



AI-Driven Drug Repurposing: A Case-Based Review With Insights From Traditional Approaches.

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ABSTRACT

Drug repurposing is an efficient strategy to identify new uses for existing drugs, reducing the time and cost typically associated with novel drug development. Traditionally, many repurposed drugs were discovered serendipitously or through clinical observation processes that, while valuable, are often slow and limited in scope. In recent years, integrating artificial intelligence (AI) into drug repurposing has transformed the landscape by enabling data-driven predictions and rapid hypothesis generation. This review explores AI-driven drug repurposing through a series of impactful case studies, including Baricitinib for COVID-19, Ketamine for cocaine use disorder, Efavirenz for Parkinson's disease, and others. These cases highlight how various AI technologies such as machine learning, natural language processing, and electronic health record mining have been used to uncover novel therapeutic indications. To enhance the value of this analysis, the review also briefly contrasts AI-based approaches with traditional repurposing examples such as Sildenafil and Thalidomide, illustrating the evolution from chance discoveries to algorithm-driven insights. By presenting these comparative case studies, this article underscores the potential of AI to revolutionise drug repurposing specifically. It concludes that while AI is not a replacement for clinical expertise, it is a powerful tool that enhances drug repurposing efforts, enabling more targeted, faster, and scalable therapeutic innovations.

KEYWORDS – Drug repurposing, artificial intelligence (AI), machine learning, traditional approaches, therapeutic innovation.

1. INTRODUCTION:

Drug repurposing—identifying new therapeutic uses for existing or previously shelved drugs—has gained increasing attention as a strategic alternative to conventional drug development [1]. Unlike traditional drug discovery, which is time-consuming, expensive, and prone to high failure rates, repurposing offers a faster and more cost-effective route to bring patient therapy [2]. This approach is particularly valuable in addressing urgent medical needs, such as emerging infectious diseases, rare disorders, and treatment-resistant conditions, where the development of new drugs may not be commercially or practically feasible [3]. The recent integration of artificial intelligence (AI) and machine learning (ML) into drug repurposing efforts has further revolutionised this field [4]. Traditional repurposing methods often rely on manual screening, serendipitous observations, or isolated mechanistic

hypotheses, which are time-intensive and limited in scope. In contrast, AI systems can analyse massive biomedical datasets including genomic, transcriptomic, proteomic, and clinical data—to uncover hidden patterns, predict drug-target interactions, and prioritise compounds for repurposing with remarkable speed and precision [5]. These technologies enable researchers to bypass many trial-and-error stages and streamline the drug development pipeline [6]. This review presents a series of case studies that demonstrate the real-world impact of AI-driven drug repurposing. Through this review, we aim to explore the evolving landscape of AI-powered drug repurposing by presenting recent and diverse case studies. We also compare AI-based approaches with traditional repurposing strategies in terms of accuracy, scalability, and translational potential to highlight how artificial intelligence is reshaping the future of therapeutic discovery and repositioning.

2. AI TECHNOLOGIES USED IN DRUG REPURPOSING

In drug repurposing, various AI techniques are employed to mine data, identify patterns, and predict new therapeutic indications for existing drugs. Below is the key AI technologies used in the process:

Machine Learning (ML)

Machine learning (ML) plays a foundational role in AI-driven drug repurposing. It involves training computational models to detect patterns in large-scale datasets, such as drug-target interactions, gene expression profiles, and chemical properties. Supervised learning techniques like random forests and support vector machines are widely used for classifying known interactions and predicting unknown therapeutic potentials. Unsupervised learning, including clustering algorithms, helps group drugs with similar bioactivity, revealing novel uses. For example, the study developed DeepDR, a machine learning framework that integrates diverse biological networks to predict drug-disease associations, demonstrating high accuracy in identifying repurposing compounds across multiple therapeutic areas [7].

2.1. Deep Learning (DL)

Deep learning (DL), a subfield of ML, involves neural networks with multiple layers capable of modelling complex, non-linear relationships in high-dimensional data. DL excels at processing unstructured biomedical information, such as raw genomic sequences, molecular structures, and transcriptomic data. This technology, when used to match disease gene expression profiles with drug-induced expression profiles, predicts therapeutic effects. The recent study demonstrated that deep neural networks trained on transcriptomic data could accurately predict the pharmacological class and repurposing potential of various compounds, highlighting the transformative value of DL in drug discovery [8].

