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Research Article

Employing Artificial Intelligence Methods in Drug Development: A New Era in Medicine

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ABSTRACT

Artificial intelligence (AI) plays a vital role in the development of pharmaceuticals. The whole drug development process, from target identification and lead optimization to clinical trials and post-marketing monitoring, has the potential to be revolutionized by AI. Data analysis is a crucial area where AI thrives. To find trends, correlations, and prospective targets for therapeutic intervention, AI systems can analyse enormous volumes of data, including electronic health records, molecular databases, academic literature, and clinical trial data. This saves time and resources by enabling researchers to decide which compounds or pathways to investigate. Lead optimization is another area where AI is essential since algorithms can screen and forecast the efficacy of new drug candidates. To improve efficacy, safety, and pharmacokinetics, the most promising leads are prioritized, and their attributes are optimized. By examining past data to pinpoint patient groupings that are most likely to respond to a certain medication, AI can also improve clinical trial design and patient selection. This advances success rates aids in the development of personalized medication and can support post-marketing surveillance by continuously scanning real-world data for adverse events or unexpected drug-drug interactions after a medicine has been licensed. This permits the quicker detection of potential safety issues and contributes to maintaining the continuous safety of licensed medications. However, some obstacles must be overcome to completely utilize AI in medication development. These include the requirement for high-quality data, assuring AI model transparency and interpretability, taking into account ethical issues, and regulatory frameworks for using AI in drug development.

1. INTRODUCTION

Drug development has been significantly impacted by artificial intelligence, which has completely changed how we find and create new medication [1]. Drug development using conventional procedures is frequently labour-intensive, expensive, and ineffective [2]. Nevertheless, AI provides a variety of tools and methodologies that help accelerate several phases of the drug discovery process, resulting in more effective and precise medicines. Early drug development is one area where AI has made important advances [3]. To find prospective medication candidates, researchers can examine enormous amounts of biological and chemical data using machine learning algorithms. Large databases may be quickly combed through by AI, which can also forecast the efficacy and toxicity of compounds and find those with the necessary attributes. Additionally, AI methods can help to streamline the clinical trial procedure [4]. AI algorithms can identify suitable patients for certain studies by examining patient data and medical records, which improves recruitment and cuts down on the time and expense needed to find qualified participants [5]. By locating pertinent biomarkers and segmenting patient populations, AI can also aid in the design of more effective trials. Additionally, AI has shown its value in forecasting the efficacy of treatment candidates. AI systems can forecast the safety and efficacy of novel substances by creating models based on existing medication trials, raising any potential issues before to the start of expensive trials [6]. This increases the likelihood of success by enabling researchers to concentrate their efforts on the most promising therapeutic candidates. Finding new uses for currently available medications is known as drug repurposing, and it is a crucial use of AI in the pharmaceutical industry. Large datasets can be analysed using AI algorithms to find possible medication interactions and therapeutic uses that conventional research

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approaches would have missed [7]. By utilizing already-approved and secure medications, this strategy conserves time and resources.

2. DRUG DISCOVERY AND IDENTIFICATION

Due to its capacity to expedite the identification and development of new medications, artificial intelligence (AI) has grown in significance in the field of drug discovery. Numerous compounds must be tested in the lab using traditional drug screening techniques, which can be time- and resource-consuming [8]. By analysing huge databases of chemical compounds and making predictions about their properties and probable biological functions, AI can help in virtual screening. This helps save time and resources by helping researchers prioritize and concentrate on the most promising options. To find prospective therapeutic targets, AI systems can examine biological data from the genomes, proteomics, and transcriptomics fields [9]. AI can reveal unique insights into the molecular causes of diseases and help identify previously undiscovered or understudied targets by integrating and analysing huge databases. Researchers can comprehend the possible efficacy and safety profiles of proposed medications by using AI-based models that predict the interactions between drug molecules and target proteins. AI can assist in prioritizing medication candidates with a higher likelihood of success and fewer negative effects by predicting the binding affinity and off-target effects, hence minimizing the need for lengthy experimental testing [10]. AI algorithms can create and test a large number of in silico analogues to optimize the attributes of lead compounds. The potency, selectivity, and pharmacokinetic features of drug candidates can be improved through this iterative approach, increasing the likelihood that they will be successful. Artificial intelligence (AI) models can evaluate the toxicity of medication candidates and forecast any potential negative effects on organs or biological systems [11]. This can minimize safety problems and cut costs by removing compounds with significant toxicity risks early in the development process.

