EUROPEAN JOURNAL OF BIOMEDICAL AND PHARMACEUTICAL SCIENCES
http://www.ejbps.com

ISSN 2349-8870
Volume: 12
Issue: 5
Year: 2025

APPLICATIONS OF GENERATIVE AI IN DRUG DISCOVERY AND DEVELOPMENT

Dr. B. Thangabalan, K. Sasikanth, *K. K. V. Sairam, K. Srimannarayana and T. Vineetha Ratnam

India.

***Corresponding Author: K. K. V. Sairam**
India.

Article Received on 25/03/2024 **Article Revised on 15/04/2025** **Article Accepted on 05/05/2025**

ABSTRACT

The use of Artificial Intelligence (AI) in the pharmaceutical industry has revolutionized the way companies approach drug discovery, development, and manufacturing. From its humble beginnings in the 1980s to the current era of deep learning and big data, AI has evolved significantly, transforming the entire process. AI has been applied to various stages of drug development, including target identification, compound selection, virtual screening, lead optimization, and drug design. The advantages of AI in drug discovery include increased efficiency, improved accuracy, and enhanced customer experience. However, there are also challenges associated with the use of AI, such as data quality, complexity of biological systems, bias in AI models, and regulatory challenges. Despite these challenges, AI has the potential to greatly accelerate the development of new drugs and improve the efficiency of the process. This abstract provides an overview of the current state of AI in drug discovery and development, its applications, advantages, and challenges, and highlights the potential of AI to revolutionize the pharmaceutical industry.

KEYWORDS: Artificial intelligence (AI); drug discovery, deep learning, drug development, deep learning, lead optimization, virtual screening, personalized medicine.

INTRODUCTION

Artificial Intelligence (AI) generative models have revolutionized the field of drug discovery and development by enabling the rapid design and optimization of new drug candidates. These models use machine learning algorithms to generate new molecular structures, predict their properties, and identify potential lead compounds. The use of AI generative models in drug discovery began in the early 2000s, with the introduction of machine learning algorithms such as neural networks and decision trees. Over the years, AI generative models have evolved to become more sophisticated and powerful, enabling the generation of more complex molecular structures and the prediction of their properties with higher accuracy.

HISTORY

History of AI in Pharmaceuticals

The use of Artificial Intelligence (AI) in the pharmaceutical industry has a rich and fascinating history that spans several decades. From its humble beginnings in the 1980s to the current era of deep learning and big data, AI has evolved significantly, transforming the way pharmaceutical companies approach drug discovery, development, and manufacturing.

Rule-Based Expert Systems

In the 1960s and 1970s, the first AI programs were developed, which were rule-based expert systems. These systems were designed to mimic human decision-making abilities by using a set of predefined rules.

1. Early Beginnings (1980s-1990s)

The first phase of AI in pharmaceuticals began in the 1980s, when researchers started exploring the use of computational models for molecular modelling and chemical structure prediction. This early work laid the foundation for the development of more sophisticated AI approaches in the future. During this period, AI was primarily used for basic tasks such as data analysis and processing.

2. Machine Learning Era (Early 2000s)

The early 2000s saw the introduction of machine learning algorithms that could analyse complex datasets and identify patterns. This marked a significant shift in the use of AI in pharmaceuticals, as companies began to apply machine learning to predict molecular interactions and optimize drug formulations. The use of machine learning enabled researchers to analyse large amounts of data, identify potential drug targets, and design new molecules with specific properties.

3. Deep Learning Era (2010s)
The 2010s witnessed the widespread adoption of deep learning techniques in pharmaceuticals, driven by advances in computing power, data storage, and the availability of large datasets. Deep learning enabled researchers to analyse complex data, such as images and genomic sequences, and make predictions with high accuracy. This led to significant breakthroughs in areas like computer-aided drug design, personalized medicine, and drug repurposing.

4. Modern AI
Today, AI is a rapidly evolving field, with applications in areas such as natural language processing, computer vision, and robotics. Modern AI systems are capable of learning from large datasets and improving their performance over time

Notable Milestones
There have been several notable milestones in the history of AI in drug discovery and development, including:
1.2014: Atomwise Launch.
The first AI-powered drug discovery platform, called "Atomwise," was launched in 2014. This platform used deep learning algorithms to analyse large datasets of chemical compounds and identify potential lead compounds.

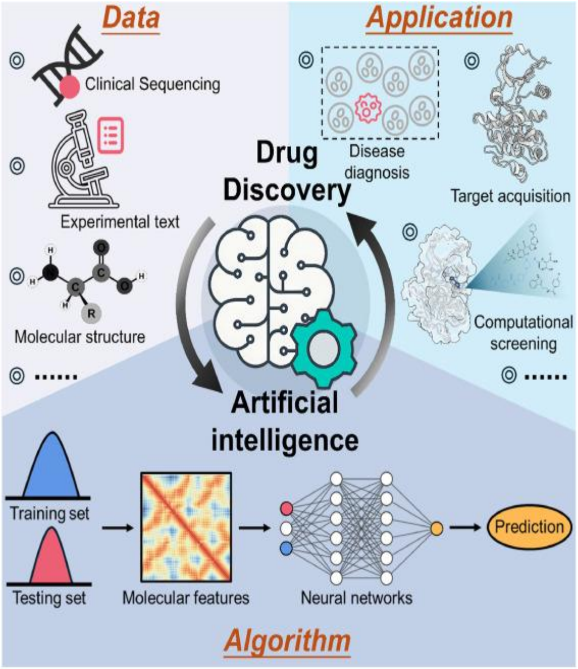
2. 2018: Verge Genomics Algorithm.
In 2018, Verge Genomics developed an algorithm to identify pathogenic genes and select drugs to target them, leading to the discovery of new drugs for neurodegenerative diseases.

3. 2018: Bayer and Merck FDA Approval:
In 2018, Bayer and Merck received FDA approval to use AI algorithms to support clinical decision-making for chronic thromboembolic pulmonary hypertension.

APPLICATIONS OF AI IN DRUG DISCOVERY:
1. Target Identification: AI can be used to identify potential drug targets by analysing large datasets of genomic and proteomic data.
2. Compound Selection: AI can analyse large libraries of chemical compounds to identify those with the highest potential as drug candidates.
3. Virtual Screening: AI can screen large libraries of compounds against a specific target, identifying those that are most likely to bind and have a therapeutic effect.
4. Lead Optimization: AI can help optimize lead compounds by predicting their pharmacokinetic and pharmacodynamic properties.
5. Lead Compound Identification: AI can be used to identify lead compounds by analysing large datasets of chemical compounds and predicting their biological activity.
6. Drug Design: AI can be used to design new drugs by generating new molecular structures and predicting their biological activity.
7. Virtual Screening: AI can be used to virtually screen large datasets of chemical compounds and identify potential lead compounds.
8. Predictive Modelling: AI can be used to build predictive models of drug efficacy and toxicity, allowing for the identification of potential issues early in the development process.
9. Clinical Trial Design: AI can be used to design clinical trials, including identifying patient populations, designing trial protocols, and predicting trial outcomes.
10. Personalized Medicine: AI can be used to develop personalized medicine approaches, including identifying individualized treatment plans and predicting patient responses to therapy.
11. Toxicity Prediction: AI can be used to predict the toxicity of potential drugs, allowing for the identification of potential issues early in the development process.
12. ADME Prediction: AI can be used to predict the absorption, distribution, metabolism, and excretion (ADME) of potential drugs, allowing for the identification of potential issues early in the development process.
13. Biomarker Discovery: AI can be used to discover biomarkers for disease diagnosis and monitoring, allowing for the development of more effective treatments.
14. Drug Repurposing: AI can be used to identify potential new uses for existing drugs, allowing for the development of new treatments for diseases.
15. Combination Therapy: AI can be used to identify potential combination therapies, allowing for the development of more effective treatments for complex diseases.

