Abstract

Elucidation of Molecular Mechanisms of *Vanda roxburghii* (Family: Orchidaceae) in the Treatment of Alzheimer’s Disease Utilizing Network Pharmacological Analysis †

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Abstract: *Vanda roxburghii* (VR), a native medicinal plant in Bangladesh belonging to the Orchidaceae family, has been previously reported to be effective against Alzheimer’s disease (AD). This study aimed to investigate the potential mechanism of the phytoconstituents of VR against AD using network pharmacology and molecular docking analysis. The phytoconstituents of VR were listed from several databases and their blood–brain barrier (BBB) permeability was predicted using SwissADME. Targets of the BBB permeable actives were predicted using SwissTargetPrediction and Similarity Ensemble Approach databases. The putative genes responsible for AD were obtained from GeneCards and DisGenet databases. The common targets for both VR and AD were scrutinized for how the protein–protein interaction (PPI) network was constructed using STRING (version 12.0) and how the core protein targets were identified using Cytoscape (version 3.10.1). Gene ontology (GO) functions and Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway enrichment analysis were performed on the target genes using DAVID 6.8. Finally, the binding interactions between the phytochemicals and targets of AD were validated by molecular docking using PyRx (version 0.8). In total, 4 phytochemicals with 328 exclusive target genes were predicted to cross the BBB. Moreover, 1046 exclusive disease targets for AD were identified and 103 shared targets of VR and AD were acquired. From the PPI network, 5 targets with higher possibilities of therapeutic activity rates of VR on AD were obtained. Furthermore, 428 biological processes, 82 cellular components, and 98 molecular functions were enriched with GO functions, and 144 KEGG pathways (including Alzheimer’s disease, apoptosis, and endocrine resistance pathways) were found enriched for VR associated with anti-AD activities and were analyzed. Molecular docking analysis further verified the definitive binding capacity of the four actives with the five target proteins (APP, JUN, ESR1, MAPK1, and MAPK3) involved in the significant KEGG pathways and GO functions. Our findings provide directions for further research on the phytochemicals of VR.

Keywords: *Vanda roxburghii*; Alzheimer’s disease; network pharmacology; molecular docking


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