GSC Biological and Pharmaceutical Sciences

eISSN: 2581-3250 CODEN (USA): GBPSC2

Cross Ref DOI: 10.30574/gscbps

Journal homepage: https://gsconlinepress.com/journals/gscbps/

(REVIEW ARTICLE)

Check for updates

Artificial Intelligence used in Drug Discovery

Ishar K Thak *, Pooja R. Hatwar, Ravindra L. Bakal, Om N. Ajmire and Gaurav P. Aswar

Shri Swami Samarth Institute of Pharmacy, At Parsodi, Dhamangaon Rly, Dist -Amravati (444709) Maharashtra, India.

GSC Biological and Pharmaceutical Sciences, 2025, 32(01), 313-320

Publication history: Received on 14 June 2025; revised on 21 July 2025; accepted on 24 July 2025

Article DOI: https://doi.org/10.30574/gscbps.2025.32.1.0295

Abstract

The integration of artificial intelligence (AI) in drug discovery has revolutionized the pharmaceutical industry, transforming the way novel therapeutics are developed. AI's ability to analyze vast amounts of data, identify patterns, and predict outcomes has accelerated the discovery process, reducing time and costs. This review highlights the role of AI in drug discovery, from target selection and validation to compound screening and lead optimization. AI-powered tools, such as machine learning algorithms and deep learning models, have been successfully applied in medical diagnoses, cellular image analysis, and chemical synthesis. The advantages of AI in drug discovery include enhanced computational power, improved accuracy, and the ability to identify potential drug candidates. However, limitations such as data quality, lack of originality, and high costs need to be addressed. Applications of AI in drug discovery include targeted therapeutic nanoparticles, drug-drug interaction identification, and clinical trial design. Future directions include the development of more sophisticated AI models, integration with omics research, and personalized medicine. AI is poised to transform the pharmaceutical industry, enabling the development of novel therapeutics and improving treatment outcomes. By leveraging AI's potential, researchers can accelerate the discovery of new drugs, reduce costs, and ultimately improve human health. As the field continues to evolve, it is essential to address the challenges and limitations associated with AI in drug discovery, ensuring the development of effective and safe therapeutics.

Keywords: Artificial intelligence; Drug discovery; Drug development; Nanorobot; Nanomedicines

1. Introduction

Chemical and biological scientists have faced a significant problem over the past 20 years, creating sophisticated and effective systems for the targeted administration of therapeutic chemicals with the highest efficiency and the lowest hazards [1]. Drug research, development, production, and distribution are just a few of the many tasks that fall within the purview of the pharmaceutical sector. The pharmaceutical value chain starts with drug discovery, which entails finding novel drug candidates [2]. One important sector that is essential to preserving lives is the pharmaceutical business. In order to solve global healthcare concerns and respond to medical disasters like the previous pandemic, it is predicated on ongoing innovation and the adoption of new technology [3]. Drug discovery has experienced a relatively late resurgence in the interest for deep learning, which already led to an unprecedented explosion of novel modeling approaches and applications [4]. The drug and biopharmaceutical industries have been limited source of inventive and novel technologies or machinery, and have led the development of novel principles or interpretations in general chemical and mechanical engineering. The pharmaceutical industry is in critical need of mechanical innovation, easing the creation of medications for human use [5]. Advancements in computational science have accelerated drug discovery and development. Artificial intelligence (AI) is widely used in both industry and academia. Machine learning (ML), an essential component in AI, has been integrated into many fields, such as data generation and analytics [6]. We have hereby practiced with an artificial intelligence (AI) system for searching marketed drugs potentially with antiviral activities against coronaviruses [7]. Nanomedicine, a combination of nanotechnology and medicine to diagnose, monitor and treat diseases, has significantly improved the treatment outcome of highly complicated and deadly diseases by

* Corresponding author: Ishar K. Thak

maintaining therapeutic dose at the target site [8]. Deep learning is a popular artificial intelligence (AI) way that has been successfully applied in medical diagnoses, cellular image analysis, chemical syntheses, classification of drugs and so on. Deep learning is a promising technology for the development and discovery of innovative drugs [9]. Drug discovery is a long and complex process that can be broadly divided into four major stages: (i) target selection and validation; (ii) compound screening and lead optimization; (iii) preclinical studies; and (iv) clinical trials [10].