Current State
Today, AI is being used in various stages of drug development, from target identification and lead optimization to clinical trials and post-marketing surveillance. AI-driven approaches have led to the discovery of promising drug candidates and the repurposing of existing drugs for new indications.

The integration of multi-omics data, collaborative AI platforms, and AI-driven personalized medicine approaches are emerging trends in AI-enabled drug discovery. These approaches have the potential to revolutionize the field of drug discovery and development, and to improve the efficiency and accuracy of the drug development process.



Advantages of Ai in drug discovery
1. Increased Efficiency: AI can automate repetitive and mundane tasks, freeing up human resources for more strategic and creative work.
2. Improved Accuracy: AI systems can process vast amounts of data quickly and accurately, reducing errors and improving decision-making.
3. Enhanced Customer Experience: AI-powered chatbots and virtual assistants can provide 24/7 customer support, helping to improve customer satisfaction and loyalty.
4. Innovation and Creativity: AI can help humans generate new ideas and solutions, leading to breakthroughs in fields such as medicine, finance, and transportation.
5. Data Analysis and Insights: AI can quickly analyse large datasets, identifying patterns and trends that humans may miss, and providing valuable insights for business decision-making.
6. Improved Healthcare: AI can help diagnose diseases more accurately and quickly, personalize treatment plans, and streamline clinical workflows.
7. Increased Safety: AI can help improve safety in various industries, such as self-driving cars, predictive maintenance, and anomaly detection.

Disadvantages of Ai in drug discovery:
1. Job Displacement: AI may displace certain jobs, particularly those that involve repetitive or routine tasks.
2. Bias and Discrimination: AI systems can perpetuate biases and discrimination if they are trained on biased data or designed with a particular worldview.
3. Dependence on Data Quality: AI is only as good as the data it is trained on, and poor data quality can lead to inaccurate or unreliable results.
4. Security Risks: AI systems can be vulnerable to cyber attacks and data breaches, particularly if they are connected to the internet.
5. Lack of Transparency: AI decision-making processes can be opaque, making it difficult to understand how decisions are made.
6. Ethical Concerns: AI raises various ethical concerns, such as the potential for AI systems to be used for surveillance, manipulation, or exploitation.
7. High Development Costs: Developing and implementing AI solutions can be expensive, particularly for small and medium-sized businesses.

FUTURE DIRECTIONS
1. Increased Adoption of Deep Learning
More widespread use of deep learning techniques, such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs), for tasks like image analysis and natural language processing.
2. Integration with Emerging Technologies
Integration of AI with emerging technologies like blockchain, Internet of Things (IoT), and quantum computing to enhance drug discovery and development.
3. Focus on Personalized Medicine
Increased use of AI for personalized medicine, tailoring treatments to individual patients based on their genetic profiles, medical histories, and lifestyle factors.
4. Expansion into New Therapeutic Areas
Application of AI in new therapeutic areas, such as gene therapy, cell therapy, and RNA-based therapies
5. Developing high-quality datasets: Initiatives to create comprehensive, standardized datasets for AI model training.
6. Improving model interpretability: Research into explainable AI (XAI) and transparent model architectures.
7. Establishing regulatory guidelines: Collaboration between regulatory agencies, industry stakeholders, and AI experts to develop guidelines and standards for AI-driven methodologies.
8. Increased Adoption in drug discovery: AI is expected to become increasingly adopted in drug discovery and development as the technology continues to evolve and improve.
9. Improved Accuracy: AI is expected to become more accurate and reliable as the technology continues to evolve and improve.
10. New Applications in drug discovery: AI is expected to be applied to new areas of drug discovery and development, such as personalized medicine and precision health.
11. Collaboration: AI is expected to facilitate collaboration between researchers, clinicians, and patients, improving the efficiency and effectiveness of drug discovery.

CHALLENGES OF AI IN DRUG DISCOVERY AND DRUG DEVELOPMENT
1. Data Quality: The quality of the data used to train AI models is crucial. If the data is noisy, incomplete, or biased, the AI model will not be able to learn effectively and may produce inaccurate results.

2. Complexity of Biological Systems: Biological systems are complex and multifaceted, making it challenging to develop AI models that can accurately capture their behaviour.
3. Bias in AI Models: AI models can inherit biases from the data they are trained on, which can lead to unfair or inaccurate results.
4. Lack of Transparency: Some AI models, such as deep learning models, are often referred to as “black boxes” because it is difficult to understand how they make decisions.
5. Regulatory Challenges: The use of AI in drug discovery and development is still a relatively new field, and there are not yet clear regulations on how to use AI in this context.
6. Integration with Traditional Methods: AI models need to be integrated with traditional methods and tools to ensure seamless workflow and decision-making.
7. Ethical Concerns: AI raises several ethical concerns, including patient privacy, informed consent, and the potential for biased results.
8. High Computational Requirements: AI models require significant computational power, which can be expensive and time-consuming.
9. Limited Expertise: There is a limited number of experts who understand both AI and drug discovery and development.
10. Cost: Developing and implementing AI models can be expensive, which can be a barrier for small companies or academic institutions.
11. Data Integration: AI requires the integration of large amounts of data from different sources, which can be challenging. The pharmaceutical industry generates vast amounts of data from various sources, including electronic health records, clinical trials, and laboratory experiments.
12. Regulatory Framework: The regulatory framework for AI in drug discovery and development is still evolving and can be unclear. Regulatory agencies, such as the FDA, are still developing guidelines for the use of AI in drug development.
13. Interpretability: AI models can be difficult to interpret, which can make it challenging to understand why a particular prediction was made. This is known as the “black box” problem, where the AI model is so complex that it is difficult to understand how it arrived at a particular decision.
14. Validation: AI models require validation to ensure that they are accurate and reliable. Validation involves testing the AI model on independent data sets to evaluate its performance and ensure that it generalizes well to new, unseen data.
15. Lack of Standardization: There is a lack of standardization in AI algorithms and models used in drug discovery and development, which can make it challenging to compare and reproduce results.
16. Scalability: AI models can be computationally intensive and require significant computational resources, which can be a challenge for large-scale drug discovery and development projects.
17. Explainability: AI models can be difficult to explain, which can make it challenging to understand why a particular prediction was made. This can be a challenge in regulatory environments where transparency and explainability are required.
18. Translational Challenges: AI models can struggle to translate from preclinical to clinical settings, which can be a challenge in drug development.
19. Collaboration: AI requires collaboration between different stakeholders, including researchers, clinicians, and industry partners, which can be a challenge in drug discovery and development.

To address these challenges, researchers and industry partners are working together to develop new methods and techniques for AI in drug discovery and development, such as.

– Developing new AI algorithms and models that are more interpretable and explainable
– Improving data quality and integration
– Developing new validation methods and protocols
– Establishing standardization and regulatory frameworks for AI in drug discovery and development
– Improving scalability and computational resources
– Developing new methods for translational research
– Fostering collaboration between different stakeholders.

These challenges highlight the AI need for careful in the field of drug discovery and development, leading to faster, more efficient, and more effective drug development processes.

By addressing these challenges, we can ensure that AI is used in a way that is safe, effective, and beneficial for patients.

