CHAPTER TITLE

**Role of Artificial Intelligence in Field of Pharmacy**

Ms. Sejal M. Khuman1, Ms. Morvi M. Raval2

**Ms. Sejal M. Khuman1**

M.Pharm,

Assistant Professor

Rofel Shri G. Bilakhia College of Pharmacy,

Rajju Shroff Rofel University, Vapi

**Ms. Morvi M. Raval2**

M.Pharm, Ph.D\*

Assistant Professor

School of Pharmacy

Dr. Subhash University, Junagadh

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**ABSTRACT**

Artificial intelligence (AI) is a field within computer science that enables machines to operate efficiently and analyze intricate data. The realm of AI in healthcare and pharmaceutical research has experienced a significant surge in research and development. This comprehensive review delves into the opportunities and challenges presented by AI in these domains. To gather relevant literature, various databases such as PubMed, Science Direct, and Google Scholar were searched using specific keywords and phrases like 'Artificial intelligence', 'Pharmaceutical research', 'drug discovery', 'clinical trial', 'disease diagnosis', etc. The focus was on selecting research and review articles published within the past five years. This article extensively examines the application of AI in disease diagnosis, digital therapy, personalized treatment, drug discovery, and the prediction of epidemics or pandemics. Deep learning and neural networks emerged as the most commonly utilized AI technologies, while Bayesian nonparametric models showed potential for clinical trial design. Natural language processing and wearable devices were employed for patient identification and clinical trial monitoring. As AI technologies continue to advance, the scientific community can anticipate rapid and cost-effective healthcare and pharmaceutical research, ultimately leading to improved services for the general public.

**Keywords:** Artificial Intelligence, Global Impact, Pharmaceutical Field

**INTRODUCTION**

Artificial intelligence (AI) refers to a collection of intelligent processes and behaviors that are developed through computational models, algorithms, or a set of rules. These processes enable machines to imitate human cognitive functions such as learning and problem-solving. [1, 2] In recent years, AI has made significant advancements in the healthcare sector, revolutionizing clinical decision-making, disease diagnosis, and automation. Furthermore, there are numerous opportunities for AI to further explore the realms of pharmaceutical and healthcare research, thanks to its ability to analyze vast amounts of data from various sources. Current studies have extensively explored the utilization of AI in healthcare and other industries. AI technologies employed in the healthcare industry include **machine learning (ML)**, **natural language processing (NLP), physical robots, and robotic process automation.** [3] ML, for instance, utilizes neural network models and deep learning techniques to analyze imaging data and identify clinically significant elements, particularly in cancer-related diagnoses. [4] ML techniques are being widely incorporated in NLP for exploring unstructured data in the database and records in the form of doctors’ notes, lab reports, etc. by mapping the essential information from various imagery and textual data which helps in decision making in diagnosis and treatment options. The ongoing disruptive innovation creates a pathway for the patients to receive a precise and rapid diagnosis and customized treatment interventions. [5] AI-based solutions have been identified which include platforms that can make use of a variety of data types viz. symptoms reported by the patients, biometrics, imaging, biomarkers, etc. With the advancements in AI, the ability to detect potential illness well ahead is made possible, leading to a greater probability to prevent as an outcome of detection at a very early stage. Physical robots are being used in various healthcare segments including nursing, telemedicine, cleaning, radiology, surgical, rehabilitation, etc. [6]