3. DRUG DESIGN DEVELOPMENT

Discovering and improving drug candidates for the treatment of diseases is the goal of the intricate and iterative process known as drug design and development. In this process, artificial intelligence has proven to be a useful tool by providing a variety of ways and procedures to help in medication development [13]. To find prospective therapeutic targets, AI systems can examine biological data from the genomes, proteomics, and metabolomics fields. AI can help in finding particular proteins, receptors, or enzymes that are crucial in the disease process by understanding the underlying biological mechanisms of diseases [14]. Researchers can analyse enormous databases of chemical compounds virtually to find possible therapeutic candidates. In order to prioritize and choose the most promising candidates for additional research, scientists can use AI to forecast the characteristics, interactions, and probable usefulness of these substances. The characteristics of these substances can be improved with the use of AI approaches. Structure-activity relationship (SAR) analysis, which predicts how changing a compound's chemical structure will influence its activity and binding to a target, is a task that AI algorithms are capable of performing [15]. Researchers can fine-tune and enhance the drug candidate's potency, selectivity, and pharmacokinetic features thanks to this iterative procedure. The potential toxicity of drug candidates can also be predicted with the aid of AI algorithms. AI algorithms can determine the possibility of harmful effects on organs or biological systems by examining past toxicity data and chemical structure information [16]. This aids researchers in early-stage chemical identification and elimination of compounds with possible safety concerns. By examining patient information, medical records, and other pertinent data sources, AI can assist in improving clinical studies. To improve enrollment and raise the likelihood of a good outcome, AI algorithms can assist in identifying the right patient demographics for certain studies [17]. AI can help the design of trials more effectively by locating pertinent biomarkers and categorizing patient populations. Figure 1 illustrates the drug design development process.

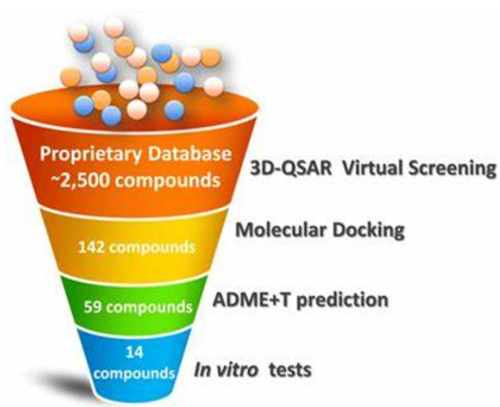

Fig. 1. The procedure for creating medication designs [12].

4. VIRTUAL TESTS USING AI

Artificial intelligence in combination with virtual human organs has several advantages. First, compared to conventional procedures that rely on animal or human studies, it enables more cost- and time-effective testing. Researchers can acquire additional information and insights by running virtual experiments in a controlled setting that is simple to repeat. Additionally, virtual testing can assist in lessening the risk to human participants and ethical issues related to animal research. Integrating unique patient data to build particular virtual organ models can also offer insights into personalized medicine, enabling more precise and focused predictions of drug reactions [19]. Overall, using artificial intelligence (AI) in conjunction with virtual human organs is a promising method for developing drugs and providing individualized care, potentially increasing the effectiveness and safety of medical research. Online tests of artificial intelligence (AI)--based virtual human organs are a developing area of medical research. In this method, computer-generated models of human organs are created, and artificial intelligence (AI) algorithms are used to simulate how the organs behave and react to various stimuli and treatments [18].

5. THE MOST USEFUL TREATMENT UTILISING AI

Healthcare professionals may now tailor patient care based on unique patient features, choose the best course of therapy, and enhance patient outcomes thanks to AI. It's crucial to remember that while AI can offer insightful information, treatment choices should always be decided in consultation with medical specialists who can take other considerations and clinical knowledge into account [20]. To find patterns and correlations, AI systems can analyse enormous volumes of patient data, including medical records, genetic data, and treatment outcomes. AI can find the treatments that have worked best for patients with comparable traits and illnesses by processing this data [21]. Utilising genetic variants, lifestyle factors, and medical history, AI can assist in customizing treatment approaches for specific patients. AI algorithms can provide personalized treatments that are more likely to be successful for each patient by taking these aspects into account. By analysing patient data and making treatment recommendations, AI can enhance healthcare providers' decisions in real time. AI systems, for instance, can evaluate a patient's symptoms, medical history, and laboratory findings to recommend the best possible treatments. Clinical trial planning and execution may benefit from AI assistance. AI algorithms can find trial candidates that are a good fit, improve trial protocols, and examine trial outcomes to find therapies that work by analysing patient data [22].