USE OF AI TOOLS

ChatGPT, a tool developed by OpenAI (San Francisco, CA, USA), was utilized to compile information and improve language readability.

CURRENT STATUS OF AI IN DRUG DISCOVERY AND DRUG DEVELOPMENT

The current status of AI in drug discovery and development is really exciting, with AI being used to revolutionize the entire process.[1] From target identification to drug design, AI is being used to analyse large datasets and identify patterns that can help scientists develop new drugs more efficiently.[2] For instance, AI can be used to predict the three-dimensional structure of proteins based on their one-dimensional amino acid sequences, which can help scientists design more effective drugs.

AI is also being used in clinical trials to help identify the right patients for trials and to monitor their progress. AI can be used to analyse large amounts of data from electronic health records and chemical informatics to identify potential new uses for existing drugs.

However, there are also some challenges to the use of AI in drug discovery and development, such as the need for high-quality data and the potential for bias in AI models.[6] Despite these challenges, the use of AI in drug discovery and development has the potential to greatly accelerate the development of new drugs and improve the efficiency of the process.

CONCLUSION

The use of Artificial Intelligence (AI) in drug discovery and development has the potential to revolutionize the entire process, from target identification to drug design. AI can analyse large datasets, identify patterns, and make predictions with high accuracy, leading to faster and more efficient drug development. While there are challenges to be addressed, such as data quality, bias, and regulatory frameworks, the benefits of AI in drug discovery and development are significant. With the continued advancement of AI technologies, we can expect to see improved drug discovery and development processes, leading to better treatments and improved patient outcomes. Ultimately, the integration of AI in drug discovery and development has the potential to transform the pharmaceutical industry and improve human health.

This review article serves as a valuable compass, guiding us through the evolving terrain of XAI's transformative impact on the field of drug discovery. By providing a comprehensive overview of the current status of XAI in drug discovery, the article highlights the potential of XAI to revolutionize the field and accelerate the development of new drugs. Ultimately, XAI has the potential to improve model performance, enhance transparency, and accelerate drug discovery, leading to the development of new and innovative treatments.

REFERENCES

1. Author Contributions: Conceptualization, D.R.S. and A.L.; methodology, D.R.S. and A.L.; software, D.R.S. and A.L.; datacuration, F.C.L., B.J.A., B.O., A.K., G.M., B.I.R., S.A.S.-G., J.A.S., G.T., C.R., H.K.R., S.R., and D.K.; writing—originaldraftpreparation, D.R.S., A.L., F.C.L., B.J.A., B.O., A.K., G.M., B.I.R., S.A.S.-G., J.A.S., G.T., C.R., H.K.R., S.R., and D.K.; writing—reviewandediting, D.R.S. and A.L.supervision, D.R.S. and A.L.; projectadministration, D.R.S. and A.L.; fundingacquisition, D.R.S.andA.L.Allauthorshavereadandagreedtothepublishedversionofthemanuscript.
2. Funding: Thisresearchwasfundedbythe Complutense University of Madrid Research Group (Innovation in Pharmacology, Nanotechnology, and personalized medicine by 3D printing). DoloresSerrano acknowledges the support received from Instituto de las Mujeres and Ministerio de Igualdad(05-12ACT-23).
3. InstitutionalReviewBoardStatement: Notapplicable.
4. InformedConsentStatement: Notapplicable.
5. Data Availability Statement: Dataisavailableinthemanuscript.
6. ConflictsofInterest: Theauthorsdeclarenoconflictsofinterest.
7. Dara, S.; Dhamercherla, S.; Jadav, S.S.; Babu, C.M.; Ahsan, M.J.MachineLearninginDrugDiscovery: AReview.Artif.Intell.Rev, 2022; 55: 1947–1999. [CrossRef][PubMed]
8. Carpenter, K.A.; Huang, X. Machine Learning-based Virtual Screening and Its Applications to Alzheimer's Drug Discovery: A Review. Curr.Pharm.Des, 2018; 24: 3347–3358. [CrossRef][PubMed]
9. Carracedo-Reboredo, P.; Linares-Blanco, J.; Rodriguez-Fernandez, N.; Cedron, F.; Novoa, F.J.; Carballal, A.; Maojo, V.; Pazos, A.; Fernandez-Lozano, C. A review on machine learning approaches and trends in drug discovery. Comput. Struct. Biotechnol. J., 2021; 19: 4538–4558. [CrossRef] [PubMed]
10. Bai, F.; Li, S.; Li, H.AIenhancesdrugdiscoveryanddevelopment.Natl. Sci. Rev. 2024; 11: nwad303.[CrossRef]
11. Hill, A.; True, J.M.; Jones, C.H. Transforming drug development with synthetic biology and AI. Trends Biotechnol, 2024; 42: 1072–1075. [CrossRef] [PubMed]
12. Niazi, S.K. The Coming of Age of AI/ML in Drug Discovery, Development, Clinical Testing, and Manufacturing: The FDA Perspectives. Drug Des. Dev. Ther, 2023; 17: 2691–2725. [CrossRef][PubMed]
13. Barrett, J.S.; Oskoui, S.E.; Russell, S.; Borens, A.Digital Research Environment(DRE) enabled ArtificialIntelligence(AI)to facilitateearlystagedrug development. Front. Pharmacol, 2023; 14: 1115356. [CrossRef]
14. Luo, Y.; Peng, J.; Ma, J. Next Decade's AI-Based Drug Development Features Tight Integration of Data and Computation. Heal. DataSci. 2022; 2022: 9816939. [CrossRef]
15. Gallego, V.; Naveiro, R.; Roca, C.; Rios Insua, D.; Campillo, N.E. AI in drug development: A multidisciplinary perspective. Mol. Divers, 2021; 25: 1461–1479. [CrossRef][PubMed]
16. Liu, Z.; Roberts, R.A.; Lal-Nag, M.; Chen, X.; Huang, R.; Tong, W. AI-based language models powering drug discovery and development. DrugDiscov. Today, 2021; 26: 2593–2607. [CrossRef][PubMed]
17. Chakravarty, K.; Antontsev, V.G.; Khotimchenko, M.; Gupta, N.; Jagarapu, A.; Bundey, Y.; Hou, H.; Maharao, N.; Varshney, J. Accelerated Repurposing and Drug Development of Pulmonary Hypertension Therapies for COVID-19 Treatment Using anAI-

