Reviving Molecules With Minds: AI-Driven Drug Repurposing Through Case-Based Intelligence

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ABSTRACT

The drug discovery process is traditionally slow and expensive, with high rates of failure during clinical trials. However, artificial intelligence (AI) has transformed this landscape by accelerating the identification of existing drugs that can be repurposed for new therapeutic indications. This innovative approach, known as AI-driven drug repurposing, utilizes advanced machine learning (ML) algorithms and deep learning (DL) models to analyze large datasets, including genomic information, patient records, and clinical trial outcomes, to predict novel drug-disease relationships. One of the most striking examples of AI's potential is the repurposing of existing antiviral drugs like remdesivir and chloroquine for COVID-19. Through AI's ability to rapidly analyze vast molecular and clinical data, these drugs were identified as potential candidates to combat the global pandemic. In oncology, AI has facilitated the exploration of metformin and statins, repurposing them for cancer treatment based on their ability to target multiple pathways involved in tumor growth. Similarly, AI in neurology has identified new applications for drugs originally developed for other conditions, offering hope for neurodegenerative diseases like Alzheimer's.

While AI promises substantial benefits in drug development, challenges such as data quality, regulatory approval, and ethical concerns must be overcome. As AI models become more refined, the potential for drug repurposing will revolutionize healthcare, reducing development timelines and providing personalized therapeutic options for patients across a variety of diseases, from rare conditions to pandemics.

Keywords

Algorithmic Pharmacovigilance, Computational Drug Repositioning, Predictive Polypharmacology, AI-Powered Indication Expansion, Deep Learning-Driven Target Mapping

INTRODUCTION

In the realm of modern drug development, time is not just money—it is survival. The conventional path to discovering a new drug spans 10–15 years, with costs soaring beyond $2.6 billion, and a clinical failure rate exceeding 90%[2]. These sobering statistics highlight the urgent need for a more agile, efficient, and intelligent approach to therapeutics[4,9]. Drug repurposing, the strategic reapplication of approved or investigational drugs for new indications, has emerged as a powerful alternative to de novo drug discovery[1]. But what is redefining this strategy in the 21st century is the integration of Artificial Intelligence (AI).

AI is transforming drug repurposing from a process once driven by serendipity into one led by algorithmic precision and computational foresight[12]. By leveraging machine learning (ML), deep neural networks, graph theory, and natural language processing (NLP), AI systems can
rapidly parse through vast oceans of biomedical data—spanning chemical libraries, protein- protein interactions, gene expression profiles, disease ontologies, adverse event databases, and patient-level clinical data[2-5].
Unlike traditional approaches, which are often hypothesis-driven and disease-centric, AI- driven repurposing is multi-dimensional, hypothesis-free, and mechanism-agnostic[6].It excels at discovering hidden pharmacological potentials through pattern recognition, unsupervised learning, and knowledge graph mining—making it possible to reposition drugs based on previously unconnected disease pathways or molecular signatures[8].
Moreover, during the COVID-19 pandemic, AI's agility was put to the test. Within weeks, platforms like BenevolentAI and Atomwise identified baricitinib, remdesivir, and others as promising candidates, accelerating clinical evaluation[3,7]. This success showcased AI's real- world utility not only in crisis response but also in combating neglected diseases, rare disorders, and polygenic conditions where traditional R&D often falters due to lack of commercial interest[1-3].
This review presents a critical exploration of how AI is deconstructing and reassembling the pharmacological universe, using real-world case studies to demonstrate its potential to democratize drug innovation, enable precision repurposing, and pave the way toward a more resilient and responsive global healthcare system[10]. Through this lens, AI is not just a tool— it is the cognitive engine of next-generation pharmacotherapy[14].

THE EVOLUTION OF DRUG REPURPOSING

Historically, drug repurposing was driven by clinical serendipity, where off-target effects or unexpected therapeutic benefits were observed during trials or post-market surveillance[9]. Examples include thalidomide (from treating morning sickness to becoming a therapy for multiple myeloma) and sildenafil (originally for angina, later repurposed for erectile dysfunction)[11,16]. While impactful, these repurposing events were anecdotal and lacked a systematic discovery framework.
Today, AI-driven drug repurposing has revolutionized the field. Through the application of machine learning, deep neural networks, systems biology, and natural language processing, AI can mine and interpret vast biomedical datasets[12]. These include genomic databases, real- world patient data, adverse drug event registries, and chemical-protein interaction networks[16]. The result is a paradigm shift—from hypothesis-driven exploration to data- driven prediction, where novel indications can be forecasted without prior mechanistic assumptions[6,9].
Traditional drug discovery follows a linear and time-intensive model, often taking 12–15 years and incurring costs exceeding $2.6 billion, with a discouraging success rate of around 10%. In contrast, AI repurposing offers a non-linear, iterative approach—compressing timelines to as little as 1–3 years, reducing costs by up to 90%, and leveraging existing safety data to improve clinical trial success rates[12].
Furthermore, AI enables targeted repurposing for specific patient subgroups, enhancing therapeutic precision and making previously overlooked compounds viable in the treatment of rare, orphan, and emerging diseases[17]. It is this integration of intelligence, speed, and scalability that positions AI as the future of drug repurposing.
Importantly, in low-resource regions, AI enables drug discovery through cost-efficient computational modeling, eliminating the need for expensive wet-lab trials[15,18]. Tools like DeepDrug, CMap, and DrugBank AI have already demonstrated successful case studies that validate these methods. AI also uncovers non-obvious drug mechanisms, including off-target immunomodulatory effects, further widening the scope of potential therapies[14]. By leveraging longitudinal patient data, it predicts both short- and long-term treatment outcomes. As AI evolves to integrate multi-omics,

wearable device data, and real-time biomarkers, its role in drug repurposing is not only transformative—it is inevitable[19].

