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A BRIEF REVIEW ON ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT: A NEW ERA IN PHARMACEUTICALS

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ABSTRACT:

Artificial intelligence (AI) is a transformative technology used in various industrial sectors including healthcare. In pharmacy practice, AI has the potential to significantly improve medication management and patient care. This review explores various AI applications in the field of pharmacy practice. This review evaluates the integration of AI tools such as IBM Watson, Medisafe, ScriptPro, and BenevolentAI into various pharmaceutical functions, including drug discovery, medication management, clinical decision support, pharmacovigilance, and inventory systems. AI applications in pharmacy contribute to optimizing operations by automating prescription verification, predicting medication adherence, minimizing dispensing errors, and enabling real-time inventory control. The integration of AI in pharmacy has the potential to improve patient safety, reduce medication errors, and enhance the overall quality of care. However, challenges such as data standardization, regulatory frameworks, and workforce development must be addressed to ensure the successful adoption of AI in pharmacy practice. This review provides insights into the current state of AI in pharmacy and its future directions.

Keywords: Artificial intelligence, machine learning, drug discovery, predictive modeling.

Introduction:

Artificial Intelligence (AI) is a broad field of computer science focused on creating machines capable of performing tasks that typically require human intelligence. These tasks include reasoning, learning, perception, natural language understanding, problem-solving, and decision-making. AI systems use algorithms, data, and computational power to simulate aspects of human cognition. AI techniques are widespread, including natural language processing, robotics, autonomous vehicles, medical diagnosis, and more. As technology evolves, AI continues to expand its capabilities and applications, raising discussions

about ethics, job displacement, and societal impacts. In the field of Artificial Intelligence (AI), researchers classify AI into several categories based on its capabilities and scope. These categories include Narrow AI (Weak AI), General AI (Strong AI), and Superintelligence, each reflecting different levels of sophistication and potential impact on human activities [1], [2], [3], [4]

These challenges demand more efficient methods, where artificial intelligence (AI) and machine learning (ML) offer a promising path toward increased efficiency and success rates in drug development, providing the pharmaceutical industry with a solution with AI/ML implementation to correct limitations while also opening up novel opportunities using new model implementations based on AI parameters. (6)

The impact of AI is particularly profound in the healthcare and pharmaceutical sectors. AI-powered technologies are being leveraged to address critical challenges in drug discovery and development, improve patient care, and enhance healthcare delivery systems [4, 5].

TEASER

Artificial intelligence-integrated drug discovery and development has accelerated the growth of the pharmaceutical sector, leading to a revolutionary change in the pharma industry. Here, we discuss areas of integration, tools, and techniques utilized in enforcing AI, ongoing challenges, and ways to overcome them. The use of artificial intelligence (AI) has been increasing in various sectors of society, particularly the pharmaceutical industry. In this review, we highlight the use of AI in diverse sectors of the pharmaceutical industry, including drug discovery and development, drug repurposing, improving pharmaceutical productivity, and clinical trials, among others; such use reduces the human workload as well as achieving targets in a short period of time. We also discuss crosstalk between the tools and techniques utilized in AI, ongoing challenges, and ways to overcome them, along with the future of AI in the pharmaceutical industry.

ARTIFICIAL INTELLIGENCE: THINGS TO KNOW:

Over the past few years, there has been a drastic increase in data digitalization in the pharmaceutical sector. However, this digitalization comes with the challenge of acquiring, scrutinizing, and applying that knowledge to solve complex clinical problems [1]. This motivates the use of AI, because it can handle large volumes of data with enhanced automation [2]. AI is a technology-based system involving various advanced tools and networks that can mimic human intelligence. At the same time, it does not threaten to replace human physical presence [3, 4] completely. AI utilizes systems and software that can interpret and learn from the input data to make independent decisions for accomplishing specific objectives. Its applications are continuously being extended in the pharmaceutical field, as described in this review. According to the McKinsey Global Institute, the rapid advances in AI-guided automation will be likely to completely change the work culture of society [5, 6].

