Artificial Intelligence in Drug Repurposing Strategies

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Abstract
Drug repurposing, also termed drug repositioning, refers to the systematic identification of new therapeutic indications for clinically approved or investigational pharmacological agents. This strategy circumvents the lengthy and resource-intensive phases of conventional de novo drug discovery, offering a substantially reduced timeline and lower attrition risk. Artificial intelligence (AI) has emerged as a transformative enabler of drug repurposing, leveraging the exponential growth of biomedical data to extract actionable drug–disease relationships at unprecedented scale. Machine learning (ML) algorithms, including supervised classifiers and ensemble methods, have been widely applied to predict drug–target interactions and adverse effect profiles. Deep learning architectures—such as convolutional neural networks, recurrent networks, and transformer-based models—enable the integration of molecular, genomic, and clinical information in high-dimensional feature spaces. Network-based approaches model the complexity of biological systems by representing proteins, diseases, and drugs as interacting nodes within multi-layered graphs, facilitating the identification of functionally relevant drug repositioning candidates. The integration of multi-omics data, electronic health records, and biomedical literature through AI frameworks has further expanded the scope of computational repurposing. Notable applications include the AI-assisted identification of baricitinib for COVID-19, the repositioning of metformin as a potential anti-cancer and neuroprotective agent, and the application of connectivity mapping to match drug-induced transcriptomic signatures with disease expression profiles. Despite considerable progress, challenges persist in model interpretability, data heterogeneity, and the translational gap between computational predictions and experimental validation. Future advances in explainable AI, federated learning, and multi-modal data integration are anticipated to substantially enhance the clinical translation of computationally repurposed therapeutics.

Keywords: Drug repurposing; Artificial intelligence; Machine learning; Deep learning; Network pharmacology; Computational drug discovery

1. Introduction

1.1. Drug Repurposing in Pharmaceutical Research

The conventional drug discovery pipeline is characterised by an average development timeline of 12–15 years and an estimated cost exceeding USD 2.5 billion per approved therapeutic entity, with overall attrition rates surpassing 90% in clinical phases [1, 2]. Drug repurposing offers a strategically compelling alternative by exploiting the established safety and pharmacokinetic profiles of existing compounds, thereby reducing development timelines to 3–12 years and significantly lowering associated

financial risk [3]. The biological rationale for repurposing is rooted in the polypharmacological nature of many drugs, whereby a single agent may modulate multiple molecular targets across distinct disease pathways [4]. Classic examples include thalidomide, originally withdrawn due to teratogenicity and subsequently repositioned for multiple myeloma and leprosy, and sildenafil, repurposed from cardiovascular therapy to pulmonary arterial hypertension [5].

1.2. Importance of Computational Approaches

The emergence of large-scale biomedical databases, high-throughput omics technologies, and electronic health records (EHR) has created an information-rich ecosystem that exceeds the analytical capacity of conventional pharmacological methods [6]. Computational approaches—encompassing cheminformatics, systems biology, and, more recently, AI—provide the methodological infrastructure to mine this data landscape for latent drug–disease associations [7]. AI, in particular, offers the capacity to model non-linear, high-dimensional biological relationships, to integrate heterogeneous data modalities, and to generate testable pharmacological hypotheses with statistical robustness [8, 9].

1.3. Scope and Objectives of the Review

This review provides a focused, analytical examination of AI methodologies applied to drug repurposing, encompassing machine learning, deep learning, and network-based systems biology approaches. The discussion covers major data resources, the computational workflow for repurposing, therapeutic applications across disease domains, and the principal challenges and future directions pertinent to the field.

2. Artificial Intelligence Approaches in Drug Repurposing

2.1. Machine Learning Models

Supervised machine learning constitutes the most extensively applied AI framework in drug repurposing. Algorithms such as random forest, support vector machines (SVM), gradient boosting (XGBoost), and logistic regression have been trained on curated drug–target interaction (DTI) datasets to classify novel compound–protein binding relationships [10]. These models encode molecular features as chemical fingerprints or physicochemical descriptors, enabling rapid large-scale screening of compound libraries against therapeutic targets [11]. Collaborative filtering approaches, analogous to recommender systems, have additionally been employed to infer drug–disease relationships from sparse interaction matrices, leveraging known therapeutic associations to predict novel ones [12]. Unsupervised methods, including k-means clustering and principal component analysis, facilitate the grouping of drugs by transcriptomic signature similarity, identifying agents with shared biological mechanisms amenable to therapeutic repurposing [13].