The role of AI in the pharmaceutical sector cannot be overlooked, as it has a wide range of applications throughout various stages. AI has a significant impact on all aspects of pharmaceutical product development, from drug discovery to product management. In the field of drug discovery, AI technologies like **machine learning (ML), deep learning**, and AI-based **quantitative structure-activity relationship (QSAR) are utilized. These algorithms, including virtual screening (VS), support vector machines (SVMs), deep neural networks (DNNs), and recurrent neural networks (RNNs)**, play a crucial role in drug screening and design. Neural networks in AI are inspired by biological neural networks, where input data is processed to generate an output response. **Artificial neural networks (ANNs**) consist of interconnected units that process information, while DNNs have multiple layers for data processing. RNNs, on the other hand, analyze data sequentially, using the output of previous analysis as input for the next phase. SVMs are employed for input data classification and regression. In pharmaceutical product development, AI is employed to select appropriate excipients, determine the development process, and ensure compliance with specifications. **Model expert systems (MES)** and ANNs are utilized in this process. In manufacturing, AI is utilized for automated and personalized manufacturing, as well as for identifying and addressing manufacturing errors. AI technologies like meta classifiers and tablet classifiers are employed to achieve the desired quality in the final product. [7]

AI has been incorporated into clinical trials to aid in subject selection and trial monitoring, resulting in a decrease in dropouts due to the close monitoring. In addition, AI technologies like ML and NLP tools are utilized in market analysis, product positioning, and product costing. Recent publications have explored the application of AI in various fields such as medicinal chemistry, healthcare, pharmaceuticals, and biomedical studies. Specifically, AI has been applied in target protein identification, computer-aided drug design, virtual screening, **in silico pharmacokinetic evaluation, and disease diagnosis,** with a focus on cancer diagnosis and treatment. [7]

This chapter discussed the role of artificial intelligence (AI) in the following areas:

1. Disease diagnosis;
2. Digital therapy/personalized treatment:
* Retina;
* Cancer;
* Other chronic disorders.
1. Drug discovery:
* Prediction of bioactivity and toxicity;
* Clinical trials:
	+ Clinical trial design, patient identification, recruitment and enrolment;
	+ Monitoring trial, patient adherence and endpoint detection.

**1. AI IN DISEASE DIAGNOSIS**

The analysis of diseases plays a crucial role in developing a compassionate treatment plan and ensuring the well-being of patients. However, the inaccuracies caused by human error pose a significant obstacle to achieving accurate diagnoses. Additionally, the misinterpretation of information further complicates the already challenging task. Artificial Intelligence (AI) offers a promising solution by enhancing accuracy and efficiency in disease analysis. Extensive research has been conducted to explore the applications of different technologies and methodologies in disease diagnosis. As the human population continues to evolve, the healthcare system faces a growing demand due to various environmental factors. [8]

Multiple diagnostic strategies are currently available, but their reliability has raised concerns. Therefore, it is crucial to prioritize the use of AI in identifying and determining the early predictive stage of diseases rather than focusing solely on treatment or diagnosis. By utilizing AI for diagnosis, early treatment can be initiated, leading to significant improvements in patients' conditions and enhanced efficiency in AI modules. [9, 10]

AI has gained significance in the field of **cancer and dementia**, [11,12] It is important to note that algorithms cannot exhibit bias if they are not self-generated or associated with existing data. To ensure statistical supervision, a relevant and specific dataset is necessary. The acceptance of AI lies not only on user input but also on the salience of the identified clusters. Unsupervised learning can be utilized for diagnosing **hepatitis**. [13] Generally, larger and diverse datasets contribute to the effectiveness of AI, although the outcome may be difficult to comprehend. Among various examples of deep learning in diagnostics, one involves the classification of **dermatological diseases** [14] and the detection of **atrial fibrillation.** [15] Cross-validation can be employed to randomly split data into multiple sets for **algorithm estimation.** [16] Accuracy, sensitivity, and specificity are three crucial aspects that AI commonly focuses on in terms of measurement.

