Computational Molecular Biology 2024, Vol.14, No.1, 20-27
http://bioscipublisher.com/index.php/cmb

Review and Progress Open Access

The Application of Artificial Intelligence in Drug Discovery: Opportunities and Challenges

Wei Wang
Institute of Life Science, Jiyang College of Zhejiang A&F University, Zhuji, 311800, China
Corresponding author email: 874202228@qq.com

Computational Molecular Biology, 2024, Vol.14, No.1 doi: 10.5376/cmb.2024.14.0003
Received: 03 Dec., 2023
Accepted: 08 Jan., 2024
Published: 20 Jan., 2024

Preferred citation for this article:
Wang W., 2024, The application of artificial intelligence in drug discovery: opportunities and challenges, Computational Molecular Biology, 14(1): 20-27 (doi: 10.5376/cmb.2024.14.0003)

Abstract With the rapid development of technology, the application of artificial intelligence (AI) in the field of drug discovery is becoming increasingly widespread, bringing unprecedented opportunities and challenges to drug research and development. This study summarizes the main applications of AI in drug discovery, including molecular design and drug screening, optimization of drug development processes, as well as clinical trial design and data analysis. It also explores the opportunities of AI in drug discovery, including accelerating the process of drug discovery and research and development, improving the accuracy and effectiveness of drugs, and reducing research and development costs and risks. These opportunities make AI an important force in promoting the progress of drug research and development. However, AI also faces some challenges in drug discovery, requiring us to fully utilize AI technology while also paying attention to its potential risks and challenges to ensure its healthy development in drug discovery. Artificial intelligence has demonstrated tremendous potential and value in drug discovery, bringing unprecedented opportunities to drug research and development. However, we should also maintain a rational and cautious attitude, conducting thorough research and addressing the challenges faced by AI in drug discovery to ensure that it can better contribute to human health.

Keywords Artificial intelligence (AI); Drug screening; Opportunities and challenges

The rapid development of artificial intelligence (AI) is bringing revolutionary changes to various fields, and the field of medicine is no exception. Especially in drug discovery and research and development, the application of artificial intelligence technology is gradually changing the traditional research and development model, providing new possibilities for the discovery of new drugs. This study aims to explore the application of artificial intelligence in drug discovery, as well as the opportunities and challenges it presents. The application of artificial intelligence technology in the field of medicine has become a hot topic (Ekins et al., 2019). From medical imaging diagnosis to personalized treatment formulation, to drug discovery and research and development, the application of artificial intelligence is providing unprecedented support and assistance to health care. Especially in the field of drug discovery, the application of artificial intelligence technology is increasingly becoming the focus of attention.

The application of artificial intelligence in drug discovery can be traced back decades, but in recent years, with the continuous advancement of technology and the accumulation of large amounts of data, its application scope and effectiveness have been greatly improved. From early drug screening and design to today's molecular simulation and virtual screening, AI technology is already playing an important role in all aspects of drug discovery. With the continuous maturity of deep learning and other technologies, the application prospect of artificial intelligence in drug discovery is broader. This study aims to comprehensively understand the application status of artificial intelligence in drug discovery and analyze the opportunities and challenges brought by it. Xu et al. (2019) hope to reveal the potential and limitations of artificial intelligence technology in the field of drug discovery through comprehensive research on existing literature and cases, so as to provide reference and reference for future research and practice. At the same time, we also expect to contribute to accelerating the drug discovery process and improving the efficiency and success rate of new drug research and development, so as to better serve the cause of human health.

1 Application in Drug Discovery

1.1 Molecular design and drug screening

Campillos et al. (2008) believe that molecular design is a key step in the drug discovery process, with the goal of finding molecular structures with specific biological activities. Traditional methods of molecular design, which rely mainly on the expertise and experience of chemists, are inefficient. AI technology can learn from large amounts of compound data and predict the biological activity of molecules through methods such as deep learning and machine learning, thereby assisting chemists to quickly screen potential drug candidates. Deep neural networks have been successfully applied to predict the biological activity of molecules. These models can predict the biological activity of new molecules by learning the structural characteristics of known active molecules, thus screening potential drug candidates. In addition, molecular generation methods based on generative adversarial networks (Gans) can also automatically generate molecular structures with specific biological activities, further expanding the scope of drug screening.

