Systematic Review of AI-Enhanced in Silico Screening of Neuroprotective Phytochemicals for Neurodegenerative Disorders

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ABSTRACT

Introduction: Neurodegenerative disorders, such as Alzheimer's, Parkinson's and Huntington's diseases, are characterized by progressive neuronal loss and lack curative therapies. Phytochemicals, with their structural diversity and multi-target bioactivity, are promising neuroprotective agents. Integrating artificial intelligence (AI) with in silico methods, like molecular docking and virtual screening, enhances drug discovery by improving the efficiency and accuracy of identifying phytochemicals targeting neurodegenerative pathways.

Aim & Objectives: This systematic literature review aims to evaluate the application of AI-assisted in silico docking and virtual screening to identify neuroprotective phytochemicals that modulate key molecular targets in neurodegenerative disorders. Objectives include assessing AI methodologies, phytochemical efficacy, pharmacokinetic profiles and network pharmacology insights.

Methods: A systematic search will be conducted across PubMed, Scopus, Web of Science and Google Scholar for peer-reviewed studies published between 2010 and 2025. Inclusion criteria will target articles using AI-driven tools (e.g., quantitative structure-activity relationship [QSAR] models, deep learning algorithms) with molecular docking platforms (e.g., AutoDock Vina, PyRx) to screen phytochemicals against targets like acetylcholinesterase (AChE), beta-secretase (BACE1) and monoamine oxidase-B (MAO-B). Data will be extracted on AI techniques, phytochemical classes, target proteins, ADMET profiles and network pharmacology interactions. Quality assessment will adhere to PRISMA guidelines and the AMSTAR-2 checklist.

Results: The review is expected to identify studies highlighting phytochemicals such as curcumin, resveratrol, bacoside A and withanolide A with high binding affinities (e.g., -7.5 to -11.0 kcal/mol) for neurodegenerative targets. AI-integrated approaches, including random forest-based QSAR and convolutional neural network-driven binding predictions, are anticipated to reduce computational time by up to 50% and improve accuracy by 25–35%. Network pharmacology is likely to reveal multi-target interactions in anti-inflammatory (NF-κB) and antioxidant (Nrf2) pathways, with favourable ADMET profiles.

Summary & Conclusion: This review will synthesize evidence on AI-enhanced in silico methodologies for identifying neuroprotective phytochemicals, highlighting their therapeutic potential. Expected findings will support preclinical validation of lead compounds while identifying gaps in standardization and experimental validation to guide future research.

Keywords: Neurodegenerative disorders, Phytochemicals, Artificial intelligence, In silico docking, Virtual screening, Network pharmacology, ADMET analysis

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