Table 1: Comparison of traditional drug discovery vs. AI-driven drug repurposing

Parameter	Traditional Drug Discovery	AI-Driven Drug Repurposing
Average time to market	12–15 years	1–3 years
Estimated cost	$2.6–3 billion USD	$300K–40 million USD
Clinical trial success rate	~10–12%	~25–35% (due to prior safety data)
Key strategy	Hypothesis-driven	Data-driven and mechanism-agnostic
Target identification	Laboratory-based, slow	Computational, network- based
Use of real-world data	Minimal	Extensive (EHRs, omics, adverse reports)
Adaptability in emergencies	Low	High (e.g., COVID-19 rapid response)
Innovation cycle	Linear	Iterative and self-improving
Therapeutic scope	Common diseases	Rare, orphan, and emerging diseases
Personalization potential	Limited	High (via AI-based patient stratification)

ROLE OF ARTIFICIAL INTELLIGENCE IN DRUG REPURPOSING

Artificial Intelligence (AI) is transforming the landscape of drug repurposing by bridging the gap between traditional drug discovery and modern, data-driven approaches[18,21]. Historically, drug repurposing relied on clinical observations, trial-and-error, or serendipitous discoveries like sildenafil's shift from a heart disease treatment to a popular erectile dysfunction medication[15]. However, AI has now elevated this practice by enabling the systematic identification of new therapeutic uses for existing drugs, leveraging vast and complex datasets that are far beyond human capabilities to analyze[19].

AI's role in drug repurposing starts with its ability to process and integrate massive, multidimensional data from diverse sources such as genomic, proteomic, transcriptomic, and metabolomic datasets, clinical trial repositories, and even real-world evidence (RWE)[16]. With the help of machine learning (ML) algorithms, AI uncovers hidden relationships between drugs, diseases, and molecular targets that were previously difficult or impossible to predict[11]. This process involves AI's use of advanced computational methods such as deep learning, which mimics the human brain's ability to process complex patterns, allowing for nonlinear predictions about drug efficacy across various diseases[18].

One of AI's core strengths is its ability to create disease-specific models using multilayered data integration, which predicts how existing drugs might interact with different disease mechanisms, particularly in complex and rare diseases[14]. For instance, AI can identify protein-drug interactions by analyzing vast chemical and biological networks, which helps find new indications for old drugs. In this process, AI tools like Graph Convolutional Networks (GCNs) enable the representation of molecules and diseases as graphs, discovering drug- receptor interactions that may have otherwise gone unnoticed[19].

Natural Language Processing (NLP) further accelerates this process by enabling AI to mine and extract actionable insights from the enormous volumes of scientific literature, identifying repurposing opportunities hidden in research papers, clinical trial reports, and patent filings[11,14]. AI can also analyze electronic health records (EHRs) and clinical data to track drug safety profiles and uncover long-term effects in diverse populations, enhancing both the repurposing speed and the personalization of therapies[19].

Another groundbreaking aspect of AI is drug-target prediction. By using Generative Adversarial Networks (GANs) and other generative models, AI can suggest new drug targets and their interactions with potential compounds based on a vast number of chemical, molecular, and biological interactions[13]. This allows researchers to hypothesize and validate repurposing opportunities faster and at a fraction of the cost and time compared to traditional methods[9,16].

AI can also help identify population-specific repurposing strategies. By integrating genomic data with patient demographic information, AI can match repurposed drugs to specific subgroups of patients who are likely to benefit the most, thus facilitating precision medicine in drug repurposing[11]. This helps ensure that repurposed drugs not only work effectively but also minimize side effects in particular populations based on genetic and phenotypic variations.

Furthermore, AI is enhancing the efficiency of clinical trials. It can optimize trial design, predict patient enrollment, identify optimal dosages, and even recommend the most promising biomarkers to track patient responses[23]. AI-powered tools also prioritize drug candidates, highlighting the compounds most likely to succeed in clinical testing based on prior knowledge and existing data, which drastically reduces both development costs and time to market[21].

AI is accelerating the repurposing of drugs not only for common diseases but also for rare and neglected diseases[25]. By mining rare disease databases and combining this information with public molecular and pharmacological databases, AI is enabling the discovery of therapeutic opportunities that were previously limited by small patient populations or lack of research funding[11,24]. In this way, AI empowers global health solutions, enabling researchers to tackle diseases that traditionally received little attention.

In summary, AI is not just a tool but a transformative force in the field of drug repurposing. It amplifies human capabilities, enabling researchers to discover novel therapeutic uses for drugs faster, cheaper, and more precisely than ever before[21]. The combination of big data, machine learning, and computational models is pushing the boundaries of innovation, opening new doors for personalized medicine, and offering a robust framework for solving some of the world's most pressing healthcare challenges[23].

KEY AI TOOLS FOR DRUG REPURPOSING

Artificial Intelligence (AI) platforms have become crucial in revolutionizing drug repurposing efforts. By leveraging the power of machine learning and data analytics, AI enables the identification of new therapeutic indications for existing drugs, drastically reducing the time and costs associated with traditional drug discovery[11]. Below are some of the most prominent AI tools and their applications in repurposing drugs for various diseases:

1. IBM Watson for Drug Discovery

IBM Watson is a widely recognized AI platform that uses natural language processing (NLP) and machine learning to analyze vast biomedical data, including clinical studies and scientific literature, enabling the identification of new drug-disease associations[7]. It's been particularly successful in repurposing drugs for cancer and neurodegenerative diseases.

