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Review Article

The role of artificial intelligence in advancing neuropharmacology

Pankaj Khuspe[1], Sitaram Kale[2], Nagnath Konapure[1], Dipali Mane[2*], Trushali Mandhare[3]

[1]Dept. of Pharmaceutics, Shriram Shikshan Sanstha's College of Pharmacy, Paniv, Maharashtra, India
[2]Dept. of Pharmacology, Shriram Shikshan Sanstha's College of Pharmacy, Paniv, Maharashtra, India
[3]Dept. of Pharmaceutical Chemistry, Navsahyadri Institute of Pharmacy, Nasrapur, Maharashtra, India

Abstract

AI is rapidly transforming the field of neuropharmacology by introducing sophisticated computational methodologies capable of addressing the multifactorial complexity of central nervous system (CNS) disorders. By integrating ML, DL, and NLP, AI enables the analysis of high dimensional biomedical data, including genomics, proteomics, metabolomics, neuroimaging, and electronic health records. These capabilities support high throughput screening, accelerate de novo drug design, and enhance target identification by uncovering subtle biological correlations and mechanistic insights that often elude traditional experimental paradigms. AI based frameworks facilitate in silico prediction of pharmacokinetics and pharmacodynamics, drug–target interactions, and blood–brain barrier permeability. This empowers researchers to develop personalized therapeutic strategies for complex neurodegenerative and neuropsychiatric disorders such as Alzheimer's disease, Parkinson's disease, schizophrenia, and major depressive disorder. Several case studies underscore AI's translational potential: Benevolent AI's application of NLP for drug repurposing in amyotrophic lateral sclerosis (ALS), Deep Genomics' AI driven discovery of RNA targeted molecules, and Atomwise's structure based compound optimization exemplify AI's impact across discovery and development pipelines. Despite its promise, the integration of AI into neuropharmacology is not without challenges. The opacity of deep learning models ("black box" problem), data heterogeneity, model generalizability, and evolving regulatory frameworks necessitate rigorous validation and interpretability efforts. This review comprehensively explores current applications, technological advancements, and future trajectories of AI in neuropharmacology. As the discipline evolves, AI stands poised as a foundational tool in the advancement of precision medicine, supporting more efficient, targeted, and individualized CNS pharmacotherapies.

Keywords: Artificial intelligence, Neuropharmacology, CNS drug discovery, Machine learning, Biomedical informatics.

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1. Introduction

Neuropharmacology, the scientific study of how drugs modulate neural function and behaviour, lies at the forefront of efforts to treat an expanding range of central nervous system (CNS) disorders, including neurodegenerative, neuropsychiatric, and neurodevelopmental conditions. Despite major advances in molecular neuroscience and pharmacological screening techniques, the development of effective CNS therapeutics remains profoundly challenging. Traditional drug discovery pipelines are hindered by low translational success, limited predictive power of animal models, and the intrinsic complexity of brain pathophysiology. Notably, over 90% of CNS targeting drug candidates fail in clinical trials, a rate significantly higher than for non CNS indications, largely due to inadequate target validation, poor blood–brain barrier (BBB) permeability predictions, and patient heterogeneity that confounds efficacy assessments.[1]

Given the multifactorial and dynamic nature of brain diseases, there is an urgent need for paradigm shifting technologies that can manage, integrate, and interpret vast, heterogeneous datasets across molecular, imaging, and clinical domains. Artificial Intelligence (AI) particularly machine learning (ML), deep learning (DL), natural language processing (NLP), and data driven predictive modelling has emerged as a disruptive force in modern drug discovery. AI's capacity to model complex, nonlinear relationships and derive actionable insights from large scale, multimodal data