2.2. Knowledge Graphs

Knowledge graphs are structured representations of entities (like drugs, genes, and diseases) and their interrelationships. These graphs provide a rich framework for AI algorithms to reason over biological relationships and discover hidden links indicative of repurposing potential. They can integrate various data sources—such as genomic databases, drug-target interaction networks, and clinical trial records—into a unified model. In one study, they used knowledge graph completion techniques to identify drug candidates for COVID-19, leveraging logical connections that would be missed using conventional statistical methods. This showcases how graph-based reasoning enhances hypothesis generation in drug repurposing [9].

2.3. Natural Language Processing (NLP)

Natural Language Processing (NLP) enables AI to extract meaningful insights from unstructured text sources such as journal articles, clinical trial reports, and EHR notes. Using techniques like entity recognition (NER) and relation extraction, NLP models can identify drug-disease relationships, mechanisms of action, and adverse effects. A prominent tool in this space is BioBERT, a domain-specific language model trained in biomedical literature. BioBERT has

outperformed traditional models in several text-mining tasks, allowing researchers to efficiently parse scientific publications and identify potential repurposing leads with high confidence [10].

2.4. Electronic Health Records (EHR) Mining

Electronic Health Records (EHRs) provide a valuable source of real-world evidence for drug repurposing. AI systems can mine EHR data to uncover patterns in drug prescriptions, patient outcomes, and disease progression. This method is particularly useful for identifying off-label drug uses and validating hypotheses generated by other AI models. For instance, the recent study combined EHR analysis with knowledge graph methods to identify potential treatments for COVID-19, demonstrating that insights derived from real patient data can complement in silico predictions and improve translational impact [9].

3. AI-BASED DRUG REPURPOSING CASE STUDIES

CASE STUDY 1: Baricitinib for COVID-19

Baricitinib, an oral Janus kinase (JAK) inhibitor originally approved for rheumatoid arthritis, emerged as a repurposing candidate for COVID-19 using artificial intelligence. Researchers at Benevolent AI utilized deep learning and knowledge graph technologies to identify baricitinib's potential to inhibit AP2-associated protein kinase 1 (AAK1) and cyclin G-associated kinase (GAK), both of which play a role in viral entry and propagation. This AI-driven prediction led to preclinical evaluations and subsequently to clinical trials, which demonstrated baricitinib's efficacy in reducing inflammatory responses in COVID-19 patients. The drug received FDA emergency use authorization in 2020, and its approval was a significant milestone in demonstrating the power of AI for repurposing existing drugs. It became a key part of treatment protocols worldwide, highlighting the impact of AI in rapidly addressing global health crises [11].

CASE STUDY 2: Ketamine for Cocaine Use Disorder

Ketamine, widely known as an anesthetic and more recently for its antidepressant effects, was identified as a repurposing candidate for cocaine use disorder (CUD) through an artificial intelligence-based prediction model. The study integrated drug-target prediction algorithms, clinical trial databases, and electronic health records to validate ketamine's potential efficacy in treating CUD. AI identified NMDA receptor modulation as a critical mechanism, which was supported by clinical observations of reduced cocaine cravings and relapse. Subsequent pilot studies showed that low-dose ketamine infusions could significantly reduce cocaine use in treatment-resistant individuals, confirming the model's prediction and demonstrating how AI can inform repurposing decisions in substance use disorders [12].

CASE STUDY 3: Efavirenz for Parkinson's Disease

Efavirenz, an antiretroviral drug originally approved as a non-nucleoside reverse transcriptase inhibitor (NNRTI) used to treat HIV/AIDS, was repurposed for Parkinson's disease based on AI-driven discovery techniques. A computational drug repositioning model was employed to screen FDA-approved compounds against targets involved in α -synuclein propagation, a hallmark of Parkinson's pathology. Efavirenz was found to activate CYP46A1, enhancing cholesterol metabolism in the brain and reducing α -synuclein accumulation. This mechanistic insight, revealed by AI and supported by preclinical studies, suggested a neuroprotective effect of efavirenz. This repositioning not only exemplifies AI's predictive power but also opens new therapeutic avenues for managing neurodegenerative diseases [13].

