Current Pharmacology Reports
https://doi.org/10.1007/s40495-024-00367-x

REVIEW

The Role of Artificial Intelligence in Revolutionizing Pharmacological Research

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Accepted: 21 August 2024

Abstract

Purpose of Review The integration of Artificial Intelligence (AI) has ushered in a transformative era in pharmacological research, offering solutions to longstanding challenges associated with high costs and protracted timelines. The primary objective of this review is to provide a comprehensive overview of the current state of AI in pharmacological research, delineate its multifaceted applications, and underscore its consequential impact.

Recent Findings In the realm of drug discovery, AI has emerged as a potent catalyst, leveraging machine learning to scrutinize vast datasets. This approach has facilitated the precise identification of potential drugs, significantly expediting the drug discovery process. Furthermore, AI has revolutionized virtual screening techniques, hastening the identification of promising drug candidates.

The applications extend to personalized medicine, where AI plays a pivotal role in recommending tailored drug regimens based on individual genetics and medical history. Simultaneously, it aids in the stratification of patient subpopulations, ensuring optimized treatments.

AI's influence is also evident in the realm of drug toxicity prediction, offering an invaluable tool for the early identification of safety concerns. The technology is set to impact pharmacological research by advancing our understanding of biological pathways, predicting long-term drug effects, enhancing regulatory compliance, and optimizing drug manufacturing processes.

Summary In summary, AI's diverse and profound applications in pharmacological research, particularly in drug development, underscore its transformative potential. However, ethical and regulatory considerations are paramount. Proposed frameworks seek to ensure the responsible adoption of AI in healthcare, recognizing the need for a balanced approach that maximizes the benefits while safeguarding ethical principles. The continued responsible harnessing of AI in pharmacological research promises to reshape the landscape of healthcare and drug development.

Keywords Artificial Intelligence · Pharmacology · Drug Discovery · Drug Repurposing · Toxicity Prediction · Personalized Medicine

Introduction

Pharmacological research has historically grappled with substantial challenges—enormous costs, extended timelines, and frequent setbacks in drug development [1, 2]. However, the infusion of Artificial Intelligence (AI) has heralded a transformative era, expediting the discovery of promising drug candidates, tailoring treatments for individuals, and proactively assessing potential toxicological risks [3, 4]. AI's significant strides in pharmacological research are notably pronounced in drug discovery, where conventional methods involved exhaustive screening of vast chemical libraries, notorious for their resource-intensive nature. In contrast, AI-driven computational models, particularly deep

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Published online: 03 September 2024

learning-based neural networks, have upended this landscape by demonstrating remarkable precision in predicting potential drug candidates [5, 6]. These advanced models meticulously pore over extensive chemical and biological datasets, distinguishing compounds with anticipated therapeutic efficacy while minimizing possible side effects.

Moreover, AI's pivotal role in personalized medicine shines brightly. By leveraging an individual's genetic makeup, medical history, and lifestyle specifics, AI algorithms adeptly customize drug regimens, aiming to minimize adverse effects and optimize therapeutic outcomes [7, 8]. This tailored approach not only enhances patient well-being but also slashes healthcare costs associated with traditional trial-and-error treatment methods.

Beyond personalized medicine, AI has emerged as an indispensable asset in foreseeing potential drug toxicities, particularly in the early stages of development. Accurate anticipation of toxicity stands as a crucial preventative measure against adverse reactions and the expensive repercussions of late-stage drug failures. AI models, exemplified by in silico toxicity prediction tools, meticulously scrutinize biological and chemical data, culminating in a comprehensive evaluation of a drug's safety profile [9, 10]. This foresight enables pharmaceutical enterprises to prioritize the advancement of safer compounds into subsequent developmental phases.

The integration of AI in pharmacological research signifies a monumental leap forward, significantly reducing the burden of traditional methods and fostering a more efficient, cost-effective, and patient-centric approach to drug development and healthcare delivery.

AI in Drug Discovery

AI's integration in drug discovery represents a pivotal evolution, reshaping traditional approaches and accelerating the quest for novel therapeutic agents [11]. Machine learning algorithms, leveraging extensive datasets encompassing chemical structures, biological targets, and disease pathways, offer a more streamlined identification of potential drug candidates. For example, the DeepChem© platform harnesses deep learning models to forecast the biological activity of compounds, thereby pinpointing promising molecules with therapeutic potential.

