

The Neuropharmacological Effects of Leaves and Fruits Essential Oils From *Litsea cubeba* Based on Network Pharmacology

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Litsea cubeba (Lauraceae) is a woody plant which is widely distributed in Vietnam. Its fruit essential oil (FEO) showed a potent effect on the central nervous system (CNS). However, the neuropharmacological effect of the leaves essential oil (LEO) has not been evaluated yet. Interestingly, both parts are used in the famous bathing remedy of Dao people – an ethnic group in Vietnam. The remedy is believed to have health benefits related to the central nervous system (steam essential oil), such as relieving the joint pain, fatigue, postpartum depression, and curing insomnia. Additionally, leaves are also a rich source of essential oil more than fruits. Therefore, the aim of this study is to investigate the interchangeability of both essential oils for the treatment of CNS disorders. Based on Jaccard index value (JIV), LEO was compared with FEO including their chemical composition which was determined by GC-MS, the potential target from molecular docking (<-6 kcal/mol), Gene Ontology (GO), pathway, and important components assessed by network pharmacology. The two essential oils shared in 11 compounds with JIV = 0.22 of all identified components but high similarity of the gene target with JIV=0.926 (shared 58 targets). In consequence, the high similarity of GO and pathways terms were shown with JIV=0.82 (Molecular Function), 0.95 (Cellular Component), 0.82 (Biological Process), and 1 (KEGG). In vitro, LEO and FEO showed the acetylcholinesterase inhibition (IC_{50} = 37.941 and 0.491 μ g/ml) and MAO-B (MIC = 4.0 and 4.0 μ l). Consequently, LEO could also affect efficiently on the central nervous system.

Awards Won:

Third Award of \$1,000