



Computational Repurposing of Drugs: A Review

N. Harikrishna¹, K. Krishna Mohan², L. Ramesh Kumar³

^{1,2,3}Government Degree College(A), Khairatabad, Hyderabad, Telangana, India

Abstract:

Drug repurposing is the modern technology for identifying the new therapeutic property of approved and operational drug. De novo drug discovery faces many challenges including clinical trials, time and cost. To overcome these aspects drug repurposing has evolved as promising approach, that has benefits like previously studied safety profiles and bypassing the early developmental changes and accelerating clinical trials by reducing the cost up to 60%.

"Omics" technologies, computational capabilities imbibed with the artificial intelligence caters the drug repurposing for new targets or pathogens. By using virtual screening, molecular docking, and sequence similarity maps, researchers can identify multiple therapeutic effects by a drug. In the year 2025, 47 drugs were approved by FDA after drug repurposing. Nearly 45 % of drugs repurposing activity in 2025 were focused on treatment of cancers. The global scale drug repurposing market has been increasing continuously and reached \$36.87 billion in 2025. In this review we focus on how drug repurposing activity enhances the use of approved drug for treatment of variety of diseases or targets.

Keywords: Drug repurposing, FDA, Artificial intelligence, De novo drug discovery, clinical trials.

1. Introduction:

Development of new drug to treat the diseases is time consuming, tedious and costly process. The success rate for development of new drug is small which takes approximately 10-15 years. Hence drug repurposing or drug reposition is one of the promising alternate approach to use the existing approved drug for treatment of other diseases. Hence Drug repurposing is used for already existing or old or banned drugs for other disease treatment. Drug repurposing in association with the computational techniques has emerged a new methodology to develop the potential treatment of new diseases (Bhagat, R. T. and Butle, S. R. 2021). Drug repurposing proved its successful applications in the treatment of infectious diseases, cancers and rare neurological conditions (Anuradha Singh, 2024). Due to emergence of new health problems, antibiotic resistance and AI forced the health sector lead to increase in the market for drug repurposing. The market for drug repurposing has been increasing continuously and estimated at USD 35.3 billion in 2024 and may reach to USD 51.8 billion by 2032 (Camps I et al., 2025).

Artificial intelligence (AI) is the technology that mimics the human intelligence and perform many tasks learning, reasoning, predictions problem solving and so on. It works based on the algorithm with help of



humans. AI has emerged as promising tool, accelerate the drug repurposing and discovery. AI helps in minimisation of off target, identification of new targets, analyses the vast data of patients and reduces side effects of drug in clinical trials.

1.1 Traditional drug development:

The traditional drug development requires extensive research work and consisting of 5 stages

1. Preclinical drug development: Effect of newly developed drug on animal models
2. Phase I : effect of newly developed drug on humans to check the adverse reactions
3. Phase II: Pharmacokinetic data of drug is obtained
4. Phase III: toxic characters and safety of drug was studied.
5. Phase IV: Drug is approved and released into the market. It is pharmacovigilance phase where post marketing survey was observed (Kulkarni VS et al 2023).

1.2 Drug repurposing stages:

Drug repurposing is approached through the two methods.

1. Experimental based methodology: Established through the in vitro or in vivo screening of drug for novel targets.
2. In silico methodology: uses the computational methods to drug repurposing via virtual screening (Khan S et al 2023).

Table 1: Differences between traditional drug discovery and drug repurposing

Character	Drug Repurposing	Traditional Drug Discovery
Safety profiles	Already available	Safety must be evaluated from scratch
Time Required to develop drug	Approximately 3–6 years	Approximately 10–15 years
Cost	Cost effective	Very high
Relies on	Computational analysis	High throughput methodologies
Risk of Failure	Low	High rate failure in clinical trials
Preclinical Studies	Limited	Extensive preclinical studies and clinical trial phases are required
Novelty	Moderate	High
Intellectual Property	Limited patent protection	Strong patent protection possible
Success Rate	Higher	Lower

23. Steps of drug repurposing:

1. **Collection of drug data and Identification of therapeutic drugs:** Collect the data of used drugs from data bases by using artificial intelligence. Data includes the name of drug, chemical structure,



mechanisms of action and safety profiles

- Identification of target of drug or disease:** Target of drug may be protein or gene of pathway or structural component of bacteria or virus etc. Data is processed for removing duplicates and standardised.
- Virtual screening:** AI screens virtually the drug target by using molecular docking. It find out the appropriate top drugs. AI also predicts efficacy of drugs and toxic profile virtually.
- Pre-clinical studies :**
- Clinical studies:** Stage I, III, III and IV (Kulkarni VS et al 2023)

In the current scenario, AI has become one of the prominent tool in drug discovery, enhancing the experimental workflows by virtual methods. AI increased the efficiency in data utilisation and data integration for drug repurposing (Herráiz-Gil, S., et al., 2025).

