

AI-DRIVEN DRUG REPURPOSING: TRANSFORMING MODERN DRUG DISCOVERY

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- Abstract

Drug repurposing has been a successful method for finding novel therapeutic uses for already-approved medications while cutting down on the time, expense, and risk involved in traditional drug research. Drug repurposing has changed dramatically as a result of recent developments in artificial intelligence (AI), which make it possible to analyse large-scale biological and pharmacological databases quickly. The prediction of drug–target interactions, therapeutic efficacy, and illness correlations has increased thanks to AI-based techniques like machine learning, deep learning, natural language processing, network pharmacology, and molecular docking. These computational methods assist precision medicine strategies, speed up compound screening, and lower drug development failure rates.

AI-driven medication repurposing has shown promise in treating a number of illnesses, including cancer, Parkinson's disease, Alzheimer's disease, uncommon disorders, and viral infections like COVID-19. AI-assisted pharmaceutical research is further supported by publicly accessible databases and bioinformatics tools like DrugBank, PubChem, ChEMBL, and Open Targets, which offer a wealth of chemical, biological, and clinical data for target discovery and predictive modelling.

Notwithstanding these developments, a number of obstacles still exist, including as inadequate clinical validation, algorithm bias, poor data quality, regulatory obstacles, and ethical issues with accountability, privacy, and transparency. AI-assisted drug repurposing and precision treatments are anticipated to be significantly improved by upcoming advancements in generative AI, digital twin technology, personalized medicine, and multi-omics integration. All things considered, AI has enormous potential to transform contemporary medication research and hasten the creation of secure, efficient, and customized treatment approaches.

- Keywords

Artificial intelligence; Drug repurposing; Machine learning; Deep learning; Precision medicine; COVID-19.

- Introduction:

It generally requires more than a decade or so and billions of dollars to move a novel medication molecule from laboratory research to clinical use. drug discovery and development is a time-consuming, costly process. Because of problems with efficacy, safety, pharmacokinetics, and toxicity, the overall success rate of conventional drug development is still quite low despite notable advances in pharmaceutical sciences^[1]. As a result, there is a growing need for alternate approaches that can lower overall costs and failure rates while speeding up therapeutic development. Drug repurposing, sometimes referred to as drug repositioning, has

become a viable method for finding novel therapeutic uses for already available or previously authorised medications ^[2].

Drug repurposing, in contrast to typical de novo drug discovery, makes use of molecules that already have documented pharmacokinetic, pharmacodynamic, and safety properties, greatly cutting down on the time and cost of medication development ^[3]. The therapeutic and financial potential of this strategy has been shown by a number of successful instances of repurposed medications, such as minoxidil, sildenafil, and thalidomide ^[2]. Drug repurposing techniques have been further transformed by recent developments in computational biology, bioinformatics, and data science. The ability of Artificial Intelligence (AI) to analyse large-scale biological datasets, predict drug–target interactions, find disease biomarkers, and more quickly and accurately optimise therapeutic candidates has drawn a lot of attention ^[4].

In order to find hidden therapeutic relationships that might not be found using traditional techniques, machine learning (ML) and deep learning (DL) algorithms can process complex biological and chemical data derived from genomics, proteomics, transcriptomics, electronic health records, and molecular databases ^[5]. Several computational techniques, such as network-based pharmacology, molecular docking, virtual screening, natural language processing, and predictive modelling, are integrated into AI-driven drug repurposing ^[6]. These methods have significantly increased the effectiveness of finding new uses for currently available medications in a variety of therapeutic domains, including cancer, neurological disorders, cardiovascular diseases, infectious diseases, and uncommon genetic abnormalities ^[7]. Additionally, AI-based models can continuously learn from freshly created datasets, improving prediction accuracy and lowering the likelihood of late-stage clinical failure ^[4].

The COVID-19 pandemic brought to light the vital significance of quick treatment discovery and greatly pushed the use of AI in medication repurposing research. Several computational techniques were used during the pandemic to find possible therapeutic candidates against SARS-CoV-2, which resulted in the quick investigation into medications like Baricitinib and Remdesivir ^[8]. By examining molecular interactions, biological pathways, and clinical records, AI-assisted platforms made it possible to quickly screen thousands of compounds, proving the usefulness of AI-driven repurposing techniques in times of public health emergency ^[9]. Despite these developments, a number of obstacles still prevent AI from being widely used in medication repurposing. Major challenges still include problems with data quality, algorithm interpretability, lack of standardised datasets, regulatory issues, and inadequate clinical validation ^[10]. Furthermore, before widespread clinical adoption can be accomplished, ethical issues with data privacy and algorithmic bias must to be carefully taken into account. However, in the near future, it is anticipated that the combination of AI with systems biology, precision medicine, and multi-omics technologies would further revolutionise contemporary drug development and customised treatment ^[4].

Thus, the goal of this study is to go over the basic ideas, computational techniques, uses, benefits, drawbacks, and prospects for AI-driven medication repurposing. Recent developments in deep learning and machine learning techniques that are influencing pharmaceutical research and therapeutic innovation are also highlighted in the review.

- Drug Repurposing

Drug repurposing, sometimes referred to as drug repositioning, is the process of finding novel therapeutic applications for currently available or previously authorised medications. Because it lowers the time, expense, and risk involved in creating new therapeutic compounds, this method has drawn a lot of interest as an alternative to traditional drug discovery ^[2]. Repurposed pharmaceuticals already have proven safety, pharmacokinetic, and pharmacodynamic profiles, enhancing the possibility of effective therapeutic application. Conventional drug development is a time-consuming and costly procedure with significant failure rates during

clinical trials^[3]. Sildenafil, Thalidomide, and minoxidil are a few well-known examples that show how effective drug repurposing techniques may be both clinically and commercially^[2,3].

1. Drug Repurposing Types

The two main categories of drug repurposing strategies are on-target and off-target. When a medication is repurposed on-target, it functions on the same biological target but is used to treat a different illness^[1]. On the other hand, off-target repurposing involves the medicine interacting with an alternative biological target to generate novel therapeutic outcomes^[1]. Drug rescue is another significant category in which previously shelved or stopped medications are reassessed for potential new clinical uses^[1]. These methods have increased treatment options for a number of illnesses, such as cancer, infectious diseases, neurological issues, and cardiovascular ailments.

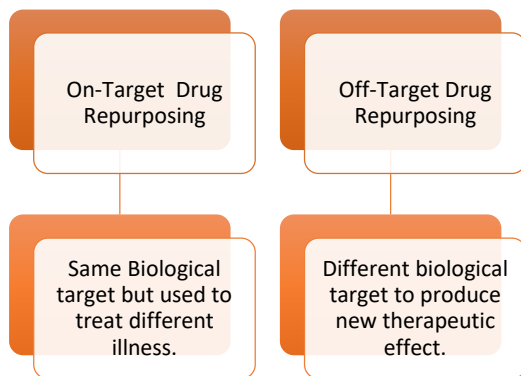


TABLE I: TYPES OF DRUG REPURPOSING

2. Methods for Repurposing Drugs

Drug repurposing research has been greatly accelerated by recent developments in computational biology, bioinformatics, and systems pharmacology. Molecular docking, virtual screening, network pharmacology, gene-expression analysis, and target prediction models are examples of contemporary methods^[6]. Researchers can use large-scale biological information and computational tools like the Connectivity Map to find connections between medications, genes, and diseases^[11]. In a similar vein, target-based prediction algorithms have made it easier to find new drug-target interactions for currently available therapeutic medicines^[12]. The efficiency and accuracy of discovering possible repurposed medication candidates have been substantially enhanced by the incorporation of machine learning and artificial intelligence tools^[4,5].

