting AI responsibly needs to be a major tenet of future research. Despite the fact that generative models provide previously unheard-of creative potential, their "black-box" nature, bias potential, and lack of interpretability continue to be major issues. [25-28]

CHALLENGES AND STRATEGIES FOR AI IN DRUG DISCOVERY:

In the field of drug discovery, artificial intelligence (AI) has revolutionary potential since it can evaluate large datasets, find drug candidates more quickly, and streamline experimental procedures. Nevertheless, despite its benefits, a number of obstacles and restrictions prevent its broad and efficient use. The quality and accessibility of data is one of the main issues. Large and varied datasets are necessary for AI algorithms, especially machine learning (ML) models, to discover significant trends. However, there are frequently insufficient, inconsistent, inadequate, or low-quality data available for drug discovery. Datasets may simply reflect a small range of chemical or biological diversity, have biases, or be improperly annotated. These restrictions lower AI models' precision and generalizability, which may result in erroneous forecasts and poor choices.

Ethical issues are a significant additional problem. AI algorithms are only as impartial and fair as the

training data. The resulting models may yield skewed results if the training data contains biases, such as an overrepresentation of particular groups or drug categories. This can lead to serious concerns about accuracy and fairness, particularly when AI predictions affect clinical research or patient care decisions. Transparent approaches, a variety of datasets, and systems to detect and address potential biases are necessary to guarantee the ethical and equitable use of AI. Researchers are using a number of approaches to deal with these issues. Data augmentation, which creates synthetic data to broaden and diversity the current datasets, is one such tactic. An encouraging strategy involves implementing explainable AI (XAI) techniques, which strive to enhance the transparency and interpretability of AI models' decision-making processes. XAI enables researchers to grasp the reasoning behind specific predictions, addressing issues related to bias and fairness while elucidating the mechanisms and assumptions that inform those projections. It's crucial to note that AI cannot replace conventional experimental techniques or human expertise. Although it can identify potential drug candidates and improve certain aspects of research, hypotheses generated by AI need to be confirmed through laboratory experiments. By combining AI with expert-led experimentation, the drug discovery process can be markedly improved, ultimately speeding up the development of effective new treatments.

CONCLUSION:

By greatly increasing the effectiveness, precision, and affordability of the pharmaceutical development process, artificial intelligence has emerged as a revolutionary force in contemporary drug design and discovery. Every phase of drug discovery, from target identification and molecular design to toxicity prediction and clinical trial optimisation, is supported by cutting-edge AI techniques like machine learning, deep learning, natural language processing, reinforcement learning, and quantum computing. Personalised medicine is made possible by these technologies, which also shorten development times and improve prediction accuracy. Widespread adoption is nevertheless hampered by issues such the scarcity of high-quality data, explainability issues, ethical dilemmas, and the requirement for experimental validation. Future studies should concentrate on strengthening regulatory frameworks, standardising evaluation techniques, enhancing model transparency, and combining AI with lab-based validation.

REFERENCES

1. Goertzel B. Artificial general intelligence: concept, state of the art, and future prospects. Artif Gen Intell 2014;5(1):1–48
2. Esteva A, Kuprel B, Novoa RA, Ko J, Swetter SM, Blau HM, Thrun S. Dermatologist-level classification of skin cancer with deep neural networks. Nature 2017;542(7639):115–8.
3. Silver D, Hubert T, Schrittwieser J, Antonoglou I, Lai M, Guez A, Hassabis D. A general reinforcement learning algorithm that master's chess, shogi, and go through self-play. Science 2018;362(6419):1140–4.
4. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discov Today 2019;24(3):773–80.
5. DiMasi JA, Grabowski HG, Hansen RW. Innovation in the pharmaceutical industry: new estimates of R&D costs. J Health Econ 2016; 47:20–33
6. Pang C, Tong HHY, Wei L, others. Advanced deep learning methods for molecular property prediction. Quant Biol 2023;11(4):395–404.
7. Jim´enez-Luna J, Grisoni F, Schneider G. Drug discovery with explainable artificial intelligence. Nat Mach Intell 2020;2(10):573–84.