AI: NETWORKS AND TOOLS :

AI involves several method domains, such as reasoning, knowledge representation, solution search, and, among them, a fundamental paradigm of machine learning (ML). ML uses algorithms that can recognize patterns within a set of data that has been further classified. A subfield of the ML is deep learning (DL), which engages artificial neural networks (ANNs). These comprise a set of interconnected sophisticated computing elements involving ‘perceptrons’ analogous to human biological neurons, mimicking the transmission of electrical impulses in the human brain [7]. ANNs constitute a set of nodes, each receiving a separate input, ultimately converting them to output, either singly or multi-linked using algorithms to solve problems [8]. ANNs involve various types, including multilayer perceptron (MLP) networks, recurrent neural networks (RNNs), and convolutional neural networks (CNNs), which utilize either supervised or unsupervised training procedures 9, 10.

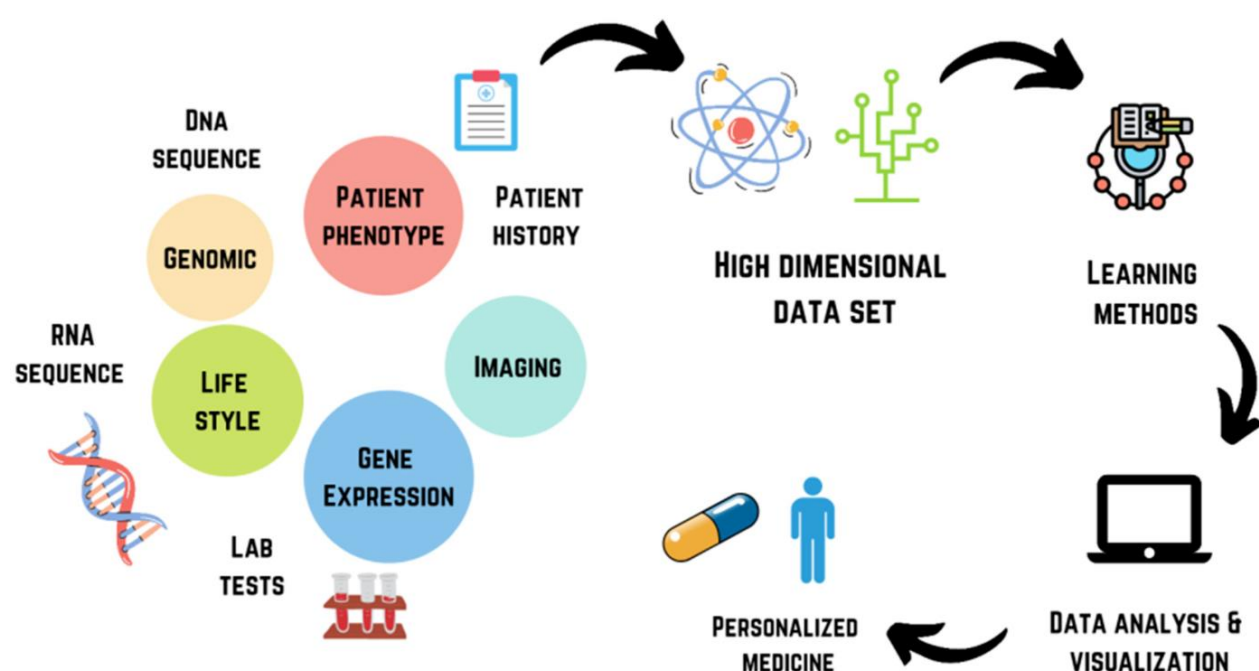


Figure. 1

The role of AI in drug discovery:

A typical drug discovery pipeline consists of multiple stages. The initial phase involves identifying new targets that demonstrate a connection to a particular disease. Next, compounds that potentially interact with these targets are discovered through high-throughput screening (HTS) of compounds libraries. These compounds are then optimized to enhance their drug-like properties. Subsequently, they undergo rigorous preclinical and clinical trials before being approved by regulatory authorities (Hughes et al., 2011). In recent decades, the pharmaceutical industry has extensively employed computer-aided drug discovery (CADD), employing both structure- and ligand-based design approaches. The development of methods, such as molecular modeling, virtual screening, and quantitative structure-activity relationship (QSAR) analysis, has enabled researchers to predict the biological activity of compounds with greater accuracy (Kirchmair et al., 2011; Yoshida and Topliss, 2000). However, CADD faces numerous challenges and limitations, including the complexity of biological systems, difficulties in accurately representing target flexibility, and the limited scope of analysis using traditional methods, which is often constrained to a narrow series of closely related compounds (Hassan Baig et al., 2016; Neves et al., 2018). In the present

era, AI has emerged as a pioneering catalyst, fundamentally altering the conventional methodologies employed in the identification, development, and delivery of potential therapeutics. This shift is being driven by AI's ability to analyze vast amounts of data. However, the exponential growth of data also presents challenges for traditional methods of data analysis. This is where the burgeoning influence of AI becomes significant, as it introduces sophisticated approaches for navigating and analyzing extensive datasets. Consequently, researchers can uncover underlying patterns, pinpoint potential drug targets, and expedite the drug discovery journey.