3. Benefits of Repurposing Drugs

Compared to conventional drug discovery techniques, drug repurposing has a number of benefits. The probability of failure during clinical development is much decreased because repurposed medications already have established safety and toxicity profiles^[1]. Furthermore, compared to de novo drug discovery, the development timeline and total cost are significantly reduced^[2]. Rapid therapeutic responses during public health catastrophes are also made possible by drug repurposing, as was shown during the COVID-19 pandemic, when numerous licensed medications were quickly tested for antiviral efficacy^[9].

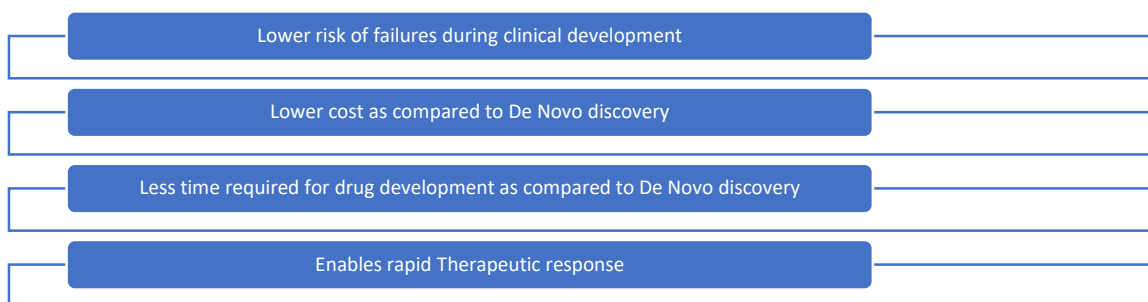


TABLE II: BENEFITS OF DRUG REPURPOSING

4. Restrictions and Difficulties

Drug repurposing has a number of drawbacks and difficulties despite its benefits. Regulatory constraints, insufficient clinical proof, intellectual property concerns, and a lack of comprehension of intricate drug-target interactions continue to be significant challenges ^[10]. Furthermore, before medicinal approval may be obtained, computational predictions frequently need substantial experimental and clinical validation ^[6]. However, it is anticipated that ongoing developments in systems biology, artificial intelligence, and precision medicine will significantly improve the efficacy and dependability of medication repurposing techniques in contemporary pharmaceutical research ^[4].

- Artificial Intelligence in Drug Discovery

1. Basic Concepts of Artificial Intelligence:

Artificial intelligence (AI) is the simulation of human intelligence by computer systems that can perform tasks like learning, reasoning, pattern recognition, prediction, and decision-making. In the pharmaceutical sciences, AI has emerged as a revolutionary technology that speeds up various stages of drug discovery and development, such as target identification, lead optimisation, toxicity prediction, clinical trial design, and drug repurposing ^[4]. Consequently, AI-based computational approaches offer a quicker and more accurate prediction models ^[13]. In order to identify hidden relationships and generate predictive models with improved accuracy, AI systems can analyse large amount of pharmacological, clinical, chemical and biological data ^[5]. Modern pharmaceutical research and precision medicine techniques have greatly benefited from the integration of AI with bioinformatics, systems biology, and big data analytics ^[4,5].

2. Machine Learning:

One important area of artificial intelligence is machine learning (ML), which allows computers to learn from datasets and enhance their predictive capabilities without the need for explicit programming ^[5]. In drug development, machine learning techniques are widely used to predict drug-target interactions, identify bioactive molecules, optimise pharmacokinetic features, and detect adverse drug reactions ^[14]. Support vector machines, random forests, decision trees, k-nearest neighbours, and naive Bayes classifiers are popular machine learning methods ^[5]. Large chemical and biological datasets can be processed effectively by these algorithms in order to identify patterns linked to treatment activity and the advancement of disease ^[15]. In virtual screening and quantitative structure-activity relationship (QSAR) research, machine learning algorithms are especially useful in predicting the biological activity of drugs based on structural features and molecular descriptors ^[4]. Additionally, by discovering possible new indications for currently available medications through the examination of molecular pathways, gene-expression profiles, and clinical datasets, ML-based algorithms have increased the effectiveness of drug repurposing ^[14]. Machine learning has become a vital technique in contemporary computational drug development due to its capacity to continuously increase prediction accuracy with growing data availability ^[5].

3. Deep learning (DL):

Deep Learning is a powerful subset of machine learning that processes extremely complicated and high-dimensional datasets using multi-layered artificial neural networks ^[7]. By automatically extracting pertinent features from unprocessed data, deep learning algorithms improve prediction performance and eliminate the need for human feature engineering. Deep learning has shown impressive results in de novo drug discovery, virtual screening, toxicity assessment, medication repurposing, and molecular property prediction in pharmaceutical research ^[16]. Deep learning algorithms may accurately find possible therapy possibilities by analysing a variety of biological information, such as proteomics, transcriptomics, genomes, and imaging data ^[7]. Convolutional neural networks (CNNs), recurrent neural networks (RNNs), and graph neural networks (GNNs) are examples of advanced architectures that have greatly improved AI systems capacity to forecast molecular interactions and biological processes ^[18]. The usefulness of deep learning in emergency pharmaceutical discovery was demonstrated during the COVID-19 pandemic when generative deep learning models were used to quickly find possible antiviral drugs targeting SARS-CoV-2 proteins ^[17].

4. The Neural Network:

Computational systems termed artificial neural networks (ANNs) draw influence from the composition and operation of the human nervous system. These networks, which process information and produce prediction outputs, are made up of interconnected neurones organised into input, hidden, and output layers ^[18]. As the neural networks can represent intricate nonlinear interactions between chemical compounds, biological targets, and therapeutic responses, they have grown in significance in pharmaceutical research ^[13]. Neural networks are extensively used in drug development for QSAR modelling, drug toxicity prediction, biomarker identification, protein structure prediction, and molecular interaction analysis ^[7]. While RNNs are used in sequence-based analyses like protein and genomic data interpretation, CNNs are very helpful for image-based analysis and molecular structure recognition ^[18]. Faster identification of promising therapeutic candidates has been made possible by the development of advanced neural network designs, which have significantly increased the accuracy and efficiency of computational drug discovery processes.

5. Natural Language Processing:

A subfield of artificial intelligence called natural language processing (NLP) makes it possible for computers to comprehend, analyse, and derive useful information from textual data and human language. By enabling automated information extraction from scientific literature, electronic health records, clinical trial databases, and pharmacovigilance reports, natural language processing (NLP) plays an important role in pharmaceutical and biomedical research ^[19]. NLP-based systems assist researchers in effectively identifying drug–disease connections, adverse drug responses, therapeutic targets, and clinical outcomes from massive text databases due to the continuously growing body of biological literature ^[20]. Deep learning techniques are used by advanced NLP models like BioBERT to enhance biomedical text mining and information retrieval ^[20]. These models support evidence-based medication discovery and repurposing studies by accurately analysing complicated medical terminology and contextual interactions. In order to improve automated literature scanning, clinical decision-making, and knowledge extraction in the pharmaceutical sciences. NLP technologies have also been combined with machine learning and deep learning frameworks ^[19]. NLP is anticipated to become more significant in AI-driven drug development and precision medicine as biomedical data continues to rise at an exponential rate.

