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ARTIFICIAL INTELLIGENCE IN DRUG REPURPOSING FOR PARKINSON'S DISEASES: A COMPREHENSIVE REVIEW

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ABSTRACT

Parkinson's disease (PD), the second most common neurodegenerative disorder, remains a major challenge in drug discovery due to its complex pathophysiology involving α-synuclein aggregation, oxidative stress, mitochondrial dysfunction, and neuroinflammation. Conventional drug development is costly, time-intensive, and limited by low success rates, highlighting the urgent need for innovative strategies. Drug repurposing, supported by artificial intelligence (AI), offers a transformative approach by leveraging existing safety profiles of approved drugs while reducing both cost and time. This review synthesizes progress between 2015 and 2025 in AI-driven methodologies, including machine learning, deep learning, and network-based frameworks, which enable systematic identification of novel drug-disease associations. Compared with traditional screening (<1% success rate), AI-guided approaches achieve substantially higher hit rates (12.5–21.4%), reduce development costs from $1.3 billion to $250,000, and shorten timelines from 15 years to approximately 4 years. Promising candidates, such as efavirenz, omaveloxolone, and cyproheptadine, demonstrate therapeutic potential by modulating disease mechanisms and offering neuroprotection. Moreover, integration of multi-omics data, knowledge graphs, and precision medicine tools has enabled accurate PD subtyping (95% accuracy), biomarker discovery, and patient stratification. Despite challenges in data integration, regulation, and clinical validation, AI-enabled drug repurposing represents a paradigm shift in PD therapeutics, paving the way for personalized treatments.

KEYWORDS: Artificial intelligence, Parkinson's disease, and Drug repurposing.

INTRODUCTION

Drug repurposing, also known as drug repositioning, is a new way of doing pharmaceutical research that finds new ways to use old drugs.[1] This method greatly lowers the risks and costs of traditional de novo drug development by using the known safety profiles and pharmacokinetic properties of FDA-approved drugs. AI-driven drug repurposing solutions are strongly endorsed by Parkinson's disease (PD), the second most common neurodegenerative disorder globally. AI technology has made this method better by making it easier to systematically analyze large biological datasets. This has led to the discovery of hidden drug-disease links that traditional methods can't find.[2] Its intricate pathophysiology encompasses multiple molecular pathways, such as α-synuclein aggregation, neuroinflammation, mitochondrial dysfunction, and oxidative stress.[3] Because traditional single-target methods for developing medications have mostly failed, we need more advanced computer methods that can deal with the complexities of Parkinson's disease.[4] Traditional screening methods are only effective less than 1% of the time. However, using AI to find new

zuses for drugs that treat Parkinson's disease has had amazing results, with success rates of 12.5% to 21.4%.[5]

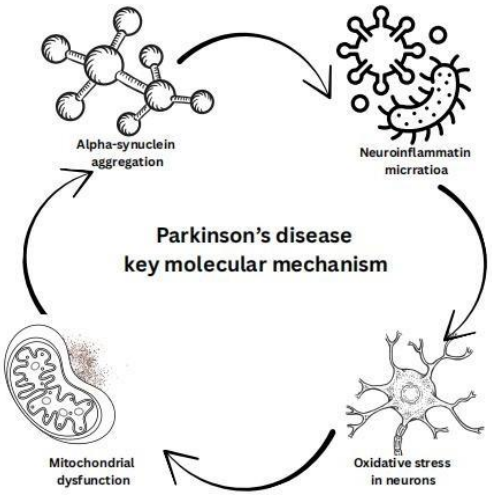

Fig. 1.