The advantages of AI technology in drug research and development are first reflected in its powerful computing power. Ching et al. (2018) Using deep learning and big data analysis, AI can simulate the interaction between molecules and biological targets, and predict the way and effect of combining drugs with organisms. This predictive ability allows researchers to make an initial assessment of a drug's effects before a trial, and thus to identify the most likely candidates for success. This not only greatly shortens the drug development cycle, but also reduces the cost of research and development. In addition to molecular design and drug screening, AI also plays an important role in other drug development processes. In the field of bioinformatics, AI technology can process massive genomics, proteomics and other big data to help researchers reveal the mechanism of drug action and targets. The understanding of these mechanisms provides a clearer direction and goal for drug development, and further improves the success rate of drug development (Figure 1).

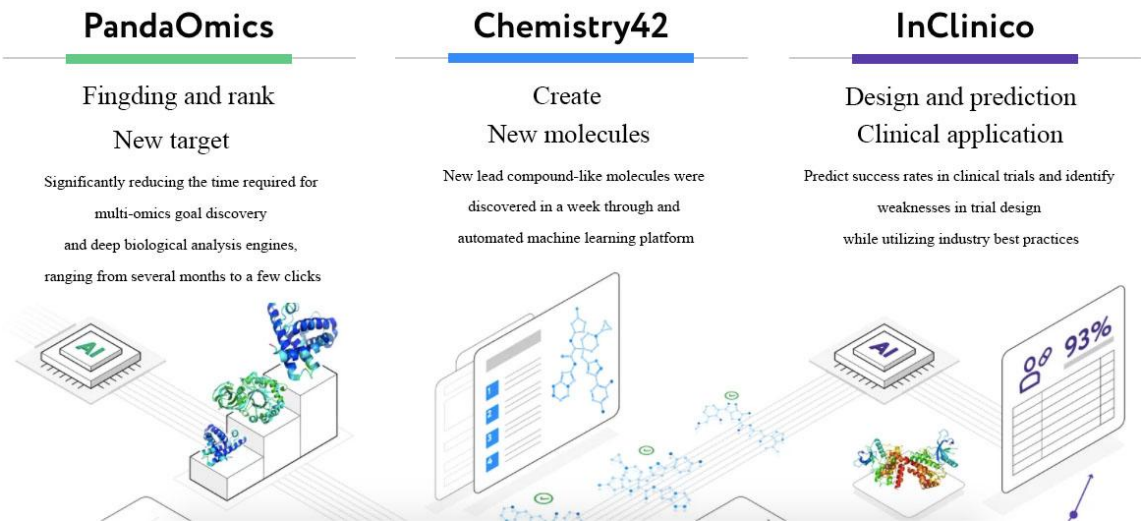

Figure 1 Analysis and screening of the drugs were performed using the AI software

1.2 Optimization of drug development process

Huang et al. (2019) proposed that AI could not only play a role in drug screening and molecular design, but also optimize the entire drug development process. The process of drug development involves many steps, including the synthesis of compounds, the testing of biological activity, and the study of pharmacokinetics. AI technology can improve the efficiency of drug development by optimizing these links. In terms of compound synthesis, AI can reduce the number and cost of experiments by predicting the synthesis route of compounds. The traditional drug discovery process is often a linear, progressive process, and the introduction of AI makes this process more flexible and efficient. AI can predict the possible results of the next experiment by analyzing the existing experimental data, so as to provide guidance for the experimenter and reduce ineffective experimental attempts.

Blanco-Gonzalez et al. (2023) introduced that the predictive model based on the graph neural network can automatically plan the optimal synthesis route according to the structure of the target molecule. In terms of biological activity testing, AI can reduce the number of experiments necessary by building predictive models. These models can predict the biological activity of compounds based on their structural characteristics, thus screening drug candidates for further experimental validation. In terms of pharmacokinetic research, AI can also predict the efficacy and safety of drugs, and predict the absorption, distribution, metabolism and excretion processes of drugs in the body by analyzing a large number of experimental data, providing a basis for the optimal design of drugs. Help researchers screen potential drug candidates at an early stage, reducing the risk and cost of late-stage clinical trials. Another important role is to provide data support and analysis. In the process of drug development, a large amount of experimental data is generated, including the structure, biological activity, pharmacokinetics and so on. AI can deeply mine and analyze these data, find the correlation and rule between the data, and provide a more comprehensive and in-depth understanding of drug development (Figure 2).