DRUG OPTIMIZATION AND DESIGN

AI-driven techniques are revolutionizing drug development by optimizing critical properties, such as solubility, stability, and bioavailability [38]. ML algorithms can analyze vast datasets of chemical structures and their associated properties to predict crucial parameters with high accuracy [39]. For example, In QSAR predictions, approximately 1000–5000 data points were used for water solubility predictions [40], whereas DL models can be used to predict drug stability under various conditions [41]. For the protein function prediction task, researchers can leverage two open databases—the UniProt Consortium [42] and the Protein Data Bank (PDB)—to gather protein sequence data from various species [43]. This data can then be used to train prediction models through processes like batch downloading, data cleaning, and pre-processing [44]. These predictive models enable researchers to rapidly identify and optimize drug candidates with improved physicochemical properties, thereby increasing their chances of successful clinical translation [5]. Furthermore, DL algorithms, such as generative adversarial networks (GANs), can be used to generate novel chemical structures with desired properties, thereby expanding the chemical space explored in the drug design process [45].

Preclinical and clinical development

Predictive modeling of pharmacokinetics (PK), pharmacodynamics (PD), and toxicity profiles are crucial for efficient drug development. AI techniques, particularly ML, have advanced these capabilities significantly. ML algorithms can analyze vast datasets of chemical structures and their associated PK/PD properties to predict key parameters such as absorption, distribution, metabolism, excretion (ADME), and drug-drug interactions. For example, DL models can accurately predict drug absorption across biological membranes, while other models can simulate drug distribution within the body [46]. Furthermore, AI can be used to predict drug reactions and toxicity profiles. ML algorithms can identify patterns and relationships between chemical structures and toxicity endpoints, enabling researchers to prioritize safer drug candidates and minimize the risk of unexpected side effects [47, 48]. AI has revolutionized clinical trial design, patient recruitment, and data analysis, leading to more efficient and effective studies. AI algorithms can analyze historical trial data to optimize the study design, such as determining the optimal sample size, selecting appropriate endpoints, and identifying the most suitable patient populations [49]. Furthermore, AI-powered platforms can significantly enhance patient recruitment by identifying and engaging potential participants through targeted advertising and personalized outreach strategies [36]. AI plays a crucial role in real-time data monitoring and analysis. ML algorithms can continuously analyze clinical trial data to identify potential safety signals, detect unexpected adverse events, and assess the efficacy of interventions in realtime [50]. This enables researchers to make informed decisions regarding study modifications, such as adjusting dosing regimens or incorporating new treatment arms, leading to faster and more efficient clinical trials (Fig. 2).

