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STRATEGICAL SURVEY AND ANALYSIS OF RECENT DRUG DISCOVERY

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ABSTRACT

The discovery of drug based on latest technologies like artificial intelligence, machine learning wich has been in the highlighted in current days and significantly which will reduce the time and cost required for developing new drugs. Thus the advancement technogies like machine learning ,artificial intelligence and deep learning technologies which will grow rapidly with drug related data set and the steps of drug development process by these methods has been analysed, In particular the pharmacists, chemists and druggists will face significant problems and issues regard to selecting and designing of potential drugs for interest of target testing, hence the major challenges which will predict and estimate the production state, the drug and its drugable interaction, generation of its novel molecular structures suitable for a target of interest.[1] Therefore, in this paper it has been reviewed recent methodologies adopted by latest technologies (AI, ML&DL), So these technologies applications will enhance the drug design interaction and new drug design process and also it has been summarized that the comprehensive process will be reported in this paper and Finally, we present the remaining challenges for the promising future on AI, ML & DL based prediction and novel drug design process.[3]

KEYWORDS: Pharmacology, AI ML, DL.

1. INTRODUCTION

Creating safe and efficient treatments for human illnesses is the main objective of drug discovery. From target selection to meticulous clinical studies, every stage of the drug development process takes a substantial amount of time and money. As costs increase gradually with every step, it is essential to ensure that appropriate drug candidates are selected for the next phase at each milestone.[5] In particular, the "hit-to-lead" process is a pivotal step in identifying promising lead compounds from hits and determining their potential as therapeutics. One of the reasons why clinical trials face side effects and lack in vivo efficacy is that single or multiple drugs often interact with multiple targets based on the concept of polypharmacology, in current days much effort was invested in drug discovery through artificial intelligence (AI), which has enabled significant and cost-effective development strategies in academia and pharmaceutical industries. The vast amounts of chemical and biological data accumulated over decades, along with technological automation through the availability of high-performance processors such as graphics processing unit computing, paved the way for AI in drug development Utilizing deep neural networks provides the advantage of understanding the very complex contexts of biological space. This is because nonlinear models can be constructed in hidden layers to extract complex patterns from multi-level representations. It also minimizes the work of manually pre-processing unformatted raw data and selecting all kinds of features.[5] Consequently, advances made in the development of deep learning based methods have led to successful outcomes for prediction of drug–target interactions and generation of novel molecules with desired properties, However, since datasets for drug development exhibit types and distributions that are different from those used in traditional AI data, such as images and texts, further attempts are still required to analyze data from a different angle and apply the latest AI ML and DL techniques.

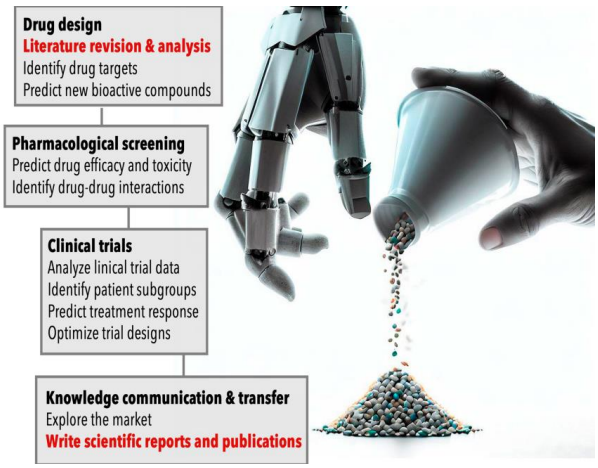

Fig 1: Graphical flowchart illustrating the development process of a pharmacologically active molecule, from design to knowledge communication and transfer.

2. Drug Discovery AI-Enabled, Its Challenges and Opportunities

With the growing accumulation of genomic and clinical data, data scientists face both challenges and opportunities when attempting to extract biologically or clinically relevant information from massive genotype and phenotype datasets.[8] In genomics, AI-based technologies and data science techniques have been utilized effectively over the past two decade.

The initial phase of drug discovery usually involves computational screening of numerous compounds to identify those with the desired cellular or biochemical effects. To enhance the speed, efficiency, and cost-effectiveness of this process, new methods are constantly being developed. A positive response during the first round of screening in a biochemical assay identifies primary "hit" compounds.