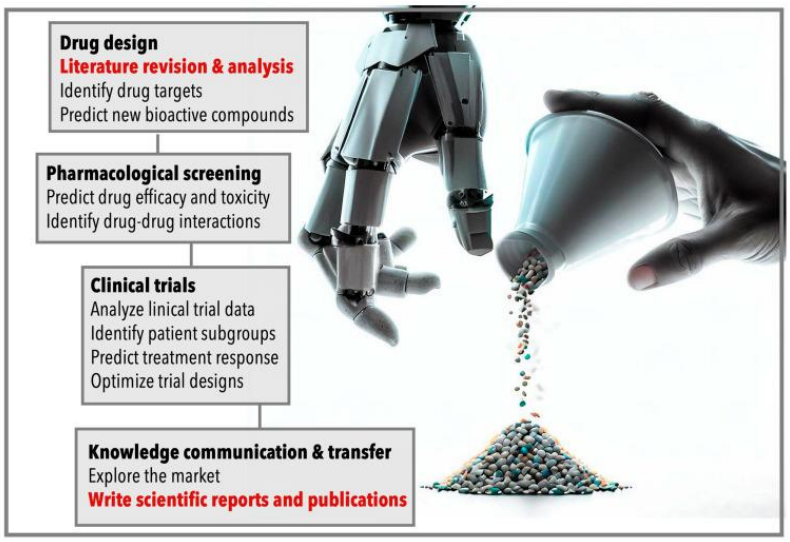

Figure 2 Through the optimization process of AI drug development

1.3 Application of artificial intelligence in clinical trial design and data analysis

Clinical trials are an integral part of the drug development process. However, the design and implementation of clinical trials often face many challenges, such as the determination of sample size, the optimization of trial design, and the complexity of data analysis. In terms of clinical trial design, AI can provide the optimal trial design scheme according to the characteristics of diseases and the nature of drugs (Aliper et al., 2016). For example, using AI algorithms to accurately calculate the sample size can reduce unnecessary sample waste while ensuring the reliability of test results. In addition, AI can also control and adjust various variables in the test process to ensure the smooth progress of the test.

In terms of data analysis, AI can efficiently process and analyze the massive data generated by clinical trials. Traditional data analysis methods are often difficult to cope with such a huge amount of data, but AI algorithms can complete the data cleaning, integration and analysis in a short time, so as to provide a more accurate and comprehensive interpretation of the test results. In addition, AI can also predict and simulate trial data to provide deeper understanding and guidance for drug development. Gupta et al. (2021) discuss the critical role of artificial intelligence, particularly artificial neural networks such as deep neural networks or recurrent networks, in drug discovery. Emphasis is placed on the significant impact of AI in quantitative structure-property relationships (QSPR) or quantitative structure-activity relationships (QSAR). AI's ability to design from scratch demonstrates its strength in generating new bioactive molecules with desired properties (Figure 3).

