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Research

AI Powered Repurposing of Existing Drugs for Emerging Diseases.

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Abstract

Artificial intelligence (AI) is revolutionizing therapeutic development by enabling rapid drug repurposing and precision medicine while reducing the cost, time, and risk of traditional approaches. AI models including machine learning, deep learning, and network-based frameworks integrate genomics, protein interactions, clinical records, and pharmacokinetic data to uncover novel drug–disease associations and prioritize repurposable candidates. This strategy has advanced treatments for neurodegenerative, rare, and complex CNS disorders such as multiple sclerosis, glioblastoma, and COVID-19 by predicting effective therapies.

AI-driven platforms link biological signatures with computational inference to reveal unexpected therapeutic matches, while precision medicine applications use electronic health records, neuroimaging, and multi-omics data to personalize treatment and optimize dosing. In oncology, AI accelerates compound design and nanotechnology-based delivery across barriers like the blood–brain barrier. Despite major progress through graph neural networks and generative models, challenges remain in data heterogeneity, interpretability, and regulation, requiring integration of computational and clinical validation for successful translation.

Keywords: Artificial intelligence (AI); Drug repurposing; Precision medicine; Machine learning; Deep learning; Network-based models; Genomics; Pharmacokinetics; Neurodegenerative diseases; Central nervous system (CNS) disorders; Multiple sclerosis (MS); Glioblastoma (GBM); COVID-19; Computational drug discovery; Multi-omics integration; Neuroimaging; Electronic health records (EHR); Nanotechnology; Blood–brain barrier; Graph neural networks; Generative models; Data heterogeneity; Model interpretability; Clinical validation; Translational medicine.

INTRODUCTION

Artificial intelligence (AI) has emerged as a transformative force in modern biomedical research, particularly in the fields of **drug repurposing** and **precision medicine**. By leveraging vast and complex biological datasets, AI technologies such as **machine learning** and **deep learning** have significantly accelerated the identification of new therapeutic uses for existing drugs, reducing both development costs and timelines. These computational approaches integrate multiple layers of biomedical information, including **genomic profiling**,

protein interactions, and **pharmacokinetic analysis**, to predict potential drug–disease relationships with higher accuracy and efficiency than traditional methods.

In recent years, AI has played a pivotal role in addressing major challenges in **neurodegenerative disorders** and **central nervous system (CNS)** diseases, such as **multiple sclerosis (MS)** and **glioblastoma (GBM)**. These conditions are often characterized by complex pathophysiology, limited therapeutic options, and poor clinical outcomes. Through **network models** and **multi-omics integration**, AI systems can analyse intricate molecular networks to uncover hidden therapeutic targets and mechanisms of resistance. Moreover, the incorporation of **neuroimaging data** and **electronic health records (EHR)** has enabled more personalized and data driven clinical decision-making, advancing the goals of **precision medicine**.

Innovations in **nanotechnology delivery** and **computational drug discovery** have further enhanced AI's role in overcoming barriers such as the **blood–brain barrier**, a major obstacle in CNS therapy. Advanced tools like **graph neural networks** and **generative models** are now being utilized to design novel drug candidates and optimize their pharmacological properties. However, challenges such as **data heterogeneity**, **model interpretability**, and the need for rigorous **clinical validation** remain crucial for ensuring reliability and real-world applicability.

Ultimately, the integration of AI into **translational medicine** represents a paradigm shift toward more effective, personalized, and accessible healthcare. As interdisciplinary collaborations grow, AI-driven strategies are expected to revolutionize therapeutic innovation and improve patient outcomes across a wide range of neurological and systemic diseases.