Integrated Biosimulation Platform. Molecules, 2021; 26: 1912. [CrossRef]
18. Burki, T. Pharma block chains AI fordrugdevelopment. Lancet, 2019; 393: 2382. [CrossRef][PubMed]
19. Lloyd, L.AIfordrugdiscovery.Nat.Rev.Urol. 2024; 21: 517. [CrossRef]
20. Sexton, J.Z.; Fursmidt, R.; O'Meara, M.J.; Omta, W.; Rao, A.; Egan, D.A.; Haney, S.A.MachineLearningandAssayDevelopmentforImage-basedPhenotypicProfilingofDrugTreatments.InAssay Guidance Manual; Markossian, S., Grossman, A., Arkin, M., Auld, D., Austin, C., Baell, J., Brimacombe, K., Chung, T.D.Y., Coussens, N.P., Dahlin, J.L., etal., Eds.; EliLilly&Companyand the National Center for Advancing Translational Sciences: Bethesda, MD, USA, 2004.
21. Sarkar, C.; Das, B.; Rawat, V.S.; Wahlang, J.B.; Nongpiur, A.; Tiewsoh, I.; Lyngdoh, N.M.; Das, D.; Bidarolli, M.; Sony, H.T.Artificial Intelligence and Machine Learning Technology Driven Modern Drug Discovery and Development.Int. J.Mol. Sci, 2023; 24: 2026.[CrossRef]
22. Hong, E.; Jeon, J.; Kim, H.U.Recentdevelopmentofmachinelearningmodelsforthepredictionofdrug-druginteractions.Korean J.Chem. Eng, 2023; 40: 276–285.[CrossRef]
23. Hao, Y.; Lynch, K.; Fan, P.; Jurtschenko, C.; Cid, M.; Zhao, Z.; Yang, H.S. Development of a Machine Learning Algorithm for DrugScreeningAnalysisonHigh-ResolutionUPLC-MSE/ QTOF Mass Spectrometry. J.Appl. Lab.Med, 2023; 8: 53–66.[CrossRef]
24. Liu, Q.; Huang, R.; Hsieh, J.; Zhu, H.; Tiwari, M.; Liu, G.; Jean, D.; ElZarrad, M.K.; Fakhouri, T.; Berman, S.; et al. Landscape Analysis of the Application of Artificial Intelligence and Machine Learning in Regulatory Submissions for Drug Development From2016to2021. Clin. Pharmacol. Ther, 2023; 113: 771–774. [CrossRef]
25. Gaudelet, T.; Day, B.; Jamasb, A.R.; Soman, J.; Regep, C.; Liu, G.; Hayter, J.B.R.; Vickers, R.; Roberts, C.; Tang, J.; et al. Utilizing graph machine learning within drug discovery and development. Brief. Bioinform, 2021; 22: bbab159. [CrossRef]
26. Liu, Q.; Zhu, H.; Liu, C.; Jean, D.; Huang, S.M.; ElZarrad, M.K.; Blumenthal, G.; Wang, Y.ApplicationofMachineLearningin DrugDevelopmentandRegulation: Current Status and Future Potential. Clin. Pharmacol. Ther, 2020; 107: 726–729.[CrossRef]
27. Reda, C.; Kaufmann, E.; Delahaye-Duriez, A. Machine learningapplicationsindrugdevelopment.Comput.Struct.Biotechnol.J., 2020; 18: 241–252.[CrossRef]
28. Rodrigues, T.; Bernardes, G.J.L. Machine learning for target discovery in drug development.Curr. Opin. Chem. Biol, 2020; 56: 16–22.[CrossRef] [PubMed]
29. Blanco-Gonzalez, A.; Cabezon, A.; Seco-Gonzalez, A.; Conde-Torres, D.; Antelo-Riveiro, P.; Pineiro, A.; Garcia-Fandino, R. The Roleof AI in Drug Discovery: Challenges, Opportunities, and Strategies. Pharmaceuticals, 2023; 16: 891. [CrossRef] [PubMed]
30. Mshani, I.H.; Jackson, F.M.; Mwanga, R.Y.; Kweyamba, P.A.; Mwanga, E.P.; Tambwe, M.M.; Hofer, L.M.; Siria, D.J.; Gonzalez- Jimenez, M.; Wynne, K.; et al.Screening of malaria infections in human blood samples with varying parasite densities and anaemicconditionsusingAI-Poweredmid-infraredspectroscopy. Malar. J., 2024; 23: 188. [CrossRef][PubMed]
31. Bittner, M.I.; Farajnia, S.AIindrugdiscovery: Applications, opportunities, andchallenges.Patterns, 2022; 3: 100529.[CrossRef]
32. Yuan, H.Y.; Tong, X.F.; Ren, Y.Y.; Li, Y.Y.; Wang, X.L.; Chen, L.L.; Chen, S.D.; Jin, X.Z.; Wang, X.D.; Targher, G.; et al.AI-based digital pathology provides newer insights into lifestyle intervention-induced fibrosis regression in MASLD: An exploratory study.Liver Int, 2024; 44: 10. [CrossRef] [PubMed]
33. Leitner, J.; Chiang, P.H.; Agnihotri, P.; Dey, S.TheEffectofanAI-Based, Autonomous, DigitalHealthInterventionUsingPrecise Lifestyle Guidance on Blood Pressure in Adults with Hypertension: Single-Arm Nonrandomized Trial.JMIR Cardio, 2024; 8: e51916. [CrossRef]
34. Khokhar, S.; Holden, J.; Toomer, C.; DelParigi, A.WeightLosswithanAI-PoweredDigitalPlatformforLifestyleIntervention. Obes.Surg, 2024; 34: 1810–1818.[CrossRef]
35. Chatterjee, A.; Pahari, N.; Prinz, A.; Riegler, M.AiandsemanticontologyforpersonalizedactivityeCoachinginhealthylifestyle recommendations: Ameta-heuristicapproach. BMCMed.Inform.Decis.Mak, 2023; 23: 278. [CrossRef]
36. AI'spotentialtoacceleratedrugdiscoveryneedsareality check.Nature, 2023; 622: 217.[CrossRef]
37. Zargaran, A.; Sousi, S.; Glynou, S.P.; Mortada, H.; Zargaran, D.; Mosahebi, A.Asystematicreviewofgenerativeadversarial networks(GANs)inplasticsurgery. J.Plast.Reconstr.AestheticSurg, 2024; 95: 377–385. [CrossRef]
38. Yoon, J.T.; Lee, K.M.; Oh, J.H.; Kim, H.G.; Jeong, J. W. Insightsand Considerationsin Development and PerformanceEvaluationofGenerativeAdversarialNetworks(GANs): WhatRadiologistsNeedtoKnow.Diagnostics, 2024; 14: 1756.[CrossRef][PubMed]
39. Schneider, P.; Walters, W.P.; Plowright, A.T.; Sieroka, N.; Listgarten, J.; Goodnow, R.A., Jr.; Fisher, J.; Jansen, J.M.; Duca, J.S.; Rush, T.S.; etal.Rethinkingdrugdesignintheartificialintelligenceera.Nat.Rev.DrugDiscov, 2020; 19: 353–364.[CrossRef][PubMed]