Subsequently, additional screening is performed to assess whether the physicochemical and pharmacological properties of the hit compounds are suitable for developing a medicine. If they pass this filter, they are designated as "leads". These leads are then refined chemically and subjected to biological screening in subsequent rounds before proceeding to clinical testing. With some luck, a lead may ultimately receive drug approval, a process that may take 12-15 years from the beginning of testing.[9]

Since the last decade, AI has been used in different areas of biological sciences, medical sciences, and general sciences. AI, also known as machine intelligence, directs computer systems' capability to learn from past data and input. AI is generally applied when a machine imitates cognitive behavior and behaves like a human. It is associated with the human brain's learning and problem-solving capabilities.[10] Due to massive multi-omics data and high-performance computer hardware availability, AI techniques were introduced as a fundamental application in various disciplines. Similarly, data digitalization has increased in the pharmaceutical sector, which has inspired the use of AI.

At the same time, automation was enhanced, and AI was empowered to handle large volumes of data. Pharmaceutical industries have collaborated with the computational industries.[11] In the last few years, progress has been made in drug discovery using AI-enabled drug discovery technologies. AI has also been used by drug discovery organizations, which has changed the drug discovery scenario in the last decade. Various AI techniques have been adopted in the different areas of drug discovery, such as virtual screening, target selection, and hit-to-lead generation.[36]

Data are required for any statistical inferences, including ML. Similarly, different models can be developed using data modalities. Data come in different forms, such as textual, image, and numerical. Extensive data analysis broadly transforms pharmaceutical and medicinal fields. Presently, data-driven digital transformation is noted in every sector, which is an emerging phenomenon.[43]

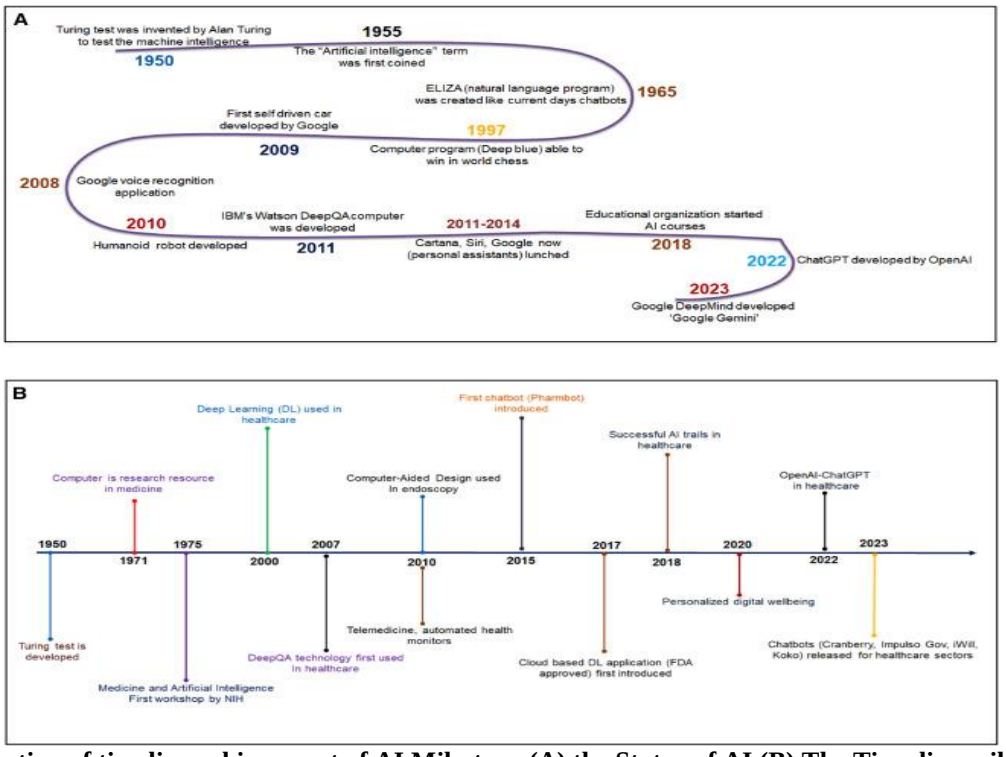

Fig 2: Illustartion of timeline achievement of AI Milestone (A) the Status of AI (B) The Time line milestone of AI in healthcare sector.

