

Antioxidant Potential of Root Extracts of *Psidium guajava* and Molecular Docking Analysis

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Natural antioxidants which are primarily derived from plants, play a crucial role in stabilising free radicals and reducing oxidative stress. *Psidium guajava*, commonly used as both a food crop and a medicinal plant, has gained attention for its health benefits. While much research has focused on its leaves and fruit, the antioxidant potential of its roots has not been extensively studied. This study aimed to evaluate the *in vitro* and *in silico* antioxidant activities of n-Hexane, Chloroform and Methanol extracts of *Psidium guajava* roots. Sequential cold maceration extraction was conducted using three solvents: n-Hexane, Chloroform, and Methanol. The total phenolic content (TPC), total flavonoid content (TFC) and total antioxidant capacity (TAC) were evaluated. While the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging was used to assess *in vitro* antioxidant activities. Each assay was performed in triplicates, and the results were analysed using one-way ANOVA followed by Tukey's post-hoc test using SPSS software to determine statistical significance ($p < 0.05$). The phytochemicals present in the extracts were identified through Gas Chromatography-Mass Spectrometry (GC-MS) analysis. The identified compounds were docked with Superoxide Dismutase (SOD) using GOLD software. Methanol extract displayed the highest TPC and TAC values (49.99 ± 0.661 mg GAE/g and 18.85 ± 1.381 mg AAE/g) respectively, while Chloroform extract showed the highest TFC value (10.84 ± 0.385 mg QE/g). Methanol and the combined (n-Hexane: Chloroform: Methanol, 1:1:1) extracts showed significantly lower IC_{50} values (1.629 ± 0.12 μ g/mL, 1.663 ± 0.10 μ g/mL respectively) compared to the standard in the antioxidant assay. The docking results showed, palmitic acid and oleic acid to exhibit the highest binding affinities towards the SOD enzyme with a PLP fitness score of 59.1739 and 56.9547 respectively. These values are higher compared to standard ligand (Ascorbic acid) which has a score of 44.496. The roots extracts of *Psidium guajava* demonstrated significant antioxidant potential, as shown by the findings of TPC, TFC, TAC, DPPH free radical scavenging activity and binding affinity towards SOD enzyme. The results suggest that these roots may prove useful in developing new antioxidant-based treatments.

Keywords: Antioxidants, DPPH, *Psidium guajava*, *In silico*, superoxide dismutase, *In vitro*