CASE STUDY 4: Drug Repurposing for Cataract Prevention in Diabetes

In a novel AI-based repurposing study, researchers sought to identify drugs that could reduce the risk of cataract extraction in diabetic patients. Machine learning algorithms analyzed large-scale clinical data to predict drug-disease interactions, and several candidate compounds were identified, including angiotensin receptor blockers and specific anti-inflammatory agents. These predictions were validated using retrospective clinical datasets, demonstrating a significant association between certain medications and reduced incidence of cataract surgery. The study showed the power of AI to identify preventive therapies by mining real-world data, offering promising strategies to manage diabetes-related complications [14].

CASE STUDY 5: Vandetanib and Everolimus for Diffuse Intrinsic Pontine Glioma (DIPG):

Vandetanib, originally approved as a tyrosine kinase inhibitor targeting VEGFR, RET, and EGFR for medullary thyroid carcinoma, and everolimus, an mTOR inhibitor used in various cancers and organ transplant rejection, were repurposed as a combination therapy to treat diffuse intrinsic pontine glioma (DIPG) – a highly aggressive and fatal pediatric brain tumor. An AI-driven platform was used to identify drugs effective against ACVR1-mutant DIPG, which represents nearly 25% of all DIPG cases. The analysis revealed that vandetanib targets ACVR1 ($K_d = 150$ nmol/L) and reduces DIPG cell viability. However, due to its poor brain penetration, combining it with everolimus, which inhibits P-gp and BCRP drug efflux transporters, enhances vandetanib delivery across the blood-brain barrier. This shows promise in orthotopic xenograft models and informed early clinical translation in pediatric patients. The study exemplifies the potential of AI in integrating genomic profiling with pharmacological data to uncover rational and effective repurposing strategies for rare diseases like DIPG [15].

CASE STUDY 6: Fragile X Syndrome – DREAM-RD Project

Fragile X Syndrome is a rare genetic disorder characterized by intellectual disability and behavioral challenges, with no FDA-approved targeted treatments currently available. In the DREAM-RD initiative, researchers applied AI/ML techniques to identify potential repurposed drugs for FXS. Utilizing a hybrid approach involving transcriptomic data analysis, gene expression signature matching, and machine learning classifiers, the study shortlisted several candidate molecules. The approach aimed to reverse disease-specific gene expression signatures using drug perturbation profiles, offering a targeted and data-driven path to drug repurposing. Although still in the early stages, this AI-based pipeline highlighted promising candidates that warrant further clinical investigation. Notably, this work is based on a preprint and has not yet undergone peer review, but it reflects an emerging trend in using AI for rare disease therapeutics [16].

TABLE 1: Overview of AI-based drug repurposing: success stories and case examples from recent literature

DRUG	ORIGINAL USE	REPURPOSED USE	AI METHOD USED	CLINICAL PHASE	OUTCOME
Baricitinib	Rheumatoid Arthritis	COVID 19	Machine learning, EHR, Clinical data	Phase 3	Successfully improved patient outcomes in COVID-19, FDA-approved for Emergency use.
Ketamine	Anesthetic	Cocaine use disorder	Machine learning, EHR	Ongoing trials	Clinical trials initiated, showing positive effects on reducing cocaine use.
Efavirenz	Antiretroviral for HIV	Parkinson's Disease	Deep learning, Genomic data	Phase 2	Demonstrated potential to reduce α -synuclein aggregation, promising effects on Parkinson's
Metformin	Type2 diabetes	Cancer (various types)	Machine learning, clinical data	Ongoing trials	Showed potential in preclinical studies, clinical trials to follow
Vendetanib + Everolimus	Cancer (Thyroid)	Diffuse intrinsic pontine glioma (DIPG)	AI-based drug repositioning	Phase 1	Ongoing trials to assess efficacy in DIPG: preclinical studies showed potential benefits.
Raloxifene	Osteoporosis, breast Cancer Prevention	FragileX syndrome (FXS)	Deep Learning, Genetic data	Early-phase trials	Early trials showed improvement in cognitive and behavioral symptoms of FXS.