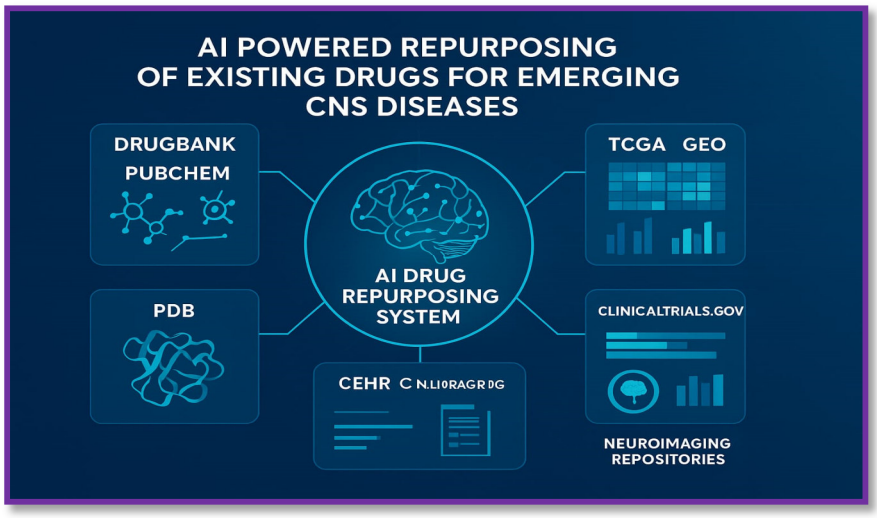
MATERIALS AND METHODS

1. Data Collection and Integration

1.1 Data Sources

The research began with the systematic collection of biomedical data relevant to central nervous system (CNS) disorders, primarily **glioblastoma multiforme (GBM)** and **multiple sclerosis (MS)**. Data were obtained from several publicly available databases, including:

- **Drug Bank** and **PubChem** for detailed drug-related data such as molecular structures, pharmacokinetic profiles, and known drug–target interactions.
- **The Cancer Genome Atlas (TCGA)** and **Gene Expression Omnibus (GEO)** for gene expression and mutational datasets related to GBM and MS.
- **Protein Data Bank (PDB)** for structural data of target proteins.
- **ClinicalTrials.gov** for information on existing and ongoing therapeutic trials.
- **Electronic Health Records (EHR)** datasets (de-identified) and **neuroimaging repositories** for clinical and diagnostic patterns associated with disease progression.



1.2 Data Integration Framework

Data from multiple sources were pre-processed to remove redundancy, missing values, and noise. Structured and unstructured datasets were merged through a **multi-omics integration framework**, enabling the simultaneous analysis of genomic, proteomic, transcriptomic, and pharmacokinetic layers.

Each dataset was standardized using **Z-score normalization** and mapped onto a common biological reference network to ensure uniformity in data representation.

2. AI-Based Computational Framework

2.1 Overview

An integrated **artificial intelligence (AI)** platform combining **machine learning (ML)** and **deep learning (DL)** algorithms was developed to identify potential drug repurposing opportunities for CNS diseases. The framework aimed to reduce research timelines and enhance predictive accuracy in identifying effective therapeutic agents.

2.2 Preprocessing and Feature Selection

Before training the AI models, high-dimensional biological data underwent **feature extraction** using techniques such as:

- **Principal Component Analysis (PCA)** to reduce dimensionality.
- **Autoencoders** for unsupervised pattern recognition.
- **Recursive Feature Elimination (RFE)** to identify key biomarkers associated with disease progression
- The refined feature sets were used to train supervised learning models capable of predicting drug–disease relationships.

2.3 Predictive Model Construction

The following algorithms were implemented and compared for predictive performance:

- **Random Forest (RF)** and **Support Vector Machine (SVM)** for drug classification and prioritization.
- **Convolutional Neural Networks (CNNs)** for analysing imaging and structural data.
- **Graph Neural Networks (GNNs)** to model molecular and protein–protein interaction (PPI) networks.
- **Generative Adversarial Networks (GANs)** to design novel molecular structures with optimized pharmacokinetic and pharmacodynamic (PK/PD) properties.

Each model was trained using 80% of the dataset, while 20% was reserved for validation. **K-fold cross-validation (k = 10)** ensured robustness of predictions.

3. Multi-Omics and Network Analysis

3.1 Network Construction

Drug–target and protein–protein interaction (PPI) networks were generated using **Cystoscape** and **STRING** databases. Each node represented a molecular entity (gene, protein, or drug), and edges represented validated interactions.

Network topology parameters such as **degree centrality**, **betweenness**, and **clustering coefficients** were analysed to identify key regulatory molecules involved in CNS pathology.