Several studies have been conducted on predictive modeling, particularly in the field of early **Parkinson's disease prediction.** [17] To aid in the diagnosis of lung diseases, a rib segmentation algorithm was developed using chest **X-ray images.** [18] However, traditional methods face limitations when it comes to segmenting X-ray images on a **rib-wise basis**. In this research, the authors have devised an algorithm that utilizes unpaired sample augmentation of chest X-ray images from pneumonia patients. Subsequently, a multi-scale network learns the image features. The study highlights that this algorithm demonstrates excellent performance in rib segmentation, which could prove valuable in the diagnosis of lung cancers and other **lung diseases.** [19] Researchers have also recently employed algorithms and machine learning techniques to identify and classify cardiac arrhythmia by **analyzing electrocardiogram signals.** [20] Additionally, tuberculosis was classified and diagnosed using an optimization **genetic algorithm** (GA) and **support vector machine (SVM)** classifier in another study. [21]

**2. AI IN DIGITAL THERAPY/PERSONALIZED TREATMENT**

AI has the potential to establish a significant correlation within the raw datasets, which can then be utilized in the diagnosis, treatment, and mitigation of diseases. Various advanced techniques used for computational understanding in this emerging field have the potential to be applied in almost every aspect of medical science. The complex clinical challenges require the acquisition, analysis, and application of extensive knowledge. The development of medical AI has aided clinicians in solving intricate clinical problems. Systems like ANNs, evolutionary computational algorithms, fuzzy expert systems, and hybrid intelligent systems can assist healthcare professionals in manipulating data. ANNs, which are based on the principles of the biological nervous system, consist of interconnected computer processors called neurons that can perform parallel computations for data processing. The first artificial neuron was created using a binary threshold function. [22] The multilayer feed-forward perceptron, with its input layer, middle layer, and output layer, emerged as the most popular model. Each neuron is connected through links with numerical weights. Paul **Werbos introduced** a new technique called ***“Backpropagation learning”*** in 1974, which has a suitable learning algorithm. [23]



Figure- AI in acquiring and analyzing data of a patient in personalizing the treatment [1]

* **AI in Retina**

The assessment of human health has been greatly enhanced by the high-resolution imaging of the retina. Through a **single photograph** of the retina, personalized data can be extracted. With the use of high-definition medicines, ophthalmologists and retinologists are able to determine a personalized therapy and establish a healthcare system that continuously improves. [24]

* **AI in cancer**

AI has become increasingly important in the field of cancer diagnosis and treatment due to its wide range of applications. In a study, gene expression data was utilized in a multilayer perceptron neural network to predict the lymphoma subtypes of non-Hodgkin lymphoma. The neural network consisted of 20,863 genes as the input layer and the lymphoma subtypes as the output layer, which included **mantle cell lymphoma (MCL), follicular lymphoma, diffuse large B-cell lymphoma (DLBCL)**, marginal zone lymphoma, and Burkitt. Remarkably, the AI neural network achieved a high level of accuracy in predicting the lymphoma subtypes. [25] AI is employed in the detection of cancer to reduce the time required while ensuring a high level of accuracy. The utilization of **AI-based PET imaging in lymphoma aids in the assessment of tumor burden,** which subsequently contributes to the characterization of the tumor, measurement of heterogeneity and prediction of treatment response. [26]

* **AI in Other Chronic Diseases**

Recently, a novel form of computer interaction has emerged known as intelligent computer-assisted instruction. This innovative approach has the potential to incorporate various AI technologies, including natural language understanding and expert systems. [90] By leveraging AI, it becomes possible to develop a personalized combination therapy by analyzing the patient's own biopsy and implementing n-of-1 medication recommendations. Given the need for regular monitoring in chronic diseases, AI can facilitate this process through virtual medical assistants. Numerous companies have already implemented such assistance, typically offering virtual coaching via text messages through mobile applications. Furthermore, AI can also provide tailored nutrition recommendations based on the individual's **gut microbiome**. Additionally, an integrated system utilizing deep learning can **predict arterial fibrillation.** [27]

1. **AI IN DRUG DISCOVERY**

If one follows traditional approaches to obtain statistical differences, it can take up to ten years to control the biological activity that has been discovered and developed .When designing a new drug, the solubility, partition coefficient, degree of ionization, and intrinsic permeability of the drug all affect target receptor binding . Algorithms, such as **Simplified Molecular Input Line Entry System (SMILES**), are used to predict binding properties. [28] The Estimation Program Interface Suite is commonly used for the determination of six physicochemical properties through **quantitative structure-property relationship (QSPR).** Deep learning and neural networks based on the ADMET predictor and ALGOPS program have been employed to predict the lipophilicity and solubility of various compounds. [29] Many undirected graphs are used to predict solubility [30]. When predicting a new chemical entity, factors such as surface area, mass, hydrogen count, refractivity, volume, log P, surface area, sum of the indices, solubility index, and rotatable bonds are taken into consideration. [31]