Sections	Key Concepts Covered	Main AI Techniques/Applications
Basic Concepts of Artificial Intelligence	Definition of AI, role in pharmaceutical sciences, AI in drug discovery and development, integration with bioinformatics and big data	Data analysis, predictive modelling, target identification, lead optimization, toxicity prediction
Machine Learning	Fundamentals of ML, learning from datasets, prediction models, QSAR studies	Support Vector Machine (SVM), Random Forest, Decision Trees, Naïve Bayes, virtual screening, drug–target interaction prediction
Deep Learning	Advanced subset of ML, multilayer neural networks, automated feature extraction	Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), Graph Neural Networks (GNNs), de novo drug design, molecular property prediction
Neural Networks	Structure and function of ANNs, computational models inspired by the human brain	ANN, CNN, RNN, QSAR modelling, toxicity prediction, biomarker identification
Natural Language Processing	Extraction and interpretation of biomedical text data, AI-based text mining	Literature mining, clinical data extraction, pharmacovigilance, BioBERT, biomedical language models
Applications in Drug Discovery	AI-assisted pharmaceutical research and therapeutic discovery	Drug repurposing, virtual screening, toxicity prediction, precision medicine, target identification
COVID-19 Applications	AI use during pandemic for rapid therapeutic discovery	Generative deep learning, antiviral drug prediction, SARS-CoV-2 target analysis
Advantages of AI in Drug Discovery	Faster analysis, improved accuracy, reduced development cost and time	Big data handling, automated prediction systems, computational screening
Challenges and Limitations	Data quality, model interpretability, clinical validation, algorithm bias	Validation of AI models, ethical concerns, reliability issues

TABLE III: SUMMARY OF THE SECTION ‘ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY’

- AI Techniques used in drug repurposing

1. Machine learning algorithms:

A key component of AI-driven drug repurposing is machine learning (ML) algorithms, which make it possible to systematically analyse massive biological and chemical datasets in order to find new drug–target and drug–disease correlations^[5]. In pharmaceutical research, supervised learning methods like Random Forest, Support Vector Machine (SVM), and Decision Trees are frequently employed for classification, regression, and pattern recognition tasks^[5,14]. To more accurately forecast possible therapy possibilities, these algorithms can process a variety of data sources, such as molecular descriptors, gene-expression profiles, protein interaction data, and clinical records^[14]. While SVMs are frequently employed for classification issues requiring complicated biological data, Random Forest models are especially good at managing high-dimensional datasets and minimising overfitting. Decision tree-based methods are appropriate for early-stage drug screening because of their interpretability and simplicity of use^[15]. ML methods are also widely used in virtual screening, pharmacokinetic and toxicity profile prediction, and quantitative structure–activity relationship (QSAR) modelling^[5]. The identification of repurposable pharmaceuticals has been greatly accelerated and decision-

making in drug discovery pipelines has been enhanced by the integration of machine learning algorithms with huge biomedical databases.

2. Deep Learning (DL):

Multi-layered neural networks are used by deep learning (DL), to simulate complex nonlinear interactions in high-dimensional datasets ^[7]. By enabling automatic feature extraction and removing the need for manual data pre-treatment, deep learning algorithms have completely transformed drug repurposing ^[16]. These models can increase prediction efficiency and accuracy by learning complex patterns from large-scale datasets like transcriptomics, proteomics, genomes, and chemical structures ^[7].

While Recurrent Neural Networks (RNNs) are useful for processing sequential data, such as protein sequences and gene-expression time series, Convolutional Neural Networks (CNNs) are frequently utilized for evaluating molecular structures, chemical pictures, and spatial biological data ^[7,18]. Graph Neural Networks (GNNs), which consider atoms and bonds as nodes and edges, respectively, have become effective methods for modelling chemical structures as graphs in more recent times ^[21]. By incorporating intricate structural and relational data, GNNs facilitate precise prediction of drug-target interactions and drug-disease relationships.

Additionally, deep learning has demonstrated promise uses in pharmacological property prediction, de novo drug development, and the discovery of new therapeutic applications ^[16]. The ability of AI systems to quickly build and repurpose medications has been significantly improved by the use of generative deep learning models, particularly in response to newly emerging disorders like COVID-19 ^[8,17].

3. Network based approaches:

In order to comprehend the complex connections between biological elements including genes, proteins, pathways, and illnesses, network-based techniques are frequently used in drug repurposing ^[6]. To find possible therapeutic options, these techniques make use of biological networks, such as drug–target interaction networks, gene regulatory networks, and protein–protein interaction (PPI) networks ^[22]. Researchers can forecast new drug-disease connections and identify underlying illness mechanisms by examining network structure, connectivity, and proximity ^[22].

When dealing with complicated and multifactorial disorders that include several molecular targets, network pharmacology is essential. These methods make it possible to find important hubs or nodes in biological networks that may be useful targets for medications ^[6]. Finding synergistic drug combinations is made easier and predictive accuracy is further improved by combining network-based approaches with machine learning and deep learning techniques ^[22]. Furthermore, by mapping relationships between medications, targets, and disease pathways, network-based models have been effectively used in drug repurposing studies for infectious illnesses, cancer, and neurodegenerative conditions ^[1,6]. These methods aid in the creation of multi-target treatment approaches and offer a systems-level understanding of pharmacological action.

4. Molecular Docking:

A popular structure-based computational method for predicting the binding affinity and interaction between a pharmacological molecule and its target protein is called Molecular Docking. It is essential for verifying possible medication candidates found using AI and machine learning techniques ^[23]. By examining the binding modalities, interaction energies, and stability of drug–target complexes, docking studies shed light on the molecular processes of pharmacological action ^[24]. Molecular docking is often used in conjunction with virtual screening approaches in drug repurposing to assess huge libraries of current medications and rank candidates according to how well they bind to particular targets ^[23]. This method expedites the discovery of prospective medicinal drugs and greatly minimizes the requirement for lengthy experimental screening. Also, docking

studies can help in understanding off-target interactions, which are crucial for recognizing new therapeutic applications of existing medication ^[24].

The association of molecular docking with AI-based predictive models improves the reliability of drug repurposing techniques by combining structural and data-driven insights.

5. Bioinformatics Integration:

Large-scale biological datasets may be collected, processed, and analysed because of bioinformatics integration, which is essential to AI-driven medication repurposing ^[6]. In order to comprehend disease mechanisms and find therapeutic targets, modern drug discovery significantly depends on bioinformatics resources including genomes, proteomics, transcriptomics, and metabolomics data. While tools like the Connectivity Map allow the detection of medication-disease links based on gene-expression profiles, databases like Drug Bank offers extensive information on drug structures, modes of action, and pharmacological qualities ^[11,25]. Similarly, by offering insights into molecular interactions and biological pathways, protein-protein interaction databases like STRING support network-based analysis ^[6]. Researchers can merge disparate datasets, identify significant trends, and create prediction models for drug repurposing by combining bioinformatics tools with AI techniques ^[6].