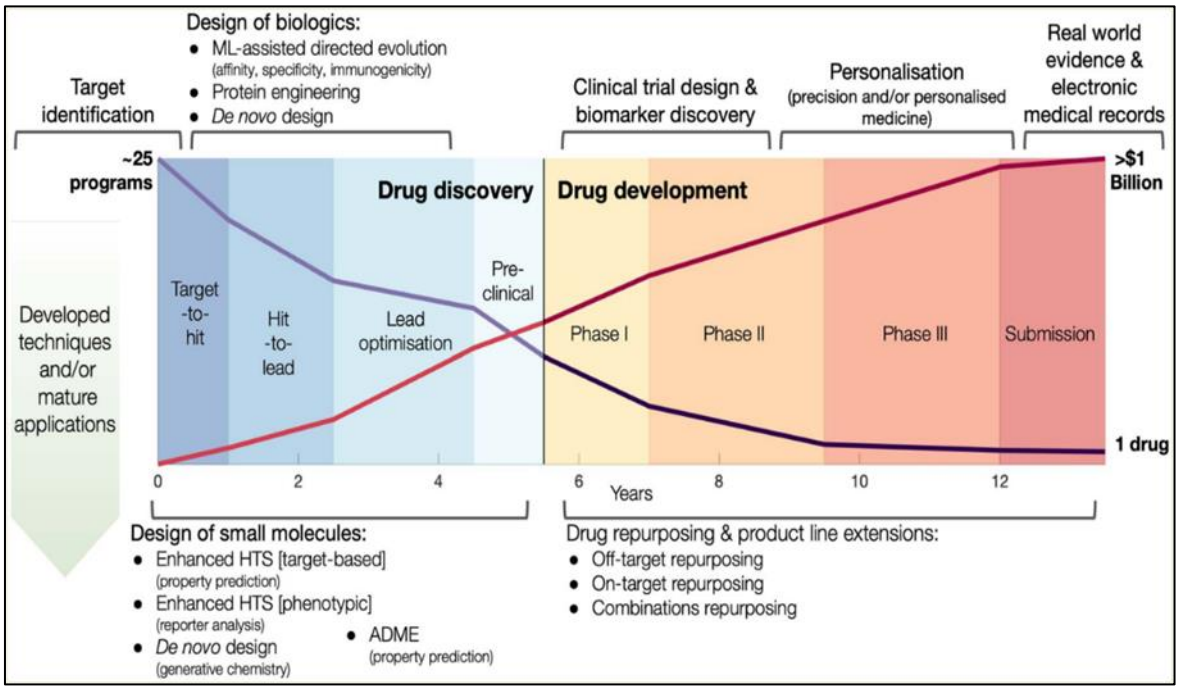

Figure 1 Drug development timeline connected to possible application areas using GML techniques [11]

2. AI in Drug Discovery

The vast chemical space, comprising >1060 molecules, fosters the development of many drug molecules. However, the lack of advanced technologies limits the drug development process, making it a time-consuming and expensive task, which can be addressed by using AI [12]. The integration of AI and big data in the field of pharmaceutics has led to the development of computational pharmaceutics, which aims to enhance drug delivery processes by utilizing multiscale modeling approaches [3]. Enhanced computational power and the development of innovative techniques in the field of AI could be used to reform drug discovery and development processes. The pharmaceutical sector has seen a dramatic increase in the digitization of information in recent years; one ongoing problem is effectively acquiring, analysing, and using this information to address complicated clinical challenges [5]. One promising technological platform for drug discovery is computational approaches. Drug design methodologies, molecular simulations, and data integration are the next steps in the drug development process, which starts with the target finding procedure [13]. AI can be used to address the time-consuming and costly medication development process that is limited by a lack of innovative technology. AI has the ability to identify hit and lead compounds, validate drug targets more quickly, and optimize drug structure design [14]. In information synthesis, artificial intelligence (AI) refers to applications that directly optimize drug development by evaluating clinically relevant data that direct the identification of novel prospective targets. Potential medications' molecular structures can be developed and optimized with AI in drug design [15]. Virtual screening of both novel chemical entities and repurposed medication candidates is one of the latest uses of artificial intelligence for COVID-19. Rapidly predicting and taking use of interrelated biological pathways or the off-target biology of currently approved medications that can be easily tested in new clinical trials has been the aim for repurposed therapeutics [16].

