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(57) Abstract :
The present invention discloses a molecular docking-based approach for identifying natural phytocompounds effective in treating Long COVID-induced brain fog. Eleven compounds were screened, of which six—luteolin, quercetin, curcumin, resveratrol, epigallocatechin gallate, and piperine—successfully docked with acetylcholinesterase (AChE), a key enzyme involved in cognitive processes. Among them, resveratrol (–12.4294 Kcal/mol) and curcumin (–12.1409 Kcal/mol) exhibited the strongest binding affinities, forming stable interactions with crucial residues such as HIS 447, TYR 337, and TRP 86. These phytochemicals demonstrated potential to restore cholinergic balance, reduce oxidative stress, and improve memory functions. The invention thus provides a natural, safe, and multi-target therapeutic strategy for alleviating cognitive impairment associated with Long COVID.

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