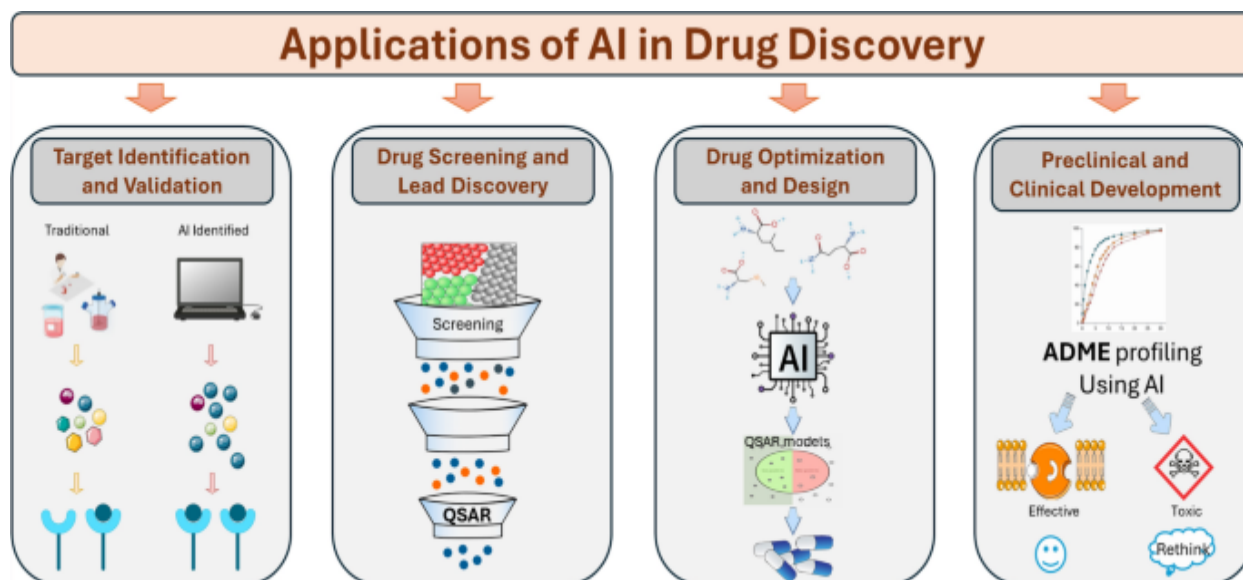


Figure. 2

Machine learning algorithms using supervised and unsupervised learning

These algorithms can be broadly categorized as supervised or unsupervised. Supervised learning, in which algorithms are trained on labeled data, is crucial for predicting drug efficacy and side effects. For instance, by training models on datasets of compounds with known activity against a specific target, researchers can predict the efficacy of new compounds [51]. Similarly, supervised learning can be used to predict potential side effects by analyzing historical data on adverse drug reactions [52]. On the other hand, unsupervised learning explores unlabeled data to identify patterns and relationships. This approach can be used to identify novel drug targets by clustering genes with similar expression patterns or by grouping compounds with similar chemical structures. Popular ML algorithms in drug discovery include random forests, which can handle high-dimensional data and provide insights into feature importance [53], SVM, which are effective for classification tasks and identifying optimal decision boundaries [54], and gradient boosting machines, which combine multiple weak learners to create a strong predictive model [55]. These algorithms are instrumental in accelerating drug discovery by enabling rapid analysis of large datasets and identifying promising drug candidates [56].

Deep learning utilizing neural networks

Deep neural networks (DNNs), particularly CNNs and RNNs, are highly effective tools in drug design. CNNs excel at processing image-like data such as molecular structures represented as 2D or 3D point clouds. They can effectively learn complex patterns within molecular structures, enabling accurate predictions of protein–ligand binding affinities and other crucial properties [57]. RNNs, however, are well suited for processing sequential data such as protein sequences or chemical reaction pathways. They can be used to predict protein–protein interactions, analyze drug-metabolizing enzymes, and generate novel drug-like molecules [58].

Natural language processing in identification of novel candidates:

NLP techniques are instrumental in mining large amounts of unstructured text data from scientific literature, patents, and electronic health records (EHRs) to discover novel drug candidates and biomarker targets. NLP algorithms can extract relevant information from scientific publications, such as experimental

results, chemical structures, and biological pathways, to identify potential drug targets and promising therapeutic strategies [62]. By analyzing patents, NLP can identify novel chemical entities, understand intellectual property landscapes, and identify potential collaborators or licensing opportunities [63].

Molecular fingerprinting:

Molecular fingerprinting is a computational technique that transforms chemical structures into compact numerical representations, such as bit vectors or feature arrays, to capture key structural and physicochemical properties. These fingerprints facilitate rapid comparison, similarity searches, and machine learning tasks, making them invaluable in drug discovery and materials science. Common types include circular fingerprints like Extended Connectivity Fingerprints (ECFP) for substructure patterns, path-based fingerprints for bond sequences, and 3D fingerprints for molecular shapes [70]. Unlike NLP, which processes human language, molecular fingerprinting encodes chemical "grammar," such as functional groups and bonds, rather than linguistic semantics. While NLP models like transformers can analyze molecules via SMILES strings, traditional fingerprinting relies on cheminformatics algorithms for applications like virtual screening and toxicity prediction. Tools such as RDKit [71], and ChemDes [72] are widely used to compute fingerprints efficiently, bridging the gap between chemistry and AI [73].

Graph neural networks :

GNNs are a powerful class of DL models specifically designed for analyzing graph-structured data, which consists of nodes (entities) and edges (relationships). Unlike traditional neural networks that process grid-like data such as images or text, GNNs excel at capturing dependencies in non-Euclidean spaces, making them particularly effective for applications like social network analysis, drug discovery, and recommendation systems. GNNs utilize a message-passing mechanism where nodes iteratively aggregate information from their neighbors, allowing them to learn meaningful representations of both local and global graph structures. Key architectures include Graph Convolutional Networks (GCNs), which apply spectral convolution; Graph Attention Networks (GATs), which use attention mechanisms to prioritize neighbor importance; and GraphSAGE, designed for scalable inductive learning [75, 76].

