Computational Evaluation of Mimosa pudica Phytoconstituents for Parkinson's Disease: A Network Pharmacology and Molecular Docking Approach

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A B S T R A C T

This study explores the therapeutic potential of phytoconstituents derived from Mimosa pudica in the treatment of Parkinson's disease (PD) using an integrative computational approach. Seventeen bioactive compounds were identified through database and literature mining and subsequently screened using pharmacokinetic and ADMET analysis to evaluate their drug-likeness and oral bioavailability. Network pharmacology revealed 261 common gene targets shared between PD and Mimosa pudica constituents. Protein-protein interaction (PPI) network analysis identified key hub targets, including SRC, AKT1, DRD2, HSP90AA1, and BCL2, which are implicated in neurodegeneration and dopaminergic signalling. Molecular docking showed high binding affinities, particularly for Myricetin-3-O-beta-D-xylopyranoside, which interacted strongly with multiple targets, including HSP90 and DRD2, suggesting potential neuroprotective and dopamine-regulating effects. These findings support Mimosa pudica as a promising source of lead compounds for PD therapeutics and demonstrate the value of in silico tools in herbal drug discovery.

Keywords:

Parkinson's disease; Mimosa pudica; network pharmacology; molecular docking; myricetin-3-O-beta-D-xylopyranoside; phytoconstituents; neuroprotection; dopaminergic synapse; HSP90; DRD