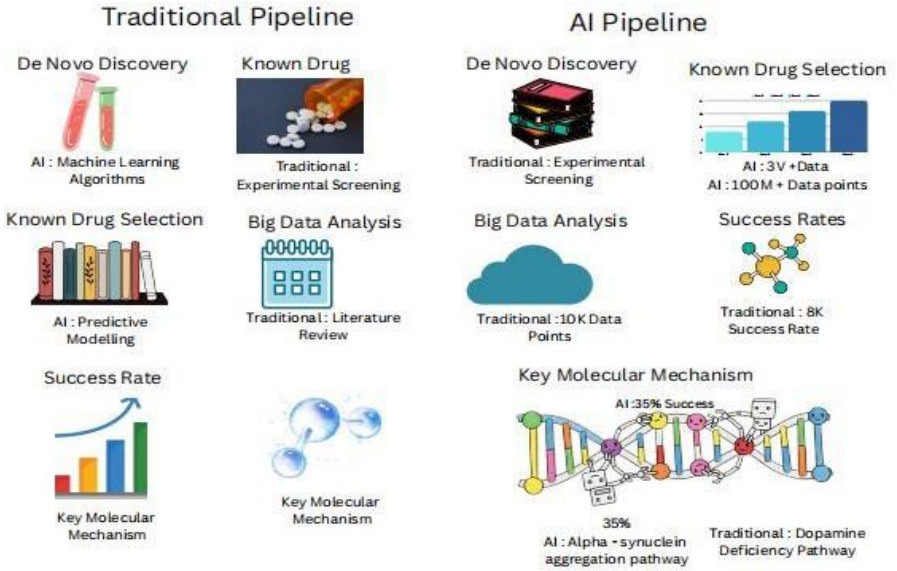

Fig. 2.

2. AI-driven computational methods in drug development

2.1 Machine learning techniques

Modern AI-driven repurposing of Parkinson's disease drugs uses a number of machine learning techniques, each of which has its own advantages for different parts of the drug development process. When used with Gaussian Process Regressors to measure uncertainty, Random Forest Regressors have been shown to be very good at predicting drug-target interactions. But other ensemble methods aren't as accurate. These hybrid models help researchers use their resources as efficiently as possible by letting them choose the best medication candidates while also judging how confident they are in their predictions.[6] Convolutional Neural Networks (CNNs) are very good at working with neuroimaging data and complex chemical structures. The capacity to identify patient subgroups predisposed to respond to particular therapeutic interventions has significant ramifications for drug repurposing. Recent research has successfully employed convolutional neural networks (CNNs) to identify disease subtypes from patient-derived stem cell images, achieving an accuracy of up to 95%. This advancement paves the way for precision medicine techniques that were previously considered unattainable.[7,8] Graph Neural Networks (GNNs) and other modern methods are good at dealing with the complicated relational data found in biological systems. These networks are great at finding complex connections between drugs, proteins, genes, and diseases in knowledge graphs. This helps make more accurate predictions for drug repurposing.[9] The End-to-End Knowledge Graph-based Drug Repurposing (EKGDR) strategy is a great example of this method. It has an AUROC of 0.9475 and an AUPR of 0.9490. Its performance metrics have been exceptional.[9]

2.2 Deep Learning Architectures

Variational Autoencoders (VAEs), which encode intricate chemical structures into low-dimensional latent

spaces while maintaining essential molecular characteristics, have proven effective in molecular representation learning. The junction tree variational autoencoder has not only explored new areas of chemical space, but it has also had great success in finding new chemical scaffolds that keep biological activity. Because of this ability, scientists have found substances that are 100 times more effective than α-synuclein aggregation inhibitors that have been documented before.[6] Sequential biological data, such as protein sequences and the temporal progression of diseases, can be effectively analyzed by recurrent neural networks (RNNs) and more advanced models like Long Short-Term Memory (LSTM) networks.[11]

2.3 Approaches Based on Networks

Network pharmacology is a key framework in AI-driven drug repurposing. It lets researchers look at drug-target-disease relationships in biological networks in a systematic way.[14] This approach acknowledges that disturbances in various interconnected pathways are responsible for most diseases, especially intricate neurodegenerative disorders such as Parkinson's disease.[13] When drug-target networks and protein-protein interaction (PPI) networks are combined, repurposing efforts have been more successful. It has been shown that drugs that target proteins that are closely linked to diseases work better. By carefully looking at FDA-approved drugs and their target profiles, researchers have found 176 possible treatment candidates for Parkinson's disease.[16]

