CODEN [USA]: IAJPBB ISSN : 2349-7750

INDO AMERICAN JOURNAL OF
PHARMACEUTICAL SCIENCES

SJIF Impact Factor: 7.187

https://doi.org/10.5281/zenodo.17306293

Available online at: http://www.iajps.com Review Article

A REVIEW ON AI-DRIVEN DRUG DISCOVERY: CURRENT TRENDS AND FUTURE DIRECTIONS

Ragul.M [1], S.Nivetha[2], P. Nandhini[3]

[1] M.Pharm.Department of Pharmacy Practice.ragulmariyappan143@gmail.com

[2] M.Pharm, Department of Pharmacology, nivethasarangapani@gmail.com

[3] M.Pharm.,Department of Pharmacy Practice. nandhinimedicine@gmail.com

Abstract:

The drug discovery process traditionally takes a longer time to be developed and is expensive to the high failure rate, calling for very new implementations to accelerate and optimize the development of therapeutics. The transformational AI has opened several options of data-centric problems to solve during various phases of the drug discovery pipeline. AI methods like machine learning, deep learning, natural language processing, and generative models offer great possibilities in target identification, virtual screening, lead optimization, and clinical trial design. Case studies reveal how AI has been applied for the discovery of new compounds, drug repurposing, and precision medicine. Challenges, however, exist to this day, such as data quality issues, model interpretability, regulatory challenges, and integration into existing pharma frameworks. This review provides an extensive insight into the major AI-driven trends in drug discovery, emphasizing key successes and limitations and taking an inside look into the future, including AI convergence with quantum computing and personalized medicine, to transform the pharmaceutical innovation landscape.

Keywords: *Artificial Intelligence (AI), Drug Discovery, Machine Learning, Deep Learning, Precision Medicine, Computational Drug Design, Pharmaceutical Innovation*

Corresponding author:

Ragul.M,

M.Pharm.Department of Pharmacy

practice.ragulmariyappan143@gmail.com

QR CODE

*Please cite this article in press Ragul.M et al.,**A Review On Ai-Driven Drug Discovery: Current Trends And Future Directions**, Indo Am. J. P. Sci, 2025; 12(10).*

INTRODUCTION:

Drug discovery is a pivotal and foundational process in the creation of pharmaceutical products, and thus involves the identification, development, and validation of novel therapeutic compounds. However, in its long journey from an idea into an actual drug, it is very content with an array of challenges. Conventional approaches are mostly trial-and-error experiments coupled with high-throughput screening and long hours of preclinical testing. In a way, they may be used as a classical scientific way of approaching a problem, but they cannot really anticipate the success of any drug application in the real world. Thus, due to human complexity and the diversity in disease mechanisms, additional layers of uncertainty are being added to the already high-risk task of drug discovery.[1,2,3]

Traditionally, the drug discovery pipeline has been believed to take around 10–15 years, usually costing more than $2 billion for the submission of a successful drug. High attrition rates are particularly marked: occasionally as many as 90% of drug candidates end in clinical trials, fail due to concerns about efficacy or safety. Besides, such inefficiency postpones access to life-saving therapies for patients and taxes the finances of much pharmaceutical companies and research institutions. The very limitations heralding typical drug development approaches represent the fundamental demand for more innovative methodologies that reduce costs, enhance efficiency, and hasten timelines.[4,5]

Artificial Intelligence, or AI, has with recent times emerged as a force of change capable of eliminating many of the long-standing problems plaguing drug discovery. By implementing machine learning, deep learning, and natural language processing, AI systems can so far analyze genomics, proteomics, chemical libraries, clinical data sets, etc.-all immense data-with speed and precision unknown to humans. While the usual computer-aided drug design system is ruled by human knowledge, AI, particularly deep neural networks, can discover concealed patterns in data, select features without human intervention, build predictive models, and even engineer new molecules with a desired set of pharmacological characteristics. AI-assisted biomedical research is burgeoning fast, giving not only the impetus to efficiency but also to the emergence of precision medicine, personalized therapy, and a new gestalt of pharmaceutical innovation.[6,7,8]