*Corresponding author: Dipali Mane
Email: dipalimanecopp@gmail.com

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makes it uniquely suited to overcome longstanding barriers in neuropharmacology. Recent developments in AI have already demonstrated measurable impact. For instance, AI assisted platforms have accelerated target identification, enabled de novo molecule generation, and improved in silico pharmacokinetic profiling. Moreover, AI has been pivotal in stratifying patients for clinical trials and identifying novel biomarkers through integrative analysis of imaging and genomic data. These capabilities represent a significant departure from conventional reductionist methods, which often fail to capture the dynamic interactions within neural systems.[2]

Despite its promise, the integration of AI into neuropharmacology is not without limitations. Challenges include the interpretability of AI models, lack of standardized datasets, data privacy concerns, and regulatory uncertainties. Nevertheless, the continuous evolution of explainable AI, federated learning, and real world validation frameworks is gradually addressing these issues.

This review provides a comprehensive overview of how AI is reshaping the landscape of neuropharmacology. It outlines current methodologies, examines emerging technologies, highlights real world applications through case studies, and discusses the challenges and future directions necessary for successful clinical translation. As the field progresses towards precision neurotherapeutics, AI is poised to serve not merely as a supplementary tool but as a cornerstone of next generation CNS drug discovery and development.[3,4]

2. AI Technologies in Neuropharmacology

Advancements in AI have catalysed a paradigm shift in neuropharmacology by enabling high throughput, data driven methodologies to interrogate complex neural systems and pharmacodynamic responses. Traditional computational methods in pharmacology such as quantitative structure activity relationship (QSAR) models and rule based systems have proven inadequate in capturing the nonlinear, multi layered nature of central nervous system (CNS) disorders. These methods often suffer from limited scalability, rigid input feature engineering, and insufficient generalizability across heterogeneous datasets. Emerging AI technologies including ML, DL, NLP, and graph neural networks (GNNs) have significantly addressed these limitations by incorporating flexible, adaptive, and scalable computational frameworks.[5]

ML forms the backbone of predictive modeling in neuropharmacology. Supervised learning algorithms (e.g., support vector machines, random forests) are used to classify disease phenotypes and predict drug response profiles using patient derived omics and imaging data. Unsupervised methods, such as k means clustering or principal component analysis (PCA), assist in uncovering latent subtypes in heterogeneous neurological disorders. However, conventional ML often depends heavily on manual feature extraction and lacks the depth to model temporal or spatial dependencies inherent in neural data.[6]

DL, particularly convolutional neural networks (CNNs) and recurrent neural networks (RNNs), offers a powerful alternative. CNNs are adept at extracting hierarchical features from high dimensional inputs like functional MRI or EEG signals, enabling improved detection of biomarkers and disease progression patterns. RNNs, including long short term memory (LSTM) networks, are applied to model time series neurophysiological data, capturing longitudinal drug effects. These architectures reduce the need for manual feature design and outperform classical ML in multi modal integration. Yet, they are often criticized for being “black box” systems, making biological interpretation difficult.[7]

NLP has emerged as a transformative tool in literature mining and real world data extraction. Using named entity recognition, relationship extraction, and context aware models like BERT, NLP systems can automatically synthesize pharmacogenomic relationships from unstructured data such as electronic health records (EHRs) and biomedical literature. This addresses a key bottleneck in traditional systematic reviews and drug repurposing pipelines, which were limited by manual curation speed and comprehensiveness.[8]

Graph Neural Networks (GNNs) represent a recent innovation particularly suited to neuropharmacology, where complex networks of interacting genes, proteins, receptors, and drugs can be naturally represented as graphs. GNNs propagate information through graph structures, capturing both local and global topological features. In drug discovery, GNNs can predict novel drug target interactions and polypharmacological effects by learning from known biochemical and disease networks. They overcome the limitations of conventional vector based models that fail to capture structural relationships.[9] AI technologies provide a robust and scalable foundation for modern neuropharmacology. While limitations such as interpretability, data sparsity, and model generalization persist, the convergence of these techniques marks a substantial departure from reductionist approaches. By enabling integrative and dynamic modeling of complex CNS systems, AI empowers a new era of precision driven neurotherapeutics and accelerates the translation of discovery into clinical intervention.[10]