6. AI KEEPS AN EYE ON POSSIBLE ADVERSE EFFECTS OF MEDICATIONS

Artificial intelligence (AI) is essential for tracking and identifying potential side effects of drugs. Researchers and healthcare practitioners can identify negative drug effects, create prediction models, and enhance patient safety outcomes by utilizing AI algorithms and data analysis. An important area where AI might help in monitoring bad medication effects is pharmacovigilance, which focuses on identifying and preventing harmful drug effects [23]. AI systems can detect potential dangers and adverse effects related to pharmaceuticals by analysing massive volumes of data, including electronic health records and clinical trial data.AI can help in anticipating the negative effects of medicine combinations as well [24-26]. When recommending various treatments to patients, these projections assist medical practitioners in making educated decisions about potential dangers. Additionally, AI has the potential to provide light on problematic drug interactions, especially when patients combine prescription and OTC drugs. Furthermore, the integration of AI with real-time monitoring systems permits ongoing patient data monitoring, enabling quick recognition of harmful effects and adverse events [27-30]. This capacity aids healthcare professionals in early intervention and treatment plan optimization to reduce harm.

7. CONCLUSIONS

Artificial intelligence plays a critical role in drug development, helping to increase decision-making processes' effectiveness, accuracy, and efficiency. Numerous facets of the pharmaceutical industry, including target identification and predictive modeling, have the potential to change, resulting in more efficient and individualized therapies. Drug development could be revolutionized by artificial intelligence (AI), which offers greater effectiveness, precision, and speed. The pharmaceutical sector has undergone radical upheaval thanks to the use of AI technology. AI integration in drug discovery and development has sped up research and improved decision-making techniques. Large data sets, including those from clinical trial data and electronic health records, can be analyzed using AI to find patterns and correlations that can be used to develop new drug targets and improve predictive modeling. It has shown promise in drug efficacy prediction, lead compound optimization, and the facilitation of adverse effects and drug interaction discovery. Despite its potential advantages, the effective use of AI in drug development depends on the accessibility of high-quality data, the resolution of ethical dilemmas, and awareness of the limitations of AI-based methods. To ensure the responsible and ethical use of AI in drug research, other difficulties must be addressed, such as data privacy and the interpretability of AI models.

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Conflicts Of Interest

The author's disclosure statement confirms the absence of any conflicts of interest.

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References

[1] F. Urbina, F. Lentzos, C. Invernizzi, and S. Ekins, "Dual use of artificial-intelligence-powered drug discovery," *Nature Machine Intelligence*, vol.4, pp.189–191, March 2022. https://doi.org/10.1038/s42256-022-00465-9

[2] A. Altharawi, M. A. Alossaimi, M. M. Alanazi, S. M. Alqahatani, and M. T. u. Qamar, "An integrated computational approach towards novel drugs discovery against polyketide synthase 13 thioesterase domain of Mycobacterium tuberculosis," *Scientific Reports*, vol.13, no.7014, pp.1-12, April 2023. https://doi.org/10.1038/s41598-023-34222-8

[3] M. Pandey, M. Fernandez, F. Gentile, O. Isayev, A. Tropsha, A. C. Stern, and A. Cherkasov, "The transformational role of GPU computing and deep learning in drug discovery," *Nature Machine Intelligence*, vol.4, pp.211–221, March 2022. https://doi.org/10.1038/s42256-022-00463-x

[4] D. Shao, Y. Dai, N. Li, X. Cao, W. Zhao, L. Cheng, et al., "Artificial intelligence in clinical research of cancers," *Briefings in Bioinformatics*, vol.22, no.1, pp.1-12, December 2021. https://doi.org/10.1093/bib/bbab523

