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Artificial Intelligence in Drug Repurposing: A Short Impact Assessment

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Abstract

Artificial intelligence (AI) in pharmaceutical repurposing has become a game-changing tool that opens new avenues for the application of new drugs that have already been approved. Traditional drug discovery is a lengthy and expensive process, whereas AI can rapidly analyze vast datasets of biological, chemical, and clinical information to predict drug-disease interactions. AI-driven techniques, such as machine learning, natural language processing, and deep learning, enable the identification of potential repurposing candidates by analyzing molecular structures, gene expression profiles, and patient data. Recent success stories include AI models identifying drugs like Baricitinib for COVID-19 and different substances for uncommon illnesses, like Fragile X syndrome. AI's capacity to streamline the process of discovering drugs speeds up therapy development, cuts costs, and improves the accuracy of matching drugs to diseases, proving to be a valuable tool in combating various illnesses. Nonetheless, issues like data quality, AI model interpretability, and the requirement for clinical validation continue to be crucial areas for additional study.

Keywords: Artificial intelligence (AI), COVID-19, fragile X syndrome, Baricitinib, AI-driven techniques

INTRODUCTION

Artificial Intelligence (AI)

Artificial Intelligence (AI) has greatly helped in drug repurposing, which involves discovering new medical uses for already existing medications. The usual process of discovering drugs is lengthy and expensive, typically lasting more than 10 years and costing billions of dollars to introduce a new drug to the market [1–3]. AI, through advanced computational methods, helps expedite this process in the following ways:

- *Data Analysis and Integration:* AI can analyze vast amounts of biomedical data, including genomic, proteomic, and clinical data, to identify potential new uses for approved drugs. Machine learning algorithms sift through these datasets to identify patterns and correlations that humans may not notice, enabling researchers to prioritize drugs that show promise for repurposing [4, 5].
- *Predictive Modeling:* AI uses machine learning models to predict how existing drugs might interact with different biological targets. By training on known drug-target interactions, these models can forecast potential new targets for existing drugs, helping researchers to focus on compounds that are most likely to work for a different condition [6–9].

NATURAL LANGUAGE PROCESSING (NLP)

AI-driven NLP techniques can scan scientific literature and patents to extract valuable information on how drugs interact with biological systems. This speeds up the identification of

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candidate drugs that have shown off-target effects or potential new mechanisms of action that could be leveraged for repurposing [10].

ACCELERATING CLINICAL TRIALS

AI is also used in optimizing clinical trial design for drug repurposing. AI can help select appropriate patient populations, predict trial outcomes, and reduce the duration of trials by better targeting the drugs' effects on specific conditions, thus lowering the costs and improving the chances of success [9, 10].

AI-DRIVEN DRUG REPURPOSING PLATFORMS

Numerous AI-powered platforms have surfaced, transforming the drug repurposing arena by employing sophisticated algorithms to discover fresh potential applications for current drugs. BenevolentAI, Insilico Medicine, and Recursion Pharmaceuticals are some of the platforms that use advanced AI technologies to search through large databases of chemical compounds and select them for further testing in various medical fields. These platforms expedite the process of discovering new drug applications by analyzing intricate biological data, gene expression patterns, and chemical interactions. AI-based systems can greatly decrease research time and costs by simplifying the drug repurposing process, resulting in quicker development of innovative treatments [11–13].

REAL-WORLD APPLICATIONS

AI technology has already been successful in repurposing drugs in practical situations. During the COVID-19 pandemic, AI was used to quickly screen existing drugs for their potential to treat the virus. For example, AI identified Remdesivir, originally developed for Ebola, as a potential treatment for COVID-19, which later received emergency approval [14].

CHALLENGES AND LIMITATIONS

- *Data quality:* AI's effectiveness in drug repurposing depends on the availability of high-quality, structured biomedical data. Inaccurate predictions may result from insufficient or low-quality data.
- *Regulatory hurdles:* Even though AI can identify promising drug candidates, regulatory approval processes still involve significant time and human oversight.
- *Biological complexity:* Understanding some diseases and drug interactions is not always simple due to the complexity of biological systems and data analysis [15–17].

These instances demonstrate how AI is increasingly impacting the simplification of drug repurposing processes, cutting down on the time and expenses linked with conventional drug discovery methods.

Drug repurposing, discovering new therapeutic purposes for current drugs, has received notable focus lately, with AI being a crucial factor. Here are a few notable recent examples of AI-driven drug repurposing studies [18–20].

