

Network Pharmacological Evaluation of Holy Basil Bioactive Phytochemicals for Identifying Novel Potential Inhibitors Against Neurodegenerative Disorder

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Abstract : Alzheimer disease is illnesses that are responsible for neuronal cell death and resulting in lifelong cognitive problems. Due to their unclear mechanism, there are no effective drugs available for the treatment. For a long time, herbal drugs have been used as a role model in the field of the drug discovery process. Holy basil in the Indian medicinal system (Ayurveda) is used for several neuronal disorders like insomnia and memory loss for decades. This study aims to identify active components of holy basil as potential inhibitors for the treatment of Alzheimer disease. To fulfill this objective, the Network pharmacology approach, gene ontology, pharmacokinetics analysis, molecular docking, and molecular dynamics simulation (MDS) studies were performed. A total of 7 active components in holy basil, 12 predicted neurodegenerative targets of holy basil, and 8063 Alzheimer-related targets were identified from different databases. The network analysis showed that the top ten targets APP, EGFR, MAPK1, ESR1, HSPA4, PRKCD, MAPK3, ABL1, JUN, and GSK3B were found as significant target related to Alzheimer disease. On the basis of gene ontology and topology analysis results, APP was found as a significant target related to Alzheimer's disease pathways. Further, the molecular docking results to found that various compounds showed the best binding affinities. Further, MDS top results suggested could be used as potential inhibitors against APP protein and could be useful for the treatment of Alzheimer's disease.

Keywords : holy basil, network pharmacology, neurodegeneration, active phytochemicals, molecular docking and simulation

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