2. Atomwise

Atomwise employs deep learning algorithms to predict how small molecules will interact with target proteins, leading to the repurposing of existing drugs for new indications[4]. This AI tool has helped in identifying repurposed drugs for Ebola and COVID-19.

3. **Insilico Medicine**Insilico Medicine uses deep learning and generative adversarial networks (GANs) for drug repurposing, focusing on aging-related diseases, cancer, and autoimmune disorders. The platform optimizes drug discovery by predicting the biological activity of molecules[16].
4. **BenevolentAI**

BenevolentAI utilizes machine learning and knowledge graphs to model complex diseases and predict the effectiveness of existing drugs. It has successfully repurposed drugs like Baricitinib for COVID-19 and autoimmune conditions[12].

5. **Exscientia**

Exscientia uses AI-driven drug design to streamline the repurposing of drugs for diseases like cancer and autoimmune conditions, significantly enhancing clinical trial efficiency and reducing drug development timelines[12].

Table 2: Overview of Key AI Tools for Drug Repurposing

Tool Name	**Key Features**	**Example of Drugs Repurposed**
IBM Watson	Uses NLP and ML to analyze biomedical data	Ibrutinib (Cancer), Irinotecan (Neurodegenerative)
Atomwise	Deep learning for molecular interaction prediction	ZMapp (Ebola), potential COVID-19 treatments
Insilico Medicine	Generative AI for drug design and repurposing	Rapamycin (Aging), Olaparib (Cancer)
BenevolentAI	Machine learning and knowledge graphs for modeling	Baricitinib (COVID-19, Autoimmune)
Exscientia	AI drug design to optimize drug repurposing	Lupus treatments, Cancer therapies

CASE STUDY 1: AI IN REPURPOSING DRUGS FOR COVID-19

The COVID-19 pandemic, caused by the SARS-CoV-2 virus, prompted an urgent global effort to identify effective treatments. Given the unprecedented speed at which the virus spread, traditional drug discovery methods, which usually take years, were far too slow[13]. Artificial intelligence (AI) tools, however, revolutionized this process by enabling rapid drug repurposing, thus providing a lifeline in the race to develop effective therapies for COVID-19.

AI platforms like Atomwise, Insilico Medicine, and BenevolentAI utilized machine learning algorithms to analyze vast amounts of data, including viral protein structures, patient demographics, and the molecular properties of existing pharmaceutical compounds[14,19]. These AI systems screened millions of drug compounds for their potential to interact with the SARS-CoV-2 virus, significantly reducing the time required for identifying promising candidates[12].

For example, BenevolentAI utilized AI to identify Baricitinib, a drug originally approved for rheumatoid arthritis, as a potential treatment for COVID-19. Its AI-driven analysis revealed that Baricitinib could block the virus's ability to enter human cells, a breakthrough that led to its expedited clinical evaluation and eventual emergency use authorization by the

FDA[18]. Another major success was Remdesivir, initially developed for Ebola but repurposed for COVID-19 after AI analysis identified its potential to inhibit viral replication. This resulted in Remdesivir being authorized for emergency use to treat COVID-19 patients, marking another AI-driven success story[12].

Furthermore, AI's role extended beyond drug identification to predicting drug efficacy using multi-omics data. AI tools employed network pharmacology to map out the complex interactions between drugs and the virus, helping to refine treatment strategies. Platforms like Exscientia contributed to the development of small molecules specifically targeting the viral spike protein, which plays a crucial role in the virus's ability to infect human cells[11].

The success of AI in repurposing drugs for COVID-19 underscores its transformative potential in drug discovery[18]. AI not only accelerated the identification of therapeutic options but also paved the way for more adaptive and efficient methods in addressing future global health crises. The repurposing of drugs like Baricitinib and Remdesivir proved that AI could significantly shorten the drug development timeline, offering hope for timely solutions during pandemics and other urgent healthcare challenges[11,19].