40. Yadalam, P.K.; Anegundi, R.V.; Ramadoss, R.; Shrivastava, D.; Almufarrij, R.A.S.; Srivastava, K.C. AI-based 3D-QSAR model of FDA-approvedrepurposeddrugsforinhibitingsclerostin. Technol.Health.Care, 2024; 32: 3007–3019. [CrossRef][PubMed]
41. Stafford, K.A.; Anderson, B.M.; Sorenson, J.; vandenBedem, H.AtomNetPoseRanker: EnrichingLigandPoseQualityfor DynamicProteinsinVirtualHigh-ThroughputScreens. J.Chem.Inf.Model.2022, 62, 1178–1189. [CrossRef][PubMed]
42. Atomwise. Availableonline: https: //www.atomwise.com(accessedon12August2024).
43. BenevolentAIDrugDiscovery. Availableonline: https: //www.benevolent.com(accessedon12August2024).
44. Beis, G.; Serafeim, A.P.; Papasotiriou, I. Data-driven analysis and druggability assessment methods to accelerate the identificationofnovel cancer targets.Comput. Struct. Biotechnol. J. 2023, 21, 46–57.[CrossRef] [PubMed]
45. DeepMind'sAlphaFoldAlgorithm. Availableonline: https: //deepmind.google/technologies/alphafold(accessedon 12August 2024).
46. Niemyska, W.; Rubach, P.; Gren, B.A.; Nguyen, M.L.; Garstka, W.; Bruno da Silva, F.; Rawdon, E.J.; Sulkowska, J.I. AlphaKnot: Server to analyze entanglement in structures predicted by AlphaFold methods.Nucleic Acids Res, 2022; 50: W44–W50.[CrossRef]
47. Efficacy and Safety of REC-2282 in Patients with Progressive Neurofibromatosis Type 2 (NF2) Mutated Meningiomas (POPLAR-NF2).Availableonline: https: //clinicaltrials.gov/study/NCT05130866?term=POPLAR&rank=2(accessedon12August2024).
48. Parvatikar, P.P.; Patil, S.; Khaparkhuntikar, K.; Patil, S.; Singh, P.K.; Sahana, R.; Kulkarni, R.V.; Raghu, A.V.Artificialintelligence: Machinelearningapproachforscreeninglargedatabase anddrugdiscovery. Antivir. Res, 2023; 220: 105740. [CrossRef]
49. Siddiqui, G.A.; Stebani, J.A.; Wragg, D.; Koutsourelakis, P.S.; Casini, A.; Gagliardi, A.ApplicationofMachineLearningAlgorithms to Metadynamics for the Elucidation of the Binding Modes and Free Energy Landscape of Drug/Target Interactions: A Case Study. Chemistry, 2023; 29: e202302375. [CrossRef]
50. Brinkhaus, H.O.; Rajan, K.; Schaub, J.; Zielesny, A.; Steinbeck, C. Open data and algorithms for open science in AI-driven molecularinformatics. Curr.Opin.Struct.Biol, 2023; 79: 102542. [CrossRef]
51. DGIdb.Availableonline: https: //www.dgidb.org(accessedon12August2024).
52. TheConnectivityMap.Availableonline: https: //www.broadinstitute.org/connectivity-map-cmap(accessedon12August2024).
53. DeepChem.Availableonline: https: //deepchem.io(accessedon13August2024).
54. Schrödinger'sMaestro Platform. Available online: on 13August 2024).
55. InsilicoMedicine.Availableonline:
56. XtalPi.Availableonline: https: //www.xtalpi.com/en(accessedon13August2024).
57. Cyclica. Availableonline: https: //cyclicarx.com/science(accessedon13August2024).
58. Le, N.Q.K.; Tran, T.X.; Nguyen, P.A.; Ho, T.T.; Nguyen, V.N. Recent progress in machine learning approaches for predicting carcinogenicityindrugdevelopment.ExpertOpin.Drug Metab.Toxicol, 2024; 20: 621–628.[CrossRef]
59. Chang, W.T.; Liu, C.F.; Feng, Y.H.; Liao, C.T.; Wang, J.J.; Chen, Z.C.; Lee, H.C.; Shih, J.Y. An artificial intelligence approach for predictingcardiotoxicityinbreastcancerpatientsreceivinganthracycline.Arch.Toxicol, 2022; 96: 2731–2737. [CrossRef][PubMed]
60. Marques, L.; Costa, B.; Pereira, M.; Silva, A.; Santos, J.; Saldanha, L.; Silva, I.; Magalhaes, P.; Schmidt, S.; Vale, N. Advancing Precision Medicine: A Review of Innovative In Silico Approaches for Drug Development, Clinical Pharmacology and PersonalizedHealthcare. Pharmaceutics, 2024; 16: 332. [CrossRef]
61. Mukherjee, D.; Roy, D.; Thakur, S.TransformingCancerCare: TheImpactofAI-DrivenStrategies.Curr.CancerDrugTargets, 2024; 24: 1–4.[CrossRef]
62. Bhinder, B.; Gilvary, C.; Madhukar, N.S.; Elemento, O.ArtificialIntelligenceinCancerResearchandPrecisionMedicine. Cancer Discov, 2021; 11: 900–915. [CrossRef] [PubMed]
63. Liu, D.; Schilling, B.; Liu, D.; Sucker, A.; Livingstone, E.; Jerby-Arnon, L.; Zimmer, L.; Gutzmer, R.; Satzger, I.; Loquai, C.; et al. Integrative molecular and clinical modeling of clinical outcomes to PD1 blockade in patients with metastatic melanoma. Nat. Med, 2019; 25: 1916–1927. [CrossRef] [PubMed]
64. Johannet, P.; Coudray, N.; Donnelly, D.M.; Jour, G.; Illa-Bochaca, I.; Xia, Y.; Johnson, D.B.; Wheless, L.; Patrinely, J.R.; Nomikou, S.; et al. Using Machine Learning Algorithms to Predict Immunotherapy Response in Patients with Advanced Melanoma.Clin. CancerRes, 2021; 27: 131–140. [CrossRef] [PubMed]
65. Dercle, L.; Fronheiser, M.; Lu, L.; Du, S.; Hayes, W.; Leung, D.K.; Roy, A.; Wilkerson, J.; Guo, P.; Fojo, A.T.; et al. Identification of Non-Small Cell Lung Cancer Sensitive to Systemic Cancer Therapies Using Radiomics.Clin. CancerRes, 2020; 26: 2151–2162. [CrossRef]
66. Blasiak, A.; Khong, J.; Kee, T.CURATE.AI: Optimizing Personalized Medicine with Artificial Intelligence. Transl. Life Sci. Innov, 2020; 25: 95–105.[CrossRef]