2.2. Deep Learning Frameworks

Deep learning has substantially expanded the representational capacity available for drug repurposing by enabling end-to-end feature learning from raw molecular graphs, sequences, and high-dimensional omics profiles [14]. Convolutional neural networks (CNN) extract spatial features from molecular images and one-dimensional chemical sequences, while recurrent neural networks (RNN), including long short-term memory (LSTM) architectures, process sequential biological data such as genomic sequences and clinical time-series [15]. Transformer-based architectures, exemplified by BERT-derived biomedical models (BioBERT, PubMedBERT), have demonstrated exceptional performance in extracting drug–disease associations from unstructured biomedical literature [16]. Generative adversarial networks (GAN) and variational autoencoders (VAE) offer the capacity to synthesise novel molecular structures or augment sparse training datasets, further enriching the AI-driven repurposing pipeline [17]. Graph neural networks (GNN), including graph convolutional networks (GCN) and graph attention networks (GAT), represent biological entities as node-embedded graphs and have shown particular utility in polypharmacology and multi-target drug repositioning [18].

2.3. Network-Based and Systems Biology Approaches

Network pharmacology integrates drug, target, and disease data within heterogeneous biological networks, enabling the systematic interrogation of drug repositioning candidates through graph-theoretic methods [19]. Random walk algorithms, network propagation, and community detection techniques are applied to identify disease modules and predict drug candidates that modulate pathologically dysregulated network regions [20]. The human interactome—encompassing protein–protein interactions (PPI), metabolic pathways, and signalling cascades—serves as the foundational graph structure upon which AI-driven network analyses are performed. Hybrid approaches combining network topology with machine learning classifiers have demonstrated superior predictive performance compared to unimodal methods, particularly in the context of multi-morbidity and disease comorbidity analyses [21].

3. Data Sources and Computational Platforms

3.1. Biomedical and Pharmacological Databases

The quality and comprehensiveness of training data are principal determinants of AI model performance in drug repurposing. Key repositories include DrugBank, which provides curated drug–target interaction data and pharmacological annotations; ChEMBL, a large-scale bioactivity database of small molecules against diverse protein targets; and the Therapeutic Target Database (TTD), which catalogues disease–target–drug relationships [22]. The STRING and BioGRID databases supply protein–protein interaction networks indispensable for network-based methodologies. Table 2 summarises major data sources and their specific roles in AI-driven repurposing workflows.

3.2. Omics Data Integration

Transcriptomic connectivity mapping, pioneered by the LINCS L1000 and Connectivity Map (CMap) initiatives, identifies drugs whose gene expression signatures reverse disease-associated expression patterns, thereby nominating repositioning candidates [23]. Gene Expression Omnibus (GEO) and ArrayExpress provide extensive repositories of publicly available transcriptomic datasets across disease contexts. Proteomic and metabolomic data from the Human Protein Atlas and MetaboLights respectively augment multi-omics integration frameworks that inform AI-driven target identification and candidate prioritisation [24].

3.3. Clinical and Real-World Datasets

Electronic health records aggregated through platforms such as the FDA Adverse Event Reporting System (FAERS),

ClinicalTrials.gov, and the UK Biobank provide pharmacovigilance signals and real-world evidence that complement experimental repurposing data [25]. NLP-based mining of these clinical datasets enables the identification of unexpected therapeutic effects and drug-disease co-occurrence patterns at population scale, substantially informing AI model training and validation.

4. AI-Driven Drug Repurposing Workflow

4.1. Target Identification and Validation

The initial phase of AI-driven repurposing involves the systematic identification of therapeutically relevant molecular targets implicated in disease pathogenesis. AI models trained on genomic, proteomic, and phenotypic association data—including genome-wide association study (GWAS) outputs and DisGeNET gene–disease mappings—rank candidate targets by biological relevance and druggability [26]. Network centrality metrics, such as betweenness and closeness centrality, are applied within PPI networks to prioritise high-impact targets amenable to pharmacological intervention.