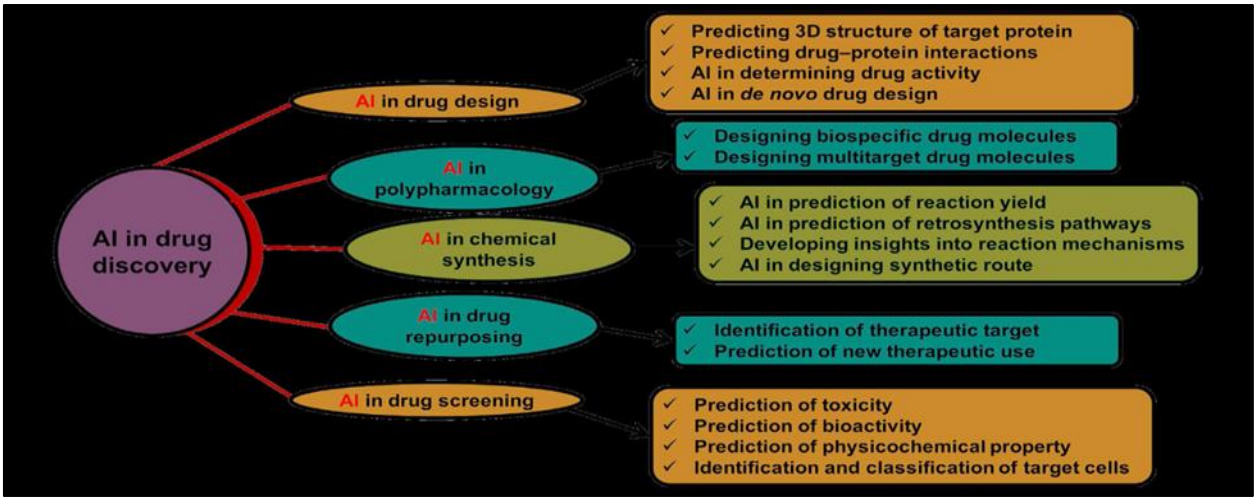

Figure 2 Artificial Intelligence's Function in Drug Discovery [17]

3. Advantages

- The pharmaceutical industry may benefit from the use of AI in de novo molecule design [12].
- The identification of lead molecules from databases has been made possible by computational techniques, which also aid in defining and elaborating the intensity of the interaction between ligands and targets [13].
- AI in community-based primary care provides a number of multifaceted benefits, from better clinical results and access to healthcare services to resource management [18].
- Users should be informed that in the future, different activity measurements for the same chemical and test may be recorded, with variations in features such the measurement time point. Since earlier releases, a number of existing data sets have undergone modifying in order to profit on the modifications in the data model and format [19].
- The foundation and core component of life science, especially medicine, is biological analysis, and the advancement of biotechnology has benefited medicine [20].

4. Disadvantages

- When evaluated against the study's data, the algorithm yielded an error rate of less than 5%; however, the primary drawback of this computational approach is that more accuracy required a larger training set [2].
- Expensive.
- Lack of originality.
- Joblessness.
- Make people lazy and emotionless [17].

5. Application

- Targeted therapeutic nanoparticles can be optimized for particular cell types and patients by integrating automation and artificial intelligence (AI) [2].
- These restrictions can be solved by AI methods like machine learning. By analysing vast amounts of data, machine learning algorithms are able to spot patterns and trends that human researchers might miss. The identification of drug-drug interactions, which occur when many medications are taken for the same or different conditions in the same patient and lead to changed effects or bad responses, is the most significant use of AI in drug discovery [21].
- Modern nano/microrobots may now go to the desired location depending on physiological parameters, like pH, increasing their effectiveness and lowering systemic side effects. When developing implantable nanorobots for controlled drug and gene delivery, factors like dose adjustment, sustained release, and control release must be taken into account. Additionally, the release of the drugs must be automated using AI tools like fuzzy logic, NNs, and integrators [12].
- AI reduces the quantity of data personnel needed for clinical trials by using strategies to collect the vast amounts of data generated by those trials. Body sensors and wearable technology are used in these technologies to

remotely record vital signs and important information, helping to satisfy patients' need for regular in-person interactions [3].