3. Knowledge-Based Graph-Based Drug discovery

3.1 Semantics Relationship Mining

Knowledge graphs have changed drug repurposing by giving researchers a way to organize and see complex biomedical interactions.[17] These graphs create huge knowledge networks that AI systems can systematically analyze by bringing together information from many sources, such as molecular databases, scientific literature, clinical records, and experimental results. The GP-KG (Genotype-Phenotype Knowledge Graph) architecture includes more than 1.2 million interactions across 61,146 elements. This helps make more accurate predictions about how medications can be repurposed. This system does very well in cross-validation tests, with AUROC values of 0.981. An AUROC of 0.868[10] also helps find FDA-approved drugs for Alzheimer's disease. DREAMwalk (Drug Repurposing via Exploring Associations using Multi-layer Random Walk) is another advanced knowledge graph technique that uses semantic multi-layer guilt-by-association concepts. This method improved the accuracy of drug-disease association predictions by as much as 16.8% when compared to the best link prediction methods. This shows that multi-layer graph analysis can find hidden therapeutic links.[17]

3.2 Multi-Omics integration

Adding multi-omics data to knowledge graph frameworks has helped us understand how diseases and treatments work better.[17] By combining clinical data with genomic, transcriptomic, proteomic, and metabolomic data, this method creates detailed pictures of disease states and treatments that are available. Recent studies[4] show that AI models trained on multi-omics data can predict medication repurposing more accurately than models trained on only one type of data. The use of phenotypic data has made drug-disease correlations and predictive accuracy better.[10]

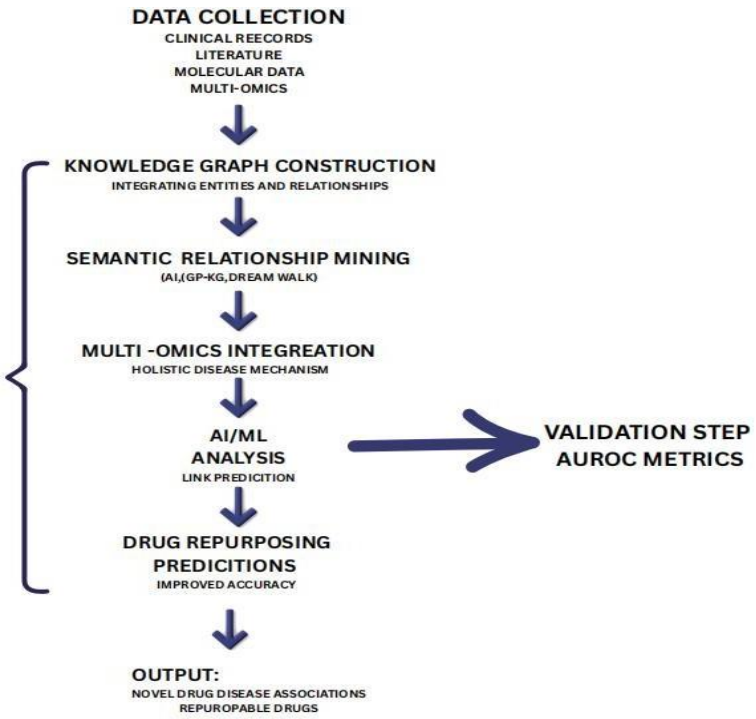

Fig. 3.

4. An sucesseful Drug Repurposing case

4.1 Alpha-synuclein-targeting therapeutic

With the FDA-approved antiviral medication Efavirenz, AI-driven medication repurposing for Parkinson's disease has advanced significantly. A comprehensive AI analysis demonstrated that efavirenz is a potent modulator of α-synuclein propagation, exhibiting substantial neuroprotective effects in both cellular and animal models of Parkinson's disease. The drug's alteration of cholesterol metabolism and its inhibition of α-synuclein dispersion via CYP46A1 modulation exemplify AI's capacity to identify novel therapeutic avenues. This finding illustrates how artificial intelligence (AI) systems can identify potential medications that conventional hypothesis-driven research methodologies might overlook.