8. Jim´enez-Luna J, Grisoni F, Schneider G. Drug discovery with explainable artificial intelligence. Nat Mach Intell 2020;2(10):573–84.
9. Chen C, Wang L, Feng Y, Yao W, Liu J, Jiang Z, Zhao L, Zhang L, Jiang J, Feng S. Spectra-descriptor-based machine learning for predicting protein–ligand interactions. Chem Sci 2025; 16:6355–65.
10. 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.
11. Lee J, Yoon W, Kim S, et al. BioBERT: a pre-trained biomedical language representation model for biomedical text mining. Bioinformatics 2020;36(4): 1234–40
12. Beltagy I, Lo K, Cohan A. SciBERT: a pretrained language model for scientific text. In: Proceedings of the 2019 conference on empirical methods in natural language processing (EMNLP); 2019. p. 3615–20
13. Popova M, Isayev O, Tropsha A. Deep reinforcement learning for de novo drug design. Sci Adv 2018;4(7): eaap7885.
14. McArdle S, Endo S, Aspuru-Guzik A, Benjamin SC, Yuan X. Quantum computational chemistry. Rev Mod Phys 2020;92(1):015003.
15. Aspuru-Guzik A, Lindoy LF, Neven H. The quantum future of drug discovery. Nat Rev Chem 2018;2(3):127–38
16. Kim H, Kim E, Lee I, Bae B, Park M, Nam H. Artificial intelligence in drug discovery: a comprehensive review of data-driven and machine learning approaches. Biotechnol Bioprocess Eng 2020;25(6):895–930.
17. Xia S, Chen E, Zhang Y. Integrated molecular modeling and machine learning for drug design. J Chem Theory Comput 2023;19(21):7478–95.
18. Tripathi MK, Nath A, Singh TP, Ethayathulla AS, Kaur P. Evolving scenario of big data and artificial intelligence (AI) in drug discovery. Mol Divers 2021;25(3): 1439–60.
19. Rifaioglu AS, Atalay V, Martin MJ, Cetin-Atalay R, Atalay A, Dogan ˘ T. Recent applications of deep learning and machine intelligence on in silico drug discovery: methods, tools and databases. Brief Bioinform 2019;20(5):1878–912.
20. Stokes JM, Yang K, Swanson K, Jin W, Cubillos-Ruiz A, Donghia NM, Collins JJ. A deep learning approach to antibiotic discovery. Cell 2020;180(4):688–702.e13.
21. Caicedo JC, Cooper S, Heigwer F, Warchal S, Qiu P, Molnar C, Carpenter AE. Data-analysis strategies for image-based cell profiling. Nat Methods 2017;14(9): 849–63.
22. Jumper, J., Evans, R., Pritzel, A., et al. (2021). Highly accurate protein structure prediction with AlphaFold. Nature, 596(7873), 583–589.
23. 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.
24. Stokes, J. M., Yang, K., Swanson, K., et al. (2020). A deep learning approach to antibiotic discovery. Cell, 180(4), 688–702.e13.
25. Vamathevan, J., Clark, D., Czodrowski, P., et al. (2019). Applications of machine learning in drug discovery and development. Nature Reviews Drug Discovery, 18(6), 463–477.
26. Zhavoronkov, A., Ivanenkov, Y. A., Aliper, A., et al. (2019). Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology, 37(9), 1038–1040.
27. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discov Today 2019;24(3):773–80.
28. Doshi-Velez F, Kim B. Towards a rigorous science of interpretable machine learning. arXiv; 2017.
29. Matta S, Lamard M, Zhang P, Le Guilcher A, Borderie L, Cochener B, Quellec G. A systematic review of generalization research in medical image classification.arXiv; 2024.
30. Ching T, Himmelstein DS, Beaulieu-Jones BK, Kalinin AA, Do BT, Way GP, Ferrero E, Agapow P-M, Zietz M, Hoffman MM, Xie W, Rosen GL, Lengerich BJ, Israeli J, Lanchantin J, Woloszynek S, Carpenter AE, Shrikumar A, Xu J, Greene CS. Opportunities and obstacles

for deep learning in biology and medicine. J R Soc Interface 2018;15(141):20170387.
31. Basu T, Engel-Wolf S, Menzer O. The ethics of machine learning in medical sciences: where do we stand today? Indian J Dermatol 2020;65(4):358–64.
32. Minh D, Wang HX, Li YF, Nguyen TN. Explainable artificial intelligence: a comprehensive review. Artif Intell Rev 2022; 55:3503

HOW TO CITE: Tark Mulani, Suchit Patel, Dr. Khushbu Patel, Dr. C. N. Patel, Review on Artificial Intelligence in Drug Discovery, Int. J. of Pharm. Sci., 2026, Vol 4, Issue 7, 5921-5931. https://doi.org/10.5281/zenodo.21713032