MULTI-PATHWAY TARGETING IN ALZHEIMER'S DISEASE: MOLECULAR DOCKING ANALYSIS OF SIX MAJOR CONSTITUENTS OF *VETIVERIA ZIZANIOIDES* WITH KEY RECEPTORS

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ABSTRACT

Alzheimer's disease (AD), a leading cause of dementia, is characterised by progressive cognitive decline and impairment in daily functioning. In this study, a molecular docking approach using AutoDock Vina was employed to evaluate the binding affinities of six major phytoconstituents from *Vetiveria zizanioides* in comparison with the standard drug donepezil. The compounds were assessed against eight key molecular targets implicated in AD pathogenesis, including GSK-3, ACHE, BuChE, NMDA, SIRT-1, TLR-4, PP2A, and BACE-1. The results demonstrated significant binding interactions, suggesting potential therapeutic relevance. Notably, the presence of aliphatic carbonyl groups was associated with strong binding affinity, while aromatic hydroxyl and methoxy groups appeared to facilitate multi-target engagement. These findings highlight the multifaceted therapeutic potential of *Vetiveria zizanioides* constituents and support further preclinical and clinical studies to develop effective multi-target-directed therapies for Alzheimer's disease.