- AI reduces the quantity of data personnel needed for clinical trials by using strategies to collect the vast amounts of data generated by those trials. Body sensors and wearable technology are used in these technologies to remotely record vital signs and important information, helping to satisfy patients' need for regular in-person interactions [3].
- The introduction of computational approaches has been very convenient in the drug discovery process, with unique benefits derived from its ability to analyse large volumes of data for security and data management. These methods are now widely recognized as a viable alternative and complement to high-throughput screening [13].
- AI uses software and systems that can analyse and learn from input data to make decisions on their own to achieve predetermined goals. As this article explains, its uses in the pharmaceutical industry are constantly expanding. The McKinsey Global Institute predicts that the swift development of AI-guided automation will probably transform society's workplace culture [14].

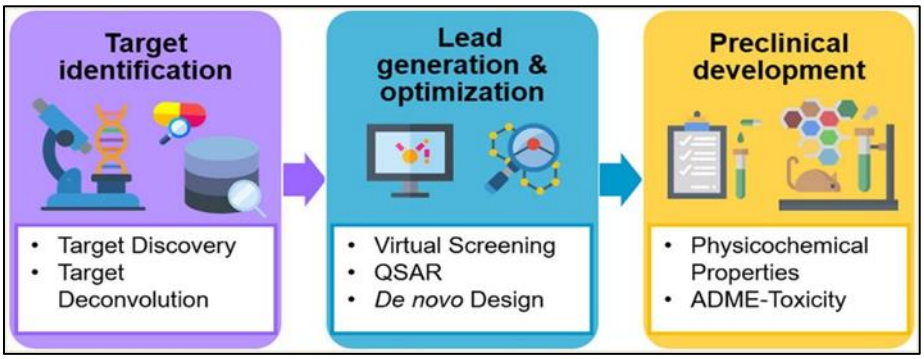

Figure 3 Uses of AI and ML in the process of finding new drugs [22]

- A macroscopic viewpoint provided by the analysis of development trends assists in identifying the variables that are driving this field's expansion as well as possible research gaps or future directions, like the potential use of AI technology to increase diagnostic precision, lower misdiagnosis rates, and produce individualized treatment [23].
- Organ-on-chip platforms have the potential to enhance and expedite efforts in rare illnesses, stratified medicine, and nanomedicine, areas that are garnering growing industrial interest, in addition to enhancing research and development efficiency generally [24].
- The development of novel delivery systems and the next generation of medications requires the use of advanced technology. This paper emphasizes the importance of TF and artificial intelligence (AI) in drug and delivery system design, as well as the possible difficult problems [25].
- The development of novel biomarkers and therapeutic targets, personalized medicine based on omics markers, and the discovery of links between medications and illnesses make it feasible to use omics research to identify new pathways and targets [26].

6. Challenges And Limitation

While the potential advantages of AI in drug discovery, a number of restrictions and difficulties need to be taken into account. The availability of appropriate data is one of the main obstacles. Large amounts of data are usually needed for training in AI-based methods. The accuracy and dependability of the results may be impacted by the fact that there is frequently a lack of available data or if the data is inconsistent or of poor quality [21]. Ineffective data integration is one issue. Diversity in datasets, which might include raw data, processed data, metadata, or candidate data, is the cause of this issue. For effective analysis, these datasets need to be gathered and compiled, but there isn't a clear procedure in place at the moment. This must be done before the drug discovery process starts because the machine learning algorithms' output will be erroneous if the data is not prepared correctly. Therefore, more effective ways to incorporate existing data into data banks prior to the start of the drug discovery process are needed [5].

Drug discovery has been greatly aided by machine learning techniques. By using these techniques, efficiency is increased and hundreds of combinations that would not have been feasible without technology are explored. As previously mentioned, algorithms are taught using input data; nevertheless, this method has certain limitations. Even while machine learning has been around for a while, the biological pathways and targets that are being found are still new.

