

## ***In vitro* and *In silico* Evaluation of Antioxidant Potential and Phytochemical Quantification of *Plectranthus amboinicus* (Lour.) Spreng Roots**

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*Plectranthus amboinicus* (Lour.) Spreng is a medicinal plant that belongs to the family *Lamiacea* and is known for its diverse pharmacological properties. Though the various parts of the plant have been extensively studied, roots remain less explored. This research aimed to evaluate phytochemical and antioxidant activities of *P. amboinicus* roots using *in vitro* and *in silico* methods. Different plant extracts of roots were made using sequential cold maceration method with n-Hexane, Chloroform and Methanol. Total Phenolic Content (TPC), Total Flavonoid Content (TFC) and Total Antioxidant Capacity (TAC) were determined while the antioxidant activity was determined using 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging method. Gas Chromatography-Mass Spectrophotometry (GC-MS) analysis was performed to identify the phytochemicals present in the root extracts. The identified phytochemicals were subjected to *in silico* molecular docking study with Superoxide dismutase (SOD) enzyme to simulate binding affinities by using GOLD Suite software. Docking results were compared and analyzed with the standard ligand binding capacity with SOD enzyme. The n-Hexane extract showed the highest TPC ( $28.22 \pm 1.155$  mg GAE/g), whereas the Methanol extract showed the highest TFC ( $21.78 \pm 0.254$  mg QE/g). The TAC assay indicated n-Hexane extract showed the highest antioxidant capacity ( $7.3490 \pm 0.446$  mg AAE/g). Nevertheless, the Methanol extract showed the best scavenging activity with the lowest  $IC_{50}$  of  $78 \pm 1.194$   $\mu$ g/mL while the standard Ascorbic acid showed  $IC_{50}$  of  $148.5 \pm 0.333$   $\mu$ g/mL. Palmitic acid ( $C_{16}H_{32}O_2$ ), Aromadendrene ( $C_{15}H_{24}$ ), and Hexanedioic acid ( $C_6H_{10}O_4$ ) were identified as the most abundant compounds present in extracts via GC-MS. Palmitic acid-SOD interaction showed a high binding potential with 3 Hydrogen bonds and 59.1739 of PLP fitness score while the standard Ascorbic acid-SOD showed only 44.496 of PLP fitness score. The study highlights the significant antioxidant potential of *P. amboinicus* root extracts. The Methanol extract exhibited the highest free radical scavenging activity, while Palmitic acid showed strong binding affinity with the Superoxide dismutase enzyme. These findings indicate that *P. amboinicus* roots possess considerable potential as a natural source of antioxidant agents. The results can be applied in the development of herbal supplements, functional foods, skincare products, and antioxidant-based therapies.

**Keywords:** *In vitro*, *In silico*, antioxidant, phytochemicals, roots, *P. amboinicus*