67. Iorio, F.; Knijnenburg, T.A.; Vis, D.J.; Bignell, G.R.; Menden, M.P.; Schubert, M.; Aben, N.; Goncalves, E.; Barthorpe, S.; Lightfoot, H.; et al. A Landscape of Pharmacogenomic Interactions in Cancer. Cell, 2016; 166: 740–754. [CrossRef]
68. Kuenzi, B.M.; Park, J.; Fong, S.H.; Sanchez, K.S.; Lee, J.; Kreisberg, J.F.; Ma, J.; Ideker, T. Predicting Drug Response and Synergy Usinga Deep Learning Model of Human Cancer Cells. CancerCell, 2020; 38: 672–684.e676. [CrossRef]
69. Sheu, Y.H.; Magdamo, C.; Miller, M.; Das, S.; Blacker, D.; Smoller, J.W.AI-assistedpredictionofdifferentialresponseto antidepressantclassesusingelectronichealthrecords. NPJDigit.Med, 2023; 6: 73. [CrossRef]
70. Arnold, P.I.M.; Janzing, J.G.E.; Hommersom, A. Machine learning for antidepressant treatment selection in depression.Drug Discov.Today, 2024; 29: 104068. [CrossRef][PubMed]
71. Liu, X.; Read, S.J.Developmentofamultivariatepredictionmodelforantidepressantresistantdepressionusingreward-relatedpredictors. Front. Psychiatry, 2024; 15: 1349576. [CrossRef]
72. Stankoski, S.; Jordan, M.; Gjoreski, H.; Lustrek, M. Smartwatch-Based Eating Detection: Data Selection for Machine Learning from Imbalanced Data with Imperfect Labels. Sensors, 2021; 21: 1902. [CrossRef]
73. Lam, B.; Catt, M.; Cassidy, S.; Bacardit, J.; Darke, P.; Butterfield, S.; Alshabrawy, O.; Trenell, M.; Missier, P.UsingWearableActivity TrackerstoPredictType2Diabetes: MachineLearning-BasedCross-sectionalStudyoftheUKBiobankAccelerometerCohort. JMIRDiabetes, 2021; 6: e23364. [CrossRef]
74. Kargarandehkordi, A.; Slade, C.; Washington, P. Personalized AI-Driven Real-Time Models to Predict Stress-Induced Blood Pressure Spikes Using Wearable Devices: Proposal for a Prospective Cohort Study.JMIR Res. Protoc, 2024; 13: e55615.[CrossRef]
75. Garbarino, S.; Bragazzi, N.L.RevolutionizingSleepHealth: TheEmergenceandImpactofPersonalizedSleepMedicine. J.Pers. Med. 2024, 14, 598. [CrossRef]
76. Schalkamp, A.K.; Peall, K.J.; Harrison, N.A.; Sandor, C. Wearable movement-tracking data identify Parkinson's disease years beforeclinicaldiagnosis. Nat.Med, 2023; 29: 2048–2056. [CrossRef]
77. Alonso, T.R.; Gagol, A.; Scherer, M.; Matji, A.; Torrado-Santiago, S.; Serrano, D.R.; Garcia-Arieta, A.; Torrado, J.J. A multivariate investigationintotherelationshipbetweenpharmaceuticalcharacteristicsandpatientpreferencesofbioequivalentibuprofen tablets.PatientPrefer. Adherence, 2018; 12: 1927–1935.[CrossRef]
78. Walsh, D.; Serrano, D.R.; Worku, Z.A.; Madi, A.M.; O'Connell, P.; Twamley, B.; Healy, A.M. Engineering of pharmaceutical cocrystalsinanexcipientmatrix: Spraydryingversushotmeltextrusion. Int.J.Pharm, 2018; 551: 241–256. [CrossRef]
79. Serrano, D.R.; Walsh, D.; O'Connell, P.; Mugheirbi, N.A.; Worku, Z.A.; Bolas-Fernandez, F.; Galiana, C.; Dea-Ayuela, M.A.; Healy, A.M.Optimisingtheinvitroandinvivoperformanceoforalcocrystalformulationsviaspraycoating.Eur.J.Pharm. Biopharm, 2018; 124: 13–27.[CrossRef]
80. Lamy, B.; Tewes, F.; Serrano, D.R.; Lamarche, I.; Gobin, P.; Couet, W.; Healy, A.M.; Marchand, S. New aerosol formulation to controlciprofloxacinpulmonaryconcentration.J.Control.Release, 2018; 271: 118–126.[CrossRef]
81. Gholap, A.D.; Uddin, M.J.; Faiyazuddin, M.; Omri, A.; Gowri, S.; Khalid, M. Advances in artificial intelligence for drug deliveryanddevelopment: Acomprehensivereview. Comput.Biol.Med, 2024; 178: 108702. [CrossRef]
82. Aundhia, C.; Parmar, G.; Talele, C.; Shah, N.; Talele, D.ImpactofArtificialIntelligenceonDrugDevelopmentandDelivery. Curr. Top. Med. Chem, 2024; inpress. [CrossRef]
83. Lou, H.; Lian, B.; Hageman, M.J.ApplicationsofMachineLearninginSolidOralDosageFormDevelopment.J.Pharm.Sci, 2021; 110: 3150–3165.[CrossRef]
84. Momeni, M.; Afkanpour, M.; Rakhshani, S.; Mehrabian, A.; Tabesh, H.Apredictionmodelbasedonartificialintelligence techniquesfordisintegrationtimeandhardnessoffastdisintegratingtabletsinpre-formulationtests.BMCMed.Inform.Decis. Mak, 2024; 24: 88. [CrossRef]
85. Serrano, D.R.; Kara, A.; Yuste, I.; Luciano, F.C.; Ongoren, B.; Anaya, B.J.; Molina, G.; Diez, L.; Ramirez, B.I.; Ramirez, I.O.; etal.3DPrintingTechnologies in Personalized Medicine, Nanomedicines, and Biopharmaceuticals. Pharmaceutics, 2023; 15: 313. [CrossRef]
86. Konta, A.A.; Garcia-Pina, M.; Serrano, D.R.Personalised3DPrintedMedicines: WhichTechniquesandPolymersAreMore Successful?Bioengineering, 2017; 4: 79. [CrossRef]
87. Yuste, I.; Luciano, F.C.; Anaya, B.J.; Sanz-Ruiz, P.; Ribed-Sanchez, A.; Gonzalez-Burgos, E.; Serrano, D.R.Engineering3D-PrintedAdvancedHealthcareMaterialsforPeriprostheticJointInfections.Antibiotics, 2023; 12: 1229.[CrossRef]
88. Anaya, B.J.; Cerda, J.R.; D'Atri, R.M.; Yuste, I.; Luciano, F.C.; Kara, A.; Ruiz, H.K.; Ballesteros, M.P.; Serrano, D.R. Engineering of 3Dprintedpersonalizedpolypillsforthetreatmentofthe metabolicsyndrome. Int.J.Pharm, 2023; 642: 123194. [CrossRef]
89. Malebari, A.M.; Kara, A.; Khayyat, A.N.; Mohammad, K.A.; Serrano, D.R. Development of Advanced 3D-Printed Solid