4. COMPARISON OF AI-DRIVEN VS TRADITIONAL DRUG REPURPOSING APPROACHES:

TABLE 2: Comparison of AI-driven vs traditional drug repurposing approaches

ASPECTS	AI-DRIVEN DRUG REPURPOSING	TRADITIONAL DRUG REPURPOSING
DISCOVERY METHODS	Machine learning, deep learning, HER mining, and network pharmacology.	Serendipity, clinical observation, literature review.
DISCOVERY SPEED	Rapid due to automation and computational screening.	Slow; relies on manual research or chance observation.
TIME REQUIRED	Weeks to months	Several years to decades
DATA DEPENDENCY	High; relies on structured/unstructured biomedical data	Low; relies on human insight and chance
COST-EFFECTIVENESS	Cost-efficient due to in silico prediction and reduced lab work	High cost due to extensive wet-lab testing and clinical trial requirements
SCALABILITY	Highly scalable across thousands of compounds and indications	Limited scalability due to manual processes.
VALIDATION NEEDS	Still requires clinical validation but benefits from strong predictive models.	Requires full validation with a higher risk of failure.
SUCCESS RATE	Increasing with better algorithms and datasets	Moderate; many leads fail in late-stage trials.
LIMITATION	Model bias, need for interpretability, data quality concerns	Unpredictable, time-consuming, narrow scope

<p>EXAMPLES</p>	<p>BARICITINIB for COVID-19, EFAVIRENZ for Parkinson's, DREAM-RD for Fragile X syndrome.</p>	<p>Thalidomide for multiple myeloma, sildenafil for erectile dysfunction</p>
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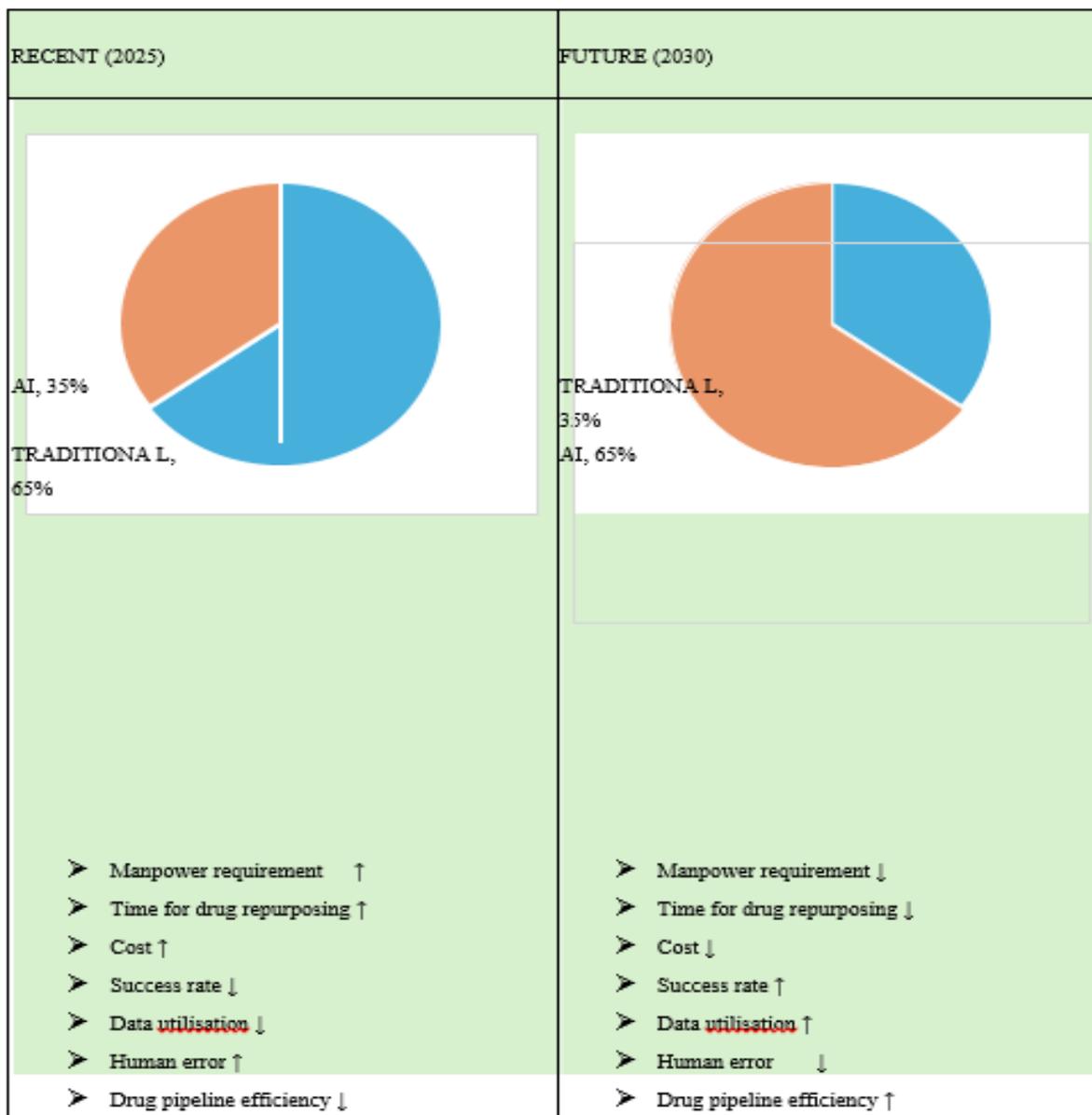