3. AI in Drug Discovery and Target Identification

AI is increasingly redefining the landscape of drug discovery and target identification in neuropharmacology, especially for complex and multifactorial conditions such as Alzheimer’s disease, Parkinson’s disease, and amyotrophic lateral sclerosis. Traditional drug discovery relies heavily on high throughput screening (HTS), molecular docking, and empirical hit to lead optimization. Although these approaches

have contributed significantly to the development of CNS targeted agents, they are limited by high failure rates, time consuming experimental cycles, and inefficiencies in accurately identifying viable drug target interactions, particularly within the complex environment of the brain.[10]

Structure based drug design (SBDD) typically employs crystallographic or homology modeled protein structures for docking potential ligands. However, its predictive accuracy is constrained by incomplete structural data, protein flexibility, and limited binding site resolution. Similarly, ligand based approaches, such as QSAR modeling, depend on curated compound libraries and predefined molecular descriptors, often failing when applied to novel chemical spaces or poorly understood targets.[12]

AI driven methods address these bottlenecks through data intensive, predictive modeling techniques. Deep learning models, such as CNNs and GCNs, can learn spatial, electronic, and topological features directly from raw molecular input either as SMILES strings, molecular graphs, or 3D coordinates eliminating the need for manual descriptor engineering. For instance, models like DeepDock and AtomNet have demonstrated high accuracy in predicting protein ligand binding affinities by capturing complex intermolecular interactions.[13]

AI integrates multi omics datasets including genomics, transcriptomics, proteomics, and connectomics to uncover novel druggable targets that are contextually relevant to disease mechanisms. For example, integrative AI platforms like Benevolent AI use knowledge graphs and natural language processing to synthesize evidence across vast biological datasets and biomedical literature, accelerating hypothesis generation for novel therapeutic targets.[14] In neurodegenerative disorders, AI's ability to model biological networks and disease progression dynamics enables the identification of targets that are not just statistically significant, but mechanistically central to disease phenotypes. AI also facilitates in silico validation through virtual screening and prioritization of compound libraries, drastically reducing the cost and time required for experimental assays.[15]

3.1. Applications in CNS pharmacology

Applications of artificial intelligence in central nervous system (CNS) pharmacology are rapidly expanding, offering advanced capabilities that enhance the efficiency and precision of drug discovery workflows. One significant application is the early stage prediction of blood brain barrier (BBB) permeability, a critical parameter for CNS active compounds, where AI models outperform traditional rule based or in vitro assays by leveraging chemical structure data and multi modal features.[10]

AI algorithms can identify targetable nodes within disease specific protein protein interaction networks by analyzing network topology and functional annotations, thus uncovering intervention points that are central to disease pathophysiology. In neuropsychiatric disorders, which are often characterized by high genetic heterogeneity, AI facilitates the deconvolution of polygenic risk architecture. By integrating large scale genomic data, it helps pinpoint functional biological pathways that may serve as therapeutic targets. Moreover, AI is instrumental in the discovery and optimization of CNS active compounds with multi target efficacy profiles, moving beyond the "one drug–one target" paradigm to more holistic therapeutic strategies suitable for complex disorders. Despite these promising applications, challenges persist. Model interpretability remains a concern, especially with deep learning systems, which are often criticized as "black boxes." Data sparsity, particularly for high quality CNS specific datasets, limits model training and validation. Additionally, algorithmic bias stemming from imbalanced training data can impact generalizability.[16] AI based systems offer scalable, data driven alternatives that overcome many of the intrinsic limitations of traditional neuropharmacological methods. The integration of these technologies into CNS drug discovery pipelines is expected to enhance target validation, improve lead optimization, and reduce attrition rates in early phase development, ultimately accelerating the path to precision neurotherapeutics.[17]