BENEVOLENTAI & BARICITINIB FOR COVID-19

One of the most well-known examples is BenevolentAI, which used AI to identify Baricitinib as a potential treatment for COVID-19. Originally an anti-inflammatory drug for rheumatoid arthritis, Baricitinib was identified through AI algorithms that analyzed drug-disease interactions. The medication was discovered to block the processes the SARS-CoV-2 virus uses to invade lung cells. This research led to clinical trials and FDA emergency use authorization for treating COVID-19 patients [21].

HEALX'S USE OF AI FOR RARE DISEASES

Healx is another company leveraging AI to repurpose drugs for rare diseases. They combine AI with drug discovery expertise to predict drug efficacy for multiple conditions. Repurposing an existing medication for the genetic condition Fragile X syndrome is one example of a success story. Healx's AI system processes vast amounts of biomedical data to identify potential drug candidates [22].

INSILICO MEDICINE – ALS AND IDIOPATHIC PULMONARY FIBROSIS (IPF)

Insilico Medicine uses AI to explore drugs for various diseases, including neurodegenerative conditions. In a study, they employed AI to identify existing drugs that could be repurposed for Amyotrophic Lateral Sclerosis (ALS) and Idiopathic Pulmonary Fibrosis (IPF). Their AI platform analyzed molecular data and suggested compounds that could target the diseases' specific biological pathways [20–22].

ATOMWISE FOR EBOLA

Atomwise, known for its AI-driven drug discovery, identified existing FDA-approved drugs that could be repurposed to treat Ebola. Their AI model, which employs deep learning, scanned through millions of compounds to identify those with potential antiviral activity against the Ebola virus. This AI-driven approach has shortened the drug identification process significantly compared to traditional methods [23, 24].

AI4COVID-19 Initiative

AI4COVID-19 is a collaborative effort involving multiple institutions that aims to utilize AI to aid in the repurposing of drugs to combat COVID-19. The project's goal is to discover current medications that may reduce the virus's effects through sophisticated AI algorithms. These AI models examine large quantities of biological, chemical, and clinical data to identify compounds with potential for therapy. Certain medications discovered using this method, like Remdesivir and Dexamethasone, have proven to be successful in treating patients with COVID-19. At the same time, AI has pinpointed additional compounds with potential, and they are now being tested in clinical trials for effectiveness and safety [25–28].

CONCLUSIONS

AI has the potential to revolutionize drug repurpose by dramatically speeding up the process, reducing costs, and identifying novel treatments for diseases, including rare and complex conditions. Yet, obstacles like data accuracy, understandability, and compliance authorization need to be resolved to fully utilize AI's potential in this area.

REFERENCES

1. Haendel M, Vasilevsky N, Unni D, Bologa C, Harris N, Rehm H, et al. How many rare diseases are there? Nat Rev Drug Discov. 2020;19(2):77–78. doi: 10.1038/d41573-019-00180-y.
2. Scherman D, Fetro C. Drug repositioning for rare diseases: knowledge-based success stories. Therapie. 2020;75(2):161–167. doi: 10.1016/j.therap.2020.02.007.
3. Roessler HI, Knoers NVAM, van Haelst MM, van Haaften G. Drug repurposing for rare diseases. Trends Pharmacol Sci. 2021;42(4):255–267. doi: 10.1016/j.tips.2021.01.003.
4. Choi RY, Aaron SC, Jayashree K-C, Michael FC, Peter JC. Introduction to machine learning, neural networks, and deep learning. Transl Vis Sci Technol. 2020;9:(2):14. doi: 10.1167/tvst.9.2.14.
5. Khurana D, Aditya K, Kiran K, Sukhdev S. Natural language processing: State of the art, current trends and challenges. Multimedia Tools and Applications 2023;82(3):3713–3744. doi: 10.1007/s11042-022-13428-4.
6. Alowais SA, Alghamdi SS, Alsuhebany N, Alqahtani T, Alshaya AI, Almohareb SN, et al. Revolutionizing healthcare: the role of artificial intelligence in clinical practice. BMC Med Educ. 2023;23:689. doi: 10.1186/s12909-023-04698-z.
7. Bajwa J, Munir U, Nori A, Williams B. Artificial intelligence in healthcare: transforming the practice of medicine. Future Healthc J. 2021;8(2):e188–e194. doi: 10.7861/fhj.2021-0095.