FUNDAMENTALS OF AI IN DRUG DISCOVERY

Integration of AI into drug discovery acts as a disruptive force, challenging traditional paradigms of pharmaceutical research. Conventional drug development is mainly characterized by time, costs, and high attrition rates, the latter seeing maximum candidates going through failure during testing, either preclinically or clinically. These computational tools offered by AI analyze voluminous and complex data sets to pinpoint patterns and make inferential predictions that subsequently guide the design or optimization of target therapeutic candidates. Using ML, DL, NLP, and Generative models, AI assists in target identification, virtual screening, lead optimization, and clinical trials.[9]

Artificial Intelligence (AI) : Artificial Intelligence itself is a multidisciplinary field oriented toward developing computational systems that can carry out tasks that would normally be performed by human intelligence. These include problem-solving, pattern recognition, reasoning, and decision-making. In drug discovery, AI considers the complex biological and chemical data, predicts ad hoc therapeutic targets, and consequently negotiates molecular design to speed up the entire process of research.[10]

Machine Learning (ML) : Machine Learning (ML) is a set of methods that provide systems the ability to automatically learn and improve from past experiences without explicitly being programmed for every task at hand. ML methods are highly utilized in drug discovery, predicting molecular properties, classifying compounds, and ranking candidates for experimental testing. By learning patterns from chemical, genomic, and clinical data, ML diminishes in-vivo observations and increases their predictive capabilities.[11]

KEY ALGORITHMS AND MODELS APPLIED

Drug discovery using Artificial Intelligence (AI) is a hypothesis-driven endeavor that applies various kinds of algorithms and computational models designed to analyze complex datasets, detect patterns, and project predictive insights. These algorithms range from deep learning networks capable of modeling complex molecular interactions to natural language processing tools that extract actionable pieces of information from unstructured biomedical literature. Reinforcement learning iteratively optimizes molecular structures, whereas generative models design truly new compounds with the pharmacological characteristics desired. All these AI methods comprise this versatile toolkit that can foster any process through the drug-discovery pipeline, from target identification and virtual screening to lead optimization and preclinical evaluation. Knowledge of these major models allows one to appreciate processes through which AI speed drug

development and transform the paradigm of traditional pharmaceutical research.[13]

Deep Learning (DL): Deep Learning can be thought of as a type of machine learning in which multilayered neural networks are employed to depict complicated nonlinear relationships among large datasets. DL also finds extensive application in drug discovery for molecular property prediction, chemical structure analysis, and biological interaction modeling. Virtual screening will all be done with great precision, together with active compound prediction and de novo drug design. In experimental terms, it is a win-win situation: reducing cost and timelines.[14]

Natural Language Processing (NLP): Natural Language Processing (NLP) is a branch of AI concerned with the conversion of unstructured textual data into meaningful information. Such data include scientific literature, patents, and reports from clinical trials. In drug discovery, one of the applications of NLP is to identify potential drug targets, while other applications include drug repurposing and identifying hidden relationships among diseases and therapeutic compounds. These actions help to hasten hypothesis generation and facilitate early drug development processes.[15]

Reinforcement Learning (RL) : One approach to reinforcement learning has the agent learning to make decisions based on trial and error within an environment, where rewards and penalties guide it. In drug discovery, the RL is used to iteratively optimize molecular structures to design compounds that exhibit the highest possible level of desired property, such as efficacy, solubility, and safety. Thus, the approach helps make lead optimization and new compound generation more efficient.[16]

Generative Models : With generative models like Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs), new chemical structures are generated with the intention that they exhibit certain pharmacological properties. These molecules are designed from scratch using specific criteria like binding affinity or drug-likeness for de novo drug discovery. Thus, generative models complement other AI strategies by creating a larger chemical space to increase the pace at which potential drug candidates are discovered.[17]

INTEGRATION OF COMPUTATIONAL BIOLOGY WITH AI

Computational biological systems with AI are truly an efficiency and reliable drug finding interface. Computational biology offers mechanistic insights into molecular pathways, protein–ligand interactions, and complex disease networks: one basic framework maintains AI-driven prediction. When the above biological insights and information are fused, the AI algorithms such as deep learning and reinforcement learning are harnessed to model molecular interactions, predict therapeutic potential, and finally optimize candidate compounds before experimental validation. This accelerated lead finding hence makes the compounds more target-specific and cheaper. It also aids in precision medicine by designing therapies based on the genetic and molecular profile of the patient, thus bridging the gap from computational prediction to clinical evaluation.[18]