4. Predictive Modeling in Pharmacokinetics and Pharmacodynamics

One of the most critical components in neuropharmacological drug development is understanding the pharmacokinetics (PK) and pharmacodynamics (PD) of candidate compounds. These parameters encompassing absorption, distribution, metabolism, excretion (ADME), and drug receptor interactions determine both efficacy and safety profiles. Traditional in vitro and in vivo approaches, though foundational, are resource intensive and often fail to capture the intricate dynamics of central nervous system (CNS) pharmacology, particularly due to the complexities of blood brain barrier (BBB) permeability and neuro specific metabolic pathways.[18] AI has increasingly been adopted to overcome these limitations by enabling data driven predictive modeling. Machine learning algorithms, particularly deep neural networks and ensemble models, have shown high accuracy in forecasting ADME properties by learning from large, heterogeneous datasets derived from cheminformatics, in vitro bioassays, and clinical pharmacokinetic studies. These models can predict time dependent plasma concentrations, tissue distribution kinetics, and metabolic biotransformation pathways under various physiological conditions.[19]

A significant advantage of AI based models is their capacity to predict BBB permeability with greater reliability than traditional rule based systems such as Lipinski's Rule of Five or simple QSAR models. AI tools like DeepTox, which employs deep learning architectures for toxicity and metabolism prediction, and ADMETlab, a comprehensive

web based platform integrating multiple ML algorithms, have been increasingly used to assess CNS drug likeness early in the pipeline. These platforms facilitate in silico screening and optimization of drug candidates, reducing the reliance on costly animal studies.[20] Ultimately, the integration of predictive AI models into PK/PD analysis enhances translational fidelity, shortens development timelines, and supports precision dosing strategies in neuropharmacology.[21]

5. Patient Stratification and Personalized Neurotherapeutics

The increasing adoption of AI in neuropharmacology has opened new avenues for precision medicine, particularly in the realm of patient stratification and individualized therapeutic interventions. Traditional approaches to classifying patients with neurological or psychiatric conditions often rely on broad diagnostic categories that fail to capture the heterogeneity inherent in these disorders. AI driven clustering algorithms, including unsupervised learning techniques such as k means, hierarchical clustering, t distributed stochastic neighbor embedding (t SNE), and self organizing maps (SOMs), have shown remarkable utility in identifying clinically meaningful subgroups within complex patient populations.[22] These models can integrate diverse data modalities ranging from neuroimaging (e.g., MRI, PET), electrophysiological signals (EEG, MEG), and transcriptomics, to longitudinal clinical and behavioral datasets to uncover latent patterns associated with disease progression, therapeutic response, or relapse risk. In disorders like Alzheimer's disease, for instance, machine learning has enabled stratification based on amyloid and tau deposition patterns, structural atrophy metrics, and cognitive decline trajectories. Similarly, in major depressive disorder and schizophrenia, clustering based on neuroimaging and genetic signatures has facilitated the identification of treatment responsive subtypes.[23]

AI enabled stratification plays a critical role in optimizing clinical trial design, minimizing placebo effects, and improving signal detection in therapeutic efficacy. This stratified approach not only enhances drug development pipelines but also supports the implementation of personalized neurotherapeutics, where treatment regimens are tailored according to an individual's unique biological and clinical profile. As AI methodologies continue to evolve, their integration into clinical neuropharmacology is expected to transform the paradigm from population based interventions to truly individualized care strategies.[24]