[5] P. A. Noseworthy, Z. I. Attia, E. M. Behnken, R. E. Giblon, K. A. Bews, et al., "Artificial intelligence-guided screening for atrial fibrillation using electrocardiogram during sinus rhythm: a prospective non-randomised interventional trial," *The Lancet*, vol.400, no.10359, pp.1206-1212, October 2022. https://doi.org/10.1016/S0140-6736(22)01637-3

[6] A. Kate, E. Seth, A. Singh, C. M. Chakole, M. K. Chauhan, et al., "Artificial Intelligence for Computer-Aided Drug Discovery," *Drug Research*, vol.73, no.70, pp.369-377, 2023. https://doi.org/10.1055/a-2076-3359

[7] F. Y. Al-Ashwal, M. Zawiah, L. Gharaibeh, R. Abu-Farha, and A. N. Bitar, "Evaluating the Sensitivity, Specificity, and Accuracy of ChatGPT-3.5, ChatGPT-4, Bing AI, and Bard Against Conventional Drug-Drug Interactions Clinical Tools," *Drug, Healthcare and Patient Safety*, vol.15, no.2023, pp.137-147, September 2023. https://doi.org/10.2147/DHPS.S425858

[8] M. Nascimben and L. Rimondini, "Molecular Toxicity Virtual Screening Applying a Quantized Computational SNN-Based Framework," *Molecules*, vol.28, no.3, pp.1-19, January 2023. https://doi.org/10.3390/molecules28031342

[9] X. He, X. Liu, F. Zuo, H. Shi, and J. Jing, "Artificial intelligence-based multi-omics analysis fuels cancer precision medicine," *Seminars in Cancer Biology*, vol.88, pp.187-200, January 2023. https://doi.org/10.1016/j.semcancer.2022.12.009

[10] S. Silva-Mendonça, A. R. S. Vitória, T. W. Lima, A. R. Galvão-Filho, and C. H. Andrade, "Exploring new horizons: Empowering computer-assisted drug design with few-shot learning," *Artificial Intelligence in the Life Sciences*, vol.4, pp.100086, December 2023. https://doi.org/10.1016/j.ailsci.2023.100086

[11] S. Yang and S. Kar, "Application of artificial intelligence and machine learning in early detection of adverse drug reactions (ADRs) and drug-induced toxicity," *Artificial Intelligence Chemistry*, vol.1, no.2, pp.100011, December 2023. https://doi.org/10.1016/j.aichem.2023.100011

[12] K. E. Khatabi, I. Aanouz, R. El-Mernissi, M. A. Ajana, T. Lakhlifi, and M. Bouachrine, "Computational modeling of acetylcholinesterase inhibitors in Alzheimer's disease," *PhytoChem & BioSub Journal*, vol.15, no.1, pp.118-128.

[13] S. Singh, D. K. Sarma, V. Verma, R. Nagpal, and M. Kumar, "Unveiling the future of metabolic medicine: omics technologies driving personalized solutions for precision treatment of metabolic disorders," *Biochemical and Biophysical Research Communications*, vol.682, pp.1-20, November 2023. https://doi.org/10.1016/j.bbrc.2023.09.064

[14] A. Joshi, S. Dubey, and P. Kumar, "Neurobioinformatics: A Novel Way For Exploring And Developing Brain Cancer Therapies," *Journal of Pharmaceutical Negative Results*, vol.13, no.9, pp.8291-8295, December 2022. https://doi.org/10.47750/pnr.2022.13.S09.973

[15] S. K. Niazi and Z. Mariam, "Recent Advances in Machine-Learning-Based Chemoinformatics: A Comprehensive Review," *International Journal of Molecular Sciences*, vol.24, no.14, pp.1-15, July 2023. https://doi.org/10.3390/ijms241411488

[16] S. Nair, "Revolutionizing Medicine: How AI Is Powering The Future Of Pharmaceutical Inventions," *Journal of Pharmaceutical Negative Results*, vol.13, no.10, pp.3811-3814, December 2022. https://doi.org/10.47750/pnr.2022.13.S10.462

[17] S. Askin, D. Burkhalter, G. Calado, and S. Dakrouni, "Artificial Intelligence Applied to clinical trials: opportunities and challenges," *Health and Technology*, vol.13, pp.203–213, February 2023. https://doi.org/10.1007/s12553-023-00738-2

[18] H. Werner, G. Tonni, and J. Lopes, "3D Physical and Virtual Models in Fetal Medicine: Applications and Procedures," *Springer Nature*, 2023.