While AI research indicated that a comprehensive analysis of molecular interaction networks holds significant therapeutic potential, traditional pharmacological knowledge failed to establish a clear connection between antiviral mechanisms and neurodegeneration. Efavirenz and nevirapine, another antiretroviral drug, were found using the same AI-driven screening method, which shows how systematic computational drug repurposing is.[3]

4.2 Neuroprotective compound

Cyproheptadine and omaveloxolone are promising therapy alternatives, according to a drug-target network analysis of FDA-approved medications. Omaveloxolone, initially formulated for the treatment of Friedreich's ataxia, demonstrates substantial neuroprotective effects and enhances cellular antioxidant responses through the activation of the Keap1-Nrf2/ARE pathway. These reactions are very important for lowering oxidative stress in people with Parkinson's disease. Cyclopeptadine, an antihistamine with established safety profiles, demonstrated remarkable efficacy in inhibiting the synthesis of interleukin-6 (IL-6) and preventing the downregulation of tyrosine hydroxylase via the MAPK/NFκB pathway.[16] These results show that network-based methods can be useful for finding drugs that work in different ways and are specific to different parts of Parkinson's disease's pathophysiology. Machine learning analysis focused on the upregulation of PINK1 expression resulted in the identification of the antiparasitic agent nitazoxanide.[18]

4.3 Beta-2 Adrenoreceptor Agonists

Salbutamol and other β2-adrenoreceptor agonists have been identified as potential neuroprotective agents for Parkinson's disease (PD) through AI-assisted epidemiological analysis. These drugs work in two ways: they reduce inflammation, which may protect dopaminergic neurons, and they change the way the SNCA gene is transcribed by adding acetyl groups to histones.[19] According to many population studies that provide strong empirical evidence for salbutamol's neuroprotective effects show that using it lowers the risk of Parkinson's disease by 34% (rate ratio of 0.66).[5]

5. Cutting-Edge AI Tools for Pharmaceutical Research.

5.1 Federated Learning Approaches

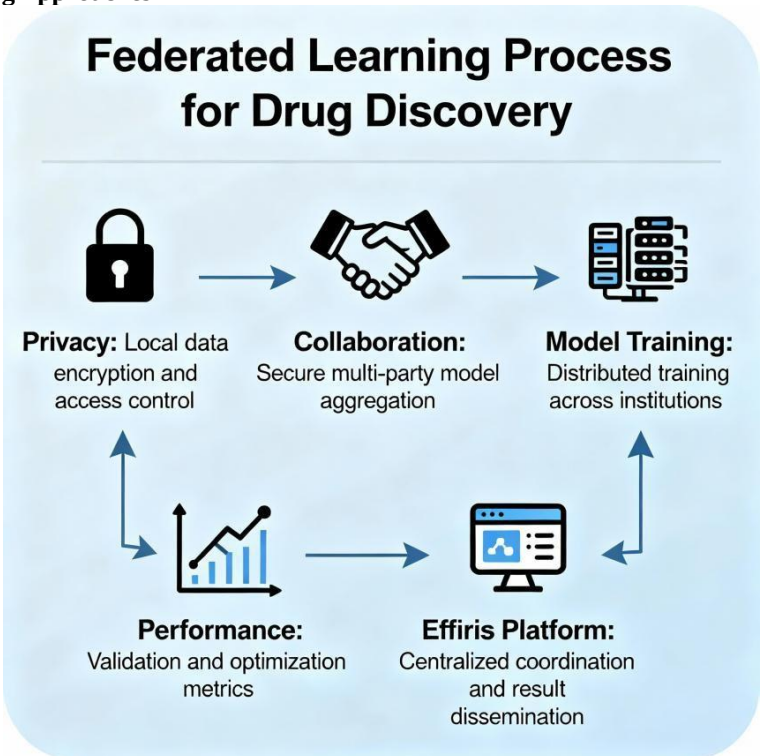

Fig. 4.