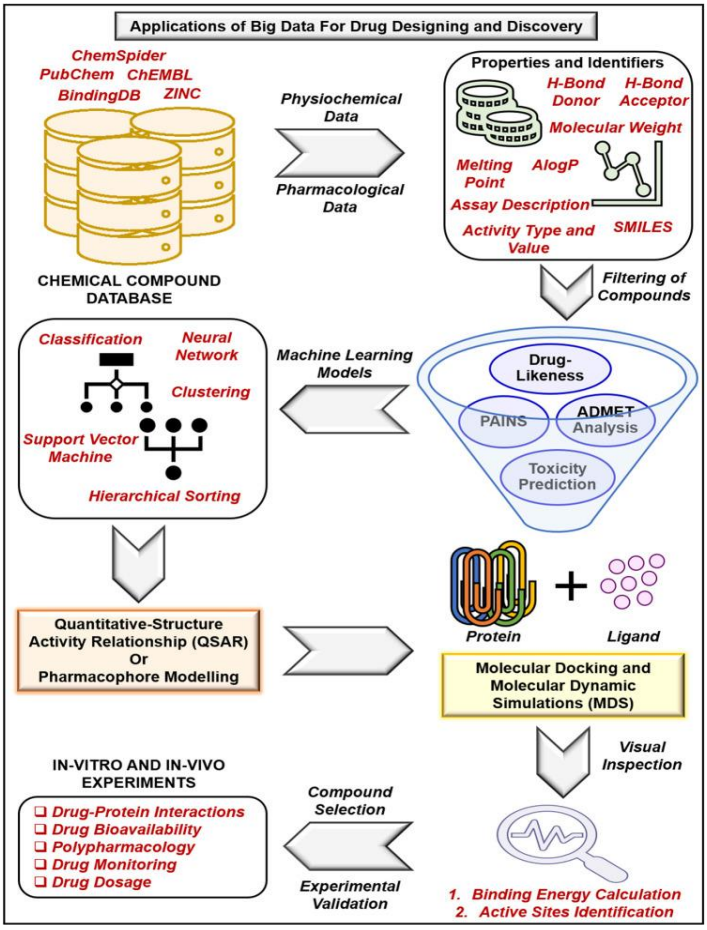

Figure 3 Application of big data in drug design and discovery

2 Opportunities for AI in Drug Discovery

2.1 Accelerate the drug discovery and development process

The traditional drug discovery process is a long and complex journey involving a large number of experiments and data analysis. Researchers need to select bioactive drug candidates from tens of thousands of compounds, and then conduct in-depth clinical trials to determine the safety and effectiveness of the drug. This process is not only time-consuming, but also costly. However, with the introduction of AI technology, the efficiency of drug discovery has been significantly improved. AI has strong deep learning and data mining capabilities, which can extract useful information from massive biomedical data. These data, including gene sequences, protein structures, disease pathogenesis, etc., are crucial for drug development. By deeply analyzing this data, AI can provide researchers with more precise research directions, reducing blindness and repetitive labor.

Jimeno and Gaulton (2018) proposed that AI-based predictive models can quickly screen potential drug candidates by analyzing the structural characteristics and biological activity of compounds, greatly reducing experimental steps and improving research and development efficiency. At the same time, AI technology can also automate and optimize the steps of drug synthesis. Through intelligent algorithms, AI can predict and optimize the synthetic route of compounds, reducing the number and cost of experiments, and further shortening the cycle of drugs from development to market. In addition, the application of AI in drug discovery is also reflected in the field of personalized medicine. By deeply analyzing patients' genetic information and disease data, AI can tailor personalized treatment programs to patients, improving treatment outcomes and quality of life. This concept of precision medicine is gradually changing the traditional drug research and development model, bringing broader development prospects for the pharmaceutical industry.

2.2 Improve the accuracy and effectiveness of drugs

The application of AI technology in drug discovery can also significantly improve the accuracy and effectiveness of drugs, and bring better treatment results to patients. LeCun (2015) showed that, on the one hand, AI can accurately predict the efficacy and side effects of drugs in different patient groups by analyzing a large number of patient data, providing strong support for individualized treatment. This concept of precision medicine is expected to help doctors develop more accurate treatment plans for patients, improve treatment effectiveness, and reduce unnecessary drug side effects.

Mayr and Klambauer (2018) argue that AI technology can also predict the biological activity of drugs by simulating their interactions with biomolecules. This prediction is far more accurate than traditional methods and can significantly improve the success rate of drug development. At the same time, AI technology can also predict and evaluate the safety of drugs, reducing the risk of drug development. The application of artificial intelligence in the field of drug discovery has brought unprecedented opportunities for drug development. By accelerating the process of drug discovery and research and development, and improving the accuracy and effectiveness of drugs, AI technology is expected to bring revolutionary changes to the pharmaceutical industry and make greater contributions to human health.

2.3 Reduce R&D costs and risks

Li et al. (2023) pointed out in their study that although drug research and development is a costly and risky activity, the application of AI technology can effectively reduce these costs and risks. Through its efficient screening and prediction capabilities, AI technology reduces the number of ineffective trial attempts and failed clinical trials, saving significant amounts of money for drug development. In addition, AI's role in real-time monitoring and analysis of experimental data helps researchers identify and solve problems in a timely manner and prevent losses caused by experimental failures.

