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Elucidating the potential mechanism of kaempferol and quercetin in ameliorating cognitive impairment using computational analysis

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Structured Abstract

Background: This study explores the neuroprotective properties of two flavonoids, kaempferol and quercetin, in alleviating cognitive impairment, which has become a public health concern due to the aging population. The researchers used in silico network pharmacology and molecular docking techniques to uncover the potential mechanisms of these compounds. Comprehensive interaction networks were constructed to integrate data from various databases related to protein-protein interactions, drug-target interactions, and disease-gene associations

Methods: 1. Screening for potential drug candidates of cognitive impairment through in silico network pharmacology 2. Identification molecular ligand receptor interaction of Kaempferol and Quercetin and protein targets by molecular docking.

Results: The molecular docking analysis revealed that kaempferol and quercetin had a high binding affinity to PTGS2 and low binding affinity to TNF, among other key proteins associated with cognitive impairment. These findings provide valuable insights for further experimental research and the development of therapeutic strategies for cognitive disorders using these natural compounds.

Conclusion: The combination of in silico network pharmacology and molecular docking was used to investigate the potential mechanisms of kaempferol and quercetin in improving cognitive impairment. Through network pharmacology analysis, key pathways related to cognitive decline were identified, and both compounds were found to modulate these pathways, suggesting their multi-target effects. Molecular docking studies revealed a high affinity between kaempferol, and quercetin and specific protein targets associated with cognitive function, which are TNF, PTGS2, FOS, and CASP3.

Keywords: Cognitive impairment, Kaempferol, Quercetin, In-silico prediction, Molecular docking

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