

# Comparison on extracted metabolites from different regions grown *Murraya koenigii* and validation by antibacterial, antioxidant, and molecular docking studies

## Abstract

*Murraya koenigii* (curry leaves) is a herbal plant native to India and is primarily used as a flavouring agent in Indian cuisine as well as in many other South Asian cuisine. This study is focused on extracting the metabolites from the *M. koenigii* leaves collected from two different locations in Tamil Nadu, India, (Sample A is Tiruvallur and Sample B is Coimbatore) and assessing its antioxidant, antibacterial properties and the compounds were docked against various targets to evaluate its biological activity. The leaves were collected from two different areas in Tamil Nadu and the secondary metabolites were extracted by using three different polarity-based solvents; hexane, chloroform, and methanol were analyzed by GC–MS. The common compounds found in three different solvents for the Tiruvallur sample were caryophyllene, humulene, and  $\beta$ -eudesmene and those from Coimbatore were caryophyllene and humulene. Gram-negative bacteria like *Chromobacterium violaceum* and *Pseudomonas aeruginosa* were used to test the antibacterial activity of extracts from *M. koenigii* leaves. Hexane extracts of both samples showed higher resistance against the selected bacteria. The antioxidant activities were evaluated using FRAP, DPPH, NOS, and ABTS assay. It was observed that Sample A exhibited more free radical scavenging activity than Sample B. Molecular docking of selected compounds from the literature was carried out against various targets like human Superoxide Dismutase I (hSOD1) [PDB ID: 5YTO], *S. aureus* DNA gyrase [PDB ID: 4PLB], Human glucose transporter 4—GLUT4 [PDB ID: 7WSN], protein kinase b [PDB ID: 2FUM], Cyclin-dependent kinase 2 [PDB ID: 6GUE], Human HER2 (ERBB2) [PDB ID: 3PP0], and Anaplastic lymphoma kinase (ALK) [PDB ID: 5FTO]. Docking studies have also been carried out for the common compounds found in three solvents of the two samples. Thus, this study represents the presence of bioactive compounds with the number of biological activities in the *M. koenigii* leaves.

## Keywords

Antibacterial; Antioxidants; Curry leaves; GC–MS; Secondary metabolites