There may not be much information available for the specific protein of interest, which would lead to little extrapolated data. The Free Energy Perturbation approach is a platform that uses computational screening to generate biological information about the protein [6]. The largest challenge for nanorobotic systems is to manipulate matter at the molecular scale and affect its dynamics and properties. This field is still in its infancy, and much work needs to be done before any significant results are obtained. Molecular robots, or bio nanorobots, have a promising future [26]. The failure rate of drug repurposing between preclinical research and clinical trials for COVID-19 can be decreased by creating reliable and efficient in vitro and in vivo models [27].

7. Future Direction

Increasing prices and decreasing efficiency are currently the pharmaceutical industry's biggest challenges when creating new drugs [1]. Through the use of advanced computational techniques, it had transformed conventional methods for drug development and discovery. To create tailored treatment, numerous pharmaceutical giants have started utilizing these advanced technologies [2]. By taking into account patient-specific factors including age, weight, genetics, and sickness state, AI algorithms will optimize medication formulations and delivery systems to enhance treatment outcomes. By forecasting the toxicity and adverse consequences of medication candidates, AI systems will transform safety evaluation [3]. Therefore, screening costs seem to be cut by up to 90% without accounting for the anticipated mechanical overhead for actually implementing dynamic learning activities [5]. The tough procedures required for the use of AI and the expected employment losses are the most significant issues with these platforms' inclusion. However, the purpose of this technology is to make the task easier rather than completely replace humans [28]. AI offers platforms and tools that improve our comprehension and strategy for treating this deadly illness. AI-based tools help pathologists diagnose cancer more reliably and accurately, which lowers error rates. Additionally, AI has proven to be quite successful in a number of medication design and development-related areas [29].

Differentiable neural computers, or DNCs, have been used to solve a variety of issues, such as determining the shortest path in graphs and answering questions. Nevertheless, drug discovery has yet to use these more sophisticated frameworks [30]. We wrap up by giving an overview of the current state of the fields of clinical pharmacology and machine learning, as well as a prediction for future developments in the integration of these two domains [31]. Clinical pharmacologists are medically qualified professionals who teach, do research, formulate policies, and provide information and guidance regarding the actions and appropriate uses of medications in people. They also apply this knowledge in clinical practice on a daily basis [32]. Further research should concentrate on appreciating how these variations impact the effectiveness and quality of health information searches [33]. The identification and optimization of therapeutic candidates will be accelerated in the not-too-distant future when MD and related techniques are regularly employed for the in silico screening of sizable libraries of small compounds [34]. The general public concurs that further effort is undoubtedly needed to improve production cost and scalability, create Good Laboratory Practice (GLP) characterisation, and improve coordination and collaboration between the public and private sectors [35]. Dynamic neural networks employ historical data to forecast a system's current and future states. Characterizing or simulating medication release from controlled release formulations may benefit from this [24]. For next drug development and nanomedicine initiatives, basket studies are probably going to offer solid underpinnings for AI-driven increases in response rates [36]. In pharmaceuticals, AI contributes significantly to drug formulation, pharmacovigilance and clinical trial design, improving outcomes while reducing time and cost. The use of AI in radiotherapy and patient-specific treatment planning is revolutionizing cancer care [37]. Future research should concentrate more on a model's influence on treatment choices, clinical and patient-reported outcomes, and cost-effectiveness in addition to its accuracy, as these factors may be more significant to patients, healthcare providers, and organizers [38].

8. Conclusion

The integration of artificial intelligence (AI) in drug discovery has revolutionized the pharmaceutical industry, transforming the way novel therapeutics are developed. AI's ability to analyze vast amounts of data, identify patterns, and predict outcomes has accelerated the discovery process, reducing time and costs. By leveraging AI-powered tools, researchers can identify potential drug candidates, optimize drug structure design, and predict toxicity and adverse consequences. While challenges and limitations exist, such as data quality and lack of originality, the benefits of AI in drug discovery are undeniable. As the field continues to evolve, AI is poised to play an increasingly important role in the development of novel therapeutics, improving treatment outcomes and reducing healthcare costs. Future research should focus on addressing the challenges and limitations associated with AI in drug discovery, ensuring the development of effective and safe therapeutics. With its vast potential, AI is set to transform the pharmaceutical industry, improving human health and saving lives.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

Reference

[1] Gupta R, Srivastava D, Sahu M, Tiwari S, Ambasta RK, Kumar P. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. Mol Divers. 2021;25(3):1315-1360. Doi: 10.1007/s11030-021-10217-3. Epub 2021 Apr 12. PMID: 33844136; PMCID: PMC8040371.