- Applications of AI-Based Drug Repurposing:

1. Cancer:

Because of its complicated pathophysiology, genetic variability, multidrug resistance, and high recurrence rates, cancer is one of the top causes of death globally and continues to pose a significant challenge to contemporary healthcare. For successful development and regulatory approval, conventional anticancer drug research frequently takes more than ten years and requires a significant financial investment. Additionally, a lot of anticancer drugs fail clinical trials due to toxicity or inadequate effectiveness. Consequently, AI-based drug repurposing has become a viable substitute approach for finding novel anticancer uses for currently available medications with established safety characteristics ^[1,4].

Large-scale biological datasets, like as genomes, proteomics, transcriptomics, metabolomics, and clinical records, are rapidly being analysed using artificial intelligence techniques like machine learning, deep learning, network pharmacology, and bioinformatics integration ^[5,6]. With the use of these technologies, scientists can find prospective treatment targets, disease-related pathways, and molecular markers linked with various cancer kinds. To predict drug sensitivity, categorize tumour subtypes, and find new drug-target interactions, machine learning techniques like Random Forest, Support Vector Machine (SVM), and Decision Trees can effectively interpret multidimensional information ^[5,14]. Through the automatic extraction of hidden patterns and nonlinear correlations from complicated biological data, deep learning algorithms enhance predictive accuracy ^[7].

Through virtual screening, network analysis, and molecular docking investigations, AI-driven systems are able to assess thousands of licensed medications and forecast their anticancer potential ^[23,24]. Large-scale screening of compounds against cancer-associated pathways has been made easier by platforms like the Drug Repurposing Hub ^[28]. Because cancer progression involves several genes, proteins, and signalling pathways interacting simultaneously, network pharmacology techniques are very helpful in the field of oncology ^[29]. Numerous medications that have been repurposed have shown notable antitumour efficacy. By activating AMP-activated protein kinase (AMPK), inhibiting the mammalian target of rapamycin (mTOR) pathway, reducing insulin-mediated tumour growth, and suppressing cancer cell proliferation, metformin which was first approved for type 2 diabetes mellitus has demonstrated potential anticancer effects ^[41,42].

Additionally, medications that can prevent angiogenesis, metastasis, inflammation, and tumour metabolism have been found by AI-assisted analysis. Currently, computational repurposing techniques are being

investigated for a number of diseases, including leukemia, glioblastoma, lung cancer, colorectal cancer, and breast cancer. It is anticipated that the future development of tailored anticancer medicines will be accelerated by the combination of AI with precision oncology.

2. Alzheimer's Disease:

Memory loss, cognitive decline, amyloid- β plaque buildup, neurofibrillary tangles, oxidative stress, mitochondrial dysfunction, and persistent neuroinflammation are the hallmarks of Alzheimer's disease (AD), a progressive neurodegenerative condition. AI-based drug repurposing is a crucial tactic for discovering new therapeutic possibilities because, despite substantial research, there are still few effective disease-modifying treatments^[30]. The intricacy of the disease pathways and the difficulties of forecasting therapy effects during clinical trials make conventional medication development for Alzheimer's disease particularly problematic. Researchers can examine complex molecular and clinical datasets linked to Alzheimer's disease etiology using artificial intelligence approaches. By examining gene-expression patterns, imaging data, and protein interaction networks, machine learning algorithms can find possible treatment targets, predict the course of a disease, and uncover disease biomarkers^[31]. By identifying hidden patterns in multidimensional datasets like genomic data and neuroimaging images, deep learning techniques significantly increase prediction accuracy^[7]. Network-based methods are also employed to find interrelated pathways related to oxidative stress, tau phosphorylation, amyloid processing, and synaptic dysfunction^[6]. Several authorized medications with neuroprotective and anti-inflammatory qualities that may halt the progression of disease have been found via AI-driven computer models. Antihypertensives, antidiabetics, anti-inflammatory medications, and anticancer medications have all been investigated in drug repurposing studies for possible therapeutic uses in Alzheimer's disease^[31]. Because of its impact on insulin signalling, mitochondrial function, oxidative stress reduction, and neuroinflammation modulation, metformin gained a lot of attention among these^[32]. Research indicates that metformin may enhance neuronal survival, encourage neurogenesis, and lessen amyloid buildup in the brain. By making it possible to identify patient-specific therapeutic targets based on genetic and molecular profiles, AI-assisted bioinformatics analyses also enhance personalized medicine techniques. The discovery of successful treatment approaches for Alzheimer's disease and other neurodegenerative disorders is anticipated to be enhanced by the integration of machine learning, systems biology, and network pharmacology.

3. Parkinson's Disease

Dopaminergic neurons in the brain's substantia nigra gradually degenerate in Parkinson's disease (PD), a chronic neurodegenerative condition. α -synuclein aggregation, mitochondrial dysfunction, oxidative stress, neuroinflammation, and poor neurotransmission are some of the main pathogenic characteristics. Current treatments do not successfully stop the progression of the disease; instead, they mostly relieve symptoms. As a result, AI-based drug repurposing has become a viable method for finding therapeutic molecules that affect illness^[34].

Parkinson's disease-related genomic, transcriptomic, proteomic, and metabolomic datasets are increasingly being analysed using artificial intelligence methods^[6]. Machine learning algorithms can categorize patient subgroups, find biomarkers associated with the course of a disease, and forecast treatment outcomes^[5]. By uncovering intricate molecular linkages involved in synapse dysfunction and neuronal degeneration, deep learning algorithms improve these investigations^[7]. Mapping the relationships between genes, proteins, signalling pathways, and environmental elements linked to Parkinson's disease pathogenesis is also made easier by network pharmacology techniques^[32]. Research has indicated that β 2-adrenoreceptor agonists may control the expression of α -synuclein and possibly lower the risk of Parkinson's disease^[33]. Numerous current medications that can alter oxidative stress, mitochondrial dysfunction, inflammatory pathways, and dopamine metabolism have been found using AI-driven computational investigations^[34]. These methods aid in the

creation of multitarget treatment plans that can deal with the complex character of Parkinson's disease. Predictive models with AI support are also helpful in finding substances that could increase dopaminergic signalling, decrease neurotoxicity, and improve neuronal survival. Additionally, the quick screening of licensed medications for neuroprotective qualities is made possible by the integration of bioinformatics databases with machine learning algorithms. It is anticipated that these computational methods will speed up the creation of tailored treatment plans and enhance Parkinson's disease long-term care.

4. Viral Infections

Due to high rates of mutation, the advent of drug-resistant viral strains, and the scarcity of efficient antiviral treatments, viral infections continue to pose serious threats to world health. AI-based drug repurposing is a desirable substitute approach for quick therapeutic identification since traditional antiviral drug research is frequently costly and time-consuming ^[27]. Rapid investigation of viral genomes, host-pathogen interactions, biochemical pathways, and pharmacological databases to find current medications with possible antiviral efficacy is made possible by artificial intelligence technologies ^[8].