FIGURE 1: AI in drug repurposing: trends from 2024 to 2030.

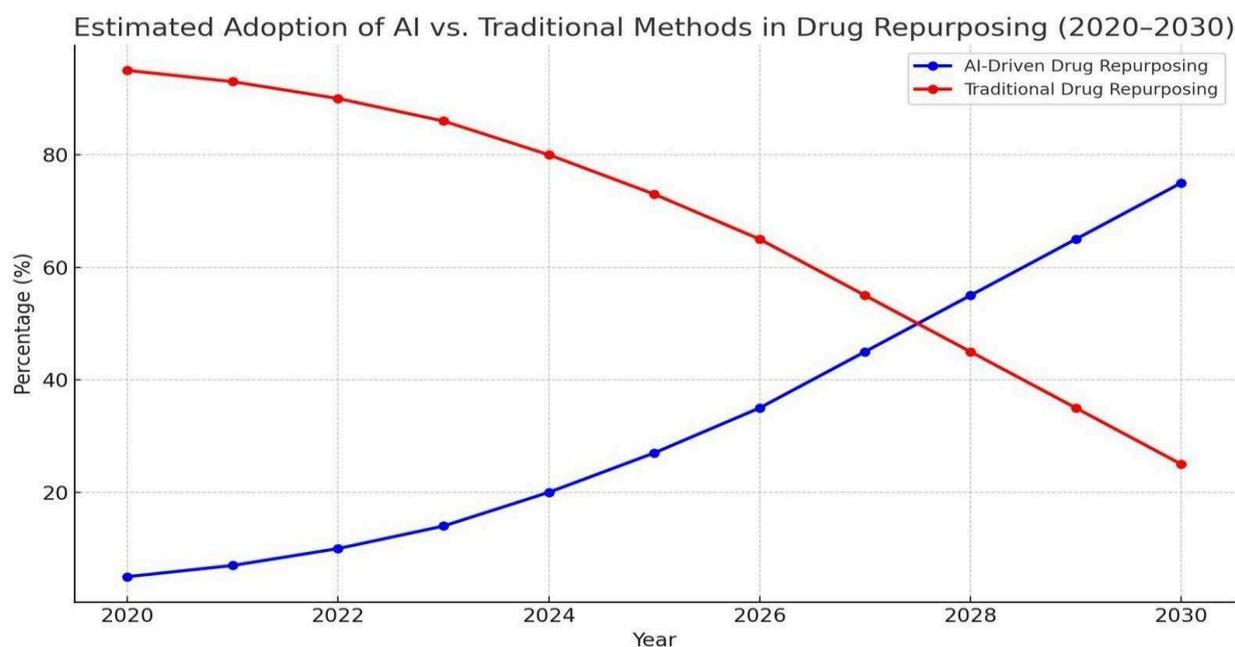


FIGURE2: Projected adoption trends of AI-based vs traditional drug repurposing approaches (2020-2030), based on recent literature and expert analysis. [9] [17].