Several AI tools and techniques exist that can be classified on the basis of neural networks, use of training data, and extraction of features, e.g., machine learning vs deep learning, supervised vs unsupervised learning, and feature selection vs dimensionality reduction, respectively. Machine learning and deep learning are related but distinct concepts within the artificial intelligence (AI) field.[11]

Table 1: The AI ML and DL Techniques and its usage in phaemalogical research.[43-57]

Technique	Methods	Process
Machine learning	Support vector machine (SVM)	It finds the best hyper plane that separates different classes with the maximum margin, allowing effective classification even in complex datasets. Identifies decision boundaries in high-dimensional data and can handle non-linear relationships. It is used for classification and regression tasks in pharmacological research.
	Random Forest	An ensemble learning method, that works by combining multiple decision trees to improve predictive accuracy, feature importance analysis, and identification of potential drug candidates. Primarily used for feature selection and classification tasks in drug discovery and toxicity prediction .
	Supervised Learning	It involves training models with labeled data to yield desired outputs, enabling accurate classification and prediction tasks through algorithms, such as neural networks, support vector machines, and random forests. Drug-target interaction prediction, virtual screening, and toxicity prediction are its main uses.
	Unsupervised Learning Principal Component Analyses (PCA)	Recursive feature elimination (RFE) is a feature selection algorithm that iteratively eliminates less important features from a dataset based on their relevance in predicting the target variable. It starts with all features and removes them one by one until the desired number of features is reached. LASSO regression, also known as L1 regularization, is a linear regression technique that performs both feature selection and regularization by adding a penalty term to the loss function. It encourages sparsity in the coefficients, effectively shrinking less important features to zero, and keeping only the most relevant features in the model. They are primarily used to select relevant molecular or clinical descriptors for drug-target interaction prediction or patient stratification.
	Dimensionality reduction principal component analysis (PCA) t-SNE (t-distributed stochastic neighbour embedding	Utilized to transform high-dimensional data into lower-dimensional representations while preserving essential information. It has value in E data exploration and visualization, feature selection, clustering and classification, noise reduction in data, and pre-processing for machine learning.
Deep Learning	Neural Networks	The Structure And Function Of Biological Neurons.
	Convolution neural networks (CNNs)	They employ convolution, a mathematical operation, to process pixel data. By breaking down images into smaller features and progressively combining them into more complex patterns, CNNs efficiently learn and extract abstract representations, minimizing overfitting. These have revolutionized image analysis tasks, enabling accurate image classification, segmentation, and object detection.
Recurrent neural networks (RNNs)	Sequence-based tasks like protein structure prediction.	

4. CONLUSIONS

In this paper the technologies like AI ML & Deep learning are analysed for drug usage and its data process in various cases.

Machine learning refers to a subset of AI techniques where computers learn from data and improve their performance without being explicitly programmed. It involves the development of algorithms and models that can automatically learn and make predictions or decisions based on data.[25-28]

On the other hand, deep learning is a subfield of machine learning that focuses on training artificial neural networks to mimic the human brain's learning process. It involves using deep neural networks, composed of multiple layers of interconnected artificial neurons, to process and analyze complex patterns in data.[35-60] Deep learning algorithms can automatically learn

hierarchical representations of data and have shown remarkable performance in tasks such as image recognition, natural language processing, and speech recognition.

In summary, machine learning is a broader concept encompassing various algorithms and techniques for training computers to learn from data. In contrast, deep learning is a specific approach within machine learning that focuses on training deep neural networks to learn and extract complex patterns from data.