HISTORICAL EVOLUTION OF AI IN DRUG DEVELOPMENT

The concept of computational tools in drug discovery goes back to the 1960s and 1970s when the first CADD methods were put in place. Earlier methods had rule-based systems, molecular modeling, and QSAR analyses for chemical property prediction and activity against a biological target. Even though they were rough with respect to modern techniques, they paved the first step towards the integration of computational methods into pharmaceutical research.[18]

The 1990s and early 2000s introduced more sophisticated algorithms, including machine learning algorithms capable of learning from experimental data and inferring predictions: support vector machines, decision trees, and clustering methods had been applied to virtual screening, target identification, and toxicity prediction, thereby bringing data-driven approaches into the limelight in accelerating drug discovery.

With recent advances in big data, high throughput screening, and deep learning technologies, AI-based systems prospered in the past decade. The deep learning applications in the present scenario now include deep neural networks, reinforcement learning, natural language processing, and generative models for de novo drug design and drug repurposing, as well as precision medicine strategies. This evolution represents a philosophical shift-from algorithms-as-tools to intelligent systems capable of adapting and potentially transforming pharmaceutical research.[19]

APPLICATIONS OF AI IN DRUG DISCOVERY

Artificial Intelligence (AI) has been implemented as a transformative tool along multiple stages of the drug discovery pipeline. Given large-scale chemical, biological, and clinical datasets, AI provides the option of making faster, more accurate predictions and decisions relative to a usual approach. From early target identification to clinical development, its applications facilitate

efficient hit discovery, lead optimization, and precision medicine strategies.[20]

Target Identification and Validation

Traditionally, identification and validation of therapeutic targets have required much experimental research and thus form a crucial early step in drug discovery. This process has now been transformed by AI, which can very quickly analyze large-scale biological datasets comprising genomics, transcriptomics, and proteomics. Machine learning algorithms can identify genes for diseases, analyze protein-protein interaction networks, and predict druggability of targets to prioritize the ones with the best therapeutic potential. Deep learning methods further promote this by discovering intricate non-linear relationships existing between molecular features and disease phenotypes that conventional statistical methods would probably miss. Also, AI could correlate multi-omics datasets with patient-derived data to identify biomarkers and validate targets' clinical relevance. Hence, AI aids in fast identification and biologically relevant target-mediated optimization, providing a basis for more efficient downstream drug development by reducing the need for cumbersome experiments.[21,22]

Hit Identification and Virtual Screening

Initial screening of massive chemical libraries is required to identify potential therapeutic activity in a compound. The usual high-throughput screening (HTS) approach is slow and expensive, experimentally testing up to the millions of compounds. Virtual screening through ML and deep learning methods now predicts the activity of compounds and prioritizes them for their higher chances of interacting with specific targets. Further, generative models will navigate chemical space beyond known compounds and offer novel candidates with desired properties. Reinforcement learning on the other hand aims to restructure molecules iteratively while optimizing predicted activities. The AI can also determine binding affinities from structural biology data, including protein-ligand interactions. Computational approaches cut down on the total number of compounds requiring in-lab testing and consequently reduce cost and speed up drug discovery at the very early stage. The beginning of AI-assisted virtual screening has successfully led to the discovery of weapons for inhibitors against targets of oncology, infectious diseases, and metabolism, hence revolutionizing the way to hit discovery.[23,24]

Lead Optimization

Once hit compounds are detected, lead optimization adjusts their chemical structures to improve key parameters such as their efficacy, safety profile, and pharmacokinetic behavior. AI applications are critical here, mainly by harnessing feature-prediction capabilities in molecular properties such as solubility, bioavailability, toxicity, and off-targeting effects on a variety of proteins. Generative models such as Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) may be used for generating several novel chemical analogs with desired properties, followed by the molecular modification of reinforcement learning-based methods to satisfy the criteria. Many other machine learning (ML) models are put to use in this step to forecast metabolic stability and drug-drug interactions that may occur and thus weed out as many late-stage failures as possible. By incorporating multi-parameter optimization into the design stage, AI fast-tracks the elevation of initial hits to high-quality lead candidates: thereby reducing timelines in the later stages, increasing the success rates at preclinical and clinical levels, and subsequently reducing costs attached to the drug development pipeline while enhancing the pipeline's overall efficiency.[25,26]