Koza et al. (2023) further explore how AI can mitigate R&D risks by deeply mining and analyzing existing data to open up new drug development ideas and strategies. In addition to the economic benefits, they also pointed out that the use of AI in the drug development process promotes cooperation and innovation across disciplines, infuses more inspiration and possibilities for drug development by integrating knowledge and technology from different fields, and promotes the continuous development and progress in the field of drug discovery. AI not only plays an important role in reducing the economics and risks of drug discovery, but also shows great potential in promoting scientific innovation and cross-field collaboration, providing new directions and strategies for future drug discovery.

3 The Challenge of AI in Drug Discovery

3.1 Data quality and privacy protection

In the field of drug discovery, one of the challenges facing AI is inconsistent data quality and privacy issues. The quality of physical medicine data, chemical data and clinical data directly affects the training effect of AI models and the accuracy and reliability of the predicted results. Issues such as missing data, inaccurate labeling, and bias have become major obstacles to the application of AI in drug discovery.

The study of Schneider et al. (2018) also emphasized that with the accumulation and application of a large amount of sensitive data, how to effectively protect data privacy has become an urgent issue. Patient data and clinical trial data involved in drug development often contain information about patient privacy, and the challenge is how to ensure data security while achieving effective sharing and utilization of data.

Weber et al. (2019) also discuss the importance of data privacy protection in AI applications, especially when dealing with sensitive data involving personal health information. They explored the use of advanced encryption techniques and anonymization methods to address the balance between data sharing and privacy protection, emphasizing the importance of promoting data sharing while ensuring that individual privacy is not violated.

3.2 Interpretability and transparency

In drug discovery, model interpretability and transparency pose one of the key challenges. Miller et al. (2019) note that the AI models on which drug discovery relies are often built based on deep learning and neural network techniques. The models created by these technologies often exist as "black boxes" whose inner workings and decision-making processes are difficult to understand intuitively, and this lack of interpretability and transparency can undermine trust and acceptance of the models' predictions.

In their study, Wilson and Martinez (2020) discuss the importance of increasing the interpretability and transparency of AI models in the field of drug discovery. In the drug discovery process, a clear understanding of the model's predictions and recommendations is essential, as it is the basis for subsequent validation and experimental activities. Meanwhile, Wilson and Martinez (2020) explore various approaches and techniques to enhance the interpretability and transparency of AI models in drug discovery applications. Together, they reveal the challenges of interpretability and transparency of AI models in drug discovery and highlight the need to enhance these attributes. This involves not only technical improvements, but also in-depth understanding and interpretation of the model's decision logic, thus enhancing the application value and practicality of the model in drug discovery. Addressing this challenge is critical to building trust in model predictions and facilitating advances in drug discovery.

3.3 Ethical and legal issues

With the widespread use of artificial intelligence (AI) in drug discovery, ethical and legal issues are emerging. Drug development is a complex and sensitive process that involves large amounts of personal information and clinical trial data. The legitimate access and use of these data is directly related to the rights of patients and the credibility of research. Therefore, it is essential to comply with relevant privacy protection laws and regulations.

The study by Hessler et al. (2022) delves into this issue and highlights the importance of compliance with privacy protection laws and regulations. They pointed out that in the process of drug development, the personal privacy information involved includes patients' identity information, health status, genetic information, etc., and the disclosure of these information may bring serious consequences to patients, such as identity theft and discrimination. Ensuring the legitimacy of data is not only a legal requirement, but also the key to maintaining patient trust and willingness to participate in research. In practice, drug discovery organizations need to take a number of measures to ensure the legitimacy and security of data, and must comply with relevant privacy laws and regulations, such as the European Union's General Data Protection Regulation (GDPR) and the U.S. Health Insurance Mobility and Accountability Act (HIPAA). These laws have made clear provisions on the collection, storage, use and sharing of data, providing legal protection for drug research and development institutions.

In the study of Sun et al. (2021), the intellectual property and patent issues that may be encountered when artificial intelligence is applied in drug discovery are discussed. Because drug development involves a large number of technological innovations and patent applications, how to protect the intellectual property of research and development results becomes a challenge, highlighting the need to develop a clear IP protection strategy and rational use of the patent system. The drug development process also requires strict adherence to ethical codes and ethical standards to ensure legal compliance with research. This includes, but is not limited to, ensuring informed patient consent, safeguarding the well-being of research subjects, and reasonably sharing research results. Solutions to the ethical and legal challenges that must be faced when using AI for drug discovery are critical to ensuring the legitimacy of scientific research, protecting patient rights, and promoting scientific and technological innovation.