REFERENCES

1. Artificial intelligence in drug discovery: recent advances and future perspectives. Jiménez-Luna J, Grisoni F, Weskamp N, Schneider G. Expert Opin Drug Discov, 2021; 16: 949–959. doi: 10.1080/17460441.2021.1909567. [DOI] [PubMed] [Google Scholar]
2. Artificial intelligence in drug discovery and development. Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Drug Discov Today, 2021; 26: 80–93. doi: 10.1016/j.drudis.2020.10.010. [DOI] [PMC free article] [PubMed] [Google Scholar]
3. Current progress and open challenges for applying deep learning across the biosciences. Sapoval N, Aghazadeh A, Nute MG, et al. Nat Commun, 2022; 13. doi:10.1038/s41467-022-29268-7. [DOI] [PMC free article] [PubMed] [Google Scholar]
4. Artificial intelligence in drug discovery: a comprehensive review of data-driven and machine learning approaches. Kim H, Kim E, Lee I, Bae B, Park M, Nam H. Biotechnol Bioprocess Eng, 2020; 25: 895–930. doi:10.1007/s12257-020-0049-y. [DOI] [PMC free article] [PubMed] [Google Scholar]
5. Artificial intelligence in cancer target identification and drug discovery. You Y, Lai X, Pan Y, et al. Signal Transduct Target Ther, 2022; 7. doi: 10.1038/s41392-022-00994-0. [DOI] [PMC free article] [PubMed] [Google Scholar]
6. Using predictive machine learning models for drug response simulation by calibrating patient-specific pathway signatures. Golriz Khatami S, Mubeen S, Bharadhwaj VS, Kodamullil AT, Hofmann-Apitius M, Domingo-Fernández D. NPJ Syst Biol Appl, 2021; 7. doi:10.1038/s41540-021-00199-1. [DOI] [PMC free article] [PubMed] [Google Scholar]
7. Machine learning approaches to drug response prediction: challenges and recent progress. Adam G, Rampášek L, Safikhani Z, Smirnov P, Haibe-Kains B, Goldenberg A. NPJ Precis Oncol, 2020; 4. doi: 10.1038/s41698-020-0122-1. [DOI] [PMC free article] [PubMed] [Google Scholar]
8. An artificial intelligence-aided virtual screening recipe for two-dimensional materials discovery. Sorkun MC, Astruc S, Koelman JV, Er S. Npj Comput Mater, 2020; 24. [Google Scholar]
9. Artificial intelligence-enabled virtual screening of ultra-large chemical libraries with deep docking. Gentile F, Yaacoub JC, Gleave J, et al. Nat Protoc, 2022; 17: 672–697. doi: 10.1038/s41596-021-00659-2. [DOI] [PubMed] [Google Scholar]
10. Impact of artificial intelligence on compound discovery, design, and synthesis. Miljković F, Rodríguez-Pérez R, Bajorath J. ACS Omega, 2021; 6: 33293–33299. doi: 10.1021/acsomega.1c05512. [DOI] [PMC free article] [PubMed] [Google Scholar]Tapping into the drug discovery potential of AI. Savage N. https://www.nature.com/articles/d43747-021-00045-7 AI., 2021; 20: 408–410. [Google Scholar]
11. Holistic models of reaction selectivity. Norrby PO. Nature, 2019; 571: 332–333. doi: 10.1038/d41586-019-02148-9. [DOI] [PubMed] [Google Scholar]
12. Crossvalidation, bootstrapping, and partial least squares compared with multiple regression in conventional QSAR studies. Cramer RD, Bunce JD, Patterson DE, Frank IE. Mol Inform, 1988; 7: 18–25. [Google Scholar]
13. Generative deep learning enables the discovery of a potent and selective RIPK1 inhibitor. Li Y, Zhang L, Wang Y, et al. Nat Commun, 2022; 13. doi:10.1038/s41467-022-34692-w. [DOI] [PMC free article] [PubMed] [Google Scholar]
14. Hit and lead discovery with explorative RL and fragment-based molecule generation. Yang S, Hwang D, Lee S, Ryu S, Hwang SJ. https://arxiv.org/abs/2110.01219 Adv Neural Inf Process Syst, 2021; 6: 7924–7936. [Google Scholar]
15. Shape-based generative modeling for de novo drug design. Skalic M, Jiménez J, Sabbadin D, De Fabritiis G. J Chem Inf Model, 2019; 59: 1205–1214. doi: 10.1021/acs.jcim.8b00706. [DOI] [PubMed] [Google Scholar]
16. Generative deep learning for targeted compound design. Sousa T, Correia J, Pereira V, Rocha M. J Chem Inf Model, 2021; 61: 5343–5361. doi: 10.1021/acs.jcim.0c01496. [DOI] [PubMed] [Google Scholar]
17. Artificial intelligence in drug metabolism and excretion prediction: recent advances, challenges, and future perspectives. Tran TT, Tayara H, Chong KT. Pharmaceutics, 2023; 15. doi: 10.3390/pharmaceutics15041260. [DOI] [PMC free article] [PubMed] [Google Scholar]
18. Machine learning in drug discovery: a review. Dara S, Dhamercherla S, Jadav SS, Babu CM, Ahsan MJ. Artif Intell Rev, 2022; 55: 1947–1999. doi: 10.1007/s10462-021-10058-4. [DOI] [PMC free article] [PubMed] [Google Scholar]
19. Artificial intelligence (AI) in drugs and pharmaceuticals. Sahu A, Mishra J, Kushwaha N. Comb Chem High Throughput Screen, 2022; 25: 1818–1837. doi: 10.2174/1386207325666211207153943. [DOI] [PubMed] [Google Scholar]
20. BioTransformer: a comprehensive computational tool for small molecule metabolism prediction and metabolite identification. Djoumbou-Feunang Y,