4.2. Drug–Target Interaction Prediction

DTI prediction constitutes the computational core of AI-based repurposing. Bipartite graph-based models, matrix factorisation algorithms, and deep neural networks are deployed to predict binding affinities between existing compounds and newly identified targets [27]. DeepDTI, GraphDTA, and MolTrans represent benchmark deep learning frameworks that have achieved state-of-the-art DTI prediction performance on standardised datasets. These models encode drug molecules as molecular graphs or SMILES representations and proteins as amino acid sequences or three-dimensional structural embeddings, facilitating the comprehensive interrogation of the drug–target interaction landscape.

4.3. Virtual Screening and Prioritisation

Following DTI prediction, AI-augmented virtual screening pipelines rank candidate drugs by predicted efficacy, selectivity, and safety profiles. Structure-based virtual screening integrates molecular docking algorithms with machine learning scoring functions to assess compound–target complementarity at atomic resolution [28]. Pharmacophore modelling and ADMET (absorption, distribution, metabolism, excretion, toxicity) prediction refine the candidate list to compounds with favourable drug-like properties. The integration of multi-criteria decision algorithms and ensemble model outputs generates a prioritised candidate portfolio for experimental validation, as illustrated in Figure 1.

5. Therapeutic Applications

5.1. Cancer and Precision Medicine

Oncology represents a primary domain for AI-driven repurposing owing to the molecular heterogeneity of cancer and the availability of large-scale pharmacogenomic datasets such as the Cancer Genome Atlas (TCGA) and the Genomics of Drug Sensitivity in Cancer (GDSC) [29]. ML models trained on transcriptomic and mutational profiles have identified clinically actionable repositioning candidates including itraconazole for basal cell carcinoma and metformin for its anti-proliferative effects across multiple tumour types. AI network analyses integrating oncogenic pathway data have further nominated approved agents capable of disrupting dysregulated signalling nodes in treatment-refractory malignancies.

5.2. Infectious Diseases and Pandemics

The SARS-CoV-2 pandemic provided compelling evidence for the clinical utility of AI-driven repurposing under emergency conditions. BenevolentAI's network-based AI platform identified baricitinib—a JAK1/JAK2 inhibitor approved for rheumatoid arthritis—as a candidate for COVID-19 management, predicting its capacity to inhibit viral endocytosis and attenuate cytokine-mediated hyperinflammation [5, 30]. This prediction was subsequently validated in randomised clinical trials, leading to emergency use authorisation. Remdesivir was similarly identified through structure-based virtual screening targeting the SARS-CoV-2 RNA-dependent RNA polymerase, demonstrating the translational potential of AI-guided repurposing in infectious disease contexts.

5.3. Neurological and Rare Diseases

Neurodegenerative diseases—including Alzheimer disease, Parkinson disease, and amyotrophic lateral sclerosis—present significant challenges for de novo drug development due to limited target tractability and the complexity of the blood–brain barrier. AI-driven transcriptomic connectivity mapping and PPI network analysis have proposed metformin, sildenafil, and several anti-inflammatory agents as repositioning candidates for Alzheimer disease, with several advancing to phase II clinical evaluation [26]. For rare diseases, where limited patient populations preclude large-scale clinical trials, AI-based repurposing using Orphanet and OMIM datasets offers a particularly valuable strategy for identifying mechanistically plausible therapeutic alternatives.

6. Challenges and Future Perspectives

6.1. Data Quality and Interpretability

A principal limitation of AI-driven repurposing is the dependence on curated, high-quality training data. Biomedical databases frequently contain incomplete, inconsistent, or biased annotations that propagate errors through downstream AI models [1, 9]. The class imbalance inherent in DTI datasets—where known interactions represent a small fraction of the biological interaction space—necessitates specialised sampling strategies and evaluation metrics. Equally critical is the interpretability of deep learning models: the black-box nature of complex neural architectures impedes mechanistic understanding of repurposing predictions, a significant barrier to regulatory acceptance and experimental prioritisation [28]. Explainable AI (XAI) frameworks, including attention mechanisms, SHAP (SHapley Additive exPlanations), and LIME (Local Interpretable Model-agnostic Explanations), are increasingly integrated into repurposing pipelines to provide feature-level explanations.