5.2 Structured based iterative learning

Structure-based machine learning has led to the discovery of strong inhibitors of α-synuclein aggregation, which is a major cause of Parkinson's disease.[6] To find drugs that stop certain protein aggregation sites from growing on their own, scientists use molecular docking simulations and iterative machine learning optimization. Because this method is iterative, it is easier to gradually improve treatment options, leading to compounds that are two orders of magnitude more powerful than known inhibitors. Our method is more than 20 times better than traditional high-throughput screening methods, with optimization rates of 12.5 to 21.4 percent. Structure-based iterative learning is also great at helping people understand how medicines work and making them stronger. AI-identified compounds have been shown to bind to target proteins with dissociation constants in the nanomolar range using surface plasmon resonance tests. This offers mechanistic insights for further enhancement and corroborates the computational predictions.[6]

5.3 Diverse Modes of AI Integration

Multi-modal AI methodologies amalgamate various data sources, including neuroimaging data, clinical records, biomarker measurements, and molecular structures, to generate comprehensive models of disease and pharmacological action.[23] These systems process medical images, lab results, and unstructured clinical notes at the same time so that they can give full evaluations of a patient's condition and how well they are responding to treatment. Recent applications have demonstrated that multi-modal AI can effectively identify Parkinson's disease subtypes based on patterns of disease progression, achieving accuracy rates of up to 95% in distinguishing between phenotypes characterized by rapid, moderate, and slow progression.[24]

6. Clinical applications and precision medicine

6.1 Disease subtyping and patient stratification

AI-driven analysis has completely changed how we understand the differences between people with PD. It has identified various disease subtypes based on genetic mechanisms, therapeutic outcomes, and trends in illness development.[25] Machine learning models have successfully identified three primary subtypes of Parkinson's disease (PD) progression: Inching Pace (PD-I), Moderate Pace (PD-M), and Rapid Pace (PD-R). These subtypes are differentiated by specific clinical characteristics and genetic markers.[24] These subgroups may respond variably to therapeutic interventions, potentially influencing the repurposing of medications. Pharmacological interventions aimed at these systems may benefit individuals with PD-R, as indicated by the activation of specific pathways linked to neuroinflammation, oxidative stress, and metabolism.[24] Transcriptomic profiling of PD progression subgroups has revealed distinct gene expression profiles, which may function as biomarkers for patient stratification and treatment selection. AI has found genes that are expressed differently and were not linked to Parkinson's disease before by looking at RNA-sequencing data. We now know more about how the disease works and what treatments might work because of this.[26]

6.2 Biomarker Identification and Validation

Artificial intelligence (AI) techniques that systematically look at multi-dimensional datasets, such as digital health data, blood-based markers, and neuroimaging, have sped up the development of biomarkers for Parkinson's disease. Deep learning models trained on nocturnal breathing patterns exhibited exceptional accuracy in diagnosing Parkinson's disease, achieving AUROC values of 0.90 and 0.85 on held-out and external test sets, respectively.[23] This breakthrough could lead to more frequent and objective evaluations of therapeutic methods by allowing people to monitor their response to therapy and the progress of their illness at home without having to go to the doctor. The AI model uses clinical rating scales ($R = 0.94$)[23] to give objective measurements that can help traditional clinical evaluations by estimating how bad and how fast Parkinson's disease (PD) is getting worse. Wearable technology, smartphone sensors, and other digital health technologies have made digital biomarkers possible. These biomarkers open up new ways to keep track of how well medications are working and how illnesses are getting worse.[28]

6.3 Predicting How People Will React to Treatment

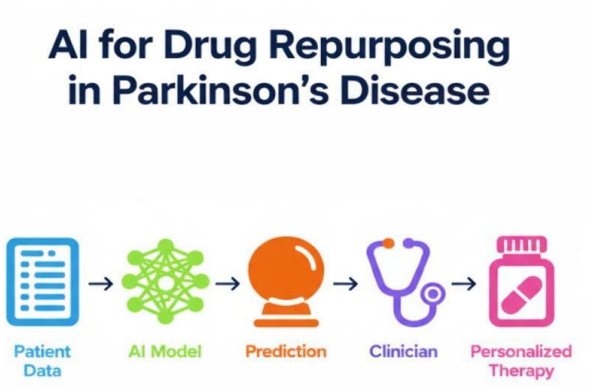

Fig. 5.