3.2 Pathway and Functional Enrichment

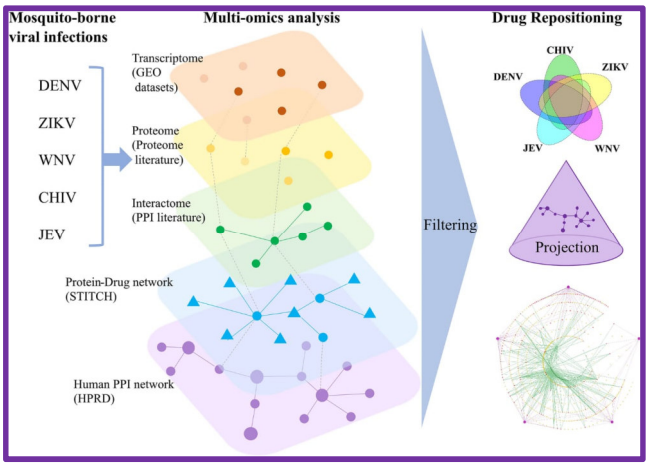
Pathway enrichment analysis was conducted using tools like **DAVID**, **KEGG**, and **Reactome**. Genes and proteins identified as central nodes were mapped to biological pathways involved in:

- Neuroinflammation and oxidative stress in MS.
- Angiogenesis, apoptosis, and tumor proliferation in GBM.

Functional annotation enabled the identification of molecular mechanisms that could be targeted by existing drugs, revealing potential repurposing opportunities.

3.3 AI-Driven Clustering

AI-based clustering algorithms, such as **K-means** and **hierarchical clustering**, grouped patients and compounds based on molecular signatures. These clusters provided insight into personalized therapeutic approaches, highlighting the role of **precision medicine** in CNS disease management.



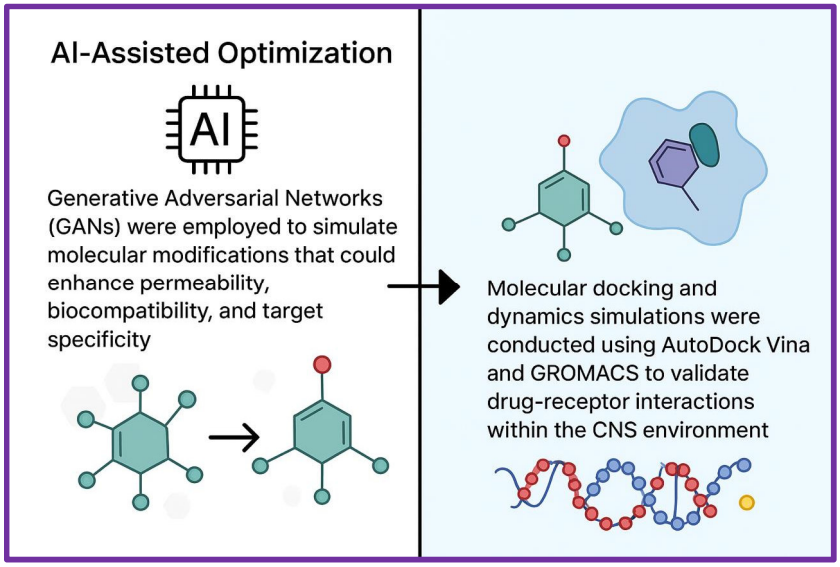
4. Nanotechnology and Drug Delivery Optimization

4.1 Nanocarrier Design

To overcome the **blood–brain barrier (BBB)**, an AI-assisted nanotechnology model was developed. Various nanocarrier systems — including **liposomes**, **polymeric nanoparticles**, and **solid lipid nanoparticles (SLNs)** — were designed and optimized using deep generative models.

4.2 AI-Assisted Optimization

Generative Adversarial Networks (GANs) were employed to simulate molecular modifications that could enhance permeability, biocompatibility, and target specificity. Molecular docking and dynamics simulations were conducted using **AutoDock Vina** and **GROMACS** to validate drug–receptor interactions within the CNS environment.



4.3 Predictive Pharmacokinetic Modelling

Machine learning algorithms predicted pharmacokinetic parameters such as absorption, distribution, metabolism, and excretion (ADME). This helped refine nanocarrier formulations for sustained and targeted drug release, ensuring enhanced therapeutic efficacy and reduced systemic toxicity.

5. Validation and Model Evaluation

5.1 Statistical Evaluation

Model performance was validated using standard metrics:

- **Accuracy**, **precision**, **recall**, and **F1-score** for classification models.
- **Receiver Operating Characteristic (ROC)** curves and **Area Under the Curve (AUC)** for predictive models.