6.2. Regulatory Considerations

The regulatory landscape for AI-derived drug repurposing candidates is evolving. Regulatory agencies, including the FDA and EMA, have issued guidance documents on the

application of AI and ML in drug development, emphasising the importance of model transparency, prospective validation, and bias assessment [13, 25]. The absence of standardised benchmarking frameworks for AI repurposing models complicates cross-study comparison and undermines confidence in computational predictions. Collaborative initiatives between regulatory bodies, academia, and industry are essential to establish validated performance metrics and data sharing standards that support the clinical translation of AI-repurposed agents.

6.3. Integration with Experimental Validation

The translational gap between computational repurposing predictions and experimental confirmation remains a critical bottleneck. High-throughput experimental assays—including cell-based phenotypic screens, patient-derived organoid models, and *in vivo* pharmacological studies—are required to empirically evaluate AI-generated candidates [14, 21]. Federated learning architectures, which enable model training across distributed clinical datasets without compromising data privacy, represent a promising strategy for expanding training data availability while maintaining regulatory compliance. Integrating AI predictions with CRISPR-based functional genomics and single-cell sequencing platforms is anticipated to substantially enhance the mechanistic validation of repurposing hypotheses.

7. Conclusion

Artificial intelligence has fundamentally transformed the drug repurposing paradigm by enabling the large-scale, data-driven identification of novel therapeutic applications for existing pharmacological agents. Machine learning, deep learning, and network-based methodologies collectively provide a comprehensive analytical toolkit capable of interrogating the full complexity of drug–disease biology. The successful AI-assisted repositioning of baricitinib for COVID-19 and the ongoing clinical evaluation of metformin and sildenafil in neurological indications exemplify the translational potential of this approach. Continued advances in explainable AI, federated learning, and multi-modal omics integration—combined with strengthened regulatory frameworks and robust experimental validation pipelines—are expected to accelerate the clinical adoption of AI-driven repurposing strategies and address critical unmet medical needs across oncology, infectious diseases, and rare disorders.