Fiamoncini J, Gil-de-la-Fuente A, Greiner R, Manach C, Wishart DS. J Cheminform, 2019; 11. doi:10.1186/s13321-018-0324-5. [DOI] [PMC free article] [PubMed] [Google Scholar]

21. A recent appraisal of artificial intelligence and in silico ADMET prediction in the early stages of drug discovery. Kumar A, Kini SG, Rathi E. Mini Rev Med Chem, 2021; 21: 2788–2800. doi: 10.2174/1389557521666210401091147. [DOI] [PubMed] [Google Scholar]
22. Computational approaches in preclinical studies on drug discovery and development. Wu F, Zhou Y, Li L, et al. Front Chem, 2020; 8. doi: 10.3389/fchem.2020.00726. [DOI] [PMC free article] [PubMed] [Google Scholar]
23. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Daina A, Michielin O, Zoete V. Sci Rep, 2017; 7. doi: 10.1038/srep42717. [DOI] [PMC free article] [PubMed] [Google Scholar]
24. Preclinical experimental models of drug metabolism and disposition in drug discovery and development. Zhang D, Luo G, Ding X, Lu C. Acta Pharm Sin B., 2012; 2: 549–561. [Google Scholar]
25. Absorption, distribution, metabolism, excretion, and toxicity evaluation in drug discovery. 14. Prediction of human pregnane X receptor activators by using naive Bayesian classification technique. Shi H, Tian S, Li Y, Li D, Yu H, Zhen X, Hou T. Chem Res Toxicol, 2015; 28: 116–125. doi: 10.1021/tx500389q. [DOI] [PubMed] [Google Scholar]
26. Techniques: application of systems biology to absorption, distribution, metabolism, excretion and toxicity. Ekins S, Nikolsky Y, Nikolskaya T. Trends Pharmacol Sci, 2005; 26: 202–209. doi: 10.1016/j.tips.2005.02.006. [DOI] [PubMed] [Google Scholar]
27. Applying machine learning techniques for ADME-Tox prediction: a review. Maltarollo VG, Gertrudes JC, Oliveira PR, Honorio KM. Expert Opin Drug Metab Toxicol, 2015; 11: 259–271. doi: 10.1517/17425255.2015.980814. [DOI] [PubMed] [Google Scholar]
28. Reliable prediction of Caco-2 permeability by supervised recursive machine learning approaches. Falcón-Cano G, Molina C, Cabrera-Pérez MÁ. Pharmaceutics, 2022; 14. doi: 10.3390/pharmaceutics14101998. [DOI] [PMC free article] [PubMed] [Google Scholar]
29. ADMET evaluation in drug discovery. 19. Reliable prediction of human cytochrome P450 inhibition using artificial intelligence approaches. Wu Z, Lei T, Shen C, Wang Z, Cao D, Hou T. J Chem Inf Model, 2019; 59: 4587–4601. doi: 10.1021/acs.jcim.9b00801. [DOI] [PubMed] [Google Scholar]
30. Drug repositioning with GraphSAGE and clustering constraints based on drug and disease networks. Zhang Y, Lei X, Pan Y, Wu FX. Front Pharmacol, 2022; 13. doi: 10.3389/fphar.2022.872785. [DOI] [PMC free article] [PubMed] [Google Scholar]