8. Brasil S, Pascoal C, Francisco R, Dos Reis Ferreira V, Videira PA, Valadão AG. Artificial intelligence (AI) in rare diseases: Is the future brighter? Genes. 2019;10(12):978. doi: 10.3390/genes10120978.
9. Jonker AH, O'Connor D, Cavaller-Bellaubi M, Fetro C, Gogou M,'t Hoen PAC, et al. Drug repurposing for rare: Progress and opportunities for the rare disease community. Front Med. 2024;17:11:1352803. doi: 10.3389/fmed.2024.1352803.
10. van der Pol Karel H, Aljofan M, Blin O, Cornel JH, Rongen GA, Woestelandt A-G, et al. Drug repurposing of generic drugs: Challenges and the potential role for government. Appl Health Econ Health Policy. 2023;21:831–840. doi: 10.1007/s40258-023-00816-6.
11. Cha Y, Erez T, Reynolds IJ, Kumar D, Ross J, Koytiger G, et al. Drug repurposing from the perspective of pharmaceutical companies. Br J Pharmacol. 2018;175(2):168–180.
12. Ekins S, Gerlach J, Zorn KM, Antonio BM, Lin Z, Gerlach A. Repurposing approved drugs as inhibitors of Kv7.1 and Nav1.8 to treat Pitt Hopkins syndrome. Pharm Res. 2019;36(9):137. doi: 10.1007/s11095-019–2671-y.
13. Sosa DN, Derry A, Guo M, Wei E, Brinton C, Altman, RB. A literature-based knowledge graph embedding method for identifying drug repurposing opportunities in rare diseases. Pac Symp Biocomput. 2020;25:463–474.
14. Esmail S, Danter WR. Artificially induced pluripotent stem cell-derived whole-brain organoid for modelling the pathophysiology of metachromatic leukodystrophy and drug repurposing. Biomedicines. 2021;9(4):440. doi: 10.3390/biomedicines9040440.
15. Cong Y, Shintani M, Imanari F, Osada N, Endo T. A new approach to drug repurposing with two-stage prediction, machine learning, and unsupervised clustering of gene expression. OMICS. 2022;26(6):339–347. doi: 10.1089/omi.2022.0026.
16. Foksinska A, Crowder CM, Crouse AB, Henrikson J, Byrd WE, Rosenblatt G, et al. The precision medicine process for treating rare disease using the artificial intelligence tool mediKanren. Front Artif Intell. 2022;5:910216. doi: 10.3389/frai.2022.910216.
17. Zhu C, Xia X, Li N, Zhong F, Yang Z, Liu L. RDKG-115: Assisting drug repurposing and discovery for rare diseases by trimodal knowledge graph embedding. Comput Biol Med. 2023;164:107262. doi: 10.1016/j.compbiomed.2023.107262.
18. Every Cure. Unlocking the hidden potential of existing drugs to save lives. 2024. Available at: https://everycure.org/. (Consulté le mars 17, 2024)
19. REPO4EU. Euro-global platform for drug repurposing. 2024. Available at: https://repo4.eu/. (Consulté le mars 18, 2024)
20. Open Targets. 2024. Available at: https://www.opentargets.org/. (Consulté le 17 mars, 2024)
21. Broad Institute. Drug Repurposing Hub. 2019. Available at https://www.broadinstitute.org/drug-repurposing-hub
22. Corsello S, Bittker J, Liu Z, et al. The Drug Repurposing Hub: a next-generation drug library and information resource. Nat Med. 2017;23:405–408. doi: 10.1038/nm.4306.
23. EURORDIS. REMEDi4ALL, an ambitious EU-funded research initiative, launches to drive forward the repurposing of medicines in Europe. 2024. Available at https://www.eurordis.org/press-release-remedi4all/. (Consulté le mars 18, 2024)
24. AFM Téléthon. I-Stem, coordinateur du consortium de recherche européen DREAMS associant intelligence artificielle, cellules souches et criblage pharmacologique pour traiter des maladies neuromusculaires. 2023. Available at: https://www.afm-telethon.fr/fr/communiques-de-presse/i-stem-coordinateur-du-consortium-de-recherche-europeen-dreams-associant
25. HealX. AI drug discovery. Rare disease treatment. 2024. Available at: https://healx.ai/. (Consulté le mars 17, 2024)
26. Biovista. Drug positioning and prioritization-drug repositioning. Biovista drug positioning and prioritization (blog). 2024. Available at: https://www.biovista.com/solutions/drug-repositioning/. (Consulté le mars 17, 2024)
27. Visibelli A, Bianca R, Ottavia S, Annalisa S. The impact of artificial intelligence in the odyssey of rare diseases. Biomedicines. 2023;11(3):887. doi: 10.3390/biomedicines11030887.
28. Wojtara M, Emaan R, Taibia R, Palak K, Heshwin S. Artificial intelligence in rare disease diagnosis and treatment. Clin Transl Sci. 2023;16(11):2106–2111. doi: 10.1111/cts.13619.