8. Figures

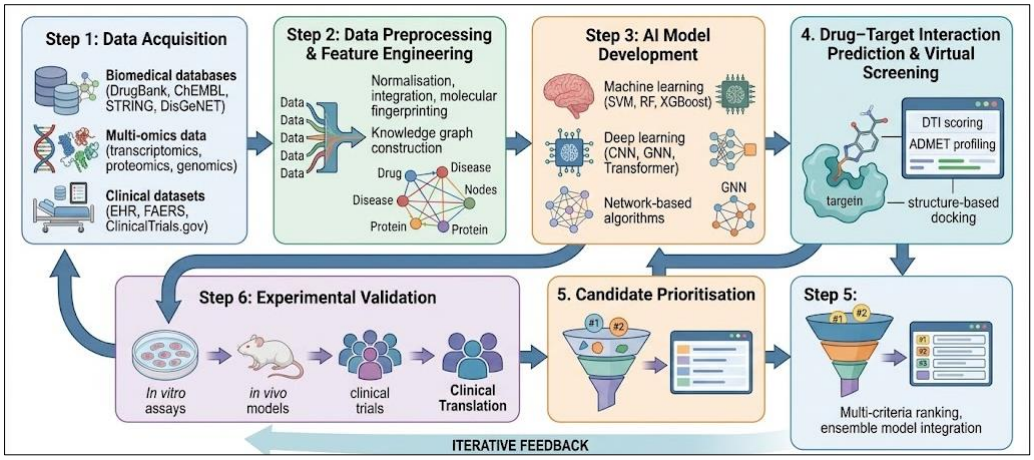

Fig 1: Workflow of Artificial Intelligence-Driven Drug Repurposing Pipeline

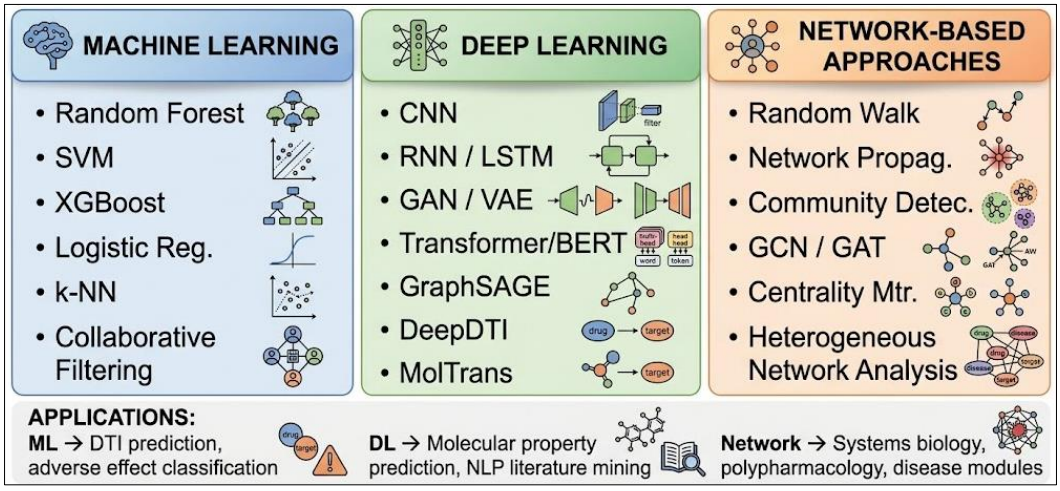

Fig 2: Major Artificial Intelligence Algorithms Used in Drug Repurposing

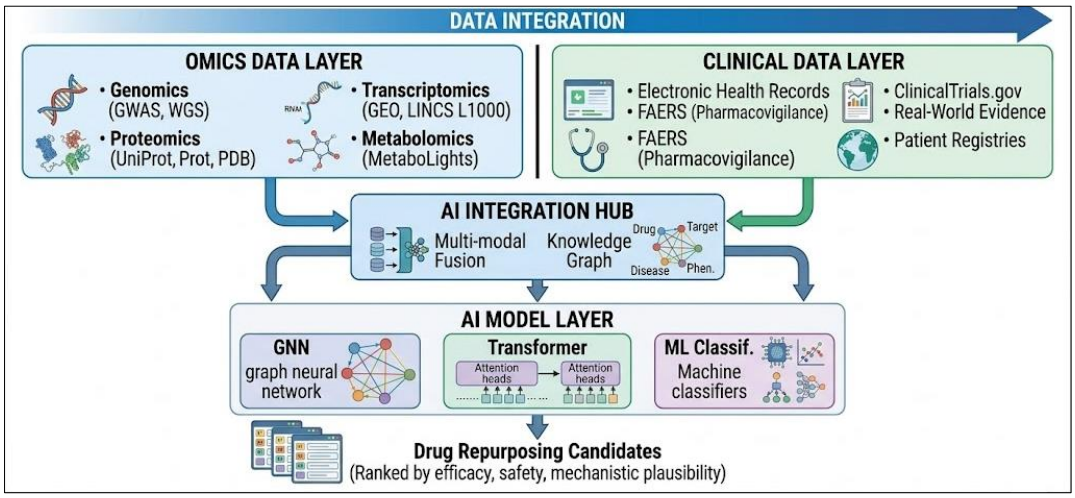

Fig 3: Integration of AI with Omics Data and Clinical Datasets for Drug Repositioning