By examining chemical structures, biological activity profiles, and molecular descriptors, machine learning algorithms are able to forecast interactions between medicinal drugs and viral proteins ^[5]. By assessing the stability and binding affinity of drug-protein complexes, molecular docking techniques provide additional validation for these predictions ^[23,24].

When it comes to finding hidden correlations in genomic and proteomic datasets related to immune responses and viral replication, deep learning techniques are especially helpful ^[7]. The identification of host cellular pathways involved in viral entrance, replication, and inflammatory responses is another common application of network pharmacology techniques ^[6]. Researchers can quickly assess hundreds of compounds and rank the most promising antiviral candidates for experimental validation thanks to AI-assisted computational screening. Influenza, hepatitis, HIV infection, Zika virus infection, Ebola virus sickness, and coronavirus infections have all been treated with these methods ^[27]. Because authorized medications already have proven safety profiles and may be used more quickly in clinical settings, drug repurposing efforts are particularly useful during virus epidemics. AI-based methods enable quick reaction to new infectious diseases and drastically shorten the time needed for therapeutic research.

5. COVID-19

The enormous potential of AI-based drug repurposing in handling international public health disasters was made evident by the COVID-19 pandemic. Researchers quickly used artificial intelligence techniques to find licensed medications that could prevent SARS-CoV-2 infection or lessen the severity of the sickness because it takes a long time to generate completely new antiviral treatments ^[8]. During the pandemic, machine learning, deep learning, molecular docking, virtual screening, network pharmacology, and other AI-assisted computational techniques were widely employed ^[27]. To find possible antiviral substances, machine learning models examined medication databases, host biological pathways, and viral genomic sequences ^[5]. Interactions between licensed medications and viral proteins like the spike protein, major protease, and RNA-dependent RNA polymerase were predicted by molecular docking studies ^[23]. Through the analysis of extensive biomedical datasets and the discovery of hidden therapeutic links, deep learning techniques substantially increased prediction accuracy ^[7].

One of the most significant repurposed antiviral medications for the treatment of COVID-19 is remdesivir. Remdesivir, which was first created to treat Ebola virus infection, works by blocking viral RNA-dependent RNA polymerase and preventing the virus from replicating ^[35]. Strong binding affinity toward SARS-CoV-2 replication machinery was shown by AI-assisted docking and computational investigations, which resulted in emergency usage authorization during the pandemic ^[35].

Another noteworthy example of AI-assisted medication repurposing is baricitinib. Baricitinib, which was first approved for rheumatoid arthritis, was discovered by AI-based predictive models as a possible COVID-19 treatment drug that could prevent viral entrance and lessen excessive inflammatory reactions ^[36,37]. Its positive benefits on lowering cytokine-mediated inflammation and enhancing patient outcomes were later validated by clinical research. These illustrations clearly highlight how AI-driven repurposing techniques could speed up the discovery of new treatments during infectious disease crises.

6. Rare Diseases

Although they only affect a small percentage of the population, rare diseases also referred to as orphan diseases affect millions of people globally. High research expenses, a lack of financial incentives, and small patient groups frequently hinder the development of new medications for uncommon diseases. As a result, AI-based drug repurposing has become a very successful and cost-effective method for finding treatments for uncommon diseases ^[38].

Researchers can examine genetic mutations, protein interactions, molecular pathways, and clinical phenotypes linked to rare diseases using artificial intelligence approaches including machine learning, network analysis, and bioinformatics integration ^[6]. Computational methods can anticipate licensed medications that may have therapeutic advantages by identifying biological pathways shared by common and unusual disorders ^[38].

By enabling patient-specific therapy predictions based on genomic and molecular traits, AI-assisted analyses also contribute to precision medicine. Identification of disease-associated targets and therapeutic candidates is further improved by integrating bioinformatics databases like DrugBank, STRING, and Connectivity Map ^[11,25,26]. Repurposed medications can greatly speed up clinical development and regulatory approval because they already have established pharmacokinetic and safety profiles ^[39]. Therefore, AI-driven drug repurposing offers a crucial tactic for meeting unmet medical needs in uncommon neurological, metabolic, and genetic illnesses.

7. Examples of successfully repurposed drugs:

The increasing significance of AI-assisted medication repurposing in contemporary therapeutic discovery is demonstrated by a number of successful examples. After AI-assisted computational analysis and molecular docking studies showed effectiveness against SARS-CoV-2 replication enzymes, Remdesivir became one of the first antiviral medications repurposed for COVID-19 treatment ^[35]. Its quick transition from computational prediction to clinical use proved that AI-driven treatment identification works well in emergency situations. Another effective example of AI-assisted repurposing is Baricitinib.

According to AI algorithms, baricitinib may prevent inflammatory cytokine signalling linked to severe COVID-19 as well as viral entry pathways ^[35,36]. Its therapeutic effectiveness in lowering inflammation and enhancing clinical outcomes was validated by later clinical research.

Originally created to treat type 2 diabetes mellitus, metformin has shown extensive therapeutic promise that extends beyond glycemic control. Metformin may be used to treat cancer, Alzheimer's disease, cardiovascular diseases, aging-related ailments, and metabolic syndromes, according to mechanistic research and AI-assisted analysis ^[32,41,42]. Its varied pharmacological effects are attributed to its capacity to control AMPK signalling, mitochondrial function, oxidative stress, inflammation, and cellular metabolism. These effective instances highlight how AI and computational technologies are revolutionizing drug discovery by increasing the therapeutic uses of already-approved medications while cutting costs and research time.

- Databases and Tools

1. DrugBank

One of the most extensive and often used bioinformatics databases for pharmaceutical research, drug development, and medication repurposing studies is DrugBank. Chemical structures, pharmacological characteristics, modes of action, molecular pathways, pharmacokinetics, toxicity profiles, and therapeutic indications are among the many drug-target details that are combined with comprehensive drug data ^[25]. The database is extremely important for AI-driven drug repurposing research because it includes data on licensed medications, exploratory compounds, nutraceuticals, and experimental treatments. DrugBank databases are widely used by artificial intelligence and machine learning techniques for molecular similarity analysis, virtual screening, drug-target interaction prediction, and the discovery of new therapeutic uses ^[5,6]. To find disease-associated targets and assess repurposable chemicals, researchers can combine DrugBank data with genomic, proteomic, and transcriptome datasets. By facilitating the examination of intricate relationships between medications, proteins, genes, and biological processes, the database also aids network pharmacology techniques ^[22]. Because its structured datasets make it easier to create deep learning algorithms and predictive computational models, Drug Bank has become especially significant in AI-assisted medicinal discovery ^[4].

Additionally, by offering comprehensive pharmacogenomic data related to treatment response and side effects, the database aids precision medicine activities. Data-driven drug discovery and repurposing tactics are greatly accelerated by Drug Bank's comprehensiveness.