[2] Narayanan RR, Durga N, Nagalakshmi S. Impact of Artificial Intelligence (AI) on Drug Discovery and Product Development. Indian Journal of Pharmaceutical Education and Research.2022;56(3):s387-s397.

[3] Vora LK, Gholap AD, Jetha K, Thakur RRS, Solanki HK, Chavda VP. Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. Pharmaceutics.2023;15:1-46.

[4] Jiménez-Luna J, Grisoni F, Weskamp N, Schneider G. Artificial intelligence in drug discovery: recent advances and future perspectives. Expert Opin Drug Discov. 2021;16(9):949-959. Doi: 10.1080/17460441.2021.1909567. Epub 2021 Apr 2. PMID: 33779453.

[5] Patel V, Shah M, Artificial intelligence and machine learning in drug discovery and development. Intelligent Medicine.2022;2(3);134-140, ISSN 2667-1026.

[6] Patel L, Shukla T, Huang X, Ussery DW, Wang S. Machine Learning Methods in Drug Discovery. Molecules.2020;25(22):5277. Doi: 10.3390/molecules25225277. PMID: 33198233; PMCID: PMC7696134.

[7] Ke YY, Peng TT, Yeh TK, Huang WZ, Chang SE, Wu SH, Hung HC, Hsu TA, Lee SJ, Song JS, Lin WH, Chiang TJ, Lin JH, Sytwu HK, Chen CT. Artificial intelligence approach fighting COVID-19 with repurposing drugs. Biomed J. 2020;43(4):355-362. Doi: 10.1016/j.bj.2020.05.001. Epub 2020 May 15. PMID: 32426387; PMCID: PMC7227517.

[8] Wilson B, Km G. Artificial intelligence and related technologies enabled nanomedicine for advanced cancer treatment. Nanomedicine (Lond). 2020;15(5):433-435. Doi: 10.2217/nnm-2019-0366. Epub 2020 Jan 30. PMID: 31997697.

[9] Bai Q, Tan S, Xu T, Liu H, Huang J, Yao X. MolAICal: a soft tool for 3D drug design of protein targets by artificial intelligence and classical algorithm. Brief Bioinform. 2021;22(3):bbaa161. Doi: 10.1093/bib/bbaa161. PMID: 32778891; PMCID: PMC7454275.

[10] Chan HCS, Shan H, Dahoun T, Vogel H, Yuan S. Advancing Drug Discovery via Artificial Intelligence. Trends Pharmacol Sci. 2019;40(8):592-604. Doi: 10.1016/j.tips.2019.06.004. Epub 2019 Jul 15. Erratum in: Trends Pharmacol Sci. 2019;40(10):801. Doi: 10.1016/j.tips.2019.07.013. PMID: 31320117.

[11] Gaudelet T, Day B, Jamasb AR, Soman J, Regep C, Liu G, Hayter JBR, Vickers R, Roberts C, Tang J, Roblin D, Blundell TL, Bronstein MM, Taylor-King JP. Utilizing graph machine learning within drug discovery and development. Brief Bioinform. 2021;22(6):bbab159. Doi: 10.1093/bib/bbab159. PMID: 34013350; PMCID: PMC8574649.

[12] 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. Doi: 10.1016/j.drudis.2020.10.010. Epub 2020 Oct 21. PMID: 33099022; PMCID: PMC7577280.

[13] Duarte Y, Márquez-Miranda V, Miossec MJ, González-Nilo F. Integration of target discovery, drug discovery and drug delivery: A review on computational strategies. Wiley Interdiscip Rev Nanomed Nanobiotechnol. 2019;11(4):e1554. Doi: 10.1002/wnan.1554. Epub 2019 Apr 1. PMID: 30932351.