9. Tables

Table 1: Major Artificial Intelligence Techniques Used in Drug Repurposing

AI Technique	Description	Key Algorithms / Tools	Application in Repurposing
Machine Learning (ML)	Learns patterns from labelled biomedical data to predict drug–target relationships	Random Forest, SVM, XGBoost, k-NN	DTI prediction, side-effect profiling
Deep Learning (DL)	Multi-layer neural architectures for feature extraction from complex molecular or omics data	CNN, RNN, GAN, Transformer	Molecular property prediction, multi-omics integration
Graph Neural Networks (GNN)	Operates on graph-structured biological networks to capture node/edge relationships	GraphSAGE, GAT, GCN	Polypharmacology, PPI-based repositioning
Natural Language Processing (NLP)	Mines biomedical literature and electronic health records for drug-disease signals	BERT, BioBERT, GPT variants	Hypothesis generation, literature mining
Network-Based Methods	Models biological systems as interaction networks to infer drug repositioning candidates	Network propagation, random walk, community detection	Disease module targeting, multi-layered network analysis
Reinforcement Learning (RL)	Agent optimises drug repositioning policy through reward-based feedback loops	Q-learning, Policy Gradient	Multi-target optimisation, lead prioritisation

Table 2: Data Sources and Databases Used in AI-Based Drug Repurposing

Database / Resource	Data Type	Relevance to AI Repurposing
DrugBank	Drug structures, pharmacology, targets, interactions	Drug–target interaction training datasets
ChEMBL	Bioactivity data for small molecules	Activity prediction, virtual screening inputs
STRING	Protein–protein interaction networks	Network-based repurposing, GNN training
DisGeNET	Gene–disease associations	Disease module identification, target validation
GEO / ArrayExpress	Gene expression profiles (transcriptomics)	Signature-based repurposing via CMap/LINCS
LINCS L1000	Drug-induced transcriptomic signatures	Connectivity mapping, drug similarity analysis
ClinicalTrials.gov	Clinical trial outcomes and indications	Real-world evidence, safety signal mining
OMIM / Orphanet	Genetic disease associations, rare disease data	Rare disease target identification
UniProt / PDB	Protein sequences and 3D structures	Structure-based docking, deep learning inputs

Table 3: Examples of Successfully Repurposed Drugs Identified Using Artificial Intelligence

Drug	Original Indication	Repurposed Indication	AI/Computational Method
Sildenafil	Angina / Hypertension	Erectile dysfunction; Pulmonary arterial hypertension	Network pharmacology; target interaction modelling
Metformin	Type 2 Diabetes	Cancer (anti-proliferative); Alzheimer disease (investigational)	ML-based phenotypic association; transcriptomic connectivity mapping
Baricitinib	Rheumatoid Arthritis	COVID-19 (JAK-STAT pathway inhibition)	AI network analysis (BenevolentAI); approved EUA 2020
Thalidomide	Morning sickness (withdrawn)	Multiple myeloma; leprosy (ENL)	Systems biology; NF-kB pathway modelling
Itraconazole	Antifungal	Basal cell carcinoma; NSCLC (Hedgehog pathway)	Deep learning–based DTI; pathway enrichment analysis
Remdesivir	Ebola (insufficient efficacy)	COVID-19 (SARS-CoV-2 RNA-dependent RNA polymerase)	Structure-based virtual screening; ML antiviral prediction
Rapamycin (Sirolimus)	Organ transplant (immunosuppression)	Longevity; TSC-associated tumours	mTOR network modelling; omics-driven repurposing

Table 4: Advantages and Limitations of Artificial Intelligence in Drug Repurposing Strategies

Advantages	Limitations
Accelerates hypothesis generation from vast multi-omics datasets	Dependence on high-quality, curated training data; inconsistencies across databases
Reduces cost and timeline relative to de novo drug discovery	Black-box nature of deep learning models limits mechanistic interpretability
Facilitates identification of novel multi-target polypharmacology	Risk of overfitting when training on small or imbalanced biomedical datasets
Enables rapid pandemic response (e.g., COVID-19 repositioning)	Lack of standardised regulatory frameworks for AI-generated candidates
Integration of heterogeneous data types (genomics, proteomics, EHR)	Translational gap between computational prediction and *in vitro*/in vivo validation
Graph and network models capture systemic biology beyond single targets	Data privacy and ethical concerns with clinical/EHR dataset utilisation
NLP enables automated mining of millions of published biomedical texts	Limited generalisability of models trained on specific disease areas or species

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