* **AI in Prediction of Bioactivity and Toxicity**

**Chem Mapper** and the similarity ensemble approach are utilized to forecast the interactions between drugs and targets. [32] The consideration can also be given to the substructure, connectivity, or a combination of both. Deep learning techniques have demonstrated enhanced performance, as they are not reliant on the 3D protein structure. Approaches such as Deep Affinity, protein, and drug molecule interaction prediction are employed. [33]

**Deep Tox**, an algorithm, surpassed all other methods by accurately identifying both static and dynamic characteristics in chemical descriptors. On the other hand, **eToxPred** was utilized to estimate the toxicity of small molecules. **TargeTox**, a drug toxicity prediction system based on biological targets, operates on the principle of guilt-by-association. [34]

A scoring function is utilized to anticipate the characteristics of newly discovered molecules. **PrOCTOR** has the capability to accurately predict if a drug would be unsuccessful in clinical trials due to its toxicity. Additionally, it has the ability to identify adverse drug events. [35] AI can provide valuable insights by incorporating computation, geometry, and evaluation in conjunction with structure-based drug discovery to forecast the protein structure. [36]

* **AI in Clinical Trials**

The high costs associated with clinical trials also have subsequent impacts on the therapeutic costs for patients. For this reason, biopharma companies incorporate the research and development costs of failed trials into the pricing of approved drugs in order to maintain profitability. The execution and conduct of clinical trials involve various processes such as trial design, patient recruitment/selection, site selection, monitoring, data collection, and analysis. Among these processes, patient recruitment and selection prove to be challenging, with 80% of trials exceeding the enrollment timeline and 30% of phase-III trials being prematurely terminated due to enrollment difficulties. Monitoring a multi-centered global trial is both expensive and time-consuming. Additionally, there are significant challenges in terms of the duration from the "last subject last visit" to data submission to regulatory agencies, as these involve extensive data collection and analysis procedures. However, the introduction of AI and digitization has been instrumental in transforming these challenges in clinical trials. [37]

* **. Clinical Trial Design, Patient Identification, Recruitment and Enrolment**

**Bayesian nonparametric models (BNMs)** have become a valuable tool in the field of clinical trial design, as well as in various other applications. This particular model offers flexibility by employing a nonparametric approach. By allowing the use of infinite-dimensional parameter sets with a limited subset of parameters, this approach effectively reduces clustering and shortens the duration of trial design. Some commonly utilized BNMs include Dirichlet process mixture models and **Markov Chain Monte Carlo (MCMC)** techniques. In the realm of clinical trial design, BNMs find numerous applications, such as dose selection in trials involving cancer patients, immuno-oncology, and cell therapy trials. Dose selection in these cases is complex due to patient heterogeneity, which can result in inaccurate dose selection and the targeting of future populations. BNMs prove to be efficient and effective tools for dose selection in such scenarios, as they take into account the variability and heterogeneity of the study subjects. [37] Bayesian nonparametric design enables **adaptive dose selection in multiple populations**, allowing for the exchange of information between populations while accounting for their heterogeneity. These models aid in the precise determination of the optimal dose, thereby minimizing any inaccuracies. [38]

* **Monitoring Trial, Patient Adherence and Endpoint Detection**

**Risk based monitoring (RBM**), an AI-enabled technique, has recently emerged as a more efficient and cost-effective alternative to traditional monitoring. A more advanced version of RBM has the potential to reduce costs and improve the efficiency and quality of data monitoring at trial sites. Through AI-assisted "smart monitoring," predictive analysis and data visualization can enhance the data quality check and performance of trial sites. Ensuring patients' compliance with adherence criteria is crucial for obtaining reliable data and achieving trial success. By utilizing video monitoring and wearable sensors, patient data can be captured automatically and continuously, thereby enhancing the efficiency of monitoring patient adherence. [39]