31. Predicting drug-disease association based on ensemble strategy. Wang J, Wang W, Yan C, Luo J, Zhang G. Front Genet, 2021; 12. doi: 10.3389/fgene.2021.666575. [DOI] [PMC free article] [PubMed] [Google Scholar]
32. Drug-disease association prediction with literature based multi-feature fusion. Kang H, Hou L, Gu Y, Lu X, Li J, Li Q. Front Pharmacol, 2023; 14. doi: 10.3389/fphar.2023.1205144. [DOI] [PMC free article] [PubMed] [Google Scholar]
33. Predicting drug-disease associations and their therapeutic function based on the drug-disease association bipartite network. Zhang W, Yue X, Huang F, Liu R, Chen Y, Ruan C. Methods, 2018; 145: 51–59. doi: 10.1016/j.ymeth.2018.06.001. [DOI] [PubMed] [Google Scholar]
34. Computational drug repositioning through heterogeneous network clustering. Wu C, Gudivada RC, Aronow BJ, Jegga AG. BMC Syst Biol, 2013; 7. doi: 10.1186/1752-0509-7-S5-S6. [DOI] [PMC free article] [PubMed] [Google Scholar]
35. PREDICT: a method for inferring novel drug indications with application to personalized medicine. Gottlieb A, Stein GY, Ruppin E, Sharan R. Mol Syst Biol, 2011; 7. doi: 10.1038/msb.2011.26. [DOI] [PMC free article] [PubMed] [Google Scholar]
36. Drug repositioning: a machine-learning approach through data integration. Napolitano F, Zhao Y, Moreira VM, Tagliaferri R, Kere J, D'Amato M, Greco D. J Cheminform, 2013; 5. doi:10.1186/1758-2946-5-30. [DOI] [PMC free article] [PubMed] [Google Scholar]
37. Guidelines for clinical trial protocols for interventions involving artificial intelligence: the SPIRIT-AI extension. Cruz Rivera S, Liu X, Chan AW, Denniston AK, Calvert MJ. Nat Med, 2020; 26: 1351–1363. doi: 10.1038/s41591-020-1037-7. [DOI] [PMC free article] [PubMed] [Google Scholar]
38. Reporting guidelines for clinical trial reports for interventions involving artificial intelligence: the CONSORT-AI extension. Liu X, Rivera SC, Moher D, Calvert MJ, Denniston AK. Nat Med, 2020; 26: 1364–1374. doi: 10.1038/s41591-020-1034-x. [DOI] [PMC free article] [PubMed] [Google Scholar]
39. Artificial intelligence for clinical trial design. Harrer S, Shah P, Antony B, Hu J. Trends Pharmacol Sci, 2019; 40: 577–591. doi: 10.1016/j.tips.2019.05.005. [DOI] [PubMed] [Google Scholar]
40. Karen Taylor, Francesca Properzi. Intelligent clinical trials. Maria Joao Cruz Intelligent clinical trials. Transforming through AI-enabled. 2020. https://www2.deloitte.com/content/dam/insights/us/articles/22934_intelligent-clinical-