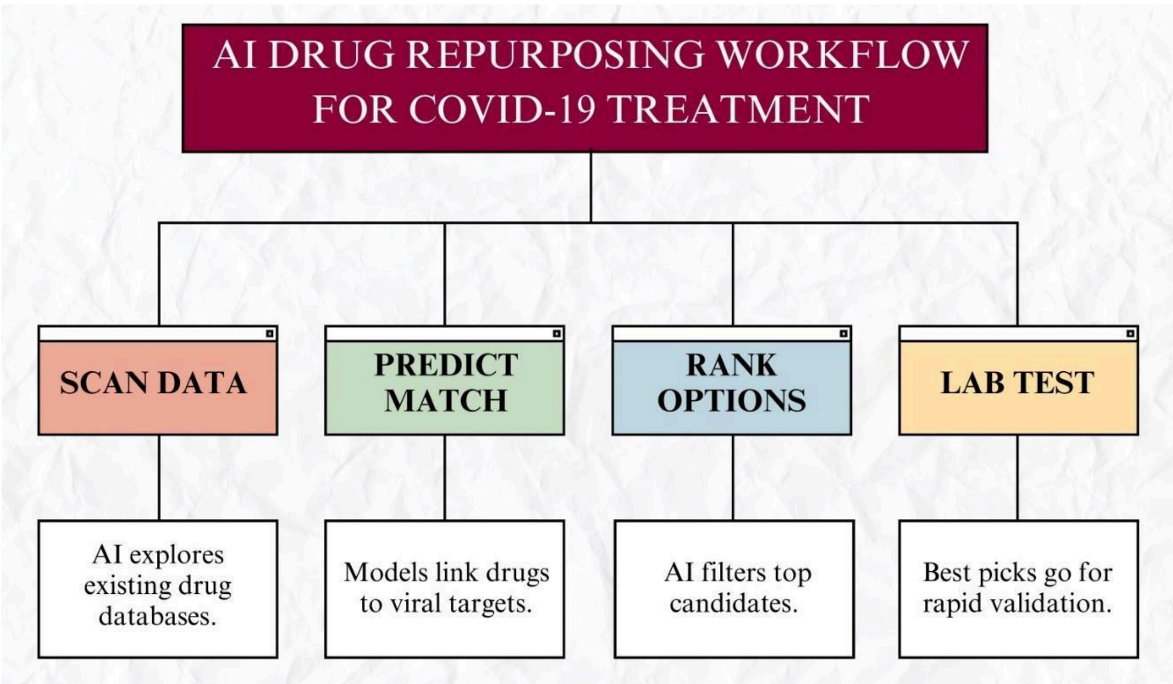

Fig. 1: **AI Drug Repurposing Workflow for COVID-19 Treatment**

CASE STUDY 2: AI IN CANCER DRUG REPURPOSING

The potential of artificial intelligence (AI) in drug repurposing for cancer treatment has revolutionized the oncology landscape[14,18]. Traditional drug discovery processes are lengthy, costly, and often unsuccessful, but AI-based platforms have significantly reduced these challenges by identifying existing drugs that may be effective in treating various cancers. AI tools analyze vast amounts of data from clinical trials, genomic databases, drug interaction profiles, and patient outcomes to uncover hidden relationships between drugs and cancer pathways[10].

One of the most promising aspects of AI in cancer drug repurposing is its ability to predict how existing drugs may interact with cancer cells at a molecular level. AI algorithms are used to analyze and predict gene-drug interactions, protein structures, and biomarkers, all of which are crucial for identifying the potential anticancer properties of existing medications[21,23]. Drugs that were initially developed for other purposes—such as metformin for diabetes or statins for cholesterol management—are now being explored for their possible anticancer effects.

Metformin—a widely used drug for managing type 2 diabetes—has been found to have potential anticancer properties, especially in cancers such as breast, colorectal, and prostate cancers[24]. AI models, including those used by IBM Watson for Drug Discovery, have identified how metformin affects AMP-activated protein kinase (AMPK), a regulator of cellular metabolism and growth. This mechanism suggests that metformin could prevent cancer cell proliferation and metastasis, especially when combined with other therapies[25].

Similarly, statins, which are prescribed to manage cholesterol, have shown promise in lung, breast, and liver cancers[20]. AI-powered platforms like Insilico Medicine use machine learning algorithms to identify how statins inhibit the mevalonate pathway, which is essential for cancer cell survival and growth. These findings have led to new clinical trials investigating statins as adjunct therapies for several cancers[12,18].

Moreover, AI platforms are exploring drugs like sildenafil, originally developed for erectile dysfunction, to treat cancers like prostate and lung cancer[21,24]. Through AI's deep learning capabilities, researchers have uncovered the antiangiogenic potential of sildenafil, inhibiting tumor vascularization, thereby preventing tumor growth and metastasis. Thalidomide, another drug with a controversial history, is being reassessed with the help of AI to treat cancers like multiple myeloma and leukemia, based on its immune-modulatory effects[13].

These case studies underscore how AI can expedite the process of drug repurposing by predicting and validating existing drugs' efficacy for various cancer types. The integration of AI into drug repurposing has not only opened doors for new treatments but also reduced the time, cost, and failure rates associated with traditional drug development, offering hope for faster, more accessible cancer therapies[20].

Table 3 : AI-driven cancer drug repurposing: case studies

Drug Name	**AI Model Used**	**Cancer Types Targeted**
Metformin	IBM Watson for Drug Discovery	Breast, Colorectal, Prostate Cancer
Statins	Insilico Medicine	Lung, Liver, Breast Cancer
Sildenafil	Atomwise	Lung, Prostate Cancer
Thalidomide	BenevolentAI	Multiple Myeloma, Leukemia
Fenofibrate	Deep Genomics	Pancreatic, Liver Cancer

CASE STUDY 3: AI IN NEUROLOGICAL DISEASE TREATMENT

Artificial Intelligence (AI) is emerging as a powerful tool in addressing the complex challenges of neurological diseases[12]. Disorders such as Alzheimer's, Parkinson's, multiple sclerosis, and epilepsy are notoriously difficult to treat due to the intricate nature of the brain and nervous system. These diseases often lack effective treatments, and the search for new therapies is hindered by slow progress, high costs, and complex disease mechanisms[15]. AI, however, offers a transformative solution by rapidly identifying drug repurposing opportunities, predicting disease progression, and personalizing treatment approaches[14].

AI models can analyze large volumes of data from multiple sources such as genomic research, neuroimaging, electroencephalography (EEG) signals, and clinical trials. By identifying hidden patterns in this data, AI can uncover new therapeutic pathways and suggest existing drugs that may have neuroprotective effects[19]. For instance, Parkinson's disease, a neurodegenerative disorder characterized by the progressive loss of dopaminergic neurons, has shown promising results with the repurposing of metformin, a drug typically used for type 2 diabetes. AI systems have analyzed the mitochondrial dysfunction and inflammation pathways in Parkinson's and found that metformin can help mitigate these issues, potentially slowing disease progression[11].