2. PubChem

The National Center for Biotechnology Information (NCBI) developed and maintains PubChem, a chemical and biological database that is accessible to the general public. Chemical compounds, molecular structures, physicochemical characteristics, biological activities, toxicity information, and bioassay results are all covered in great detail ^[43]. One of the biggest chemical knowledge archives, PubChem is widely used in AI-based pharmaceutical research and computational drug discovery. PubChem datasets are often used by machine learning and deep learning models to examine biological activity profiles, structural fingerprints, and chemical descriptors in virtual screening and drug repurposing research ^[4,5]. Large-scale PubChem data can be processed by AI algorithms to assess pharmacological characteristics of compounds, find possible treatment options, and forecast drug-target interactions ^[23]. PubChem chemical structure data is also a major source of information for molecular docking studies, which simulate drug-protein interactions. Multidimensional analysis of chemical and biological data is made easier by PubChem's support for integration with various bioinformatics tools. For QSAR modelling, toxicity prediction, cheminformatics analysis, and network pharmacology research, the database is very helpful ^[6]. Furthermore, its open accessibility encourages teamwork and extensive computational studies in contemporary pharmaceutical sciences.

3. ChEMBL

The European Bioinformatics Institute (EBI) created ChEMBL, a manually curated bioactivity database with comprehensive data on drug-like compounds, bioactive molecules, molecular targets, and pharmacological actions that have been verified by experimentation ^[44]. The database is extremely useful for AI-driven pharmaceutical research since it combines chemical, biological, and pharmacological data taken from scholarly publications and drug discovery investigations. ChEMBL is widely utilized in machine learning and deep learning applications for virtual screening, drug-target interaction research, quantitative structure-activity relationship (QSAR) modelling, and biological activity prediction ^[5]. Inhibitory concentration (IC₅₀), binding affinity, potency, and pharmacokinetic characteristics are examples of experimentally observed bioactivity data that are provided by the database and

are crucial for the creation of predictive computational models. ChEMBL datasets are used to train AI systems that can anticipate the therapeutic uses of medications and uncover hidden molecular linkages ^[16].

By allowing researchers to examine relationships between drugs, proteins, pathways, and diseases, the database also enables network pharmacology and systems biology techniques ^[6]. To speed up contemporary drug discovery and repurposing procedures, ChEMBL is often coupled with cheminformatics software, molecular docking tools, and bioinformatics platforms. ChEMBL continues to be a valuable tool in AI-assisted medication development because of its extensive curated datasets and superior bioactivity data.

4. Open Targets

An open-access bioinformatics platform called Open Targets was created to facilitate the methodical discovery, verification, and ranking of therapeutic drug targets ^[45]. The platform establishes connections between genes, diseases, and therapeutic drugs by integrating large-scale genomic, transcriptomic, proteomic, pathway, and clinical datasets. Because of its capacity to integrate several biological evidence sources into a single computational framework, it is extensively utilized in AI-based drug discovery and drug repurposing research. Open Targets data is used by AI and machine learning techniques for pathway analysis, biomarker discovery, disease-associated target prediction, and repurposable drug identification ^[6]. In order to discover important molecular targets implicated in the progression of disease, the platform integrates protein interactions, genetic connections, signalling pathways, and clinical evidence to support network-based analysis ^[22].

Precision medicine techniques can be facilitated and therapy prediction accuracy increased by AI-driven computational models created with Open Targets datasets. Because Open Targets allows for the systematic investigation of target-disease relationships, it is especially useful in the research of complex diseases like cancer, neurological disorders, autoimmune diseases, and infectious diseases ^[45]. In order to improve multidimensional analysis of biomedical data, the platform also facilitates integration with other bioinformatics databases and computational tools. It is a potent tool for expediting AI-assisted therapeutic discovery and drug repurposing research due to its open-access nature and large biological datasets.

Database/Tool	Key Features	Role in AI-Based Drug Repurposing	Website
DrugBank	Drug structures, mechanisms, pharmacokinetics, targets, interactions	Used for drug–target prediction, virtual screening, network pharmacology, and machine learning studies	https://go.drugbank.com/
PubChem	Chemical structures, bioassays, molecular properties, toxicity data	Supports molecular docking, QSAR studies, virtual screening, and AI-based compound analysis	https://pubchem.ncbi.nlm.nih.gov/
ChEMBL	Bioactive molecules, IC50 values, target data, pharmacological activities	Used in machine learning, deep learning, QSAR modelling, and drug–target interaction prediction	https://www.ebi.ac.uk/chembl/
Open Targets	Gene–disease associations, pathway analysis, clinical and genomic data	Supports AI-driven target prioritization, biomarker discovery, and precision medicine	https://www.opentargets.org/

TABLE IV: DATABASES/TOOLS USED IN AI BASED DRUG REPURPOSING

- Advantages of AI in Drug Repurposing

1. Faster Screening

The ability of artificial intelligence (AI) to speed up the screening and identification of possible therapeutic options is one of its main benefits for drug repurposing. While AI-driven computational tools may quickly examine vast chemical and biological datasets in a much shorter amount of time, conventional drug development methods can need several years of experimental investigation and significant financial commitment ^[4,4]. Thousands of compounds may be screened at once, drug-target interactions can be predicted, and attractive candidates for additional experimental validation can be found using machine learning and deep learning algorithms ^[5,7]. AI-assisted virtual screening techniques assess the binding affinity, pharmacological activity, and therapeutic potential of current medications using molecular docking, predictive modelling, and network pharmacology ^[23,24].

AI-based computer screening techniques made it possible to quickly identify repurposable medications like baricitinib and remdesivir during the COVID-19 pandemic, highlighting the significance of AI in emergency pharmaceutical discovery ^[8,35,36]. By recognizing hidden chemical patterns and forecasting biological activity from massive datasets, deep learning models might further expedite the drug discovery process ^[7,7]. These capabilities increase the effectiveness of pharmaceutical research and significantly shorten the time needed for initial drug screening.

2. Reduced Failure Rates

By increasing prediction accuracy in preclinical and clinical stages, AI-based medication repurposing considerably lowers drug development failure rates. Because many compounds fail owing to toxicity, poor effectiveness, or unfavourable pharmacokinetic features, traditional drug discovery techniques are linked to high attrition rates ^[4]. In order to more correctly predict drug behaviour, safety profiles, and therapeutic effects, artificial intelligence systems can examine multidimensional biological and clinical datasets ^[5]. By detecting possible side effects, pharmacological interactions, and toxicity patterns prior to clinical testing, machine learning models can reduce late-stage failures ^[51]. Using transcriptomic, genomic, and proteomic data, deep learning techniques also make it easier to anticipate pharmacological characteristics and treatment responses ^[16,16].

By prioritizing the most promising compounds for experimental validation, AI-assisted predictive models increase overall success rates and lower research expenses ^[13]. Furthermore, repurposed medications already have established pharmacokinetic and safety profiles, which further reduces the likelihood of clinical trial failure ^[1,2]. Because of these benefits, AI-assisted repurposing is a more dependable and cost-effective approach than conventional de novo drug development.

3. Precision Market Support

By facilitating the creation of patient-specific treatment plans, artificial intelligence significantly contributes to the advancement of precision medicine. The goal of precision medicine is to customize care based on each patient's unique genetic, molecular, environmental, and clinical traits ^[53]. Large-scale genomic, transcriptomic, proteomic, and electronic health record information can be analysed by AI algorithms to find biomarkers, predict therapeutic responses, and choose the best medications for each patient ^[54]. Predicting treatment outcomes, classifying patients based on genomic profiles, and identifying disease subtypes are all common uses for machine learning algorithms ^[5]. Through the analysis of intricate biomedical datasets and the discovery of hidden connections between illness development and treatment effectiveness, deep learning techniques further enhance customized medicine ^[7]. AI-assisted medication repurposing is especially useful for rare diseases like cancer, where the disease's heterogeneity necessitates individualized treatment strategies ^[29,38].

