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AI-DRIVEN DRUG TARGET IDENTIFICATION IN NEURODEGENERATION: APPLICATIONS IN ALZHEIMER'S, PARKINSON'S, AND ALS RESEARCH

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ABSTRACT

Neurodegenerative diseases — including Alzheimer's disease (AD), Parkinson's disease (PD), and amyotrophic lateral sclerosis (ALS) — represent the greatest unmet therapeutic need in neurology, with no currently approved disease-modifying therapies for AD or ALS and limited options for PD. The extraordinarily high failure rate of neurodegenerative drug candidates — approximately 99% for AD clinical trials — reflects incomplete understanding of disease mechanisms and inadequate target validation at the preclinical stage. Artificial intelligence, encompassing machine learning network analysis, protein structure prediction, knowledge graph mining, and molecular dynamics simulation, is transforming the drug target identification process for neurodegenerative diseases by enabling the integration of genomic, proteomic, transcriptomic, and clinical data at scales previously impossible. This review analyses 40 studies of AI-driven target identification in neurodegeneration

published between 2019 and 2024. Knowledge graph-based target identification approaches have generated candidate targets with network-level validation in AD and PD, several of which have advanced to preclinical or clinical evaluation. AlphaFold2 protein structure predictions have enabled structure-based drug design for neurodegeneration-related proteins previously considered undruggable. Implications for neuropharmacological research capacity development are discussed.

Keywords: neurodegeneration; Alzheimer's disease; drug target identification; artificial intelligence; knowledge graph; AlphaFold; protein structure; drug discovery

1. INTRODUCTION

The clinical and social burden of neurodegenerative diseases is extraordinary: Alzheimer's disease alone affects 55 million individuals globally, with annual costs estimated at USD 1.3 trillion; Parkinson's disease affects 10 million; and ALS, while less prevalent, is universally fatal within 2–5 years of diagnosis with no approved disease-modifying therapy (WHO, 2023; GBD 2016 Neurology Collaborators, 2017). Despite decades of research investment, the neurodegenerative drug development pipeline has been characterised by an exceptionally high clinical trial failure rate: 99.6% for Alzheimer's disease trials over the past two decades, reflecting both the complexity of neurodegenerative pathophysiology and the inadequacy of preclinical target validation strategies.

The failure of single-target drug development approaches — focused sequentially on amyloid-β, tau, and inflammatory targets in AD — has driven a paradigm shift toward multi-target network approaches, in which drug target identification is framed as a network medicine problem: identifying nodes and edges in the

molecular interaction network of neurodegenerative disease whose perturbation would produce beneficial therapeutic effects across multiple pathological mechanisms simultaneously (Barabási et al., 2011). This reframing is inherently suited to AI-driven analysis: biological networks are too complex and multidimensional for human intuition to navigate effectively, but machine learning and graph algorithms can identify therapeutic targets through principled analysis of protein-protein interaction networks, gene regulatory networks, and multi-omics integration.

The AlphaFold2 protein structure prediction system — which has now generated predicted structures for virtually all human proteins with near-experimental accuracy — has dramatically expanded the structural druggability landscape for neurodegeneration, enabling structure-based design against targets previously classified as unstructured or undruggable. This review evaluates the current evidence for AI-driven target identification in neurodegeneration and the translational potential of candidate targets identified through these approaches.

2. MATERIALS AND METHODS

A systematic search of PubMed, Scopus, and bioRxiv identified 40 studies of AI-driven drug target identification specifically applied to Alzheimer's disease, Parkinson's disease, or ALS published between 2019 and 2024. Inclusion required original research, AI methodology (machine learning, knowledge graph, network analysis, or protein structure prediction), and reporting of target candidates with at least one level of experimental or computational validation. Studies were categorised by AI methodology, disease focus, and validation level of identified targets.

3. RESULTS

Knowledge graph-based target identification — mining networks of biological and clinical relationships extracted from literature, databases, and EHRs — identified 8–24 candidate targets per disease across included studies. Validation against Mendelian randomisation, genome-wide association study, and network proximity analyses supported 30–60% of identified candidates. For AD specifically, knowledge graph approaches identified TREM2, BIN1, and PICALM as high-confidence network targets with convergent multi-omics support — all subsequently validated in independent experimental studies. In PD, LRRK2 network interactions and GBA lysosomal pathway targets were consistently identified across multiple AI approaches.

AlphaFold2 structure predictions were applied to target identification in 11 of 40 included studies, enabling structure-based virtual screening against previously unstructured neurodegeneration-related proteins including TDP-43, FUS, and α-synuclein aggregation-prone regions. Virtual screening of >100 million compounds against AlphaFold2-predicted binding sites generated nanomolar-affinity candidate molecules for multiple ALS-related targets — results not achievable without the structural predictions.

4. DISCUSSION

AI-driven target identification for neurodegenerative diseases demonstrates significant promise, with knowledge graph approaches generating biologically validated candidate targets at scales impossible through traditional hypothesis-driven research. The convergence of knowledge graph mining, multi-omics integration, and AlphaFold2-enabled structure-based design represents a qualitative advance in the target identification toolkit for neurodegenerative drug discovery. However, the translational gap between computationally identified

targets and clinically validated drugs remains substantial: of the AI-identified neurodegenerative targets reviewed, only a small proportion have advanced to clinical-stage evaluation, reflecting the extraordinary biological complexity and clinical heterogeneity of neurodegenerative diseases.

For biomedical research institutions in Uzbekistan and Central Asia — including Tashkent State Medical University — AI-driven target identification represents an opportunity to contribute to global neurodegeneration research without requiring the large experimental infrastructure investments of traditional drug discovery, leveraging computational approaches that are increasingly accessible through cloud computing platforms and open-source AI frameworks.

5. CONCLUSION

AI-driven drug target identification — encompassing knowledge graph mining, multi-omics network analysis, and AlphaFold2-enabled structure-based design — is generating biologically validated neurodegenerative disease target candidates at scales and with methodological rigour not achievable through traditional approaches. For Alzheimer's disease, Parkinson's disease, and ALS, AI target identification has identified high-confidence candidates with convergent multi-omics support and structural druggability, several of which have advanced to clinical evaluation. For biomedical research institutions in Uzbekistan, AI-driven computational neuropharmacology represents an accessible research frontier with significant contribution potential. Future priorities include integration of Central Asian population genomic data into neurodegenerative disease knowledge graphs and development of regional computational neuroscience research infrastructure.

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