In Alzheimer's disease, AI is enabling the identification of amyloid plaques and tau tangles, two hallmark features of the disease, much earlier than traditional methods. AI algorithms are also being used to predict the potential of donepezil—a widely used drug for Alzheimer's—as a combination therapy to stimulate neurogenesis and enhance cognitive function in patients. AI's ability to predict which existing drugs could slow the progression of these diseases opens new avenues for faster clinical trials and more effective treatments[18].

Additionally, AI tools are being used to address issues in stroke recovery. AI platforms can predict the most effective drug therapies for promoting neuroplasticity and brain regeneration after a stroke[11]. One such drug, N-acetylcysteine (NAC), traditionally used for treating respiratory conditions, is being explored for its potential to reduce oxidative stress in post-stroke patients and protect neuronal tissue from further damage[18].

In epilepsy, AI is enhancing the identification of seizure triggers, which can lead to more personalized drug regimens. For instance, drugs like gabapentin, originally developed for nerve pain, are being investigated for their ability to modulate neuronal excitability and provide better seizure control in epilepsy patients[19,23]. By analyzing patient-specific data through AI- driven models, therapies can be tailored to optimize seizure management, minimizing side effects and improving patient quality of life.

AI's integration into neurological disease treatment offers several key advantages, including the ability to identify novel therapeutic options, reduce time-to-market for drug repurposing, and personalize therapies based on individual patient profiles[22]. Through its ability to analyze massive datasets and predict outcomes more efficiently than traditional methods, AI is poised to make a significant impact on the treatment of some of the world's most challenging neurological diseases[21].

BENEFITS OF AI IN DRUG REPURPOSING

The integration of Artificial Intelligence (AI) into the field of drug repurposing offers a multitude of transformative benefits, significantly altering the traditional approach to drug discovery and development. As the world faces pressing global health challenges, AI's ability to accelerate the process of identifying new uses for existing drugs provides both economic and clinical advantages. Here are several unique benefits of using AI in drug repurposing:

1. **Accelerated Drug Development**: AI algorithms can sift through vast datasets, including molecular structures, patient data, clinical trials, and genetic information, at speeds unimaginable for human researchers[12,19]. This capability dramatically reduces the time needed to identify viable repurposing candidates, often cutting the process from years to months. By leveraging historical clinical data and known drug profiles, AI systems can predict the efficacy of existing drugs for new diseases, eliminating much of the lengthy trial-and-error process typical of traditional drug discovery[17].
2. **Cost-Efficiency**: Drug repurposing, by nature, is a cost-effective approach compared to developing new drugs from scratch. AI enhances this by predicting the most promising drug candidates with precision, avoiding

unnecessary investments in drug candidates that are less likely to succeed. By reducing research and development (R&D) costs, AI provides a more cost-efficient pathway to market, especially important when dealing with rare diseases or urgent global health crises, such as pandemics[11].

3. **Improved Success Rates**: Traditional drug discovery faces a high failure rate, especially during clinical trials. However, AI's ability to analyze comprehensive data sets, including biological, pharmacological, and clinical datasets, significantly improves the likelihood of success[20]. AI's predictive models can identify off-target effects, drug-disease interactions, and patient-specific responses, leading to more informed, targeted treatment options and a higher probability of success in clinical trials[21].
4. **Enhanced Precision Medicine**: AI's power lies in its ability to analyze patient-specific data, including genetic profiles, comorbidities, and prior drug responses[15]. This allows for personalized medicine, where drug repurposing can be tailored to individual patients or specific subpopulations[21]. AI-driven insights can identify which drugs, when repurposed, will be most effective for specific genetic variants or disease phenotypes, resulting in better patient outcomes and fewer adverse effects[25].
5. **Targeting Unmet Medical Needs**: AI's data-crunching capabilities enable the identification of drug repurposing opportunities for diseases with no current treatment options or where existing therapies are insufficient[19]. For example, AI has been used to find repurposed drugs for rare diseases, antimicrobial resistance, and even emerging infectious diseases like COVID-19, where conventional drug discovery might take too long to meet urgent medical needs[7,19]. By analyzing patterns across multiple data points, AI can pinpoint potential treatments that would otherwise go unnoticed.
6. **Optimizing Clinical Trials**: AI can optimize the clinical trial process by identifying the most appropriate candidates for specific trials. Through predictive analytics, AI can streamline patient recruitment by matching participants based on their genetic makeup, disease subtype, and medical history[12]. This not only improves the efficiency of trials but also increases the likelihood of success, as patient populations are more accurately aligned with the drug being tested.
7. **Repurposing Existing Drugs for Drug-Resistant Diseases**: AI has a unique role in combating the rise of drug-resistant diseases, particularly in areas like antibiotics and cancer therapies. AI models can analyze historical data from drug resistance patterns and propose novel uses for existing drugs[4,8]. For example, metformin, commonly used for diabetes, has shown promise in repurposing for cancer treatment due to its ability to modulate cellular metabolism, offering a new approach to overcoming resistance in chemotherapy[19].
8. **Speed in Pandemic Response**: AI's role in rapid drug repurposing was particularly evident during the COVID-19 pandemic. AI technologies rapidly identified existing antiviral drugs such as remdesivir and chloroquine for potential use in COVID-19 treatment by analyzing global databases of drug properties and known viral pathways. This swift action demonstrated how AI can be pivotal in responding to global health emergencies by quickly finding potential therapies from the already available drug arsenal[11].
9. **Cross-Disciplinary Insights**: One of the unique advantages of AI is its ability to integrate insights from various disciplines, such as genetics, pharmacology, biochemistry, and data science. This enables a holistic view of drug-disease interactions, which is essential for successful drug repurposing[18]. AI platforms like Insilico Medicine and Atomwise combine biological data with computational models, offering an interdisciplinary approach to discover new therapeutic indications for old drugs[11].
10. **Regulatory Efficiency**: Regulatory approval processes for repurposed drugs are generally less time-consuming than for new drug molecules, as these drugs have already passed safety assessments[11,18]. AI accelerates this further by identifying repurposing candidates that are already well-characterized in terms of their pharmacokinetics and toxicity profiles, making it easier for regulators to assess their potential in new

indications. AI can also predict potential regulatory hurdles by assessing compliance with existing safety guidelines, allowing for smoother regulatory approval[19].