By facilitating the examination of gene-drug-disease relationships and signalling pathways linked to specific patients, network pharmacology and bioinformatics integration also contribute to precision medicine ^[6]. Therefore, AI-driven predictive models make it easier to choose the best therapeutic approaches while reducing side effects and enhancing clinical results.

4. Big Data Handling

Another significant benefit of AI in drug repurposing is its capacity to process and evaluate large biomedical datasets. Large volumes of data from genomes, proteomics, metabolomics, transcriptomics, clinical trials, imaging studies, and electronic health records are produced by contemporary pharmaceutical and medical research ^[55]. Such big and multidimensional datasets are frequently difficult for conventional analytical techniques to handle effectively. However, large-scale biological and clinical data can be quickly processed, integrated, and interpreted using artificial intelligence algorithms ^[4]. From heterogeneous datasets, machine learning and deep learning algorithms may predict therapeutic links, find hidden correlations, and extract important patterns ^[5,56]. AI systems can enhance drug discovery and repurposing research by integrating data from many bioinformatics databases, including DrugBank, PubChem, ChEMBL, and Open Targets ^[23,43,44,45]. Additionally, real-time monitoring of patient records, illness development, adverse drug reactions, and treatment responses is made possible by big data analytics, which enhances decision-making in pharmaceutical research and healthcare administration ^[55]. Additionally, AI-driven computational models improve the accuracy of data interpretation and make it easier to automate difficult analytical activities that would otherwise take a lot of manual labour ^[58]. Therefore, by speeding up therapeutic identification, enhancing predictive accuracy, and bolstering evidence-based precision medicine techniques, the combination of AI with big data technologies is revolutionizing contemporary drug discovery.

Parameter	Traditional Drug Discovery	AI-Assisted Drug Discovery
Time Required	Typically requires 10–15 years for development and approval	Significantly reduces discovery and screening time through computational prediction
Cost of Development	Extremely expensive due to extensive laboratory and clinical studies	Reduces overall cost by prioritizing promising candidates computationally
Screening Process	Manual and high-throughput experimental screening	Automated virtual screening using AI and machine learning algorithms
Drug Failure Rate	High failure rates during clinical trials	Predictive AI models help reduce failures
Data Handling Capacity	Limited ability to process multidimensional biomedical data	Efficient handling of large-scale genomics, proteomics, and clinical datasets
Target Identification	Primarily based on conventional biological experiments	AI predicts novel drug–target interactions and disease associations
Precision Medicine Support	Limited personalization of therapies	Enables patient-specific therapeutic prediction and biomarker analysis
Use of Omics Data	Difficult integration of genomics and proteomics data	AI efficiently integrates multi-omics datasets for therapeutic discovery
Molecular Design	Requires extensive medicinal chemistry optimization	Generative AI can design and optimize novel molecules computationally
Clinical Decision Support	Mostly dependent on clinician expertise and standard protocols	AI-assisted predictive analytics supports clinical decision-making
Drug Repurposing Capability	Slower identification of alternative therapeutic uses	Rapid identification of repurposable drugs using computational analysis
Major Limitations	Long timelines, high costs, low success rates	Data quality issues, algorithm bias, regulatory and ethical concerns

Future Scope	Incremental improvement in conventional methodologies	Integration with generative AI, digital twins, and precision medicine
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TABLE V: COMPARISON OF TRADITIONAL VS AI-ASSISTED DRUG DISCOVERY

- Challenges and Limitation

1. Data Quality Issues

Artificial intelligence (AI) has made significant strides in medication repurposing, but its clinical applicability and dependability are still hampered by a number of issues. The availability and quality of biomedical data required to train AI models is one of the main issues. Large-scale datasets from genomes, proteomics, transcriptomics, electronic health records, clinical trials, and bioinformatics databases are crucial to AI-driven medication repurposing techniques^[4,49]. However, model performance and forecast accuracy may be adversely affected by these datasets frequent heterogeneity, incompleteness, inconsistency, or poor annotation^[52]. Computational analysis is further complicated by inconsistent data integration, missing clinical information, and experimental procedure variability^[6].

False predictions, inaccurate drug-target relationships, and poor reproducibility of results might emerge from biased or inaccurate datasets^[53]. Furthermore, AI models that were trained on little or poor-quality datasets may experience excessive fitting, which limits their capacity to generalize across various demographics and medical situations^[5]. Therefore, the availability of high-quality, curated, and standardized biological data is crucial to the success of AI-assisted drug repurposing.

2. Algorithm Bias

Another significant drawback of AI-based drug repurposing and healthcare applications is algorithm bias. Biased or inaccurate data might result in biased predictions and uneven therapy effects since machine learning models rely heavily on the datasets used during training^[54]. A lack of representation of particular ethnic groups, age groups, genders, or disease populations in biomedical databases might lead to bias^[55]. Because of this, AI algorithms might show lower prediction accuracy for some patient populations, which could result in suggestions for treatment that are not appropriate. Algorithmic bias can lead to differences in patient care, diagnosis, and treatment choices in healthcare systems^[54].

Because deep learning models underlying decision-making processes are hard to understand, they are frequently referred to as "black-box" systems, which further reduces transparency and confidence in predictions made by artificial intelligence^[7]. Therefore, the dependability, equity, and clinical acceptability of AI-assisted drug repurposing techniques may be impacted by the existence of hidden biases in training datasets. As a result, the creation of clear, comprehensible, and objective AI systems has grown in importance within contemporary biomedical and pharmacological research.

3. Lack of Clinical Validation

Many computational predictions lack adequate experimental and clinical validation, despite the fact that AI models can effectively anticipate possible therapy options. Though effective computational predictions do not always translate into clinical efficacy, AI-driven medication repurposing studies often produce promising in silico outcomes^[13,56]. Because biological systems are so complicated, it is impossible to fully anticipate many pharmacokinetic, pharmacodynamic, and toxicological aspects using computational methods alone. Due to inadequate efficacy, unanticipated side effects, or subpar therapeutic results, many AI-identified medication candidates fail preclinical or clinical trials^[46]. Furthermore, the validation of AI-generated

predictions is hindered by the scarcity of high-quality clinical trial data^[58]. It can be costly and time-consuming to conduct extensive laboratory experiments, animal research, and multicenter clinical trials for validation studies^[8].

Therefore, to increase dependability and translational success in medication repurposing applications, AI predictions must be integrated with experimental pharmacology and clinical research.

4. Regulatory Concerns

Another significant obstacle to the application of AI in medication repurposing and healthcare systems is regulatory issues. Before approving AI-assisted treatment techniques, regulatory bodies like the US Food and Drug Administration (FDA) require solid scientific proof of safety, efficacy, reproducibility, and transparency^[57]. However, standardization and validation are challenging because many AI algorithms are constantly changing due to adaptive learning processes. Clinical implementation and approval processes are made more difficult by the absence of widely recognized regulatory frameworks for AI-based healthcare technology^[58]. Furthermore, AI-assisted pharmaceutical research continues to raise serious questions about data privacy, cybersecurity, informed consent, and accountability^[59].