**CONCLUSION**

The pharmaceutical sector is continuously progressing with its technological advancements, and the integration of AI presents a valuable opportunity to reduce both the cost and time associated with drug development. The effectiveness of AI in disease diagnosis is clearly illustrated through the utilization of deep learning, neural networking, and unsupervised learning techniques. These advanced AI tools possess the capability to analyze unorganized data and establish connections with acquired knowledge to accurately forecast the outcome, thereby proving valuable in predicting specific disease diagnoses. AI has demonstrated its significance in various areas, including intelligent computer-assisted instruction (ICAI), case-based reasoning, vector regression technique, and clinical decision support for monitoring chronic disease progress and optimizing therapy. The vector regression technique aids in identifying connections between variables, while ICAI assists in providing informative answers to patients during computer-assisted instruction. Case-based reasoning helps solve problems based on past experiences, and clinical decision support offers patient-specific information to healthcare teams for disease monitoring and treatment. These technologies play a crucial role in developing personalized treatments, which is a constant challenge. Additionally, techniques like Radiomics, which predicts outcomes and toxicity in individual patients' radiation therapy, and high-resolution imaging of the retina contribute to the examination of human health. In the field of pharmaceutical research and development, the primary objective is to discover and bring new drugs to the market, which is a lengthy and costly process. AI has the potential to streamline this process, starting from target selection to clinical trials. The drug discovery process begins with identifying biological molecules that can modify the disease. Computer-aided drug design and quantitative structure-activity relationship (QSAR) or quantitative structure-property relationships (QSPR) are utilized to determine the physicochemical and pharmacokinetic properties of thousands of synthetic molecules generated for targeting specific diseases. Deep learning and neural networks, based on the ADMET predictor and ALGOPS program, are employed to predict the lipophilicity and solubility of new chemical entities (NCEs). AI technologies like Chem Mapper and similarity ensemble approach are utilized to predict drug-target interactions. In terms of toxicity testing, AI plays a crucial role. Hence, the implementation of AI-powered methods will unlock numerous prospects across different domains of healthcare and pharmaceutical research, potentially revolutionizing future investigations.