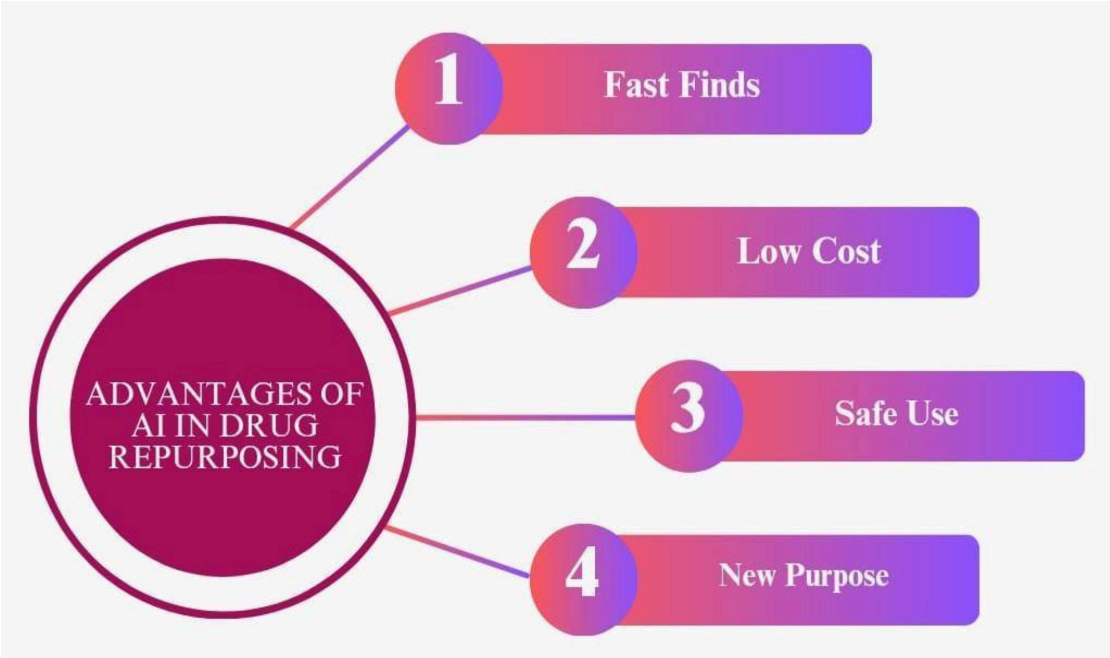

Fig. 2: **Advantages of AI in Drug Repurposing**

CHALLENGES AND LIMITATIONS OF AI IN DRUG REPURPOSING

Despite the transformative potential of Artificial Intelligence (AI) in drug repurposing, its widespread adoption is not without significant challenges and limitations. The integration of AI into the drug discovery and repurposing processes presents a complex landscape filled with technical, ethical, and regulatory obstacles[15]. Understanding these challenges is crucial for advancing AI-driven drug repurposing from an experimental phase to a more robust and reliable application. Below are some of the key challenges:

1. **Data Quality and Availability**: AI's effectiveness depends heavily on the quality and volume of data it can access[15]. The success of AI models is directly tied to the availability of high-quality, comprehensive datasets that span genetic, clinical, pharmacological, and demographic information. Unfortunately, such data is often siloed, incomplete, or fragmented across institutions, making it difficult for AI to derive accurate and actionable insights. Furthermore, unstructured data, such as clinical notes or medical images, can be challenging to process and require advanced AI techniques to interpret effectively[18].
2. **Bias in AI Models**: One of the major concerns with AI is the bias embedded in training data. AI systems are only as unbiased as the data they are trained on. If the data lacks diversity, the AI model may produce skewed results that are not applicable to all populations, particularly marginalized or underserved groups[18]. This is a significant concern in drug repurposing, as biased algorithms may fail to identify effective treatments for specific genetic profiles or ethnic groups, potentially exacerbating healthcare disparities[11].
3. **Interpretability of AI Models**: While AI models, especially deep learning algorithms, can provide highly accurate predictions, they often operate as "black boxes," meaning their decision-making processes are not

transparent[4,18]. This lack of interpretability can be problematic when healthcare providers and regulators need to understand how a particular drug was repurposed for a new indication. In drug repurposing, understanding the underlying rationale for the AI's predictions is crucial for building trust among clinicians, patients, and regulatory bodies[15].