Evaluating the dependability and clarity of intricate deep learning systems presents additional difficulties for regulatory bodies, particularly when algorithms function as opaque "black-box" models^[53]. Therefore, to guarantee the safe and efficient use of AI in drug repurposing, it is essential to create clear regulatory rules and standardized validation processes.

5. Ethical Considerations

Precision medicine and AI-driven drug repurposing both heavily rely on ethical considerations. Concerns about informed permission, privacy protection, confidentiality, and ethical data sharing are raised by the use of massive patient data in AI applications^[59]. Additionally, if biased datasets are utilized for model training, AI systems may unintentionally perpetuate current healthcare gaps^[55]. Thus, fairness, accountability, openness, and explainability of AI algorithms have become important ethical issues in biological research^[60]. Clinicians may not fully comprehend how therapy recommendations are created due to the lack of transparency associated with some deep learning models^[53].

Patients and medical professionals may become less trusting of AI-assisted decision-making as a result. Implementing AI technologies in healthcare systems is also still hampered by ethical concerns about who owns biomedical data, who is responsible for algorithmic failures, and how to use patient data appropriately^[59]. For AI to be successfully included into future drug repurposing methods, transparent algorithms, ethically sound AI frameworks, and fair healthcare legislation must be developed.

- Future Perspective

1. Generative AI

It is anticipated that generative artificial intelligence (AI) would revolutionize pharmaceutical research and drug repurposing in the future. Generative AI systems can create new molecular structures, forecast biological activities, and develop drug candidates with better therapeutic qualities, in contrast to traditional AI models that mainly examine pre-existing datasets^[61]. By learning intricate chemical patterns from vast biomedical datasets, deep learning-based generative models may quickly discover possible molecules^[7,62]. These methods improve the efficiency of finding repurposable medicinal agents while drastically cutting the time and expense involved in traditional drug discovery. Promising uses of generative AI have already been shown in computational biology and medicinal chemistry, such as the quick identification of kinase inhibitors and the optimization of

molecular structures for particular disease targets ^[61]. Personalized and precision-based therapies may be developed more quickly if generative AI is integrated with molecular docking, network pharmacology, and bioinformatics platforms ^[6,23]. Furthermore, it is anticipated that future developments in explainable AI and reinforcement learning will enhance the predicted accuracy, interpretability, and dependability of generative models in drug repurposing applications.

2. Digital Twins

Another new development with great promise for AI-assisted drug repurposing and personalized medicine is digital twin technology. A virtual computing model that mimics a patient's biological, physiological, and clinical traits is called a digital twin ^[63]. These models simulate illness progression and treatment responses by integrating real-time clinical data, genetic information, imaging results, and physiological characteristics. Before actual clinical administration, researchers and clinicians may be able to assess treatment outcomes, forecast patient-specific medication reactions, and refine therapeutic approaches thanks to AI-driven digital twins ^[64]. Such technology has the potential to enable tailored healthcare methods, enhance treatment efficacy, and lessen adverse medication reactions. Predictive modelling and decision-making in complicated diseases like cancer and cardiovascular problems may be further improved by integrating digital twin systems with machine learning and big data analytics ^[49,50].

Therefore, the use of digital twins in the future could transform precision medicine and hasten the creation of safer and more potent repurposed treatments.

3. Personalized Medicines

By facilitating the creation of patient-specific treatment plans based on genetic, molecular, and clinical traits, artificial intelligence is anticipated to greatly advance personalized medicine. Instead of using broad therapeutic techniques, personalized medicine concentrates on choosing the best course of action for each patient ^[47]. Large-scale biomedical information, such as transcriptome data, proteomic signatures, genetic profiles, and electronic health records, can be analysed by AI algorithms to find biomarkers and forecast treatment outcomes ^[65]. The use of machine learning and deep learning algorithms to categorize disease subtypes, forecast treatment results, and determine the best medication combinations for specific patients is growing ^[5,7]. AI-assisted tailored medicine may reduce needless treatments and harmful drug reactions while increasing therapeutic efficacy ^[66]. Personalized computational models can help identify medications that can be repurposed for particular biological pathways and patient populations in drug repurposing research ^[6]. As a result, it is anticipated that combining AI with precision medicine techniques would enhance clinical results and revolutionize healthcare systems in the future.

4. Integration with Genomics and Proteomics

Future medication repurposing research is expected to be significantly improved by the integration of artificial intelligence with genomes, proteomics, and other multi-omics technologies. To provide a thorough understanding of disease causes and treatment targets, multi-omics techniques integrate data from genomes, transcriptomics, proteomics, metabolomics, and epigenomics ^[67]. These extremely complicated datasets can be effectively processed by AI algorithms to find possible therapeutic targets, disease-associated pathways, and hidden biological patterns. Drug-target interactions, treatment efficacy, and disease progression can all be predicted more accurately when machine learning models are combined with omics technology ^[68]. Precision medicine applications could be supported by AI-assisted genomic and proteomic data processing, which could also help identify patient-specific therapy regimens and biomarkers ^[69].

Additionally, it is anticipated that developments in AI-driven protein structure prediction tools, like AlphaFold, will transform structural biology and hasten the discovery of new therapeutic targets ^[70]. Therefore, integrating AI with proteomics and genomics has enormous potential to improve knowledge of complicated diseases, increase the accuracy of therapeutic predictions, and speed up the development of novel repurposed medications in the future.

• Conclusion

By increasing the speed, effectiveness, and precision of therapeutic discovery, artificial intelligence (AI) has become a game-changing strategy in contemporary medication repurposing. While AI-driven computational tools allow for the quick identification of possible treatment candidates utilizing available biological and pharmacological data, conventional drug development is frequently linked to high prices, long timeframes, and significant failure rates ^[4,5]. The prediction of drug-target interactions has been greatly improved by machine learning, deep learning, network pharmacology, molecular docking, and bioinformatics integration. These methods have also made it easier to find drugs that can be repurposed for a variety of diseases, including cancer, neurodegenerative disorders, rare diseases, and viral infections like COVID-19 ^[6,8,22,23].

With notable examples like remdesivir, baricitinib, and metformin, AI-assisted drug repurposing has shown significant promise, underscoring the clinical significance of computational therapeutic discovery ^[35,36,41]. By facilitating effective data analysis and target discovery, the availability of extensive databases like DrugBank, PubChem, ChEMBL, and Open Targets has further expedited AI-based pharmaceutical research ^[23,43,44,45]. Despite these developments, there are still a number of obstacles to overcome, such as problems with data quality, algorithm bias, a lack of clinical validation, moral dilemmas, and legal restrictions ^[53,54,57,59].

It is anticipated that advancements in generative AI, digital twin technology, customized medicine, and multi-omics integration would further transform precision therapies and drug repurposing ^[61,63,67,70]. Thus, ongoing integration of AI with clinical research, experimental pharmacology, and regulatory frameworks may enhance translational success and make it easier to design safer, quicker, and more successful treatment approaches in the future.

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