5. DISCUSSION

The integration of artificial intelligence into drug repurposing workflows represents a transformative phase in pharmaceutical development. By examining six diverse case studies, this review highlights how AI is accelerating the identification of new indications for existing drugs while enhancing precision in targeting diseases with unmet therapeutic needs. From Baricitinib’s rapid redeployment for COVID-19 to Ketamine’s repositioning in substance use disorders, the synergy between computational models and real-world data has redefined traditional repurposing paradigms.

A significant advantage of AI-driven drug repurposing lies in its ability to process vast datasets—ranging from molecular structures to electronic health records (EHRs)—uncovering hidden therapeutic potentials with unmatched speed and accuracy. Unlike traditional methods, which often rely on serendipity or labor-intensive screening, AI methods like machine learning, knowledge graphs, and deep learning enable hypothesis-free identification of drug candidates [17][18]. For instance, the case of Efavirenz for Parkinson’s

disease demonstrates how AI, through network pharmacology and mechanistic modelling, can predict novel neuroprotective roles. However, still challenges remain. Issues such as data quality, standardization, and the “black box” nature of some AI algorithms continue to limit model performance and clinical trust [19]. The regulatory landscape is also struggling to keep pace with the integration of AI into therapeutic decision-making, and clinical validation remains a bottleneck. For example, many AI-predicted drug candidates, such as Ketamine for cocaine use disorder, require extensive in vitro, in vivo, and clinical testing before clinical adoption.

Despite these challenges, the success stories presented in this review illustrate that AI is not merely a tool but rather a central driver of therapeutic innovation. The application of AI in rare diseases, as demonstrated by the DREAM-RD project for Fragile X Syndrome, showcases its potential to address gaps left by conventional pharmaceutical pipelines. Looking forward, AI-enabled drug repurposing is expected to become more dynamic and personalized. Real-time mining of global health data and adaptive learning models are set to guide individualized therapeutic decisions [20].

In conclusion, AI-driven drug repurposing has moved beyond chance discoveries, shifting toward intentional, data-driven strategies. As technological capabilities continue to evolve, AI will not only uncover new uses for existing drugs but will also play a central role in advancing precision medicine and tackling diseases that have long been neglected.

6. CONCLUSION

Artificial intelligence has emerged as a transformative force in the field of drug repurposing, offering unprecedented opportunities to revolutionize how therapeutic candidates are identified and validated. The case studies reviewed in this article illustrate AI's power in accelerating the repositioning of existing drugs for new indications, with notable successes in areas such as COVID-19, neurological disorders, and rare diseases. By leveraging AI-driven approaches like machine learning, deep learning, and EHR mining, researchers can now predict, validate, and optimize drug candidates with greater efficiency and accuracy than traditional methods.

While the challenges related to data quality, algorithm transparency, and regulatory approval remain, the continued integration of AI into drug repurposing workflows holds immense promise. The ability to mine vast amounts of clinical and molecular data, along with the potential for personalized treatments, will pave the way for more rapid, cost-effective, and impactful drug development. As we look toward the future, AI's role in drug repurposing is set to expand, with advancements in real-time data analysis, adaptive learning algorithms, and the incorporation of patient-specific data. Now, due to technological advancements, traditional approaches yield comparatively lower repurposing data. However, with AI, researchers can uncover significantly more repurposing opportunities not only for existing drugs but also for upcoming compounds—transforming how we approach both present and future drug discovery. Ultimately, as AI technologies continue to evolve, they will not only uncover new uses for existing drugs but also create more targeted and efficient therapeutic strategies, marking a new era in medicine. The convergence of AI and drug repurposing not only holds the potential to address pressing global health needs but also positions “AI as a key player in the next wave of pharmaceutical innovation”

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