Table 2: Drug repurposed drugs and their applications

S.No	Name of the Drug	Usage	Drug repurposed for	Reference
1	Amphotericin B	Anti-fungal:	methicillin resistant <i>Staphylococcus aureus</i>	Farid, N., et al., (2023).
2	Aspirin	Pain and inflammation	Cardiovascular disease and cancers	Tapas Kumar Mohapatra et al., 2019
3	Methotrexate	Anti-cancer	Autoimmune disorders- Rheumatoid Arthritis, Psoriasis	Herfarth, H. H., et al., (2016).
4	Curcumin	Anti-inflammatory and anti-oxidant	Cancer, Arthritis	Agarwal B and Harikumar K.B . 2009
5	Amantidine	Against influenza	Parkinsons disease	Khan S et al., 2023
6	Ambroxol	Respiratory disease	Parkinsons disease	Simon R.W Stott et al., 2021
7	Azithromycin	Bacterial infection	Zika virus	Anuradha Singh, 2024
8	Chloroquine	Anti-malarial	Cancer, anti-Corona virus	Anuradha Singh, 2024
9	Ivermectin	Anti-parasitic	Influenza, Zika and Dengue viruses	Anuradha Singh, 2024
10	Valproic acid	Epilepsy	Cancer	Dhirendra Singh 2021



One Day National Seminar on

“Advances in Life Sciences for Diversity, Applications, and Human Welfare”

(ALSDAHW – 2025)

Organized by Department of Microbiology & Department of Biotechnology

M.V.S. Government Arts & Science College (Autonomous), Mahabubnagar-509001

E-ISSN: 2229-7677 • Website: www.ijSAT.org • Email: editor@ijSAT.org

11	Novobiocin	Anticoumarin antibiotic used against MRSA	Zika virus and Corona virus	S. G. Viveiros Rosa, (2020).
12	Minoxidil	Anti hypertensive	Hair growth	Okuyama R. 2023.
13	Boswellic acids	Anti-inflammatory (Boswellia)	Arthritis, inflammatory bowel disease	Abdel-Tawab, M., etal 2013
14	Artemisinin	Anti malarial	Cancer	Lai, H. C., 2013

Tools used in drug repurposing:

Data based used for drug repurposing	AI tools used in the drug repurposing
ChEMBL	AlxFuse
ChemDB	DeepICL
Pubchem	WISER
Drug target	MUSE115
Bindingg DB	ASGARD
Drug Bank	HiSIF-DTA
Drug Target Commons (DTC)	Hyper Synergy
STITCH	Deep CE
Therapeutic Target Database (TTD)	KGE_NFM
Pharm KGB	DEEP drug
L10000	PREDICT
GDSC	Drug Rep
Toxicogenomics Database	Zaira Chem

(Z. Wan, et al ., 2025, Anuradha Singh, 2024)

Challenges in Drug repurposing:

Even though the Drug repurposing using AI is a great advantage in the field of drug discovery but many challenges has to be addressed.

Quality of data:

AI is trained with the already available data in the data bases. These input data is crucial for outcome. Any missing data, bias and noise results in the inaccurate outcome or prediction. The biological data is very complex and effect of drug may varies on the different tissues. This complexity makes hurdles in the prediction of drug repurposing using AI (Keramida, P., 2025). Hence, the data generated should be accurate which improves analysis by AI. Further, lack of accessibility to the training datasets also hinders the reproducibility and validation (Anokian E., 2024).



Ethical consideration:

Large biological data set usage for AI prediction has concern reliable safety for privacy of individuals. The data of patients regards with sensitive genetic or behavioural information raises the ethical concerns. Hence stringent laws should be framed to protect the sensitive data (Anokian E., 2024).

Collaboration:

Lacking of collaboration between the research institutes and industries is one of the major challenge for implementation of AI for drug repurposing. The problem can be addressed through the collaboration between the stakeholders, which enables the AI to enhance the efficiency, accuracy, and impact in drug discovery. High-performance computing and cloud computing are plays key role in the AI-driven drug discovery. AI tools efficiently handles the large genomic or proteomic or other data for drug repurposing. (Anokian E., 2024, Keramida, P., 2025).

Conclusion:

AI driven Drug repurposing is playing a pivotal role in the acceleration of drug discovery for unmet targets other than actual target discovered led to fulfil the gap. It not only reduces the financial burden but also time and work flow. The drugs used for repurpose already have gone through safety profiles, hence decreases the risk of failure and enhance the success rate by 30%. The AI driven drug repurposing, improved by advent of data mining and Machine learning, enable analysis of public data extensively and predicts the new drug target and uncovering valuable insights from structural data

References:

1. Pinzi, L., Bisi, N., & Rastelli, G. (2024). How drug repurposing can advance drug discovery: Challenges and opportunities. *Frontiers in Drug Discovery*, 4, 1460100. <https://doi.org/10.3389/fddsv.2024.1460100>
2. Bhagat, R. T., & Butle, S. R. (2021). Drug repurposing: A review. *Journal of Pharmaceutical Research International*, 33(31B), 161–169. <https://doi.org/10.9734/jpri/2021/v33i31B31704>
3. Khan, S., Agnihotri, J., Patil, S., & Khan, N. (2023). Drug repurposing: A futuristic approach in drug discovery. *Journal of Pharmaceutical and Biological Sciences*, 11(1), 66–69. <https://doi.org/10.18231/j.jpbs.2023.011>
4. Kulkarni, V. S., Alagarsamy, V., Solomon, V. R., Jose, P. A., & Murugesan, S. (2023). Drug repurposing: An effective tool in modern drug discovery. *Russian Journal of Bioorganic Chemistry*, 49(2), 157–166. <https://doi.org/10.1134/S1068162023020139>
5. Camps, I., Künzel, S. R., Schubert, M., & Singh, R. K. (2025). Editorial: Opportunities and challenges in drug repurposing. *Frontiers in Pharmacology*, 16, 1709217. <https://doi.org/10.3389/fphar.2025.1709217>
6. Aggarwal, B. B., & Harikumar, K. B. (2009). Potential therapeutic effects of curcumin, the anti-inflammatory agent, against neurodegenerative, cardiovascular, pulmonary, metabolic, autoimmune



- and neoplastic diseases. *The International Journal of Biochemistry & Cell Biology*, 41(1), 40–59. <https://doi.org/10.1016/j.biocel.2008.06.010>
7. Herfarth, H. H., Kappelman, M. D., Long, M. D., & Isaacs, K. L. (2016). Use of methotrexate in the treatment of inflammatory bowel diseases. *Inflammatory Bowel Diseases*, 22(1), 224–233. <https://doi.org/10.1097/MIB.0000000000000589>
 8. Singh, D., Gupta, S., Verma, I., Morsy, M. A., Nair, A. B., & Ahmed, A.-S. F. (2021). Hidden pharmacological activities of valproic acid: A new insight. *Biomedicine & Pharmacotherapy*, 142, 112021. <https://doi.org/10.1016/j.biopha.2021.112021>
 9. Roozbeh, F., Saeedi, M., Alizadeh-Navaei, R., Hedayatzadeh-Omran, A., Merat, S., Wentzel, H., & Shamshirian, A. (2021). Sofosbuvir and daclatasvir for the treatment of COVID-19 outpatients: A double-blind, randomized controlled trial. *Journal of Antimicrobial Chemotherapy*, 76(3), 753–757. <https://doi.org/10.1093/jac/dkaa502>
 10. Herráiz-Gil, S., Nygren-Jiménez, E., Acosta-Alonso, D. N., León, C., & Guerrero-Aspizua, S. (2025). Artificial intelligence-based methods for drug repurposing and development in cancer. *Applied Sciences*, 15(5), 2798. <https://doi.org/10.3390/app15052798>
 11. Rosa, S. G. V., Fierro, I. M., & Santos, W. C. (2020). Repositioning and investigational drugs for Zika virus infection treatment: A patent review. *Expert Opinion on Therapeutic Patents*, 30(11), 847–862. <https://doi.org/10.1080/13543776.2020.1805747>
 12. Okuyama, R. (2023). Advancements in drug repurposing: Examples in psychiatric medications. *International Journal of Molecular Sciences*, 24(13), 11000. <https://doi.org/10.3390/ijms241311000>
 13. Keramida, P., Syrigos, N. K., Kouvela, M., Poulakou, G., Charpidou, A., & Fiste, O. (2025). AI-driven drug repurposing: Applications and challenges. *Medicines*, 12(4), 28. <https://doi.org/10.3390/medicines12040028>
 14. Anokian, E., Bernett, J., Freeman, A., List, M., Santamaría, L. P., Tanoli, Z., & Bonnin, S. (2024). Machine learning and artificial intelligence in drug repurposing—Challenges and perspectives. *Drug Repurposing*, 1, e20240004. <https://doi.org/10.58647/DRUGREPO.24.1.0004>
 15. Abdel-Tawab, M., Werz, O., & Schubert-Zsilavec, M. (2011). *Boswellia serrata*: An overall assessment of in vitro, preclinical, pharmacokinetic and clinical data. *Clinical Pharmacokinetics*, 50, 349–369. <https://doi.org/10.2165/11586800-000000000-00000>
 16. Lai, H. C., Singh, N. P., & Sasaki, T. (2013). Development of artemisinin compounds for cancer treatment. *Investigational New Drugs*, 31, 230–246. <https://doi.org/10.1007/s10637-012-9873-z>
 17. Wan, Z., Sun, X., Li, Y., Chu, T., Hao, X., Cao, Y., & Zhang, P. (2025). Applications of artificial intelligence in drug repurposing. *Advanced Science*, 12(1), 2411325. <https://doi.org/10.1002/advs.202411325>