The contributions of generative AI models in drug discovery are particularly striking. Generative Adversarial Networks (GANs) and Variational AutoEncoders (VAEs) have opened avenues for generating novel chemical structures with therapeutic promise [6]. This innovative approach has led to groundbreaking discoveries, such as AI-designed antibiotics like halicin, demonstrating efficacy against drug-resistant bacteria. AI's generative capabilities allow researchers to traverse a broader chemical space, potentially unveiling compounds that might have eluded detection via traditional methods.

Moreover, AI's role in optimizing virtual screening methods for drug discovery is remarkable [12]. Virtual screening, entailing computational evaluations of expansive chemical libraries, has witnessed a significant efficiency boost through AI-driven approaches. Machine learning models predict the binding affinity between compounds and target proteins, enhancing the accuracy and speed of this process. As a result, candidates with higher probabilities of success are prioritized, expediting the identification of potential therapeutic agents.

The amalgamation of AI into drug discovery not only accelerates the identification of potential candidates but also enhances the precision and efficiency of the entire process, offering promising avenues for the discovery of novel drugs and therapeutic solutions (Fig. 1).

AI in Drug Repurposing

AI's burgeoning role in drug repurposing signifies a transformative leap in biomedical innovation, leveraging its prowess to analyze expansive datasets and unveil novel therapeutic uses for existing drugs [13]. By mining a wealth of electronic health records and genetic information, AI algorithms adeptly unravel unforeseen connections between established drugs and fresh therapeutic indications. A compelling example is the rediscovery of thalidomide, originally formulated as a sedative, which found new life as a treatment for multiple myeloma, thanks to AI-driven data analysis.

Moreover, the application of natural language processing (NLP) techniques within AI has been instrumental in driving drug repurposing initiatives [14]. NLP's efficacy lies in its ability to extract invaluable information from scientific literature and clinical records, uncovering concealed relationships and pertinent data buried within the vast expanse of biomedical literature. This enables researchers to efficiently navigate through extensive textual data, extracting crucial insights that inform strategies for drug repurposing.

The fusion of AI and data-driven methodologies presents a promising avenue to expedite the discovery of drug repurposing opportunities [13, 14]. This integrated approach offers a cost-effective and time-efficient means to bring forth new treatment options, propelling them into the forefront of medical research and clinical practice. The synergy between AI's analytical capabilities and data-driven strategies holds immense potential to unlock novel therapeutic avenues, enriching the landscape of available treatments and positively impacting patient care.