4 Future and Outlook

The application of artificial intelligence in drug discovery has made remarkable progress. Through molecular design and drug screening, optimization of the drug development process, and the application of AI in clinical trial design and data analysis, AI technology has become an important tool for accelerating drug discovery and development. Many research institutions and biotechnology companies are actively exploring the application of

AI in drug discovery, and have achieved a series of encouraging results (Du et al., 2022). However, AI still faces a number of challenges in drug discovery, including data quality and privacy protection, interpretability and transparency, and ethical and legal issues. Addressing these challenges requires interdisciplinary cooperation and joint efforts, including strengthening data quality control and privacy protection mechanisms, improving the interpretability and transparency of AI models, and complying with relevant ethical norms and laws and regulations.

In the face of the many challenges in the field of drug discovery, international cooperation and sharing of data resources have become particularly important. Governments, research institutions and companies should work together to develop data standards and sharing agreements, and establish mechanisms for sharing data across national borders. An open data platform and database should be established to integrate and share various types of drug research and development data to provide broader data resource support for global drug discovery research (Liang et al., 2020). In addition, international personnel exchanges and cooperation should be strengthened to jointly train and introduce researchers with interdisciplinary backgrounds and AI expertise, and promote the innovative application of AI in drug discovery. In the future, the application of AI in drug discovery will show the following trends. AI technology will be more popular and mature, including deep learning, transfer learning, reinforcement learning and other technologies will be more widely used, and combined with traditional drug discovery methods, to achieve more efficient drug screening and optimization. The application of personalized medicine and precision medicine therapy will be more prominent. Through the analysis of patients' genomic data, clinical manifestation data and drug metabolism data, combined with artificial intelligence technology, personalized drug compatibility and treatment plan design can be achieved to improve the accuracy and effectiveness of drug therapy.

Applications in clinical trial design and data analysis will also be further strengthened. By simulating clinical trial process, optimizing sample selection and data analysis methods, improve the efficiency and success rate of clinical trials, and accelerate the marketing and clinical application of new drugs. The application of drug safety evaluation and drug side effect prediction will also become a research hotspot in the future. By integrating various types of biomedical data and pharmaceutical chemistry data, combined with artificial intelligence technology, rapid prediction and evaluation of drug safety and side effects can be achieved to provide a more comprehensive.

References

Aliper A., Plis S., Artemov A., Ulloa A., Mamoshina P., and Zhavoronkov A., 2016, Deep learning applications for predicting pharmacological properties of drugs and drug repurposing using transcriptomic data, Molecular Pharmaceutics, 13(7): 2524-2530.
https://doi.org/10.1021/acs.molpharmaceut.6b00248
PMid:27200455 PMCid:PMC4965264

Blanco-González A, Cabezón A, Seco-González A, Conde-Torres D, Antelo-Riveiro P., Piñeiro Á, Garcia-Fandino R.,2023, The Role of AI in Drug Discovery: Challenges, Opportunities, and Strategies. Pharmaceuticals (Basel), 16(6): 891.
https://doi.org/10.3390/ph16060891
PMid:37375838 PMCid:PMC10302890

Campillos M., Kuhn M., Gavin A.C., Jensen L.J., and Bork P., 2008, Drug target identification using side-effect similarity, Science, 321(5886): 263-266.
https://doi.org/10.1126/science.1158140
PMid:18621671

Ching T., Himmelstein D.S., Beaulieu-Jones B.K., Kalinin A.A., Brian T Do B.T., Way G.P., Ferrero E., Agapow P., Zietz M., Hoffman M.M., Xie W., Rosen G.L., Lengerich B.J., Israeli J., Lanchantin J., Woloszynek S., Carpenter A.E., Shrikumar A., Xu J.B., Cofer E.M., Lavender C.A., Srinivas C Turaga S.C., Alexandari A.M., Lu Z.Y., Harris D.J., DeCaprio D., Qi Y.J., Kundaje A., Peng Y.F., Wiley L.K., Segler M.H.S., Boca S.M., Swamidass S.J., Huang A., Gitter A., and Greene C.S., 2018, Opportunities and obstacles for deep learning in biology and medicine, Journal of The Royal Society Interface, 15(141): 20170387.
https://doi.org/10.1098/rsif.2017.0387
PMid:29618526 PMCid:PMC5938574

Du H., Wu Y.F., and Du X., 2022, Dvances in application of Artificial Intelligence in new drug research and development, Progress in Pharmaceutical Sciences, 46(11): 875-880.