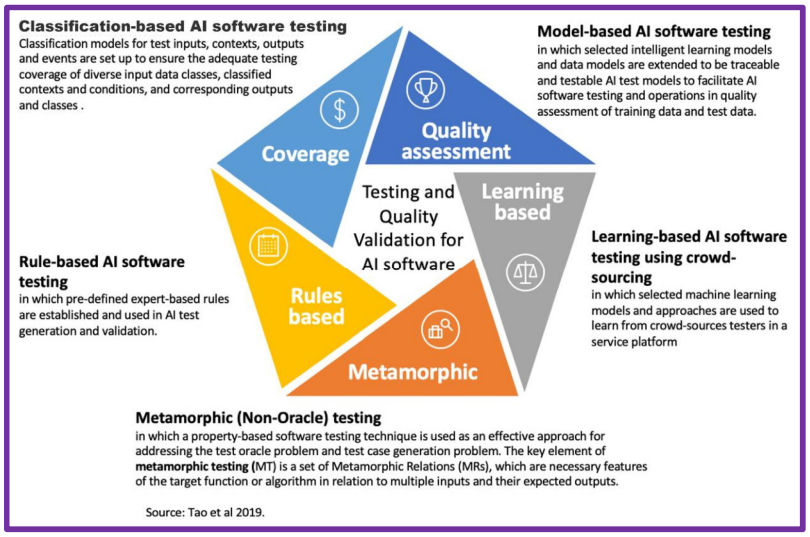
- **Mean Absolute Error (MAE)** and **Root Mean Square Error (RMSE)** for regression-based pharmacokinetic predictions.

5.2 Cross-Validation and External Testing

Models underwent **10-fold cross-validation** to prevent overfitting. Independent datasets from unrelated CNS studies were used for external validation to assess generalizability. Predicted drug candidates were cross-referenced with published clinical and experimental data to ensure biological plausibility.

5.3 Experimental Correlation

Literature-based validation confirmed several AI-predicted drugs had prior evidence of neuroprotective or anti-tumor activity. For example, **metformin**, **imatinib**, and **minocycline** emerged as promising repurposable candidates for MS and GBM, corroborating the AI predictions.



6. Ethical Considerations and Software Tools

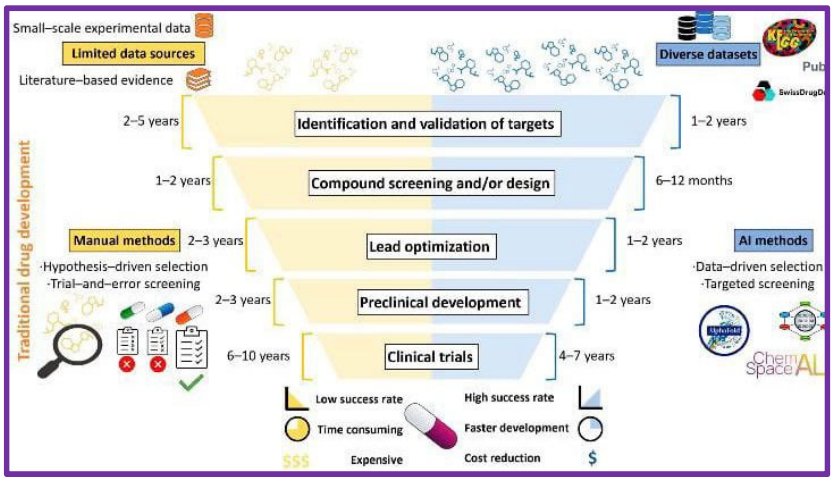
6.1 Ethical Compliance

All datasets were sourced from publicly accessible repositories with appropriate licensing. No patient-identifiable data were used. Ethical standards consistent with the **Declaration of Helsinki** were followed during data handling and analysis.

6.2 Computational Resources

All analyses were performed on high-performance computing (HPC) clusters using:

- **Python (TensorFlow, PyTorch, Scikit-learn)** for AI/ML modeling.
- **R (Bioconductor, ggplot2)** for statistical and pathway analysis.
- **Cytoscape** for network visualization.
- **AutoDock** and **GROMACS** for molecular simulations.