Generative AI:

Gen-AI tools such as ChatGPT hold significant potential in healthcare education and clinical practice. In pharmacy, they could enhance efficiency by assisting with prescription reviews, drug interaction checks, and adverse reaction monitoring, ultimately improving patient care. However, their application in pharmacy education remains underexplored, with limited research on implementation challenges, underscoring the need for further investigation [81]. Beyond assisting in clinical tasks, generative AI can also synthesize large datasets to train predictive models, expanding its utility in medical research. Among these AI techniques, GANs stand out as a powerful DL framework composed of two competing neural networks—a generator that creates synthetic data and a discriminator that evaluates its authenticity. Through iterative adversarial training, the generator refines its outputs to produce highly realistic data, enabling applications in medical imaging, super-resolution, and data augmentation [82]. For example, Super-Resolution GAN has demonstrated success in enhancing low-resolution images, proving valuable in medical diagnostics and video surveillance [83].

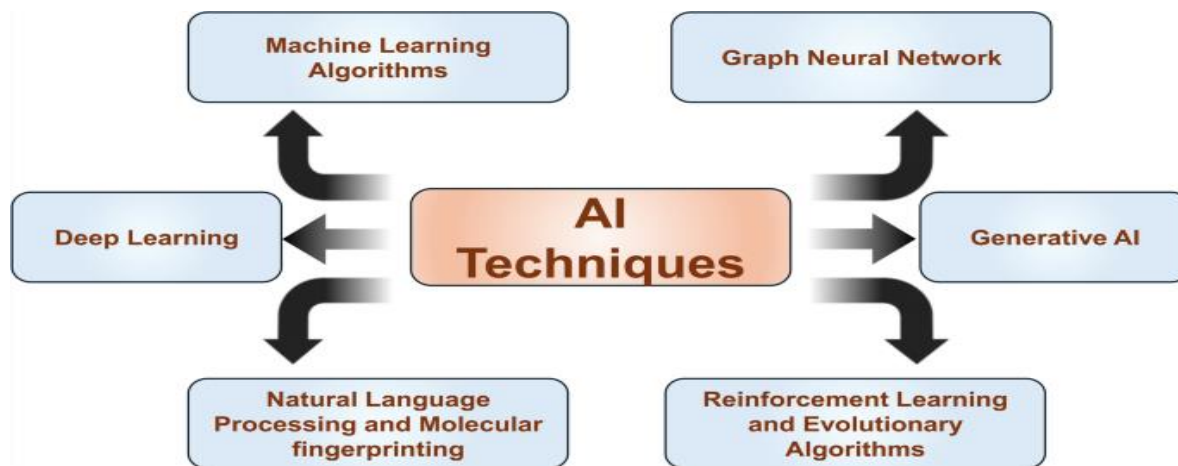


Figure. 3

Integration and workflow disruption:

Implementing AI requires restructuring traditional R&D workflows. Most pharma companies still rely heavily on wet lab experiments, and integrating AI into existing pipelines necessitates new infrastructure, retraining of staff, and a shift in research culture [110]. Collaboration between data scientists and biologists is often hampered by disciplinary divides and a lack of mutual understanding. Regulatory bodies such as the FDA are still developing frameworks to assess AI-driven drug candidates. Unlike traditional methods, AI-generated molecules or biomarkers may not fit neatly into existing regulatory categories, slowing approvals and raising legal uncertainty [111].

Reproducibility and validation:

AI models are often trained on retrospective data, but their performance in prospective or real-world applications remains limited. Many models fail to generalize outside their training environments, and reproducibility is hampered by lack of standardized reporting or access to proprietary datasets [112].

CHALLENGES AND STRATEGIES FOR AI IN DRUG DISCOVERY :

Artificial Intelligence (AI) holds transformative potential in the field of drug discovery, offering the ability to analyze vast datasets, identify drug candidates faster, and optimize experimental processes. However, despite its advantages, several challenges and limitations hinder its widespread and effective application. One of the primary challenges is the availability and quality of data [113]. AI algorithms, particularly machine learning (ML) models, require large and diverse datasets to learn meaningful patterns [114]. However, in many cases, the data available for drug discovery are limited, incomplete, inconsistent, or of poor quality [108]. Datasets may lack proper annotation, contain biases, or represent only a narrow spectrum of chemical or biological diversity. Such limitations reduce the accuracy and generalizability of AI models, potentially leading to unreliable predictions and misguided decisions.

