

Network Pharmacology and Molecular Docking Analysis of *Moringa oleifera* in Alzheimer's Disease

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- *Moringa oleifera* exhibits multi-target therapeutic potential against Alzheimer's disease.
- Network pharmacology identified key molecular targets associated with neuroinflammation, cell survival, and synaptic function.
- Several *M. oleifera* metabolites demonstrated docking affinities comparable to reference inhibitors for AKT1, SRC, and EGFR.
- These findings provide a computational basis for the neuroprotective effects of *M. oleifera* and support further validation through molecular dynamics simulations and experimental studies.

INTRODUCTION

- Alzheimer's disease (AD) is a leading cause of dementia with limited disease-modifying therapies.
- Moringa oleifera* exhibits antioxidant, anti-inflammatory, and neuroprotective activities.
- The molecular targets and mechanisms of *M. oleifera* in AD remain unclear.
- This study employed network pharmacology and molecular docking to identify the bioactive compounds, key targets, and signaling pathways involved in its potential anti-AD effects.

METHODS

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graph TD; MO[Moringa oleifera] --> ID1[Identification of bioactive compound using literature, Knapack, INPPAT 2.0, and relevant literature]; AD[Alzheimer's Disease] --> ID2[Identification of associated genes using GeneCards]; ID1 --> ID3[Identification of compound-target genes using Swiss Target Prediction (STP) and Similarity Ensemble Approach (SEA)]; ID2 --> OG((Overlapping genes)); ID3 --> OG; OG --> PPI[Protein-protein Interaction (PPI) Network using STRING]; OG --> V1[Visualization and identification of core gene target using Cytoscape]; PPI --> V1; V1 --> V2[Visualization of compound-target gene]; V1 --> FE[Functional Enrichment Analysis using Shiny Go]; V2 --> CTP[Compound-target protein interaction by Autodock Vina];
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RESULTS

A. Identification of Compounds-Target Genes and AD-associated Genes

We obtained 64 compounds and 992 target genes. In parallel, 1,040 AD-associated genes were retrieved from database. Integration of both datasets identified 382 overlapping genes.

MO compound: 601, AD genes: 658, Overlap: 382

B. Protein-Protein Interaction (PPI) Network

Protein–protein interaction (PPI) network was constructed using Cytoscape. Hub genes and top 10 core genes were identified. Top 10 core genes including AKT1, JUN, SRC, STAT3, TP53, HIF1A, IL6, NFKB1, GAPDH, and EGFR.

C. Compound-Target Interaction (CTI) network

C. KEGG Pathway Enrichment Analysis

Biological Process, Cellular Component, Molecular Function

D. Molecular Docking

Based on hub gene ranking and expression profiles from AlzData, AKT1, SRC, and EGFR were selected for molecular docking analysis.

No	Protein	Compound	Binding Affinity (kcal/mol)
1	AKT1	mk2206*	-10.7
2	AKT1	Ellagic acid	-9.9
3	SRC	Dasatinib*	-9.3
4	SRC	Isorhamnetin	-9.2
5	EGFR	Gefitinib*	-8.2
6	EGFR	Myricetin	-8.3

*reference inhibitor

CONCLUSIONS

- An integrated network pharmacology approach identified AKT1, SRC, and EGFR as key therapeutic targets of *Moringa oleifera* in Alzheimer's disease.
- Functional enrichment analysis suggested that these targets are involved in pathways regulating neuroinflammation, cell survival, and synaptic function.
- Several *M. oleifera* bioactive compounds exhibited binding affinities comparable to reference inhibitors, supporting their potential as multi-target therapeutic candidates.
- These findings provide a computational basis for the neuroprotective effects of *M. oleifera* and warrant further validation through molecular dynamics simulations and experimental studies.

REFERENCES

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