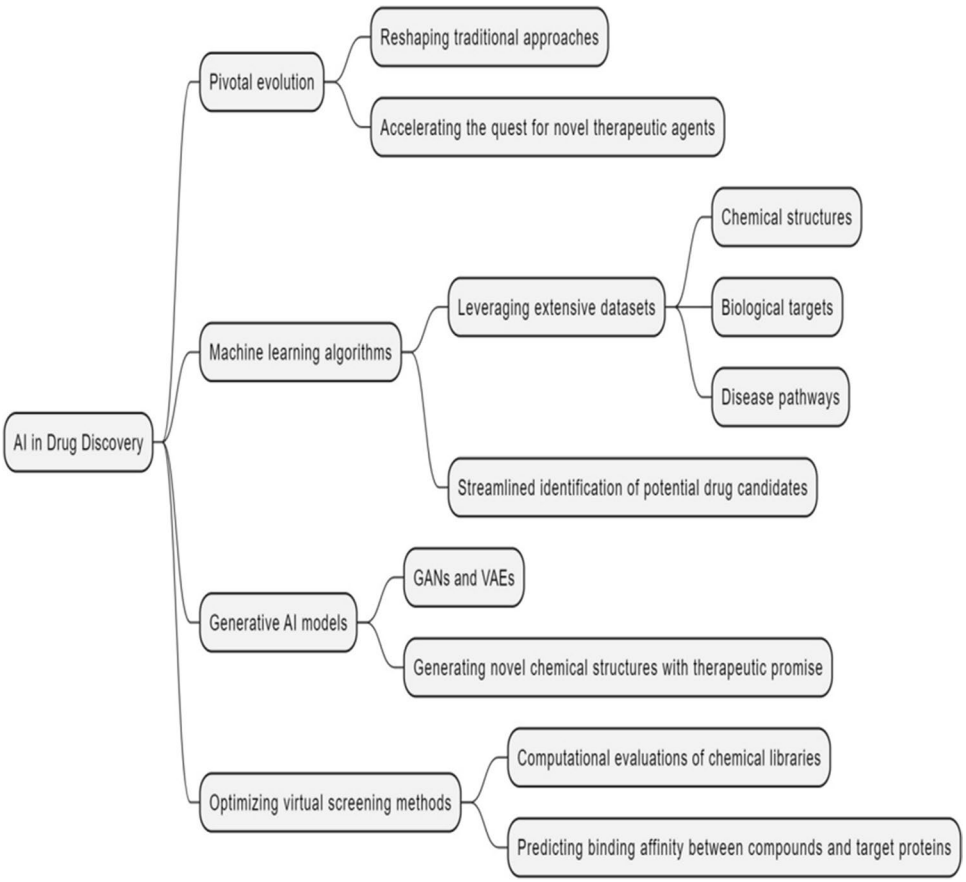

Fig. 1 AI can be integrated into drug discovery and can revolutionize the traditional approaches It can accelerate the quest for novel therapeutic agents. Machine learning algorithms leverage extensive datasets to streamline the identification of potential drug candidates. Generative AI models, such as GANs and VAEs, enable the generation of novel chemical structures with therapeutic promise. Additionally, AI optimizes virtual screening methods by enhancing the accuracy and speed of computational evaluations of chemical libraries. This integration of AI into drug discovery enhances the precision and efficiency of the entire process, offering promising avenues for the discovery of novel drugs and therapeutic solutions

AI in Toxicity Prediction

The realm of drug development hinges on predicting and mitigating potential adverse effects to ensure the creation of safe and effective pharmaceuticals. AI models, especially those rooted in deep learning, have emerged as pivotal tools, showcasing exceptional prowess in foreseeing adverse effects by analyzing both chemical structures and biological data. The Tox21 Challenge stands as a testament to AI's capability, leveraging advanced techniques to forecast toxicity across various assays, a critical step in identifying safe drug candidates [15].

Moreover, AI's applications extend beyond general toxicity prediction; it has been instrumental in addressing organ-specific adverse effects, such as cardiac and hepatic toxicity, which pose significant concerns in drug development [16]. These AI-driven models facilitate the early identification and mitigation of potential safety issues associated with specific organs, contributing substantially to the comprehensive safety assessment of drug candidates. This proactive approach enhances the overall safety profile evaluation, minimizing risks and bolstering confidence in drug development.

AI's predictive capabilities transcend traditional toxicity assessments by encompassing diverse data sources [17]. Machine learning models adeptly incorporate information from gene expression profiles, cellular responses, and clinical data to offer a multifaceted evaluation of a drug's safety profile. This integration of multiple data types augments the accuracy and robustness of toxicity predictions, presenting a valuable asset for pharmaceutical researchers and regulators alike.

The amalgamation of AI techniques not only enhances the accuracy of toxicity assessments but also empowers the pharmaceutical industry to proactively address safety concerns at multiple levels of drug development. By leveraging AI's capacity to analyze diverse datasets and predict potential adverse effects, stakeholders can streamline the drug development process, mitigating risks and ensuring the creation of safer pharmaceuticals for patient well-being.

AI in Personalized Medicine

The advent of personalized medicine signifies a monumental shift in healthcare, centering on tailoring treatment strategies to individual patients based on their unique genetic blueprint, medical history, and lifestyle. The integration of artificial intelligence (AI) into personalized medicine heralds a patient-centric era, facilitating the identification of

personalized treatment options and optimizing healthcare outcomes.

AI-driven methodologies, such as genomic data analysis and predictive modeling, serve as cornerstones in personalized medicine [18]. These techniques harness extensive datasets to unravel intricate associations between genetic variations and disease susceptibility. For example, AI algorithms proficiently predict a patient's response to a particular cancer therapy by scrutinizing their genetic mutations [18]. By identifying genetic markers linked to treatment response or resistance, clinicians gain insights to tailor therapies, enhancing efficacy, and minimizing adverse events.