7. Pharmacology in Systems Biology and Networks

7.1 Multi-target drug discovery

Network pharmacology approaches, which acknowledge that successful therapies for complex illnesses like Parkinson's disease typically involve the simultaneous regulation of several targets, have significantly changed the way medications are repurposed.[31] The intricate interactions among numerous cellular pathways in neurodegenerative diseases render the transition from single-target to network-based therapy development particularly significant. Researchers have combined protein-protein interaction (PPI) networks and drug-target databases to find drugs that might change network modules that are important for diseases.[32] Compounds that target core regulatory proteins are prioritized due to

research indicating that medications affecting densely connected nodes (hubs) in disease networks possess a greater likelihood of efficacy. Systems biology techniques show that autophagy-related pathways are important parts of many neurodegenerative diseases, such as Parkinson's disease.[32]

7.2 Pathway enrichment and mechanism discovery

AI-driven drug repurposing workflows now often use Gene Ontology (GO) and KEGG pathway investigations to systematically find molecular pathways and biological processes that could be affected by new drugs.[31] The mechanistic conclusions derived from these analyses guide rational strategies for drug combination and selection. Several drugs that affect the PI3K/AKT pathway are being tested because recent studies have shown that this signaling pathway is a key target for treating Parkinson's disease.[31] Network pharmacology studies show that curcumin, a naturally occurring drug that is safe, protects neurons mainly by turning on the PI3K/AKT signaling pathway. This discovery gives curcumin a molecular basis for its potential as a treatment for Parkinson's disease. Several genes in the inositol phosphate biosynthesis pathway (INPP5F, IP6K2, ITPKB, and PPIP5K2) have been proposed as potential candidates associated with Parkinson's disease, and machine learning analysis of GWAS data has identified this pathway as a novel therapeutic target.[34]

7.3 Drug Combination Techniques

Network-based techniques have made it possible to rationally develop therapeutic combination therapy by finding drugs that work on different nodes in sickness networks.[32] This approach is especially pertinent to Parkinson's disease (PD), as addressing the various degenerative mechanisms that lead to neurodegeneration may necessitate a multimodal therapeutic strategy. AI analysis of drug interaction networks shows that combinations of repurposed drugs work better together than alone. These combinations offer comprehensive treatment coverage by concentrating on various facets of Parkinson's disease pathophysiology, including α-synuclein aggregation, neuroinflammation, and mitochondrial dysfunction. Polypharmacology networks have shown that many effective Parkinson's disease treatments work on more than one target. This means that drugs with similar multi-target properties might be good candidates for repurposing.[35]

8. Challenges and future perspectives

8.1 Problems with Data Integration and Quality

Data integration, quality assurance, and cross-platform standardization are still big problems, even though AI-driven drug repurposing has come a long way.[29] Different types of data sources, like scientific articles, clinical records, and molecular databases, often use different formats, terms, and quality standards. So, we need advanced ways to harmonize data. The Observational Medical Outcomes Partnership's (OMOP) Common Data Model is one way to make healthcare data the same across many countries and institutions. This might make it easier to test and train AI models. Many healthcare systems and research institutions are still in the early stages of putting these guidelines into action. The number of people with rare diseases like Parkinson's disease (PD) may be very small, and the datasets may not show how the disease changes over time. The absence of data and selection biases persist as challenges in the development of AI models.[30] Federated learning approaches provide partial solutions by safeguarding data privacy and facilitating access to larger, more diverse datasets.[22]