**REFERENCES**

1. Subrat Kumar Bhattamisra , Priyanka Banerjee, Pratibha Gupta, Jayashree Mayuren , Susmita Patra and Mayuren Candasamy , Artificial Intelligence in Pharmaceutical and Healthcare Research. Big Data Cogn. Comput. 2023, 7- 10.
2. Chen, M.; Decary, M. “Artificial intelligence in healthcare: An essential guide for health leaders. In Healthcare Management Forum”; SAGE Publications: Los Angeles, CA, USA, 2020.
3. Bajwa, J.; Munir, U.; Nori, A.; Williams, B. Artificial intelligence in healthcare: Transforming the practice of medicine. Futur. Healthc. J. 2021, 8, 188–194.
4. Davenport, T.; Kalakota, R. The potential for artificial intelligence in healthcare. Futur. Healthc. J. 2019, 6, 94–98.
5. Esteva, A.; Robicquet, A.; Ramsundar, B.; Kuleshov, V.; Depristo, M.; Chou, K.; Cui, C.; Corrado, G.; Thrun, S.; Dean, J. A guide to deep learning in healthcare. Nat. Med. 2019, 25, 24–29.
6. Hussain, A.; Malik, A.; Halim, M.U.; Ali, A.M. The use of robotics in surgery: A review. Int. J. Clin. Pract. 2014, 68, 1376–1382.
7. Paul, D.; Sanap, G.; Shenoy, S.; Kalyane, D.; Kalia, K.; Tekade, R.K. Artificial intelligence in drug discovery and development. Drug Discov. Today 2021, 26, 80–93.
8. Menschner, P.; Prinz, A.; Koene, P.; Köbler, F.; Altmann, M.; Krcmar, H.; Leimeister, J.M. Reaching into patients’ homes— Participatory designed AAL services: The case of a patient-centered nutrition tracking service. Electron. Mark. 2011, 21, 63–76.
9. Obeng, O.; Paul, S. Understanding HIPAA compliance practice in healthcare organizations in a cultural context. In Proceedings of the 25th Americas Conference on Information Systems 2019, Cancún, Mexico, 15–17 August 2019.
10. Spohrer, J.; Banavar, G. Cognition as a Service: An Industry Perspective. AI Mag. 2017, 36, 71–86.
11. Mazzocco, T.; Hussain, A. Novel logistic regression models to aid the diagnosis of dementia. Expert Syst. Appl. 2012, 39, 3356–3361.
12. Lu, J.; Song, E.; Ghoneim, A.; Alrashoud, M. Machine learning for assisting cervical cancer diagnosis: An ensemble approach. Futur. Gener. Comput. Syst. 2020, 106, 199–205.
13. Singh, A.; Mehta, J.C.; Anand, D.; Nath, P.; Pandey, B.; Khamparia, A. An intelligent hybrid approach for hepatitis disease diagnosis: Combining enhanced k -means clustering and improved ensemble learning. Expert Syst. 2020, 38, e12526.
14. Mishra, S.; Yamasaki, T.; Imaizumi, H. Supervised classification of Dermatological diseases by Deep learning. arXiv 2018, arXiv:1802.03752.
15. Jin, Y.; Qin, C.; Huang, Y.; Zhao, W.; Liu, C. Multi-domain modeling of atrial fibrillation detection with twin attentional convo-lutional long short-term memory neural networks. Knowl.-Based Syst. 2020, 193, 105460.
16. Wong, T.T. Performance evaluation of classification algorithms by k-fold and leave-one-out cross validation. Pattern Recognit. 2015, 48, 2839–2846.
17. Prashanth, R.; Roy, S.D.; Mandal, P.K.; Ghosh, S. High-Accuracy Detection of Early Parkinson’s Disease through Multimodal Features and Machine Learning. Int. J. Med. Inform. 2016, 90, 13–21.
18. . Wang, H.; Zhang, D.; Ding, S.; Gao, Z.; Feng, J.; Wan, S. Rib segmentation algorithm for X-ray image based on unpaired sample augmentation and multi-scale network. Neural Comput. Appl. 2021, 1–15.
19. Wang, H.; Zhang, D.; Ding, S.; Gao, Z.; Feng, J.; Wan, S. Rib segmentation algorithm for X-ray image based on unpaired sample augmentation and multi-scale network. Neural Comput. Appl. 2021, 1–15.
20. augmentation and multi-scale network. Neural Comput. Appl. 2021, 1–15. [CrossRef] 51. Qaisar, S.M.; Khan, S.I.; Srinivasan, K.; Krichen, M. Arrhythmia classification using multirate processing metaheuristic optimization and variational mode decomposition. J. King Saud Univ.—Comput. Inf. Sci. 2022; in press.