Furthermore, AI's role extends to identifying patient subgroups more likely to benefit from specific treatments [19]. Analyzing clinical and genetic data empowers AI algorithms to categorize patients into distinct groups exhibiting varied treatment responses. This stratification aids healthcare providers in selecting tailored treatment strategies for each subgroup, optimizing treatment outcomes by aligning therapies with specific patient profiles.

The application of AI in personalized medicine transcends treatment decision-making; it extends to optimizing drug dosages for desired therapeutic effects while mitigating side effects [20]. Real-time analysis of patient data enables AI systems to dynamically adapt treatment regimens based on individual responses, ensuring therapy evolves alongside each patient's unique needs. This adaptive approach maximizes treatment efficacy while minimizing adverse effects, enhancing patient well-being.

The integration of AI into personalized medicine signifies a paradigm shift, propelling healthcare towards individualized, precise, and adaptive treatments. AI's ability to interpret vast datasets and discern nuanced patient characteristics fosters tailored therapies, optimizing treatment outcomes and steering healthcare towards a more patient-centric and effective future.

Recent Breakthroughs and Future Directions

The collaboration between artificial intelligence (AI) and pharmacological research has ignited a profound era of innovation and efficacy, reshaping drug discovery and development. AI-powered drug screening platforms, exemplified by Atomwise© and BenevolentAI©, stand as transformative tools that have remarkably expedited the identification of potential drug candidates [21, 22]. These platforms leverage advanced machine learning algorithms to scrutinize extensive datasets encompassing chemical structures, biological data, and historical drug development information. This empowers researchers to pinpoint promising compounds with heightened probabilities of success, accelerating the drug discovery process.

Furthermore, AI's impact extends to optimizing drug formulations, aiming for improved efficacy and patient compliance [23, 24]. Through predictive modeling and data analytics, AI contributes to refining drug delivery systems, enhancing drug stability, and mitigating side effects. This optimization process augments patient outcomes and fosters more effective pharmaceutical interventions.

Looking toward the future, AI-driven pharmacological research is poised to revolutionize the pharmaceutical industry on various fronts. One promising trajectory involves the development of AI systems adept at comprehending complex biological pathways [25]. These systems offer in-depth insights into disease mechanisms, paving the way for the identification of novel drug targets and the fine-tuning of drug designs with heightened precision.

Moreover, AI is anticipated to play a pivotal role in predicting long-term drug effects, a critical aspect in assessing the safety and efficacy of pharmaceuticals over extended periods [26]. AI-driven predictive modeling enables the anticipation of potential adverse effects, guiding the design of clinical trials and contributing to more informed decision-making throughout the drug development lifecycle.

AI's potential in regulatory compliance is also on the horizon, offering assistance in ensuring adherence to rigorous standards and guidelines in drug development [27]. This involvement streamlines the approval process, reducing both time and costs associated with bringing new drugs to market, expediting access to innovative therapies for patients.

Additionally, AI is positioned to make significant strides in drug manufacturing by optimizing production processes and enhancing quality control [28]. AI-driven process optimization holds the promise of increased efficiency and reduced manufacturing costs, benefiting both the pharmaceutical industry and patients by ensuring higher-quality pharmaceutical products.

The evolving landscape of AI-driven pharmacological research holds tremendous promise, promising breakthroughs that will fundamentally redefine drug development, manufacturing, and regulatory compliance, ultimately revolutionizing patient care and treatment accessibility.

Ethical and Regulatory Considerations

The burgeoning integration of artificial intelligence (AI) in pharmacological research has ignited a profound discourse surrounding ethical and regulatory considerations that demand meticulous attention. These multifaceted considerations encompass critical dimensions, including data privacy, algorithmic bias, transparency, and validation in AI-driven drug development, becoming focal points of extensive discussions within scientific and regulatory communities.

Data privacy emerges as a paramount concern as AI systems necessitate access to sensitive patient information and proprietary data [29]. Balancing the imperative to safeguard patient privacy while enabling data sharing for research remains a significant challenge. Regulatory bodies such as the European Medicines Agency (EMA) and the FDA are actively engaged in formulating guidelines to ensure AI-driven research complies with stringent data privacy regulations, aiming to protect patient confidentiality while facilitating essential research endeavors.