8.2 Frameworks for Validation and Regulation

Clinical drug development workflows cannot incorporate AI techniques without comprehensive regulatory frameworks that guarantee safety, efficacy, and repeatability while promoting innovation.[36] The FDA has started to give advice on how to use AI in drug research and clinical trials, but it is still working on a full set of rules for AI-driven drug repurposing. Clinical validation of AI-identified therapeutic candidates necessitates meticulously designed trials that incorporate the distinctive attributes of repurposed medications and their anticipated mechanisms of action.[29] Standard clinical trial methodologies may not optimally validate network-based hypotheses identified through AI techniques or multi-target therapies. One area of ongoing research that has important implications for clinical translation is the creation of machine learning models that can explain how they make predictions. In drug development applications, where physicians and regulatory agencies necessitate clear elucidations of AI decision-making processes, explainable AI (XAI) has gained prominence.[37]

8.3 The Integration of New Technologies

Quantum computing, an advanced technology that facilitates more intricate molecular simulations and optimization techniques, holds the potential to substantially enhance AI's capabilities in drug discovery.[30] Initial applications indicate that the functions of virtual screening and molecular design may expand considerably. Large Language Models (LLMs) trained on biomedical literature are starting to show promise when it comes to mechanistic reasoning and coming up with new ideas for repurposing drugs.[1] These models can analyze extensive scientific literature to uncover previously unidentified drug-disease relationships and generate testable hypotheses subject to empirical validation. Digital twins of patients and disease models[30] are a new way of thinking that could make treatment better and make it easier to predict how drugs will work.

9. CONCLUSION

The convergence of artificial intelligence and drug repurposing has redefined the therapeutic landscape for Parkinson’s disease. By integrating machine learning, deep learning, and network-based approaches, AI has

achieved unprecedented improvements in drug discovery efficiency—enhancing success rates, lowering costs, and significantly reducing development timelines. Beyond identifying promising repurposed candidates such as efavirenz, omaveloxolone, and cyproheptadine, AI methodologies have advanced precision medicine through accurate disease subtyping, biomarker discovery, and patient stratification. These innovations enable more tailored treatment strategies, aligning therapeutic interventions with individual patient profiles. Furthermore, the incorporation of multi-omics integration, knowledge graphs, and systems biology provides deeper mechanistic insights into disease pathways, uncovering novel targets and drug combinations. However, challenges persist in data harmonization, regulatory validation, and clinical translation, underscoring the need for standardized frameworks and explainable AI models to ensure safety and efficacy. Looking ahead, emerging technologies such as federated learning, digital twins, and quantum computing hold the potential to further revolutionize the field. Collectively, evidence demonstrates that AI-powered drug repurposing is not only a cost-effective and time-efficient strategy but also a transformative paradigm for developing next-generation, personalized therapies for Parkinson's disease and other neurodegenerative disorders.

10. Future Aspects

Future advancements in AI-driven drug repurposing for Parkinson's disease (PD) hold tremendous potential to transform therapeutic discovery and personalized care. Continued integration of **multi-omics platforms**—including genomics, proteomics, metabolomics, and real-world clinical data—will enhance the precision of mechanistic predictions and help identify highly specific molecular signatures for early diagnosis. The emergence of **federated learning**, enabling secure collaboration across global medical institutions, is expected to generate larger, more diverse datasets that reduce bias and improve model robustness.

Advancements in **explainable AI (XAI)** will play a crucial role in increasing transparency, helping clinicians and regulators better understand the scientific rationale behind AI-generated drug recommendations. Cutting-edge technologies such as **quantum computing** and **digital twin simulations** may offer unprecedented capabilities in simulating disease progression, predicting patient-specific treatment responses, and optimizing repurposing pipelines. As regulatory frameworks evolve and harmonized data standards become widely adopted, clinical translation of AI-identified candidates—either as monotherapies or in multi-target drug combinations—will accelerate. Altogether, these innovations will pave the way for faster, safer, and more personalized therapeutic strategies for Parkinson's disease in the coming decade.

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