Another major concern involves ethical considerations [115]. AI systems are only as fair and unbiased as the data they are trained on. If the training data contain biases, such as an overrepresentation of certain populations or drug types, the resulting models may produce skewed outcomes. This can raise significant issues of fairness and accuracy, especially when AI predictions influence decisions in clinical research or

patient care. Ensuring the ethical and fair use of AI requires transparent methodologies, diverse datasets, and mechanisms to identify and correct potential biases [116].

To address these challenges, researchers are adopting several strategies. One such strategy is data augmentation, which involves generating synthetic data to expand and diversify the existing datasets. This can help mitigate data scarcity and improve the robustness of ML models by exposing them to a wider range of scenarios [117]. Another promising approach is the adoption of explainable AI (XAI) methods [118], which aim to make the decision-making process of AI models transparent and interpretable. XAI allows researchers to understand why a particular prediction was made, addressing concerns related to bias and fairness and helping to clarify the mechanisms and assumptions underlying the projections [119].

Importantly, AI is not a replacement for traditional experimental methods or human expertise [120]. While it can predict potential drug candidates and streamline aspects of research, AI-generated hypotheses must be validated through laboratory experiments. By integrating AI with expert-driven experimentation, the drug discovery process can be significantly optimized, ultimately accelerating the development of effective new therapies [121].

CONCLUSION

The integration of AI in drug design and discovery has ushered in a transformative era for the pharmaceutical industry. AI models contribute significantly to key processes including target identification, drug design, lead identification, drug repurposing, lead optimization, and toxicity prediction, substantially accelerating the development pipeline. AI-powered approaches are proving invaluable in identifying drug repurposing candidates, an especially vital area in the context of emerging diseases and pandemics. By enabling more accurate predictions, analyzing large-scale data sets, and simulating complex molecular interactions, AI holds the potential to significantly reduce the time, cost, and failure rates traditionally associated with drug development. However, challenges remain, including data quality, interpretability of models, and the need for collaboration between AI experts and domain-specific researchers. Nevertheless, as AI continues to evolve and mature, its role in drug discovery is poised to enhance the precision, efficiency, and success of developing new therapeutic agents, ultimately improving patient outcomes globally.

REFERENCES:

1. S.J. Russell, N. Peter : Artificial intelligence: a modern approach Pearson (2016)
2. B. Goertzel: Artificial general intelligence: concept, state of the art, and future prospects *Artif Gen Intell*, 5 (1) (2014), pp. 1-48, [10.2478/jagi-2014-0001](https://doi.org/10.2478/jagi-2014-0001)
3. N. Bostrom *Superintelligence: paths, dangers, strategies* Oxford University Press (2014)
4. M. Tegmark *Life 3.0: being human in the age of artificial intelligence* Knopf (2017)
5. Sahoo, B. M.; Ravi Kumar, B. V. V.; Sruti, J.; Mahapatra, M. K.; Banik, B. K.; Borah, P. Drug Repurposing Strategy (DRS): Emerging Approach to Identify Potential Therapeutics for Treatment of Novel Coronavirus Infection. *Frontiers in Molecular Biosciences* **2021**, DOI: 10.3389/fmolb.2021.628144