DosagePediatricFormulationsforHIVTreatment. Pharmaceuticals, 2022; 15: 435. [CrossRef][PubMed]
90. Ayyoubi, S.; Cerda, J.R.; Fernandez-Garcia, R.; Knief, P.; Lalatsa, A.; Healy, A.M.; Serrano, D.R.3Dprintedsphericalmini-tablets: Geometryversuscompositioneffectsincontrollingdissolutionfrompersonalisedsoliddosageforms. Int. J.Pharm, 2021; 597: 120336.[CrossRef] [PubMed]
91. Cerda, J.R.; Arifi, T.; Ayyoubi, S.; Knief, P.; Ballesteros, M.P.; Keeble, W.; Barbu, E.; Healy, A.M.; Lalatsa, A.; Serrano, D.R. Personalised 3D Printed Medicines: Optimising Material Properties for Successful Passive Diffusion Loading of Filaments for FusedDeposition Modelling of Solid Dosage Forms. Pharmaceutics, 2020; 12: 345. [CrossRef]
92. Vora, L.K.; Gholap, A.D.; Jetha, K.; Thakur, R.R.S.; Solanki, H.K.; Chavda, V.P.ArtificialIntelligenceinPharmaceuticalTechnologyandDrugDeliveryDesign.Pharmaceutics, 2023; 15: 1916.[CrossRef][PubMed]
93. Obeid, S.; Madzarevic, M.; Krkobabic, M.; Ibric, S. Predicting drug release from diazepam FDM printed tablets using deep learning approach: Influence of process parameters and tablet surface/volume ratio. Int. J. Pharm, 2021; 601: 120507. [CrossRef][PubMed]
94. Alhijjaj, M.; Nasereddin, J.; Belton, P.; Qi, S. Impact of Processing Parameters on the Quality of Pharmaceutical Solid DosageFormsProduced by Fused Deposition Modeling (FDM). Pharmaceutics, 2019; 11: 633. [CrossRef]
95. Elbadawi, M.; McCoubrey, L.E.; Gavins, F.K.H.; Ong, J.J.; Goyanes, A.; Gaisford, S.; Basit, A.W. Harnessing artificial intelligence forthenextgenerationof3Dprintedmedicines. Adv.DrugDeliv.Rev, 2021; 175: 113805. [CrossRef]
96. Chen, S.; Li, T.; Yang, L.; Zhai, F.; Jiang, X.; Xiang, R.; Ling, G.Artificialintelligence-drivenpredictionofmultipledruginteractions. Brief.Bioinform, 2022; 23: bbac427.[CrossRef]
97. Patel, S.; Patel, M.; Kulkarni, M.; Patel, M.S. DE-INTERACT: A machine-learning-based predictive tool for the drug-excipient interactionstudyduringproductdevelopment-Validationthroughparacetamolandvanillinasacasestudy.Int.J.Pharm, 2023; 637: 122839. [CrossRef]
98. Matji, A.; Donato, N.; Gagol, A.; Morales, E.; Carvajal, L.; Serrano, D.R.; Worku, Z.A.; Healy, A.M.; Torrado, J.J. Predicting the criticalqualityattributesofibuprofentabletsviamodellingofprocessparametersforrollercompactionandtabletting.Int. J. Pharm, 2019; 565: 209–218. [CrossRef]
99. Mansuri, A.; Volkel, M.; Mihiranga, D.; Feuerbach, T.; Winck, J.; Vermeer, A.W.P.; Hoheisel, W.; Thommes, M.Predicting self-diffusion coefficients in semi-crystalline and amorphous solid dispersions using free volume theory. Eur. J. Pharm. Biopharm. 2023, 190, 107–120. [CrossRef] [PubMed]
100. HughesJP, ReesS, KalindjianSB, PhilpottKL.Principlesofearlydrugdiscovery.BrJPharmacol, 2011; 162: 1239-1249[PMID: 21091654DOI: 10.1111/j.1476-5381.2010.01127.x]
101. BohrH.Chapter3-Drugdiscoveryandmolecularmodelingusingartificialintelligence.AIHealth2020; 61-83[DOI: 10.1016/b978-0-12-818438-7.00003-4]
102. EkinsS, PuhlAC, ZornKM, LaneTR, RussoDP, KleinJJ, HickeyAJ, ClarkAM.Exploitingmachinelearningforend-to-enddrugdiscoveryand development. Nat Mater, 2019; 18: 435-441 [PMID: 31000803DOI: 10.1038/s41563-019-0338-z]
103. ZhangL, TanJ, HanD, ZhuH.Frommachinelearningtodeeplearning: progressinmachineintelligenceforrationaldrugdiscovery.DrugDiscov Today, 2017; 22: 1680-1685 [PMID: 28881183DOI: 10.1016/j.drudis.2017.08.010]
104. LavecchiaA.Deeplearningindrugdiscovery: opportunities, challengesandfutureprospects.DrugDiscovToday, 2019; 24: 2017-2032[PMID: 31377227DOI: 10.1016/j.drudis.2019.07.006]
105. GaultonA, BellisLJ, BentoAP, ChambersJ, DaviesM, HerseyA, LightY, McGlincheyS, MichalovichD, Al-LazikaniB, OveringtonJP.ChEMBL: a large-scale bioactivity database for drug discovery. Nucleic Acids Res, 2012; 40: D1100-D1107 [PMID: 21948594DOI: 10.1093/nar/gkr777]
106. KimS.ExploringChemicalInformationinPubChem.CurrProtoc, 2021; 1: e217[PMID: 34370395DOI: 10.1002/cpz1.217]
107. AshrafFB, AkterS, MumuSH, IslamMU, UddinJ.Bio-activitypredictionofdrugcandidatecompoundstargetingSARS-Cov-2usingmachine learning approaches. PLoS One, 2023; 18: e0288053 [PMID: 37669264DOI: 10.1371/journal.pone.0288053]
108. MayrA, KlambauerG, UnterthinerT, HochreiterS.DeepTox: ToxicityPredictionusingDeepLearning.FrontEnvironSci, 2016; 3[DOI: 10.3389/fenvs.2015.00080]
109. WuZ, RamsundarB, FeinbergEN, GomesJ, GeniesseC, PappuAS, LeswingK, PandeV.MoleculeNet: abenchmarkformolecularmachinelearning. Chem Sci, 2018; 9: 513-530 [PMID: 29629118DOI: 10.1039/c7sc02664a]
110. WallachHA, DzambaMI.AtomNet: adeepconvolutionalneuralnetworkforbioactivitypredictioninstructure-baseddrugdiscovery.arXiv; 2015
111. MarrB.HowisAIusedinhealthcare—5powerfulreal-worldexamplesthatshowthelatestadvances.Forbes; 2018.
112. TheCONVERGE®Platform.Lastaccessed: April23, 2024.Availablefrom: https: //www.vergegenomics.com/approach

113. FDA Grants Breakthrough Device Status to Healthcare AI Software.Last accessed April 23, 2024. Available from:
114. Artificialintelligencedecodescancerpathologyimages.LastaccessedApril23, 2024.Availablefrom: https://www.novartis.com/stories/artificial-intelligence-decodes-cancer-pathology-images
115. Machinelearningpoisedtoacceleratedrugdiscovery.LastaccessedApril23, 2024.Availablefrom: https://www.novartis.com/stories/machine-learning-poised-accelerate-drug-discovery
116. CyclicaDrivesDrugDiscoveryThroughAI-AugmentedIntegratedNetworkofCloud-BasedTechnologiestogetherwithBayer.Lastaccessed April 23, 2024. Available from:
117. HarveyA.Theroleofnaturalproductsindrugdiscoveryanddevelopmentinthenewmillennium.IDrugs, 2010; 13: 70-72. [PMID: 20127553]
118. BegleyCG, EllisLM.Drugdevelopment: Raisestandardsforpreclinicalcancerresearch.Nature, 2012; 483: 531-533[PMID: 22460880DOI: 10.1038/483531a]
119. Korinek M, Hsieh PS, Chen YL, Hsieh PW, Chang SH, Wu YH, Hwang TL. Randialic acid B and tomentosolic acid block formylpeptidereceptor1inhumanneutrophilsandattenuatepsoriasis-likeinflammationinvivo.BiochemPharmacol, 2021; 190: 114596[PMID: 33964283DOI: 10.1016/j.bcp.2021.114596]
120. Tingaud-SequeiraA, CarnevaliO, Cerdà J. Cathepsin Bdifferentialexpressionandenzymeprocessingandactivityduring Fundulusheteroclitus embryogenesis. Comp Biochem Physiol A Mol Integr Physiol, 2011; 158: 221-228 [PMID: 21059400DOI: 10.1016/j.cbpa.2010.11.002]
121. WingenderE.TheTRANSFACprojectasanexampleofframeworktechnologythatsupportstheanalysisofgenomicregulation.BriefBioinform, 2008; 9: 326-332 [PMID: 18436575DOI: 10.1093/bib/bbn016]
122. BaigMH, AhmadK, RabbaniG, DanishuddinM, ChoiI.ComputerAidedDrugDesignanditsApplication totheDevelopmentofPotentialDrugs for Neurodegenerative Disorders. Curr Neuropharmacol, 2018; 16: 740-748 [PMID: 29046156DOI: 10.2174/1570159X15666171016163510]
123. DanaD, GadhiyaSV, StSurinLG, LiD, NaazF, AliQ, PakaL, YaminMA, NarayanM, GoldbergID, NarayanP.DeepLearninginDrugDiscovery and Medicine; Scratching the Surface. Molecules, 2018; 23 [PMID: 30231499DOI: 10.3390/molecules23092384]
124. Urban G, Bache KM, Phan D, Sobrino A, Shmakov AK, Hachey SJ, Hughes C, Baldi P. Deep Learning for Drug Discovery and CancerResearch: AutomatedAnalysisofVascularizationImages.IEEE/ACMTransComputBiolBioinform, 2019; 16: 1029-1035[PMID: 29993583DOI: 10.1109/TCBB.2018.2841396]
125. Lim J, Ryu S, Park K, Choe YJ, Ham J, Kim WY. Predicting Drug-Target Interaction Using a Novel Graph Neural Network with 3DStructure-EmbeddedGraphRepresentation.JChemInfModel, 2019; 59: 3981-3988[PMID: 31443612DOI: 10.1021/acs.jcim.9b00387]
126. ChenZ, LiuX, HoganW, ShenkmanE, BianJ.Applicationsofartificialintelligenceindrugdevelopmentusingreal-worlddata.DrugDiscovToday, 2021; 26: 1256-1264 [PMID: 33358699DOI: 10.1016/j.drudis.2020.12.013]
127. LavecchiaA, DiGiovanniC.Virtualscreeningstrategiesindrugdiscovery: acriticalreview.CurrMedChem, 2013; 20: 2839-2860[PMID: 23651302DOI: 10.2174/09298673113209990001]
128. SivakumarB, KaliappanI.Leaddrugdiscoveryfromimidazolinonederivativeswith Aurorakinaseinhibitors.PHAR, 2023; 70: 1529-1540[DOI: 10.3897/pharmacia.70.e114935]
129. MaloN, HanleyJA, CerquozziS, PelletierJ, NadonR.Statisticalpracticeinhigh-throughputscreeningdataanalysis.NatBiotechnol, 2006; 24: 167-175 [PMID: 16465162DOI: 10.1038/nbt1186]
130. DaraS, DhamercherlaS, JadavSS, BabuCM, AhsanMJ.MachineLearninginDrugDiscovery: AReview.ArtifIntellRev, 2022; 55: 1947-1999 [PMID: 34393317DOI: 10.1007/s10462-021-10058-4]
131. ShockleyKR, GuptaS, HarrisSF, LahiriSN, PeddadaSD.QualityControlofQuantitativeHighThroughputScreeningData.FrontGenet, 2019; 10: 387[PMID: 31143201DOI: 10.3389/fgene.2019.00387]
132. BeheiN, TryhubchakO, PryymakB.Developmentofamlodipineandenalaprilcombinedtabletsbasedonqualitybydesignandartificialneural network for confirming of qualitative composition. PHAR, 2022; 69: 779-789 [DOI: 10.3897/pharmacia.69.e86876]
133. KrausVB.Biomarkersasdrugdevelopmenttools: discovery, validation, qualificationanduse.NatRevRheumatol, 2018; 14: 354-362[PMID: 29760435DOI: 10.1038/s41584-018-0005-9]
134. PuL, NaderiM, LiuT, WuHC, MukhopadhyayS, BrylinskiM.eToxPred: amachinelearning-basedapproachtoestimatethetoxicityofdrugcandidates. BMC Pharmacol Toxicol, 2019; 20: 2 [PMID: 30621790DOI: 10.1186/s40360-018-0282-6]
135. MakKK, PichikaMR.Artificialintelligenceindrugdevelopment: presentstatusandfutureprospects.DrugDiscovToday, 2019; 24: 773-780[PMID: 30472429DOI: 10.1016/j.drudis.2018.11.014]
136. HarrerS, ShahP, AntonyB, HuJ.ArtificialIntelligenceforClinicalTrialDesign.Tre