4. **Regulatory Hurdles**: The regulatory landscape for AI-driven drug repurposing is still in its infancy, and many regulatory bodies have yet to establish clear guidelines for approving AI-based repurposing approaches[11]. The FDA and EMA, for example, are cautious in their approval of AI-based methodologies for drug repurposing, especially given the potential for unforeseen side effects or interactions when drugs are repurposed for conditions they were not originally designed to treat. Regulatory bodies need to define protocols for validating AI predictions and ensuring the safety and efficacy of repurposed drugs[13].
5. **Complexity of Disease Mechanisms**: Diseases such as cancer, neurological disorders, and autoimmune conditions often have complex, multifactorial mechanisms that are not easily modeled by AI. Drug repurposing efforts are limited by the lack of comprehensive understanding of the pathophysiology of many diseases. For instance, the heterogeneity of diseases like Alzheimer's disease complicates AI's ability to pinpoint which existing drugs will be effective across all patients[7-8]. AI can struggle with diseases that have multiple etiologies or high genetic diversity among patients.
6. **Lack of Standardization**: In drug discovery, data standardization is a critical issue. Different institutions, researchers, and databases may use inconsistent methods for storing and sharing data, resulting in difficulties for AI systems to integrate and analyzedata effectively[17]. For drug repurposing, standardization of drug-related data, such as dosage forms, chemical structures, and clinical outcomes, is essential for ensuring that AI systems can produce reliable and reproducible results.
7. **Ethical and Legal Concerns**: The application of AI in drug repurposing raises several ethical and legal questions. For example, how should intellectual property rights be managed when a repurposed drug is found through AI, especially if the original patent holder of the drug is different from the AI developers? Moreover, informed consent for the use of patient data in AI-driven studies needs to be addressed, particularly when personal and health information is involved in training AI models. Additionally, data privacy concerns, especially regarding sensitive health data, must be handled with extreme care[11-12].
8. **Integration with Existing Healthcare Systems**: For AI-driven drug repurposing to be truly effective, it must integrate seamlessly into existing healthcare systems, including pharmaceutical R&D pipelines, clinical workflows, and patient management systems[11,18]. Many healthcare institutions lack the infrastructure needed to adopt AI technologies effectively. The interoperability of AI systems with different platforms, including electronic health records (EHR) and drug development databases, remains a challenge[17].
9. **Over-reliance on AI Predictions**: While AI has shown great promise in drug repurposing, there is a risk of over-relying on its predictions[12]. AI should be viewed as a complementary tool rather than a replacement for human expertise. There is still the need for expert validation to ensure the AI's findings are clinically relevant. Over- reliance on AI could lead to misguided repurposing efforts or failure to consider other critical aspects of drug development, such as long-term safety and patient-centered outcomes[23,25].
10. **Cost of Implementation**: While AI promises to reduce long-term costs associated with drug discovery, the initial investment in AI infrastructure, including data collection, training models, and hiring AI specialists, can be prohibitively expensive for smaller pharmaceutical companies and academic institutions[21]. The costs associated with obtaining high-quality data, validating AI models, and ensuring compliance with regulatory standards may outweigh the immediate benefits, particularly in the early stages of drug repurposing[12].

ETHICAL CONSIDERATIONS IN AI-DRIVEN DRUG REPURPOSING

AI-driven drug repurposing presents numerous ethical challenges that must be addressed to ensure its responsible and equitable use in healthcare[11]. A primary concern is data privacy. With the use of sensitive patient data, the risk of unauthorized access and misuse increases. Ensuring robust data protection measures, such as encryption and anonymization, is vital to safeguarding patient confidentiality[19]. Additionally, informed consent becomes crucial, as patients need to understand how their health data will be used in AI systems for drug repurposing.

Another ethical issue is bias in AI models[14]. If AI systems are trained on biased or incomplete datasets, the resulting drug repurposing suggestions could lead to discriminatory outcomes, with certain groups being overlooked or harmed[17]. Ensuring diversity and representation in training data is necessary to avoid such disparities. Furthermore, AI-driven repurposing can sometimes expedite drug development, bypassing certain clinical trial stages, raising questions about whether the repurposed drugs have been sufficiently tested for safety and efficacy[15]. Clear regulatory oversight is essential to ensure that safety standards are maintained.

Lastly, accountability in the case of adverse events is a concern. If AI systems cause harm, it may be unclear who is responsible—whether it is the developers of the AI model, the healthcare providers, or the pharmaceutical companies. This ambiguity calls for clear legal frameworks to address liability and accountability[15].

Table 4 : Ethical Issues in AI-Driven Drug Repurposing

Ethical Issue	**Impact**
Data privacy and security	Risk of data breaches and unauthorized access to sensitive patient information.
Bias in AI models	Potential for AI models to make biased decisions, leading to unfair treatment outcomes.
Informed consent	Patients may not fully understand how their data is used in the AI-driven drug repurposing process.
Regulatory approval	Risk of bypassing crucial clinical trials, compromising safety and efficacy testing of repurposed drugs.
Accountability	Uncertainty about responsibility when AI-driven repurposing leads to negative health outcomes.

FUTURE DIRECTIONS IN AI-DRIVEN DRUG REPURPOSING

The future of AI-driven drug repurposing holds vast potential, transforming the landscape of pharmaceutical development and healthcare[11,18]. As AI technology continues to advance, we can expect more sophisticated models that can analyze multidimensional data—from genomics and proteomics to clinical trial results and patient records[13]. This deeper data integration will lead to more accurate predictions for potential repurposed drugs, helping to identify therapies that were previously overlooked. In particular, multimodal AI—the use of different types of data such as images, genetic sequences, and electronic health records—will offer a comprehensive approach to finding new uses for existing drugs[23].

One of the most promising future trends is the use of deep learning algorithms in personalized medicine. By leveraging AI to examine an individual's genetic makeup, lifestyle factors, and medical history, repurposed drugs can be tailored to match the unique needs of individual patients. This could result in faster, safer, and more effective treatment options, improving patient outcomes and reducing side effects[22].