trials/DI_Intelligent-clinical-trials.pdf https://www2.deloitte.com/content/dam/insights/us/articles/22934_intelligent-clinical-trials/DI_Intelligent-clinical-trials.pdf

41. Artificial intelligence in medical imaging: threat or opportunity? Radiologists again at the forefront of innovation in medicine. Pesapane F, Codari M, Sardanelli F. https://eurradiolexp.springeropen.com/articles/10.1186/s41747-018-0061-6. Eur Radiol Exp, 2018; 2 doi: 10.1186/s41747-018-0061-6. [DOI] [PMC free article] [PubMed] [Google Scholar]
42. The use of artificial intelligence in pharmacovigilance: a systematic review of the literature. Salas M, Petracek J, Yalamanchili P, et al. Pharmaceut Med, 2022; 36: 295–306. doi: 10.1007/s40290-022-00441-z. [DOI] [PubMed] [Google Scholar]
43. Key use cases for artificial intelligence to reduce the frequency of adverse drug events: a scoping review. Syrowatka A, Song W, Amato MG, et al. Lancet Digit Health, 2022; 4: 137–148. doi: 10.1016/S2589-7500(21)00229-6. [DOI] [PubMed] [Google Scholar]
44. Artificial intelligence, real-world automation and the safety of medicines. Bate A, Hobbiger SF. Drug Saf, 2021; 44: 125–132. doi: 10.1007/s40264-020-01001-7. [DOI] [PubMed] [Google Scholar]
45. A new era in pharmacovigilance: toward real-world data and digital monitoring. Lavertu A, Vora B, Giacomini KM, Altman R, Rensi S. Clin Pharmacol Ther, 2021; 109: 1197–1202. doi: 10.1002/cpt.2172. [DOI] [PMC free article] [PubMed] [Google Scholar]
46. Artificial intelligence and the future of the drug safety professional. Danysz K, Cicirello S, Mingle E, et al. Drug Saf, 2019; 42: 491–497. doi: 10.1007/s40264-018-0746-z. [DOI] [PMC free article] [PubMed] [Google Scholar]
47. Improving drug safety with adverse event detection using natural language processing. Botsis T, Kreimeyer K. Expert Opin Drug Saf, 2023; 1–10. doi: 10.1080/14740338.2023.2228197. [DOI] [PubMed] [Google Scholar]
48. Adverse drug event detection and extraction from open data: a deep learning approach. Fan B, Fan W, Smith C, Garner HS. Inf Process Manag, 2020; 57: 102131–102110. [Google Scholar]
49. Precision medicine, AI, and the future of personalized health care. Johnson KB, Wei WQ, Weeraratne D, et al. Clin Transl Sci, 2021; 14: 86–93. doi: 10.1111/cts.12884. [DOI] [PMC free article] [PubMed] [Google Scholar]
50. Artificial intelligence and personalized medicine. Schork NJ. Cancer Treat Res, 2019; 178: 265–283. doi: 10.1007/978-3-030-16391-4_11. [DOI] [PMC free article] [PubMed] [Google Scholar]
51. Rise of the machines? Predicting brivaracetam response using machine learning. Terman SW. Epilepsy Curr, 2022; 22: 111–113. doi: 10.1177/15357597211049052. [DOI] [PMC free article] [PubMed] [Google Scholar]
52. Personalised dosing using the CURATE.AI algorithm: protocol for a feasibility study in patients with hypertension and type II diabetes mellitus. Mukhopadhyay A, Sumner J, Ling LH, et al. Int J Environ Res Public Health, 2022; 19. doi: 10.3390/ijerph19158979. [DOI] [PMC free article] [PubMed] [Google Scholar]
53. Evolution of support vector machine and regression modeling in chemoinformatics and drug discovery. Rodríguez-Pérez R, Bajorath J. J Comput Aided Mol Des, 2022; 36: 355–362. doi: 10.1007/s10822-022-00442-9. [DOI] [PMC free article] [PubMed] [Google Scholar]
54. Identification of potential histone deacetylase1 (HDAC1) inhibitors using multistep virtual screening approach including SVM model, pharmacophore modeling, molecular docking and biological evaluation. Krishna S, Lakra AD, Shukla N, Khan S, Mishra DP, Ahmed S, Siddiqi MI. J Biomol Struct Dyn, 2020; 38: 3280–3295. doi: 10.1080/07391102.2019.1654925. [DOI] [PubMed] [Google Scholar]
55. Comparing different supervised machine learning algorithms for disease prediction. Uddin S, Khan A, Hossain ME, Moni MA. BMC Med Inform Decis Mak, 2019; 19. doi: 10.1186/s12911-019-1004-8. [DOI] [PMC free article] [PubMed] [Google Scholar]
56. Machine learning for predicting lifespan-extending chemical compounds. Barardo DG, Newby D, Thornton D, Ghafourian T, de Magalhães JP, Freitas AA. Aging (Albany NY), 2017; 9: 1721–1737. doi: 10.18632/aging.101264. [DOI] [PMC free article] [PubMed] [Google Scholar]
57. Applications of machine learning in drug discovery and development. Vamathevan J, Clark D, Czodrowski P, et al. Nat Rev Drug Discov, 2019; 18: 463–477. doi: 10.1038/s41573-019-0024-5. [DOI] [PMC free article] [PubMed] [Google Scholar]
58. Machine learning techniques for personalised medicine approaches in immune-mediated chronic inflammatory diseases: applications and challenges. Peng J, Jury EC, Dönnes P, Ciurtin C. Front Pharmacol, 2021; 12. doi: 10.3389/fphar.2021.720694. [DOI] [PMC free article] [PubMed] [Google Scholar]
59. .Drug-target interaction prediction based on protein features, using wrapper feature selection. Abbasi Mesrabadi H, Faez K, Pirgazi J. Sci Rep, 2023; 13. doi: 10.1038/s41598-023-30026-y. [DOI] [PMC free article] [PubMed] [Google Scholar]
60. A comprehensive review of feature based methods for drug target interaction prediction. Sachdev K, Gupta MK. J Biomed Inform, 2019; 93. doi: 10.1016/j.jbi.2019.103159. [DOI] [PubMed] [Google Scholar]