[14] 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. Doi: 10.1016/j.drudis.2020.10.010. Epub 2020 Oct 21. PMID: 33099022; PMCID: PMC7577280.

[15] Farghali H, Kutinová Canová N, Arora M. The potential applications of artificial intelligence in drug discovery and development. Physiol Res. 2021;70(Suppl4):S715-S722. Doi: 10.33549/physiolres.934765. PMID: 35199553; PMCID: PMC9054182.

[16] Keshavarzi Arshadi A, Webb J, Salem M, Cruz E, Calad-Thomson S, Ghadirian N, Collins J, Diez-Cecilia E, Kelly B, Goodarzi H, Yuan JS. Artificial Intelligence for COVID-19 Drug Discovery and Vaccine Development. Front Artif Intell. 2020;3:65. Doi: 10.3389/frai.2020.00065. PMID: 33733182; PMCID: PMC7861281.

[17] Krosuri P, Pravallika G, Paravathi G, Sumanasri J, Akhila C, Srinikitha SK, Gnana G. Artificial intelligence in drug discovery, Journal of Xidian University.2023;17:734-753.

[18] Xiques-Molina W, Lozada-Martinez ID, Fiorillo-Moreno O, Hernández-Lastra AL, Bermúdez V. Operational Advantages of Novel Strategies Supported by Portability and Artificial Intelligence for Breast Cancer Screening in Low-Resource Rural Areas: Opportunities to Address Health Inequities and Vulnerability. Medicina (Kaunas). 2025;61(2):242. Doi: 10.3390/medicina61020242. PMID: 40005359; PMCID: PMC11857370.

[19] Mendez D, Gaulton A, Bento AP, Chambers J, De Veij M, Félix E, Magariños MP, Mosquera JF, Mutowo P, Nowotka M, Gordillo-Marañón M, Hunter F, Junco L, Mugumbate G, Rodriguez-Lopez M, Atkinson F, Bosc N, Radoux CJ, Segura-Cabrera A, Hersey A, Leach AR. ChEMBL: towards direct deposition of bioassay data. Nucleic Acids Res. 2019;47(D1):D930-D940. Doi: 10.1093/nar/gky1075. PMID: 30398643; PMCID: PMC6323927.

[20] Chen S, Li Z, Zhang S, Zhou Y, Xiao X, Cui P, Xu B, Zhao Q, Kong S, Dai Y. Emerging biotechnology applications in natural product and synthetic pharmaceutical analyses. Acta Pharm Sin B. 2022 Nov;12(11):4075-4097. Doi: 10.1016/j.apsb.2022.08.025. Epub 2022 Sep 5. PMID: 36386468; PMCID: PMC9643291.

[21] 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;16(6):891. Doi: 10.3390/ph16060891. PMID: 37375838; PMCID: PMC10302890.

[22] Vatansever S, Schlessinger A, Wacker D, Kaniskan HÜ, Jin J, Zhou MM, Zhang B. Artificial intelligence and machine learning-aided drug discovery in central nervous system diseases: State-of-the-arts and future directions. Med Res Rev. 2021;41(3):1427-1473. Doi: 10.1002/med.21764. Epub 2020 Dec 9. PMID: 33295676; PMCID: PMC8043990.

[23] Chen S, Wu C, Zhang Z, Liu L, Zhu Y, Hu D, Jin C, Fu H, Wu J, Liu S. The role of artificial intelligence in aortic valve stenosis: a bibliometric analysis. Front Cardiovasc Med. 2025;12:1521464. Doi: 10.3389/fcvm.2025.1521464. PMID: 40013126; PMCID: PMC11860872.

[24] Esch EW, Bahinski A, Huh D. Organs-on-chips at the frontiers of drug discovery. Nat Rev Drug Discov. 2015;14(4):248-60. Doi: 10.1038/nrd4539. Epub 2015 Mar 20. PMID: 25792263; PMCID: PMC4826389.

[25] Hassanzadeh P, Atyabi F, Dinarvand R. The significance of artificial intelligence in drug delivery system design. Adv Drug Deliv Rev. 2019;151-152:169-190. Doi: 10.1016/j.addr.2019.05.001. Epub 2019 May 6. PMID: 31071378.