Algorithmic bias stands as another critical issue in AI-driven pharmacological research. AI algorithms, if not carefully developed, can inadvertently perpetuate biases present in training data, potentially leading to disparities in healthcare outcomes [30, 31]. Addressing and mitigating biases in AI models and ensuring fairness in their application have become pivotal goals. Ongoing research explores methods to identify and rectify bias in healthcare AI, striving to ensure equitable healthcare delivery.

Transparency and validation emerge as pivotal pillars for the responsible integration of AI in drug development [32]. Clear documentation of AI algorithms and their decision-making processes is imperative to comprehend their outputs. Regulatory agencies like the FDA emphasize the significance of transparency, interpretability, and validation in AI-driven medical devices. These guidelines underscore the necessity for transparent methodologies to ensure the reliability and accountability of AI applications in drug development.

To tackle these concerns, regulatory agencies are advocating comprehensive frameworks to guide the ethical deployment of AI technologies [32]. For instance, the FDA's Pre-Certification Program aims to assess the quality and safety of software products utilizing AI and machine learning. This initiative seeks to strike a balance between fostering innovation and regulating AI technologies, ensuring adherence to high standards of safety, effectiveness, and ethical considerations.

The evolving landscape of AI integration in pharmacological research demands a delicate balance between harnessing innovation and addressing ethical and regulatory challenges. Stakeholders across scientific, regulatory, and technological domains are actively collaborating to establish robust frameworks that uphold ethical standards, promote transparency, mitigate biases, and safeguard patient privacy, ensuring the responsible and ethical application of AI in advancing drug development.

Conclusion

The infusion of Artificial Intelligence (AI) into pharmacological research represents a monumental shift, heralding a new epoch in drug discovery and development. The far-reaching impact of AI across drug discovery, repurposing, toxicity prediction, and personalized medicine signifies its transformative potential. As AI evolves, it promises to redefine drug development, rendering it more efficient, cost-effective, and tailored to individual patient needs. Yet, to fully harness its potential, collaborative efforts among the scientific community, regulatory bodies, and industry stakeholders are imperative to navigate the ethical and regulatory challenges accompanying this groundbreaking technology.

AI's integration into pharmacological research has sparked a renaissance in drug discovery and development. Its capability to expedite drug candidate identification, tailor treatment plans, and predict toxicities stands poised to revolutionize the pharmaceutical landscape, enhancing efficiency and cost-effectiveness. The evolving field of AI in pharmacology holds tremendous promise in overcoming longstanding challenges entrenched in drug development.

In the realm of drug discovery, AI has become indispensable. Its prowess in analyzing vast datasets, generating novel chemical structures, and refining virtual screening processes accelerates the identification of potential therapeutic agents, offering solutions to pivotal hurdles in drug development.

AI's emergence as a pivotal tool in toxicity prediction is monumental, promising substantial enhancements in safety assessment for drug candidates. By mitigating costly setbacks associated with drug development, AI significantly contributes to minimizing risks and improving drug safety profiles.

The revolutionizing impact of AI on personalized medicine signifies a paradigm shift. Its capacity to identify patient-specific treatment options, optimize dosages, and minimize adverse effects propels healthcare toward greater effectiveness and patient-centeredness.

The ongoing synergy between AI and pharmacological research holds the promise of continued breakthroughs spanning drug discovery, formulation, regulatory compliance, and drug manufacturing. These advancements bear the potential to transform the pharmaceutical landscape, driving efficiency, cost-effectiveness, and patient-centered care.

However, as AI continues to reshape pharmacological research, navigating the ethical and regulatory terrain remains critical. Balancing the utilization of AI's potential for drug discovery with the imperative of responsible, ethical, and legally compliant practices is pivotal. This balance ensures healthcare advancement while safeguarding patient rights and safety in an evolving landscape. Collaborative efforts are essential to harness the transformative potential of AI while ensuring its ethical and responsible application in shaping the future of pharmacological research and healthcare.

Acknowledgements The author would like to thank all staff members of Department of Pharmacy, Vishwakarma University for their support and constructive criticism in the preparation of manuscript.