21. Hrizi, O.; Gasmi, K.; Ben Ltaifa, I.; Alshammari, H.; Karamti, H.; Krichen, M.; Ben Ammar, L.; Mahmood, M.A. Tuberculosis Disease Diagnosis Based on an Optimized Machine Learning Model. J. Heal. Eng. 2022, 2022, 8950243.
22. Jain, A.; Mao, J.; Mohiuddin, K. Artificial neural networks: A tutorial. Computer 1996, 29, 31–44.
23. Mandal, L.; Jana, N.D. Prediction of Active Drug Molecule using Back-Propagation Neural Network. In Proceedings of the 8th International Conference System Modeling and Advancement in Research Trends (SMART) 2019, Moradabad, India, 22–23 November 2019; pp. 22–26
24. Schmidt-Erfurth, U.; Sadeghipour, A.; Gerendas, B.S.; Waldstein, S.M.; Bogunovi´c, H. Artificial intelligence in retina. Prog. Retin. Eye Res. 2018, 67, 1–29.
25. Carreras, J.; Hamoudi, R. Artificial Neural Network Analysis of Gene Expression Data Predicted Non-Hodgkin Lymphoma Subtypes with High Accuracy. Mach. Learn. Knowl. Extr. 2021, 3, 720–739.
26. Hasani, N.; Paravastu, S.S.; Farhadi, F.; Yousefirizi, F.; Morris, M.A.; Rahmim, A.; Roschewski, M.; Summers, R.M.; Saboury, B. Artificial Intelligence in Lymphoma PET Imaging: A Scoping Review (Current Trends and Future Directions). PET Clin. 2022, 17, 145–174.
27. Li, X.; Liu, H.; Du, X.; Zhang, P.; Hu, G.; Xie, G.; Guo, S.; Xu, M.; Xie, X. Integrated Machine Learning Approaches for Predicting Ischemic Stroke and Thromboembolism in Atrial Fibrillation. In AMIA Annual Symposium Proceedings; American Medical Informatics Association: Chicago, IL, USA, 2016; Volume 2016, p. 799
28. Hessler, G.; Baringhaus, K.-H. Artificial Intelligence in Drug Design. Molecules 2018, 23, 2520.
29. Lusci, A.; Pollastri, G.; Baldi, P. Deep Architectures and Deep Learning in Chemoinformatics: The Prediction of Aqueous Solubility for Drug-Like Molecules. J. Chem. Inf. Model. 2013, 53, 1563–1575.
30. Kumar, R.; Sharma, A.; Siddiqui, M.H.; Tiwari, R.K. Prediction of human intestinal absorption of compounds using artificial in-telligence techniques. Curr. Drug Discov. Technol. 2017, 14, 244–254.
31. Chai, S.; Liu, Q.; Liang, X.; Guo, Y.; Zhang, S.; Xu, C.; Du, J.; Yuan, Z.; Zhang, L.; Gani, R. A grand product design model for crystallization solvent design. Comput. Chem. Eng. 2020, 135, 106764.
32. Lounkine, E.; Keiser, M.J.; Whitebread, S.; Mikhailov, D.; Hamon, J.; Jenkins, J.L.; Lavan, P.; Weber, E.; Doak, A.K.; Côté, S.; et al. Large-scale prediction and testing of drug activity on side-effect targets. Nature 2012, 486, 361–367.
33. Feng, Q.; Dueva, E.; Cherkasov, A.; Ester, M. Padme: A deep learning-based framework for drug-target interaction prediction. arXiv 2018, arXiv:1807.09741.
34. Lysenko, A.; Sharma, A.; A Boroevich, K.; Tsunoda, T. An integrative machine learning approach for prediction of toxicity-related drug safety. Life Sci. Alliance 2018, 1, e201800098.
35. Gayvert, K.M.; Madhukar, N.S.; Elemento, O. A Data-Driven Approach to Predicting Successes and Failures of Clinical Trials. Cell Chem. Biol. 2016, 23, 1294–1301.
36. Wan, F.; Zeng, J. Deep learning with feature embedding for compound—Protein interaction prediction. bioRxiv 2016, 086033.
37. Kolluri, S.; Lin, J.; Liu, R.; Zhang, Y.; Zhang, W. Machine Learning and Artificial Intelligence in Pharmaceutical Research and Development: A Review. AAPS J. 2022, 24, 19.
38. Li, M.; Liu, R.; Lin, J.; Bunn, V.; Zhao, H. Bayesian Semi-parametric Design (BSD) for adaptive dose-finding with multiple strata. J. Biopharm. Stat. 2020, 30, 806–820.
39. Harrer, S.; Shah, P.; Antony, B.; Hu, J. Artificial Intelligence for Clinical Trial Design. Trends Pharmacol. Sci. 2019, 40, 577–591.