6. Case Studies

6.1. Case study 1: BenevolentAI and ALS drug repurposing

AI has emerged as a pivotal enabler of drug repurposing strategies, particularly for complex neurodegenerative diseases such as amyotrophic lateral sclerosis (ALS), where conventional drug discovery approaches are often slow and prone to failure. A compelling demonstration of this paradigm shift is evident in the work conducted by Benevolent AI, which harnessed an AI driven platform to identify novel therapeutic indications for existing drugs. Utilizing a proprietary biomedical knowledge graph, the company integrated vast volumes of structured and unstructured data spanning peer reviewed publications, clinical trial reports, biochemical pathways, and transcriptomic datasets to extract mechanistically relevant insights. In this specific case, Benevolent AI's platform employed NLP and machine learning algorithms to traverse complex biological associations. Through this integrative computational approach, the Janus kinase (JAK) inhibitor baricitinib, originally approved for rheumatoid arthritis, was identified as a candidate for repurposing in ALS. The platform highlighted baricitinib's potential to modulate neuroinflammatory pathways implicated in ALS pathology, particularly by interfering with aberrant JAK STAT signaling involved in microglial activation and neuronal degeneration. Following the AI guided prediction, baricitinib advanced rapidly to preclinical validation and early phase clinical investigation, representing a significant acceleration compared to traditional drug discovery timelines. This case underscores the transformative role of AI in hypothesis generation, data synthesis, and rational repurposing of pharmacological agents for CNS disorders. By systematically uncovering latent therapeutic potential within existing pharmacopoeia, AI systems such as BenevolentAI offer a scalable solution for addressing urgent unmet needs in neuropharmacology.[25,27]

6.2. Case study 2: Deep genomics and RNA based neurotherapeutics

The convergence of AI with RNA biology has enabled a new frontier in neuropharmacology, particularly in the design and development of RNA targeted therapeutics for rare neurological diseases. Deep Genomics, a biotechnology company at the forefront of this convergence, has developed an AI powered platform known as the AI Workbench capable of analyzing massive RNA sequence datasets to predict the functional consequences of genetic variants and design antisense oligonucleotides (ASOs) with therapeutic potential. Unlike conventional bioinformatics tools, which often rely on limited rule based algorithms, Deep Genomics' platform leverages deep learning architectures trained on experimental transcriptomic and genomic data. This system processed over 69 billion RNA interactions to identify patterns of aberrant splicing associated with pathogenic mutations. The AI models predict not only the likelihood of a splicing defect but also the potential for its correction using customized ASOs, which are short, synthetic nucleotide sequences designed to modulate RNA function by targeting specific pre mRNA elements. In the context of neuropharmacology, this approach is particularly promising due to the high prevalence of splicing related dysfunction in rare neurodevelopmental and neurodegenerative disorders. By enabling high

throughput target discovery and therapeutic design, the AI Workbench has expedited the transition from genetic insight to preclinical candidate development. A notable outcome includes the identification of lead ASOs for previously untreatable monogenic CNS disorders, representing a paradigm shift in precision neurotherapeutics. This case exemplifies how AI is not merely augmenting, but fundamentally redefining, the landscape of RNA based drug discovery in neurology.[28,29]

7. Challenges and Limitations

Despite the growing momentum of AI applications in neuropharmacology, several critical challenges hinder its seamless integration into clinical and translational workflows. These limitations pertain primarily to algorithmic transparency, data quality and interoperability, and the evolving landscape of regulatory compliance.[30]

7.1. Model interpretability

One of the foremost obstacles in deploying AI driven models, particularly DL architectures, in neuropharmacology is the issue of interpretability. Deep neural networks often function as "black box" systems, offering high predictive performance but limited explanatory insight into their decision making processes. In clinical and pharmacological contexts, where decisions directly impact patient outcomes and regulatory approval, such opacity is problematic. Without transparent reasoning or mechanistic pathways, stakeholders including clinicians, regulatory authorities, and pharmaceutical developers may lack confidence in adopting AI generated outputs for therapeutic development or patient stratification. Emerging approaches such as attention mechanisms, explainable AI (XAI) frameworks, and saliency mapping aim to address this gap, but their application in neuroscience remains limited and requires further validation.[31]