Ekins S., Puhl A.C., Zorn K.M., Lane T.R., Russo D.P., Klein J.J., and Hickey A.J., 2019, Exploiting machine learning for end-to-end drug discovery and development, Nature Reviews Drug Discovery, 18(8): 435-441.
https://doi.org/10.1038/s41563-019-0338-z

Gupta R, Srivastava D, Sahu M, Tiwari S, Ambasta RK, Kumar P. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. Mol Divers. 2021 Aug;25(3):1315-1360.
https://doi.org/10.1007/s11030-021-10217-3
PMid:33844136 PMCid:PMC8040371

Hessler G, and Baringhaus K.H., 2018, Artificial Intelligence in Drug Design, Molecules, 23(10): 2520.
https://doi.org/10.3390/molecules23102520
PMid:30279331 PMCid:PMC6222615

Huang F., Yang H.F., and Zhu X., 2021, Progress in the application of artificial intelligence in new drug discovery, Progress in Pharmaceutical Sciences, 45(7): 502-511.

Jimeno A., and Gaulton A., 2018, The role of artificial intelligence in drug discovery and development. Drug Discovery Today, 23(9): 1538-1548.
https://doi.org/10.1016/j.drudis.2018.05.010
PMid:29750902 PMCid:PMC6078794

Koza J.R., Bennett F.H., Andre D., Keane M.A., and Dean K., 2001, Automated synthesis of analogs to peptides: A genetic programming approach to ligand design. Science, 294(5543): 1317-1321.

LeCun Y., Bengio Y., and Hinton G., 2015, Deep learning. Nature, 521(7553): 436-444.
https://doi.org/10.1038/nature14539
PMid:26017442

Li S.X., Li Y.H., Lin Z., Zhang Y., Yang Y.W., Qu Z., Li Y.C., Huo G.T., Lv J.J., 2023, Research progress in application of artificial intelligence during process of drug Discovery, Drug Evaluation Research, 46(9): 2030-2036.

Liang L., Deng C.L., Zhang Y.M., Hua Y., Liu H.C., Lu T., and Cheng Y.D., 2020, Application and challenges of artificial intelligence in drug discovery, Progress in Pharmaceutical Sciences, 44(1): 18-27.

Mayr A., and Klambauer G., 2018, Deep learning in drug discovery, Molecular Informatics, 37(3-4): 1800119.

Schneider P., Walters W.P., Plowright A.T., Sieroka N., Listgarten J., Goodnow Jr, R. A., and Schneider, G., 2018, Rethinking drug design in the artificial intelligence era, Nature Reviews Drug Discovery, 19: 353-364.
https://doi.org/10.1038/s41573-019-0050-3
PMid:31801986

Stokes J.M., Yang, K., Swanson K., Jin W.G., Cubillos-Ruiz A., Donghia N.M., MacNair C.R., French S., Carfrae L.A., Bloom-Ackermann Z., Tran V.M., Chiappino-Pepe A., Badran A.H., Andrews I.A., Chory E.J., Church G.M., Brown E.D., Jaakkola T.S., Barzilay R., and Collins J.J., 2020, A deep learning approach to antibiotic discovery, Cell, 180(4): 688-702.
https://doi.org/10.1016/j.cell.2020.01.021
PMid:32084340 PMCid:PMC8349178

Sun Y.J., Li C.Y., and Zeng X.Q., 2019, Application of artificial intelligence in drug discovery, China Medical Herald, 16(33): 162-166.

Weber G.M., Mandl K.D., and Kohane I.S., 2019, Finding the Missing Link for Big Biomedical Data. JAMA, 321(24): 2471-2472.

Xu Y.J., Dai Z.W., Chen F.J., Gao S.S., Pei J.F., and Lai L.H., 2019, Deep learning for drug-induced liver injury. Journal of Chemical Information and Modeling, 59(10): 2085-2093.
https://doi.org/10.1021/acs.jcim.5b00238
PMid:26437739