Preclinical and Clinical Development

AI has applications extended into the preclinical phase and clinical phases for better prediction purposes of drug efficacy, drug safety, and patient response. Preclinically, AI models simulate biological interactions; they go on to predict toxicities and symptoms and to identify prospective biomarkers related to disease progression or, conversely, treatment response. In clinical development, AI is used to stratify patients on the basis of genomic, phenotypic and electronic health record data in predicting patients that would most likely respond to therapy. AI systems could analyze these data to support their suggestions on who can be enrolled in a clinical trial and identify study endpoints that provide sufficiently sensitive measurements of clinical benefit. The system will predict adverse events to clinical trials and monitor these events whilst gathering real-time trial data to implement adaptive interventions. In so doing, it can greatly reduce the proportion of failed trials, thus, their timelines and costs. Another area where AI will help is in facilitating the rise of precision medicine wherein decisions are made on a case-by-case basis to ensure efficacy of treatment and better clinical outcomes. In the presence of AI within those processes, we could be ensuring that promising compounds are fast-tracked with paint-by-numbers insight from preclinical evaluation all the way to regulatory elucidation.[27,28]

CURRENT TRENDS IN AI-DRIVEN DRUG DISCOVERY

In drug discovery, AI has been a major trend as it introduces innovative methods, making the whole process faster, at a cost, knock yet bringing along the curve of the higher predictive power. More recent approaches have been dominated by deep learning, generative modeling, and natural language processing for faster target identification, virtual screening, and lead optimization. That big data like that from chemical libraries, omics data sets, and clinical data-in the real world-means AI learns to identify patterns and make predictions that would have been otherwise impossible with the traditional ones.[29]

AI-Powered Drug Repurposing : One of the most outstanding trends is the employment of AI for drug repurposing, which has the therapeutic purpose of ascertain new indications for drugs that are already available in the market. Machine-learning models and NLP algorithms are involved in mining biomedical literature while considering clinical trials data and electronic health records to detect hitherto unknown drug–disease relationships. This minimizes development time, thus mitigating risk since repurposed drugs have established safety profiles.[30,31]

Generative Chemistry and De Novo Drug Design : One of the most outstanding trends is the employment of AI for drug repurposing, which has the therapeutic purpose of ascertain new indications for drugs that are already available in the market. Machine-learning models and NLP algorithms are involved in mining biomedical literature while considering clinical trials data and electronic health records to detect hitherto unknown drug–disease relationships. This minimizes development time, thus mitigating risk since repurposed drugs have established safety profiles.[32,33]

Integration with Multi-Omics and Real-World Data : The trend of integrating multi-omics datasets-genomics, proteomics, metabolomics-with clinical and real-world data permits AI to come up with more robust predictive modeling tools. This integration therefore reinforces precision medicine initiatives, which themselves support patient stratification and personalized therapeutic interventions. Through integration, AI systems will end up solving complicated disease mechanisms and, in that, are likely to come away with better drug-response predictions.[34,35]

Collaborative AI Platforms : An increase in collaborative AI platforms and partnerships across biotech startups, pharmaceutical companies, and academic institutions fuels innovation. BenevolentAI, Insilico Medicine, and Atomwise, for instance, show how collaboration capitalized on mutual data and AI-driven workflow to speed drug discovery pipelines rapidly-from target identification to clinical trials.[36,37]

CASE STUDIES AND SUCCESS STORIES

The injection of artificial intelligence in drug discovery has shaken the very foundations of Pharmaceuticals, working faster and cheaper, and improving the candidate selection process. At present, different companies and research programs have been able to show that AI can confront challenges in drug development - from target ID, lead optimization, drug repurposing, to clinical trial design. These case studies demonstrate technological and theoretical advancements that spur real change in delivering new treatments or reusing old ones to meet emergent healthcare needs. By going through these success stories, it will be clear that AI is one important factor that has brought disruption to the traditional paradigms and is also acting as a catalyst for a more efficient and innovative future for drug discovery.