Additionally, the integration of AI with real-world data (RWD) from wearables and patient- reported outcomes will allow AI systems to continuously monitor the effectiveness of repurposed drugs in real-world conditions, making it easier to identify successful therapies post-market[21]. This real-time data will drive adaptive clinical trials, reducing the time and cost of traditional clinical testing.

Furthermore, AI models will likely evolve to assess drug interactions and synergy, enabling the discovery of new combination therapies that can be more effective than individual drugs alone[22,25]. This could dramatically expand the scope of repurposing, allowing for multi- drug treatments that are customized for complex conditions like cancer and chronic diseases.

The collaboration between AI developers, pharma companies, and regulatory bodies will also be crucial to ensure that the process remains ethically sound, adheres to safety standards, and accelerates the regulatory approval of repurposed drugs. The future of AI in drug repurposing promises not only to reduce development costs and time but also to broaden the therapeutic landscape for many unmet medical needs, offering patients quicker access to life-saving treatments[21-22].

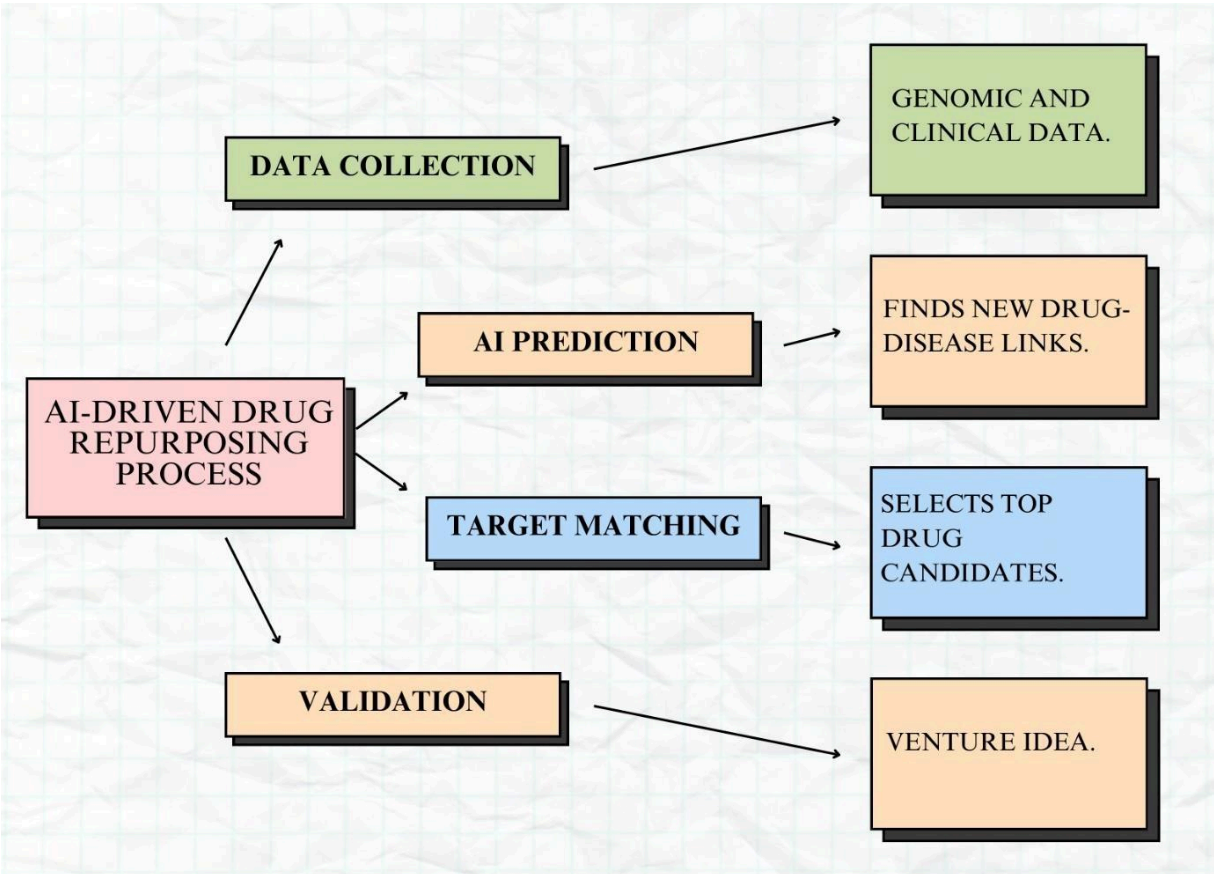

Fig . 3: AI-Driven Drug Repurposing Process

CONCLUSION

Artificial Intelligence (AI) is revolutionizing drug repurposing by accelerating the identification of new uses for existing drugs, drastically reducing time and costs compared to traditional methods. Through advanced data analysis, predictive modeling, and machine learning, AI offers unprecedented efficiency in finding treatments for complex diseases, from COVID-19 to cancer and neurological disorders. The ability to repurpose drugs quickly makes AI a vital tool in addressing urgent global health challenges and provides a more personalized, targeted approach to treatment.

Despite its potential, AI-driven drug repurposing faces challenges such as data quality, algorithmic biases, and regulatory hurdles. These obstacles need careful consideration and robust solutions to ensure the technology's safe and equitable application. Looking to the future, AI's integration with genomics and personalized medicine will likely lead to more precise, cost-effective treatments, reshaping the landscape of healthcare. The continuous advancement of AI in drug discovery promises a transformative shift, offering hope for faster, more accessible, and effective therapies worldwide.

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