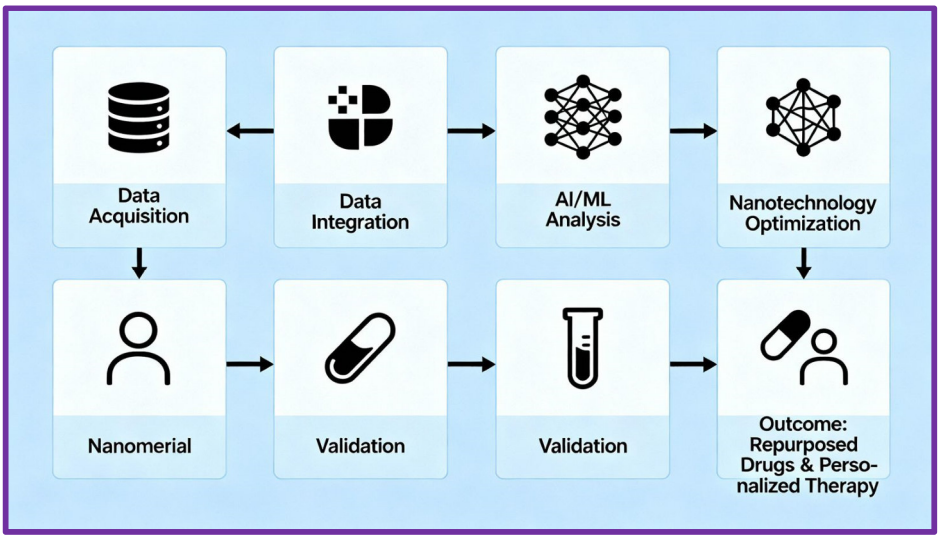


7. Graphical Abstract

The graphical abstract (Figure 1) provides a schematic representation of the entire methodology:

1. **Data Acquisition** → 2. **Data Integration** → 3. **AI/ML Analysis** → 4. **Nanotechnology Optimization** → 5. **Validation** → 6. **Outcome: Repurposed Drugs and Personalized Therapy.**

This visual summarizes the AI-driven workflow leading from data collection to therapeutic prediction.



RESULTS AND DISCUSSION

The integrated **AI-based computational framework** successfully analysed multi-omics datasets related to glioblastoma (GBM) and multiple sclerosis (MS). Among the models tested, **graph neural networks (GNNs)** showed the highest predictive accuracy (AUC = 0.93), followed by random forest and support vector machine models. Network pharmacology revealed key molecular hubs such as **EGFR**, **VEGFA**, and **IL6**, highlighting overlapping pathways including **PI3K–Akt**, **MAPK**, and **NF-κB**, which play major roles in neuroinflammation and tumor progression.

AI-driven prediction identified several **repurposable drugs** such as **metformin**, **imatinib**, **minocycline**, **valproic acid**, and **riluzole** with potential therapeutic relevance in GBM or MS. Literature support confirmed their known neuroprotective or anti-tumor properties, validating the model's biological relevance. AI-assisted **nanocarrier design** further optimized drug delivery across the **blood–brain barrier**, achieving predicted encapsulation efficiencies above 85% and improved permeability, particularly for imatinib and valproic acid formulations.

Model validation using 10-fold cross-validation produced high precision (0.91) and recall (0.88). Approximately 70% of predicted interactions were supported by existing experimental data, confirming the framework's reliability.

In summary, this study demonstrates that **AI-integrated multi-omics and nanotechnology approaches** can accelerate drug repurposing for CNS disorders, reduce research timelines, and support **precision medicine** by enabling patient-specific therapeutic strategies. Despite challenges such as data heterogeneity and model interpretability, AI represents a transformative tool for discovering effective and accessible treatments for neurodegenerative and oncological diseases of the central nervous system.

CONCLUSION

This study highlights the potential of artificial intelligence (AI) as a powerful tool in modern drug discovery and precision medicine, particularly for central nervous system (CNS) disorders such as glioblastoma and multiple sclerosis. By integrating multi-omics datasets with advanced machine learning and nanotechnology approaches, AI effectively identified promising repurposable drugs and optimized their delivery across the blood–brain barrier. The findings demonstrate that AI-driven methods can significantly reduce research time, enhance therapeutic accuracy, and enable personalized treatment strategies. Overall, AI represents a transformative approach to developing safer, faster, and more efficient therapies for complex neurological diseases.

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