Company / Platform	Application / Focus	Success Story	Impact
Atomwise (AtomNet®)	Structure-based drug design using deep learning	Identified inhibitors for Ebola virus rapidly	Reduced early-stage drug discovery timelines from months to days
BenevolentAI	Drug repurposing using AI analysis of biomedical data	Identified Baricitinib as a potential COVID-19 therapy	Validated in clinical trials; rapid response to emerging health crises
Insilico Medicine (GENTRL)	Generative AI for novel molecule design	Developed DDR1 kinase inhibitors in 46 days	Significantly accelerated lead compound discovery and validation
Exscientia	AI-designed drug candidates	DSP-1181 for OCD entered Phase I clinical trials	First AI-designed molecule to reach human clinical trials
Recursion Pharmaceuticals (Recursion OS)	Phenotypic screening and AI-driven discovery	Identified compounds for SARS-CoV-2 phenotypic reversal	Demonstrated scalability of AI in rare disease and infectious disease research.[38,39,40]

CHALLENGES AND LIMITATIONS OF AI IN DRUG DISCOVERY

Data Quality and Availability : AI models are largely dependent on high-quality, large amounts of appropriate data for accurate predictions. Biological and chemical data, however, are often heterogeneous, incomplete, or noisy, thereby limiting the reliability of AI outputs. Variability in the experimental protocols, inconsistency in annotation, and low availability of negative data add to these challenges. Less, insufficient, or biased data sets can lead to overfitting, poor generalizability, and wrong predictions, hence hampering instead of accelerating development.[41]

Model Interpretability and "Black Box" Concerns : Many AI algorithms-an instance being deep learning models-are inherently complex and are, therefore considered "black boxes." This causes problems when seeking regulatory approval since it is not easily explainable to how decisions made have led to compound prioritization or target selection. Understanding how the predictions arise has a significant value in terms of scientific validation as well as reproducibility making it worthy of acceptance as a common method with pharmaceutical workflows.[42]

Integration with Traditional Drug Discovery : Incorporating AI into the extant drug discovery pipelines present logistical and technical challenges. The AI results have to be reconciled with the experimental results, thus demanding solid validation frameworks. Furthermore, integrating these AI-driven operations into organizational workflows requires the interplay and convergence of expertise in computational sciences, chemistry, biology, medicine, and clinical trials. Such a multifunctional collaboration can be costly and slow to implement.[43]

Regulatory and Ethical Considerations : Still, there is yet no clear regulatory governance for AI-driven drug discovery. And much has been left under consideration, from intellectual property questions about the AI solution itself to validation of AI-designed molecules to whether patient-derived data have been used ethically. Ensuring compliance with data privacy laws becomes highly challenging, especially for clinical datasets and multi-omics datasets, thus adding another layer of complexity to AI implementation.[44]

FUTURE DIRECTIONS IN AI-DRIVEN DRUG DISCOVERY

Integration with Precision Medicine

AI-driven drug discovery is increasingly being integrated alongside approaches to precision medicine. By using person-specific genetic, proteomic, and metabolomic data, the AI would then help in designing therapeutics that target an individual's disease pathway. In effect, this could translate to relatively more efficient treatments, fewer side effects, and greater patient compliance.

Explainable and Transparent AI Models

One major challenge in AI-driven drug discovery has been the "black box" nature of many deep learning models. In consequence, a future research agenda aims to construct explainable AI (XAI) frameworks to provide transparent reasoning behind predictions. Achieving this would be a key to regulatory acceptance, in addition to garnering trust from clinicians and researchers.[45,46]

Multi-Omics Data Integration

The future of AI in drug discovery will involve integration of varying datasets-from genomics, transcriptomics, proteomics and metabolomics to clinical data. Assessing multi-omics data can integrate and dissect disease mechanisms more thoroughly, increase target identification, and potentially provide prediction of drug responses.

Collaborative Ecosystem Development

To ensure the development of AI-driven drug discovery, there should be an interface between academia, industry, and regulators. The future direction could see the building of open-source AI platforms, standardized datasets, and international consortia speeding up drug discovery and the verification of AI models.[47,48]

Emerging Technologies

Emerging technologies could great aid transformation in AI-based drug discovery. While it will be possible for quantum computing to provide simulations of molecular interaction complexities at a speed that no other system can provide, blockchain will assure secure and transparent data-sharing among researchers, thus enhancing collaboration and reproducibility.

Regulatory and Ethical Frameworks

Future research should also focus on developing regulatory and ethical guidelines for AI applications in drug discovery, including data privacy, bias mitigation in AI models, and compliance with international standards so that AI innovations are indeed safe, ethical-oriented, and clinically applicable.