7.2. Data heterogeneity

Neuropharmacology is inherently multi dimensional, involving diverse data types such as neuroimaging, electrophysiology, molecular profiles, behavioural metrics, and clinical annotations. Integrating such heterogeneous, high throughput datasets poses significant technical and computational challenges. Disparities in data quality, resolution, formats, and sampling methods complicate model training and validation, often resulting in overfitting or diminished generalizability. Standardization of data acquisition protocols, development of cross platform ontologies, and robust feature harmonization techniques are essential to enable effective multi modal AI modelling.[32]

7.3. Regulatory oversight

The regulatory environment governing AI applications in neuropharmacology remains nascent and fragmented. Unlike traditional therapeutics, AI algorithms evolve through iterative learning, making it difficult to establish fixed validation metrics or static performance baselines. Regulatory agencies such as the FDA and EMA are beginning to draft frameworks for Software as a Medical Device (SaMD) and algorithmic transparency, but specific guidance for AI driven drug discovery and clinical trial optimization in the CNS domain is still under development. The lack of standardized protocols for evaluating AI model safety, efficacy, and reproducibility continues to be a bottleneck in achieving full clinical translation.[33]

8. Future Prospects

The future of neuropharmacology is poised to be fundamentally reshaped by the convergence of AI with emerging biomedical technologies such as advanced neuroimaging, wearable biosensors, and digital phenotyping. These synergistic domains offer the potential to unlock unprecedented insights into brain function and disease progression, facilitating the development of more precise and dynamic pharmacological interventions.[34] The integration of AI with neuroimaging modalities such as functional MRI (fMRI), positron emission tomography (PET), and diffusion tensor imaging (DTI) is enabling real time analysis of brain activity patterns, structural connectivity, and receptor level interactions. Machine learning algorithms can detect subtle neuroanatomical or functional changes predictive of early stage pathology, thereby supporting earlier diagnosis and drug intervention points. Additionally, the fusion of AI with wearable technologies allows for continuous, longitudinal monitoring of neurological and behavioral parameters in real world settings. These high resolution datasets can be algorithmically transformed into digital biomarkers, facilitating adaptive dosing strategies and more personalized neuropharmacological therapies.[35]

One of the most promising frontiers lies in AI driven digital twin modeling. By integrating patient specific multi omics data, neural dynamics, and pharmacokinetic/pharmacodynamic profiles, AI can simulate individualized brain models that respond virtually to candidate compounds. These "in silico patients" have the potential to revolutionize preclinical research by reducing reliance on animal models and accelerating hypothesis testing in a controlled, scalable manner. AI enabled platforms will increasingly support simulation based regulatory submissions, closed loop neurostimulation systems, and augmented reality assisted cognitive interventions. As these innovations mature, AI is expected to underpin a paradigm shift toward predictive, preventive, and precision neuropharmacology in the coming decade.[36]

9. Conclusion

Artificial intelligence is emerging as a cornerstone in the evolution of neuropharmacology, offering unprecedented capabilities to decode complex neural processes, optimize drug discovery, and enable precision based interventions. Through the integration of multi omics data, clinical phenotypes, and real world evidence, AI driven platforms are

accelerating the identification of novel therapeutic targets and refining the design of CNS active compounds. Importantly, AI enhances predictive modeling of pharmacokinetics, stratifies patient populations based on individual risk profiles, and informs adaptive clinical trial designs. Nevertheless, the full realization of AI's potential in neuropharmacology depends on overcoming persistent challenges. These include the need for model interpretability, harmonization of diverse data sources, standardization of validation protocols, and the development of ethical frameworks for AI assisted decision making in clinical contexts. Additionally, interdisciplinary collaboration among neuroscientists, pharmacologists, computer scientists, and regulatory bodies will be essential to ensure translational impact. In summary, while obstacles remain, the synergistic application of AI technologies offers a compelling path forward. By bridging the gap between computational intelligence and neurobiological complexity, AI stands poised to transform neuropharmacology into a more predictive, personalized, and effective discipline, ultimately improving outcomes for patients with neurological and psychiatric disorders.

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None.

11. Conflict of Interest

None.

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