[26] Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discov Today. 2019;24(3):773-780. Doi: 10.1016/j.drudis.2018.11.014. Epub 2018 Nov 22. PMID: 30472429.

[27] Zhou Y, Wang F, Tang J, Nussinov R, Cheng F. Artificial intelligence in COVID-19 drug repurposing. Lancet Digit Health. 2020;2(12):e667-e676. Doi: 10.1016/S2589-7500(20)30192-8. Epub 2020 Sep 18. PMID: 32984792; PMCID: PMC7500917.

[28] Sarkar C, Das B, Rawat VS, Wahlang JB, Nongpiur A, Tiewsoh I, Lyngdoh NM, Das D, Bidarolli M, Sony HT. Artificial Intelligence and Machine Learning Technology Driven Modern Drug Discovery and Development. Int J Mol Sci. 2023;24(3):2026. Doi: 10.3390/ijms24032026. PMID: 36768346; PMCID: PMC9916967.

[29] Iqbal J, Cortés Jaimes DC, Makineni P, Subramani S, Hemaida S, Thugu TR, Butt AN, Sikto JT, Kaur P, Lak MA, Augustine M, Shahzad R, Arain M. Reimagining Healthcare: Unleashing the Power of Artificial Intelligence in Medicine. Cureus. 2023;15(9):e44658. Doi: 10.7759/cureus.44658. PMID: 37799217; PMCID: PMC10549955.

[30] Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug Discov Today. 2018;23(6):1241-1250. Doi: 10.1016/j.drudis.2018.01.039. Epub 2018 Jan 31. PMID: 29366762.

[31] Badillo S, Banfai B, Birzele F, Davydov II, Hutchinson L, Kam-Thong T, Siebourg-Polster J, Steiert B, Zhang JD. An Introduction to Machine Learning. Clin Pharmacol Ther. 2020;107(4):871-885. Doi: 10.1002/cpt.1796. Epub 2020 Mar 3. PMID: 32128792; PMCID: PMC7189875.

[32] Zhavoronkov A, Vanhaelen Q, Oprea TI. Will Artificial Intelligence for Drug Discovery Impact Clinical Pharmacology? Clin Pharmacol Ther. 2020 Apr;107(4):780-785. Doi: 10.1002/cpt.1795. Epub 2020 Mar 3. PMID: 31957003; PMCID: PMC7158211.

[33] Fu Y, Han P, Wang J, Shahzad F. Digital pathways to healthcare: a systematic review for unveiling the trends and insights in online health information-seeking behavior. Front Public Health. 2025 Feb 12;13:1497025. Doi: 10.3389/fpubh.2025.1497025. PMID: 40013047; PMCID: PMC11860893.

[34] De Vivo M, Masetti M, Bottegoni G, Cavalli A. Role of Molecular Dynamics and Related Methods in Drug Discovery. J Med Chem. 2016 May 12;59(9):4035-61. Doi: 10.1021/acs.jmedchem.5b01684. Epub 2016 Feb 8. PMID: 26807648.

[35] Dickherber A, Morris SA, Grodzinski P. NCI investment in nanotechnology: achievements and challenges for the future. Wiley Interdiscip Rev Nanomed Nanobiotechnol. 2015;7(3):251-65. Doi: 10.1002/wnan.1318. Epub 2014 Nov 27. PMID: 25429991.

[36] Ho D, Peter w, Kee T. Artificial intelligence in Nanomedicine, Nanoscale horizons.2018;4:1-13.

[37] khanderao GJ, Bakal RL, Kubde JA, Hatwar PR and Karule VG. A comprehensive review of Artificial Intelligence. GSC Advanced Research and Reviews, 2025, 23(03), 020-025. Article DOI: https://doi.org/10.30574/gscarr.2025.23.3.0155

[38] Mane SA, Bakal RL, Hatwar PR. Artificial Intelligence in Pharmaceutical Research, Journal of Drug Delivery and Therapeutics. 2025; 15(6):260-267 DOI:http://dx.doi.org/10.22270/jddt.v15i6.7234