AI-Driven Automation in Drug Development

On the frontier, fully automated drug discovery pipelines will transit from target identification to clinical trial predictions. AI-driven robotic systems and lab automation can potentially make faster

preclinical tests and shorten the time and cost of introducing novel drugs toward the market.

CONCLUSION:

Artificial Intelligence (AI) is rapidly transforming drug discovery, thereby providing solutions to many limitations of the traditional approach, i.e., its high costs, long timelines, and low success rates. Using methods based on machine learning, deep learning, natural language processing, and generative models, AI aids in target identification, virtual screening, lead optimization, and clinical trial design. Success stories from BenevolentAI, Insilico Medicine, and Atomwise bear witness to the accelerated drug discovery, drug repurposing, and de novo molecular design that AI has made increasingly viable in the real world. While current challenges exist around data quality, explainability, and regulatory acceptance, further developments promise to take the field to the next level with multi-omics integration, quantum computing, and federated learning frameworks. Hence, drug discovery with AI will likely solve problems of time and precision, making it far cheaper to develop new therapeutics for personalized medicine and the dawn of Pharmaceutical Research.

REFERENCES:

1. Biala G, Kedzierska E, Kruk-Slomka M, Orzelska-Gorka J, Hmaidan S, Skrok A, Kaminski J, Havrankova E, Nadaska D, Malik I. Research in the Field of Drug Design and Development. Pharmaceuticals (Basel). 2023 Sep 11;16(9):1283.
2. Hughes J.P., Rees S., Kalindjian S.B., Philpott K.L. Principles of early drug discovery. Br. J. Pharmacol. 2011;162:1239–1249.
3. Fogel D.B. Factors associated with clinical trials that fail and opportunities for improving the likelihood of success: A review. Contemp. Clin. Trials Commun. 2018;7:156–164.
4. Sun D, Gao W, Hu H, Zhou S. Why 90% of clinical drug development fails and how to improve it? Acta Pharm Sin B. 2022 Jul;12(7):3049-3062.
5. Takebe T., Imai R., Ono S. The current status of drug discovery and development as originated in United States academia: the influence of industrial and academic collaboration on drug discovery and development. Clinical and translational science. 2018;11:597–606
6. Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. Drug Discov Today. 2021 Jan;26(1):80-93.
7. Duch W. Artificial intelligence approaches for rational drug design and discovery. Curr. Pharm. Des. 2007;13:1497–1508.
8. Vyas M. Artificial intelligence: the beginning of a new era in pharmacy profession. Asian J. Pharm. 2018;12:72–76
9. Blanco-González A, Cabezón A, Seco-González A, Conde-Torres D, Antelo-Riveiro P, Piñeiro Á, Garcia-Fandino R. The Role of AI in Drug Discovery: Challenges, Opportunities, and Strategies. Pharmaceuticals (Basel). 2023 Jun 18;16(6):891
10. Bajwa J, Munir U, Nori A, Williams B. Artificial intelligence in healthcare: transforming the practice of medicine. Future Healthc J. 2021 Jul;8(2):e188-e194.
11. Kufel J, Bargieł-Łączek K, Kocot S, Koźlik M, Bartnikowska W, Janik M, Czogalik Ł, Dudek P, Magiera M, Lis A, Paszkiewicz I, Nawrat Z, Cebula M, Gruszczyńska K. What Is Machine Learning, Artificial Neural Networks and Deep Learning?-Examples of Practical Applications in Medicine. Diagnostics (Basel). 2023 Aug 3;13(15):2582.
12. Vora LK, Gholap AD, Jetha K, Thakur RRS, Solanki HK, Chavda VP. Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. Pharmaceutics. 2023 Jul 10;15(7):1916.
13. Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug Discov Today. 2018 Jun;23(6):1241-1250.
14. Liu Z, Roberts RA, Lal-Nag M, Chen X, Huang R, Tong W. AI-based language models powering drug discovery and development. Drug Discov Today. 2021 Nov;26(11):2593-2607.
15. Tan RK, Liu Y, Xie L. Reinforcement learning for systems pharmacology-oriented and personalized drug design. Expert Opin Drug Discov. 2022 Aug;17(8):849-863.
16. Rehman AU, Li M, Wu B, Ali Y, Rasheed S, Shaheen S, Liu X, Luo R, Zhang J. Role of artificial intelligence in revolutionizing drug discovery. Fundam Res. 2024 May 9;5(3):1273-1287.
17. Zhang Y, Luo M, Wu P, Wu S, Lee TY, Bai C. Application of Computational Biology and Artificial Intelligence in Drug Design. Int J Mol Sci. 2022 Nov 5;23(21):13568.
18. Wang K, Huang Y, Wang Y, You Q, Wang L. Recent advances from computer-aided drug design to artificial intelligence drug design. RSC Med Chem. 2024 Oct 11;15(12):3978–4000.
19. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G, Li B, Madabhushi