Author contributions N.B planned the study and wrote the main manuscript M.U.K and S. A. performed the Literature review and analysis

Declarations

Informed consent As the present manuscript is a review article, no informed consent is required or applicable.

Disclosure The Authors declare that they have no conflict of research with any person or organization.

Research involving Human Participants and/or Animals This article does not contain any studies with human or animal subjects performed by any of the authors.

References

1. Dahlin JL, Inglese J, Walters MA. Mitigating Risk in Academic Preclinical Drug Discovery. Nat Rev Drug Discovery. 2015;14(4):279–94. https://doi.org/10.1038/nrd4609.
2. Scannell JW, Blanckley A, Boldon H, Warrington B. Diagnosing the Decline in Pharmaceutical R&D Efficiency. Nat Rev Drug Discovery. 2012;11(3):191–200. https://doi.org/10.1038/nrd3681.
3. Aliper A, Plis S, Artemov A, Ulloa A, Mamoshina P, Zhavoronkov A. Deep Learning Applications for Predicting Pharmacological Properties of Drugs and Drug Repurposing Using Transcriptomic Data. Mol Pharmaceutics. 2016;13(7):2524–30. https://doi.org/10.1021/acs.molpharmaceut.6b00248.
4. Gawehn E, Hiss JA, Schneider G. Deep Learning in Drug Discovery. Mol Informatics. 2016;35(1):3–14. https://doi.org/10.1002/minf.201501008.
5. Schneider P, Walters WP, Plowright AT. Rapid Hit to Lead: Medicinal Chemistry Strategies for the Discovery of Small-Molecule Lead Compounds. Cell Chem Biol. 2018;25(1):66–79. https://doi.org/10.1016/j.chembiol.2017.11.012.
6. Stokes JM, Yang K, Swanson K, Jin W, Cubillos-Ruiz A, Donghia NM, Collins JJ. A Deep Learning Approach to Antibiotic Discovery. Cell. 2020;180(4):688–702. https://doi.org/10.1016/j.cell.2020.01.021.
7. Gottlieb A, Stein GY, Ruppin E, Sharan R. PREDICT: A Method for Inferring Novel Drug Indications with Application to Personalized Medicine. Mol Syst Biol. 2018;14(6):e7910. https://doi.org/10.15252/msb.20177910.
8. Miotto R, Li L, Kidd BA, Dudley JT. Deep Patient: An Unsupervised Representation to Predict the Future of Patients from the Electronic Health Records. Sci Rep. 2018;6(1):1–10. https://doi.org/10.1038/s41598-018-21058-z.
9. Harel S, Radin A, Pachter L. Model-Based Transcriptome-Wide Analysis of Neural Substrates for Pharmacological Properties of Drugs. Nat Commun. 2021;12:3759. https://doi.org/10.1038/s41467-021-23913-4.
10. Judson R, Richard A, Dix DJ, et al. ACToR—Aggregated Computational Toxicology Resource. Toxicol Appl Pharmacol. 2015;233(1):7–13. https://doi.org/10.1016/j.taap.2007.02.001.
11. Merkle D. DeepChem: A Genome-Scale Chemoinformatics Library. J Chem Inf Model. 2018;58(2):609–15. https://doi.org/10.1021/acs.jcim.7b00677.
12. Goh GB, Hodas NO, Vishnu A. Deep Learning for Computational Chemistry. J Comput Chem. 2017;38(16):1291–307. https://doi.org/10.1002/jcc.24764.
13. Hipp J, Smith S, Bauer-Mehren A, et al. Curated Crowdsourced Information for Enhancing Pharmacovigilance and Adverse Drug Event Detection. J Biomed Inform. 2019;93:103139. https://doi.org/10.1016/j.jbi.2019.103139.
14. Hao J, Peng S, Zou B. Integrating Artificial Intelligence into Medical Informatics and Pharmacoinformatics. Comput Struct Biotechnol J. 2019;17:664–75. https://doi.org/10.1016/j.csbj.2019.05.008.
15. Huang R, Xia M, Sakamuru S. Modelling the Tox21 10 K Chemical Profiles for In Vivo Toxicity Prediction and Mechanism Characterization. Nat Commun. 2016;7:10425. https://doi.org/10.1038/ncomms10425.