6. Mak K-K, Wong Y-H, Pichika MR. Artificial Intelligence in Drug Discovery and Development. In: Hock FJ, Pugsley MK, editors. Drug discovery and evaluation: safety and pharmacokinetic assays. Cham: Springer International Publishing; 2024. p. 1461–98.
7. Vora LK, et al. Artificial intelligence in pharmaceutical technology and drug delivery design. *Pharmaceutics*. 2023;15(7):1916.
8. Ramesh A. Artificial intelligence in medicine. *Ann. R. Coll. Surg. Engl.* 2004;86:334–338. doi: 10.1308/147870804290. [[DOI](#)] [[PMC free article](#)] [[PubMed](#)] [[Google Scholar](#)]
9. Miles J., Walker A. The potential application of artificial intelligence in transport. *IEE Proc. -Intell. Transport Syst.* 2006;153:183–198. [[Google Scholar](#)]
10. Smith R.G., Farquhar A. The road ahead for knowledge management: an AI perspective. *AI Mag.* 2000;21 17–17. [[Google Scholar](#)]
11. Lamberti M.J. A study on the application and use of artificial intelligence to support drug development. *Clin. Ther.* 2019;41:1414–1426. doi: 10.1016/j.clinthera.2019.05.018. [[DOI](#)] [[PubMed](#)] [[Google Scholar](#)]
12. Beneke F., Mackenrodt M.-O. Artificial intelligence and collusion. *IIC Int. Rev. Intellectual Property Competition Law*. 2019;50:109–134. [[Google Scholar](#)]
13. Steels L., Brooks R. Routledge; 2018. The Artificial Life Route to Artificial Intelligence: Building Embodied, Situated Agents. [[Google Scholar](#)]
14. Bielecki A., Bielecki A. Foundations of artificial neural networks. In: Kacprzyk Janusz., editor. Models of Neurons and Perceptrons: Selected Problems and Challenges. Springer International Publishing; 2019. pp. 15–28. Polish academy of sciences, Warsaw, Poland. [[Google Scholar](#)]
15. Kalyane D. Artificial intelligence in the pharmaceutical sector: current scene and future prospect. In: Tekade Rakesh K., editor. The Future of Pharmaceutical Product Development and Research. Elsevier; 2020. pp. 73–107. [[Google Scholar](#)]
16. J.P. Hughes, S. Rees, S.B. Kalindjian, K.L. Philpott Principles of early drug discovery *Br. J. Pharmacol.*, 162 (2011), pp. 1239-1249
17. J. Kirchmair, S. Distinto, K. Roman Liedl, P. Markt, J. Maria Rollinger, D. Schuster, G. Maria Spitzer, G. Wolber Development of anti-viral agents using molecular modeling and virtual screening techniques
18. Vidhya KS, et al. Artificial intelligence’s impact on drug discovery and development from bench to bedside. *Cureus*. 2023;15(10):e47486.
19. Singh S, et al. Artificial intelligence and machine learning in pharmacological research: bridging the gap between data and drug discovery. *Cureus*. 2023;15(8):e44359.
20. Piir G, et al. Best practices for QSAR model reporting: physical and chemical properties, ecotoxicity, environmental fate, human health, and toxicokinetics endpoints. *Environ Health Perspect.* 2018;126(12):126001.
21. Vora LK, et al. Artificial intelligence in pharmaceutical technology and drug delivery design. *Pharmaceutics*. 2023;15(7):1916.

22. Paul D, et al. Artificial intelligence in drug discovery and development. *Drug Discov Today*. 2021;26(1):80–93.
23. Wu K, et al. Predicting pharmacodynamic effects through early drug discovery with artificial intelligence-physiologically based pharmacokinetic (AI-PBPK) modelling. *Front Pharmacol*. 2024;15:1330855
24. Chow S-C, Liu J-P. *Design and analysis of clinical trials: concepts and methodologies*, vol. 507. Hoboken: Wiley; 2008.
25. Vamathevan J, et al. Applications of machine learning in drug discovery and development. *Nat Rev Drug Discov*. 2019;18(6):463–77.
26. Toni E, et al. Machine learning techniques for predicting drug-related side effects: a scoping review. *Pharmaceuticals (Basel)*. 2024;17(6):795.
27. Breiman L. Random forests. *Mach Learn*. 2001;45(1):5–32.
28. Awad M, Khanna R. Support vector machines for classification. In: *efficient learning machines: theories, concepts, and applications for engineers and system designers*. Berkeley, CA: Apress; 2015. p. 39–66.
29. Alzubaidi L, et al. Review of deep learning: concepts, CNN architectures, challenges, applications, future directions. *J Big Data*. 2021;8(1):53.
30. Grisoni F, et al. Bidirectional molecule generation with recurrent neural networks. *J Chem Inf Model*. 2020;60(3):1175–83.
31. Agarwal P, Searls DB. Literature mining in support of drug discovery. *Brief Bioinform*. 2008;9(6):479–92.
32. Kosonocky CW, et al. Mining patents with large language models elucidates the chemical function landscape. *Digital Discovery*. 2024;3(6):1150–9.
33. Li Z, et al. Fingerprinting interactions between proteins and ligands for facilitating machine learning in drug discovery. *Biomolecules*. 2024;14(1):72.
34. Landrum G. Rdkit documentation. Release. 2013;1(1–79):4.
35. Dong J, et al. ChemDes: an integrated web-based platform for molecular descriptor and fingerprint computation. *J Cheminform*. 2015;7(1):60.
36. Dong J, et al. ChemDes: an integrated web-based platform for molecular descriptor and fingerprint computation. *J Cheminform*. 2015;7:60.
37. Zaidan AM. The leading global health challenges in the artificial intelligence era. *Front Public Health*. 2023;11:1328918.
38. Wu Z, et al. A comprehensive survey on graph neural networks. *IEEE Trans Neural Networks Learn Syst*. 2020;32(1):4–24.
39. Lan L, et al. Generative adversarial networks and its applications in biomedical informatics. *Front Public Health*. 2020;8:164.
40. E. Topol *Deep medicine: How artificial intelligence can make healthcare human again* Basic Books (2019)
41. K.H. Yu, A.L. Beam, I.S. Kohane Artificial intelligence in healthcare *Nat Biomed Eng*, 2 (10) (2018), pp. 719-731, [10.1038/s41551-018-0305-z](https://doi.org/10.1038/s41551-018-0305-z)
42. S. Matta, M. Lamard, P. Zhang, A. Le Guilcher, L. Borderie, B. Cochener, G. Quéllec A systematic review of generalization research in medical image classification
43. J.K. Yella, S. Yaddanapudi, Y. Wang, A.G. Jegga Changing trends in computational drug repositioning *Pharmaceuticals*, 11 (2018), p. 57