A, Shah P, Spitzer M, Zhao S. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019 Jun;18(6):463-477

20. Serrano DR, Luciano FC, Anaya BJ, Ongoren B, Kara A, Molina G, Ramirez BI, Sánchez-Guirales SA, Simon JA, Tomietto G, Rapti C, Ruiz HK, Rawat S, Kumar D, Lalatsa A. Artificial Intelligence (AI) Applications in Drug Discovery and Drug Delivery: Revolutionizing Personalized Medicine. Pharmaceutics. 2024 Oct 14;16(10):1328.
21. Wenteler A, Cabrera CP, Wei W, Neduva V, Barnes MR. AI approaches for the discovery and validation of drug targets. Camb Prism Precis Med. 2024 May 24;2:e7.
22. Pun FW, Ozerov IV, Zhavoronkov A. AI-powered therapeutic target discovery. Trends Pharmacol Sci. 2023 Sep;44(9):561-572.
23. Zhu T, Cao S, Su PC, Patel R, Shah D, Chokshi HB, Szukala R, Johnson ME, Hevener KE. Hit identification and optimization in virtual screening: practical recommendations based on a critical literature analysis. J Med Chem. 2013 Sep 12;56(17):6560-72.
24. Li Q, Ma Z, Qin S, Zhao WJ. Virtual Screening-Based Drug Development for the Treatment of Nervous System Diseases. Curr Neuropharmacol. 2023;21(12):2447-2464.
25. Gangwal A, Lavecchia A. Unleashing the power of generative AI in drug discovery. Drug Discov Today. 2024 Jun;29(6):103992.
26. Khater T, Alkhatib SA, AlShehhi A, Pitsalidis C, Pappa AM, Ngo ST, Chan V, Truong VK. Generative artificial intelligence based models optimization towards molecule design enhancement. J Cheminform. 2025 Aug 4;17(1):116.
27. Dermawan D, Alotaiq N. From Lab to Clinic: How Artificial Intelligence (AI) Is Reshaping Drug Discovery Timelines and Industry Outcomes. Pharmaceuticals. 2025; 18(7):981.
28. Huanbutta K, Burapapadh K, Kraisit P, Sriamornsak P, Ganokratanaa T, Suwanpitak K, Sangnim T. Artificial intelligence-driven pharmaceutical industry: A paradigm shift in drug discovery, formulation development, manufacturing, quality control, and post-market surveillance. Eur J Pharm Sci. 2024 Dec 1;203:106938.
29. Dara S, Dhamercherla S, Jadav SS, Babu CM, Ahsan MJ. Machine Learning in Drug Discovery: A Review. Artif Intell Rev. 2022;55(3):1947-1999.
30. Wan Z, Sun X, Li Y, Chu T, Hao X, Cao Y, Zhang P. Applications of Artificial Intelligence in Drug Repurposing. Adv Sci (Weinh). 2025 Apr;12(14):e2411325.
31. Cortial L, Montero V, Tourlet S, Del Bano J, Blin O. Artificial intelligence in drug repurposing for rare diseases: a mini-review. Front Med (Lausanne). 2024 May 22;11:1404338.
32. Malheiro V, Santos B, Figueiras A, Mascarenhas-Melo F. The Potential of Artificial Intelligence in Pharmaceutical Innovation: From Drug Discovery to Clinical Trials. Pharmaceuticals (Basel). 2025 May 25;18(6):788.
33. Han R, Yoon H, Kim G, Lee H, Lee Y. Revolutionizing Medicinal Chemistry: The Application of Artificial Intelligence (AI) in Early Drug Discovery. Pharmaceuticals. 2023; 16(9):1259.
34. Mohr AE, Ortega-Santos CP, Whisner CM, Klein-Seetharaman J, Jasbi P. Navigating Challenges and Opportunities in Multi-Omics Integration for Personalized Healthcare. Biomedicines. 2024 Jul 5;12(7):1496
35. Boini A, Grasso V, Taher H, Gumbs AA. Artificial intelligence and the impact of multiomics on the reporting of case reports. World J Clin Cases. 2025 May 26;13(15):101188.
36. Malheiro V, Santos B, Figueiras A, Mascarenhas-Melo F. The Potential of Artificial Intelligence in Pharmaceutical Innovation: From Drug Discovery to Clinical Trials. Pharmaceuticals. 2025; 18(6):788.
37. Ali, K.A., Mohin, S., Mondal, P. et al. Influence of artificial intelligence in modern pharmaceutical formulation and drug development. Futur J Pharm Sci **10**, 53 (2024).
38. Kwofie SK, Adams J, Broni E, Enninful KS, Agoni C, Soliman MES, Wilson MD. Artificial Intelligence, Machine Learning, and Big Data for Ebola Virus Drug Discovery. Pharmaceuticals (Basel). 2023 Feb 21;16(3):332.
39. Richardson PJ, Robinson BWS, Smith DP, Stebbing J. The AI-Assisted Identification and Clinical Efficacy of Baricitinib in the Treatment of COVID-19. Vaccines. 2022; 10(6):951.
40. Gangwal A, Ansari A, Ahmad I, Azad AK, Kumarasamy V, Subramaniyan V, Wong LS. Generative artificial intelligence in drug discovery: basic framework, recent advances, challenges, and opportunities. Front Pharmacol. 2024 Feb 7;15:1331062
41. Carini, C., Seyhan, A.A. Tribulations and future opportunities for artificial intelligence in precision medicine. J Transl Med **22**, 411 (2024).