[19] M. Cellina, M. Cè, M. Alì, G. Irmici, S. Ibba, et al., "Digital Twins: The New Frontier for Personalized Medicine?," *Applied Sciences*, vol.13, no.13, pp.1-16, July 2023. https://doi.org/10.3390/app13137940

[20] D. Gala and A. N. Makaryus, "The Utility of Language Models in Cardiology: A Narrative Review of the Benefits and Concerns of ChatGPT-4," *International Journal of Environmental Research and Public Health,* vol.20, no.15, pp.1-14, July 2023. https://doi.org/10.3390/ijerph20156438

[21] R. Sawhney, A. Malik, S. Sharma, and V. Narayan, "A comparative assessment of artificial intelligence models used for early prediction and evaluation of chronic kidney disease," *Decision Analytics Journal*, vol.6, pp.100169, March 2023. https://doi.org/10.1016/j.dajour.2023.100169

[22] T. Doherty, Z. Yao, A. A. l. Khleifat, H. Tantiangco, S. Tamburin, et al., "Artificial intelligence for dementia drug discovery and trials optimization," *Alzheimer's & Dementia*, pp.1-12, July 2023. https://doi.org/10.1002/alz.13428

[23] V. Kumar, S. K. Bharti, D. Shukla, A. Suryavanshi, K. K. Jangde, et al., "Pharmacovigilance in Digital Era: Real-World Data and Safety Monitoring," *Chhattisgarh Journal of Science and Technology*, vol.19, no.2, pp.-319-334, 2022.

[24] T. N. K. Hung, N. Q. K. Le, N. H. Le, L. V. Tuan, T. P. Nguyen, et al., "An AI-based Prediction Model for Drug-drug Interactions in Osteoporosis and Paget's Diseases from SMILES," *Molecular Informatics*, vol.41, no.6, pp.2100264, June 2022. https://doi.org/10.1002/minf.202100264

[25] G. Ali, M. M. Eid, O. G. Ahmed, M. Abotaleb, A. M. Z. Alaabdin, and B. A. Buruga, "Artificial intelligence in Corneal Topography: A Short Article in Enhancing Eye Care," *Mesopotamian Journal of Artificial Intelligence in Healthcare*, vol.2023, pp.31-34, June 2023. https://doi.org/10.58496/MJAIH/2023/006

[26] R. Doshi, K. K. Hiran, M. Gök, E. M. El-kenawy, A. Badr, and M. Abotaleb, "Artificial Intelligence's Significance in Diseases with Malignant Tumours," *Mesopotamian Journal of Artificial Intelligence in Healthcare*, vol.35, pp.35-39, July 2023. https://doi.org/10.58496/MJAIH/2023/007

[27] K. Guo, H. Tao, Y. Zhu, B. Li, C. Fang, et al., "Current applications of artificial intelligence-based computer vision in laparoscopic surgery," *Laparoscopic, Endoscopic and Robotic Surgery*, vol.6, no.3, pp.91-96, September 2023. https://doi.org/10.1016/j.lers.2023.07.001

[28] M. M. Mijwil, AH. Al-Mistarehi, M. Abotaleb, E. M. El-kenawy, A. Ibrahim, A. A. Abdelhamid, and M. E. Eid, "From Pixels to Diagnoses: Deep Learning's Impact on Medical Image Processing-A Survey," *Wasit Journal of Computer and Mathematics Science*, vol.2, no.2, pp.8-14, September 2023. https://doi.org/10.31185/wjcms.178

[29] N. L. Bragazzi, H. Dai, G. Damiani, M. Behzadifar, M. Martini, and J. Wu, "How Big Data and Artificial Intelligence Can Help Better Manage the COVID-19 Pandemic," *International Journal of Environmental Research and Public Health*, vol.17, no.9, pp.3176, May 2020. https://doi.org/10.3390/ijerph17093176

[30] B. S. Shukur and M. M. Mijwil, "Involving Machine learning as Resolutions of Heart Diseases," *International Journal of Electrical and Computer Engineering*, vol.13, no.2, pp.2177-2185, April 2023. http://doi.org/10.11591/ijece.v13i2.pp2177-2185