ndsPharmacolSci2019; 40: 577-591[PMID: 31326235DOI: 10.1016/j.tips.2019.05.005]
137. HutsonM.HowAIisbeingusedtoaccelerateclinicaltrials.Nature, 2024; 627: S2-S5[PMID: 38480968DOI: 10.1038/d41586-024-00753-x]
138. JohnsonKB, WeiWQ, WeeraratneD, FrisseME, MisulisK, RheeK, ZhaoJ, SnowdonJL.PrecisionMedicine, AI, andtheFutureofPersonalized Health Care. Clin Transl Sci, 2021; 14: 86-93 [PMID: 32961010DOI: 10.1111/cts.12884]
139. SchorkNJ.ArtificialIntelligenceandPersonalizedMedicine.CancerTreatRes, 2019; 178: 265-283[PMID: 31209850DOI: 10.1007/978-3-030-16391-4_11]
140. MichelhaughSA, JanuzziJLJr.UsingArtificialIntelligencetoBetterPredictandDevelopBiomarkers.HeartFailClin, 2022; 18: 275-285[PMID: 35341540DOI: 10.1016/j.hfc.2021.11.004]
141. SiegertMJ, PriscuJC, AlekhinaIA, WadhamJL, LyonsWB.Preface.PhilosTransAMathPhysEngSci, 2016; 374[PMID: 26667919DOI: 10.1098/rsta.2015.0145]
142. HousehMS, AldosariB, AlanaziA, KushnirukAW, BoryckiEM.BigData, BigProblems: AHealthcare Perspective. Stud Health TechnolInform, 2017; 238: 36-39 [PMID: 28679881]
143. MehrabiN, MorstatterF, SaxenaN, LermanK, GalstyanA.ReducingBiasinAI: ASurveyonSourcesofBiasandMitigationStrategies.2019 Preprint. Available from: arXiv: 1908.09635 [DOI: 10.48550/arXiv.1908.09635]
144. LiptonZC.TheMythosofModelInterpretability.2016Preprint.Availablefrom: arXiv: 1606.03490[DOI: 10.48550/arXiv.1606.03490]
145. ZitnikM, NguyenF, WangB, LeskovecJ, GoldenbergA, HoffmanMM.MachineLearningforIntegratingDatainBiologyandMedicine: Principles, Practice, and Opportunities. Inf Fusion, 2019; 50: 71-91 [PMID: 30467459DOI: 10.1016/j.inffus.2018.09.012]
146. WachterS, MittelstadtB, RussellC.CounterfactualExplanationsWithoutOpeningtheBlackBox: AutomatedDecisionsandtheGDPR. SSRNJ[DOI: 10.2139/ssrn.3063289]
147. ZhavoronkovA.ArtificialIntelligenceforDrugDiscovery, BiomarkerDevelopment, andGenerationofNovelChemistry.MolPharm, 2018; 15: 4311-4313[PMID: 30269508DOI: 10.1021/acs.molpharmaceut.8b00930]
148. DraperP, FarkasS.ArtificialIntelligenceandDeepLearninginPathology: ATutorialontheBasicPrinciplesandRecentAdvances.2019Preprint. Available from: arXiv, 1901.00515 [DOI: 10.48550/arXiv.1901.00515]
149. HiwaleM, WalambeR, PotdarV, KotechaK.Asystematicreviewofprivacy-preservingmethodsdeployedwithblockchainandfederatedlearning for the telemedicine. Healthc Anal (NY), 2023; 3: 100192 [PMID: 37223223DOI: 10.1016/j.health.2023.100192]
150. YadavS, SinghA, SinghalR, YadavJP.Revolutionizingdrugdiscovery: The impact of artificial intelligenceonadvancementsinpharmacology and the pharmaceutical industry. Intelligent Pharm, 2024; 2: 367-380 [DOI: 10.1016/j.ipha.2024.02.009]
151. YangF, Zhang Q, JiX, Zhang Y, Li W, Peng S, Xue F. Machine Learning Applicationsin Drug Repurposing. Interdiscip Sci, 2022; 14: 15-21. [PMID: 35066811DOI: 10.1007/s12539-021-00487-8]
152. VidhyaKS, SultanaA, MNK, Rangareddy H. ArtificialIntelligence’s Impacton Drug Discoveryand Development From Benchto Bedside. Cureus, 2023; 15: e47486[PMID: 37881323DOI: 10.7759/cureus.47486]