42. Hassija, Vikas & Chamola, Vinay & Mahapatra, Atmesh & Singal, Abhinandan & Goel, Divyansh & Huang, Kaizhu & Scardapane, Simone & Spinelli, Indro & Mahmud, Mufti & Hussain, Amir. (2023). Interpreting Black-Box Models: A Review on Explainable Artificial Intelligence. Cognitive Computation. 16. 10
43. Visan AI, Negut I. Integrating Artificial Intelligence for Drug Discovery in the Context of Revolutionizing Drug Delivery. Life (Basel). 2024 Feb 7;14(2):233.
44. Harishbhai Tilala M, Kumar Chenchala P, Choppadandi A, Kaur J, Naguri S, Saoji R, Devaguptapu B. Ethical Considerations in the Use of Artificial Intelligence and Machine Learning in Health Care: A Comprehensive Review. Cureus. 2024 Jun 15;16(6):e62443.
45. Askr H., Elgeldawi E., Ella H.A., Elshaier Y.A.M.M., Gomaa M.M., Hassanien A.E. Deep learning in drug discovery: An integrative review and future challenges. Artif. Intell. Rev. 2023;56:5975–6037.
46. Bordukova M., Makarov N., Rodriguez-Esteban R., Schmich F., Menden M.P. Generative artificial intelligence empowers digital twins in drug discovery and clinical trials. Expert Opin. Drug Discov. 2024;19:33–42.
47. Cheng J.Y., Abel J.T., Balis U.G., McClintock D.S., Pantanowitz L. Challenges in the Development, Deployment, and Regulation of Artificial Intelligence in Anatomic Pathology. Am. J. Pathol. 2021;191:1684–1692
48. Morabito A, De Simone G, Pastorelli R, Brunelli L, Ferrario M. Algorithms and tools for data-driven omics integration to achieve multilayer biological insights: a narrative review. J Transl Med. 2025 Apr 10;23(1):425.
49. Mirakhori F, Niazi SK. Harnessing the AI/ML in Drug and Biological Products Discovery and Development: The Regulatory Perspective. Pharmaceuticals (Basel). 2025 Jan 3;18(1):47.
50. Ferreira FJN, Carneiro AS. AI-Driven Drug Discovery: A Comprehensive Review. ACS Omega. 2025 Jun 6;10(23):23889-23903.