61. .Deep convolutional neural networks: Outperforming established algorithms in the evaluation of industrial optical coherence tomography (OCT) images of pharmaceutical coatings. Wolfgang M, Weißensteiner M, Clarke P, Hsiao WK, Khinast JG. Int J Pharm X., 2020; 2. doi:10.1016/j.ijpx.2020.100058. [DOI] [PMC free article] [PubMed] [Google Scholar]
62. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. Gupta R, Srivastava D, Sahu M, Tiwari S, Ambasta RK, Kumar P. https://link.springer.com/article/10.1007/s11030-021-10217-3. Mol Divers, 2021; 25: 1315–1360. doi: 10.1007/s11030-021-10217-3. [DOI] [PMC free article] [PubMed] [Google Scholar]
63. Feature selection strategies for drug sensitivity prediction. Koras K, Juraeva D, Kreis J, Mazur J, Staub E, Szczurek E. Sci Rep, 2020; 10. doi: 10.1038/s41598-020-65927-9. [DOI] [PMC free article] [PubMed] [Google Scholar]
64. A review of feature selection methods for machine learning-based disease risk prediction. Pudjihartono N, Fadason T, Kempa-Liehr AW, O'Sullivan JM. Front Bioinform, 2022; 2. doi: 10.3389/fbinf.2022.927312. [DOI] [PMC free article] [PubMed] [Google Scholar]
65. Machine learning and feature selection for drug response prediction in precision oncology applications. Ali M, Aittokallio T. Biophys Rev, 2019; 11: 31–39. doi: 10.1007/s12551-018-0446-z. [DOI] [PMC free article] [PubMed] [Google Scholar]
66. Machine learning feature selection for predicting high concentration therapeutic antibody aggregation. Lai PK, Fernando A, Cloutier TK, et al. J Pharm Sci, 2021; 110: 1583–1591. doi: 10.1016/j.xphs.2020.12.014. [DOI] [PubMed] [Google Scholar]
67. Machine learning for drug-target interaction prediction. Chen R, Liu X, Jin S, Lin J, Liu J. Molecules, 2018; 23. doi: 10.3390/molecules23092208. [DOI] [PMC free article] [PubMed] [Google Scholar]
68. Recommendation techniques for drug-target interaction prediction and drug repositioning. Alaimo S, Giugno R, Pulvirenti A. Methods Mol Biol, 2016; 1415: 441–462. doi: 10.1007/978-1-4939-3572-7_23. [DOI] [PubMed] [Google Scholar]
69. Using feature selection technique for drug-target interaction networks prediction. Yu W, Jiang Z, Wang J, Tao R. Curr Med Chem, 2011; 18: 5687–5693. doi: 10.2174/092986711798347270. [DOI] [PubMed] [Google Scholar]
70. Privacy and artificial intelligence: challenges for protecting health information in a new era. Murdoch B. BMC Med Ethics, 2021; 22. doi: 10.1186/s12910-021-00687-3. [DOI] [PMC free article] [PubMed] [Google Scholar]
71. You can't have AI both ways: balancing health data privacy and access fairly. Bak M, Madai VI, Fritzsche MC, Mayrhofer MT, McLennan S. Front Genet, 2022; 13. doi: 10.3389/fgene.2022.929453. [DOI] [PMC free article] [PubMed] [Google Scholar].
72. Artificial intelligence in pharmacology research and practice. van der Lee M, Swen JJ. Clin Transl Sci, 2023; 16: 31–36. doi: 10.1111/cts.13431. [DOI] [PMC free article] [PubMed] [Google Scholar]
73. The impact of artificial intelligence on data system security: a literature review. Raimundo R, Rosário A. Sensors (Basel), 2021; 21. doi: 10.3390/s21217029. [DOI] [PMC free article] [PubMed] [Google Scholar]
74. Integrating artificial intelligence into health care through data access: can the GDPR act as a beacon for policymakers? Forcier MB, Gallois H, Mullan S, Joly Y. J Law Biosci, 2019; 16: 317–335. doi: 10.1093/jlb/lsz013. [DOI] [PMC free article] [PubMed] [Google Scholar]
75. Artificial intelligence (AI) in pharmacy: an overview of innovations. Raza MA, Aziz S, Noreen M, Saeed A, Anjum I, Ahmed M, Raza SM. Innov Pharm, 2020; 13. doi: 10.24926/iip.v13i2.4839. [DOI] [PMC free article] [PubMed] [Google Scholar]
76. Machine learning and artificial intelligence in pharmaceutical research and development: a review. Kolluri S, Lin J, Liu R, Zhang Y, Zhang W. AAPS J., 2022; 24. doi:10.1208/s12248-021-00644-3. [DOI] [PMC free article] [PubMed] [Google Scholar]