44. T. Ching, D.S. Himmelstein, B.K. Beaulieu-Jones, A.A. Kalinin, B.T. Do, G.P. Way, E. Ferrero, P.-M. Agapow, M. Zietz, M.M. Hoffman, W. Xie, G.L. Rosen, B.J. Lengerich, J. Israeli, J. Lanchantin, S. Woloszynek, A.E. Carpenter, A. Shrikumar, J. Xu, ..., C.S. Greene
45. Opportunities and obstacles for deep learning in biology and medicine
46. S. Tsuji, T. Hase, A. Yachie-Kinoshita, T. Nishino, S. Ghosh, M. Kikuchi, K. Shimokawa, H. Aburatani, H. Kitano, H. Tanaka Artificial intelligence-based computational framework for drug-target prioritization and inference of novel repositionable drugs for Alzheimer's disease
47. R. Gómez-Bombarelli, J.N. Wei, D. Duvenaud, J.M. Hernández-Lobato, B. Sánchez-Lengeling, D. Sheberla, J. Aguilera-Iparraguirre, T.D. Hirzel, R.P. Adams, A. Aspuru-Guzik Automatic chemical design using a data-driven continuous representation of molecules
48. T. Basu, S. Engel-Wolf, O. Menzer The ethics of machine learning in medical sciences: where do we stand today?
49. H. Shima, W. Khernamnuai, K. Kannan, M.C. Cohen Strategic best response fairness in fair machine learning Proceedings of the 2022 AAAI/ACM conference on AI, ethics, and society; New York, NY, USA. 7–9 February 2022, Association for Computing Machinery (ACM), New York, NY, USA (2022), p. 664
50. L. Taylor, G. Nitschke Improving deep learning with generic data augmentation Proceedings of the 2018 IEEE symposium series on computational intelligence, SSCI 2018; Piscataway, NJ, USA. 18–21 November 2018, Institute of Electrical and Electronics Engineers Inc., Piscataway, NJ, USA (2019), pp. 1542-1547
51. D. Minh, H.X. Wang, Y.F. Li, T.N. Nguyen Explainable artificial intelligence: a comprehensive review Artif Intell Rev, 55 (2022), pp. 3503-3568, [10.1007/s10462-021-10088-y](https://doi.org/10.1007/s10462-021-10088-y)
52. A.B. Arrieta, N. Díaz-Rodríguez, J. Del Ser, A. Bennetot, S. Tabik, A. Barbado, S. Garcia, S. Gil-Lopez, D. Molina, R. Benjamins, others Explainable artificial intelligence (XAI): concepts, taxonomies, opportunities and challenges toward responsible AI
53. Inf Fusion, 58 (2020), pp. 82-115, [10.1016/j.inffus.2019.12.012](https://doi.org/10.1016/j.inffus.2019.12.012)