16. Begoli E, Williams M, Drown R. AI Applications in Drug Development and Toxicology. Drug Discovery Today. 2020;25(9):1636–43. https://doi.org/10.1016/j.drudis.2020.06.012.
17. Rodgers AD, Zhu H, Fourches D, Rusyn I. Computational Approaches in Cheminformatics, Toxicoinformatics, and Bioinformatics for Chemical Toxicity Prediction. In Computational Toxicology: Humana Press; 2017. p. 221–72.
18. Cheng F, Desai RJ, Handy DE, Wang R, Schneeweiss S, Barabási AL. Network-Based Approach to Prediction and Population-Based Validation of In Silico Drug Repurposing. Nat Commun. 2018;9(1):1–11. https://doi.org/10.1038/s41467-018-05090-2.
19. Shah ND, Montori VM, Krumholz HM, Tu K, Alexander GC, Jackevicius CA, Ross JS. Responding to an FDA Warning—Geospatial Analysis of Rosiglitazone Prescriptions. N Engl J Med. 2019;363(21):2081–4. https://doi.org/10.1056/NEJMc0900445.
20. Hengartner MP, Kos M. Artificial Intelligence for Personalized Antidepressant Treatment: Let's Get the Basics Right. Mol Psychiatry. 2019;24(3):369–70. https://doi.org/10.1038/s41380-018-0343-9.
21. Wallach I, Dzamba M, Heifets, A. AtomNet: A deep convolutional neural network for bioactivity prediction in structure-based drug discovery. ArXiv,abs/1510.02855 2015.
22. Swanson DR. Artificial Intelligence and Data Mining: New Paradigms for Drug Discovery. Drug Dev Res. 2018;79(7):291–4. https://doi.org/10.1002/ddr.21435.
23. Langer R. Drug Delivery and Targeting. Nature. 2019;523(7560):316–21. https://doi.org/10.1038/nature14588.
24. Madabushi R, Wang Y. Discovering In Vitro and In Vivo Parameters for Drug Development with Artificial Intelligence: A Primer. Clin Pharmacol Ther. 2019;106(2):186–91. https://doi.org/10.1002/cpt.1495.
25. Schwaller P, Probst D, Vaucher AC, Laino T. Neural-Network-Based Predictions of Organic Reactions: Synthetic Feasibility, Retrosynthesis, and Reaction Optimization. Chem Rev. 2020;120(18):11070–128. https://doi.org/10.1021/acs.chemrev.9b00715.
26. Chen X, Liu M, Zhang J. Computational Models for Predicting Drug-Drug Interactions. Curr Pharm Des. 2019;25(42):4451–61. https://doi.org/10.2174/1381612825666191220164219.
27. Rupp M. Computational Chemistry for the Design of Efficient Organic Photovoltaics. Annu Rev Phys Chem. 2019;70:261–83. https://doi.org/10.1146/annurev-physchem-042018-052749.
28. Gopalakrishnan K, Mistry M, Sarma AV, Suresh P. Digital Twin of Pharmaceutical Continuous Manufacturing—a Review. Curr Opin Chem Eng. 2020;28:81–9. https://doi.org/10.1016/j.coche.2020.07.010.
29. European Medicines Agency. European Medicines Agency Roadmap to 2025. 2021. https://www.ema.europa.eu/en/documents/regulatory-procedural-guideline/roadmap-2025-achie

ving-ema-vision-2025-european-medicines-agency_en.pdf. Accessed 15 Oct 2023.
30. Obermeyer Z, Powers B, Vogeli C, Mullainathan S. Dissecting Racial Bias in an Algorithm Used to Manage the Health of Populations. Science. 2019;366(6464):447–53. https://doi.org/10.1126/science.aax2342.
31. Zou J, Schiebinger L, Bhattacharya S, et al. AI in Health: State of the Art, Challenges, and Future Directions. Yearb Med Inform. 2019;28(1):16–26. https://doi.org/10.1055/s-0039-1677913.
32. FDA. Proposed Regulatory Framework for Modifications to Artificial Intelligence/Machine Learning (AI/ML)-Based Software as a Medical Device (SaMD). 2019. https://www.fda.gov/media/122535/download. Assessed 15 October 2023.