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LCMS based Dereplication Guided Identification and Purification of Novel Metabolites using Silica Matrix from *Dysoxylum malabaricum*

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ABSTRACT

The present work aimed to investigate the phytoconstituents of *Dysoxylum malabaricum* (Meliaceae) bark through dereplication studies. A dereplication protocol based on LCMS-DNP database was developed for the rapid recognition of compounds from the crude extract. The extraction of shade-dried bark was done by methanol-dichloromethane (1:1) at room temperature. The crude extract was obtained after filtration and evaporation of the solvent under reduced pressure and further lyophilized. Later it was suspended in distilled water and fractionated sequentially by hexane, ethyl acetate, and chloroform. The highest extractive content was enriched in the ethyl acetate fraction. A portion of ethyl acetate was subjected to LCMS profiling along with cytotoxicity assay and a comparative study was done on the LCMS spectra and DNP database. Further this extract was subjected to bioassay-guided fractionation using column chromatography. Five novel compounds were isolated from most active fraction, purified via HPLC and their structure was characterized by NMR, HRESIMS and stereochemistry was determined by ECD calculations. The compounds were confirmed as cycloartane triterpenoids and evaluated for their cytotoxic potential against the panel of breast cancer cell lines and human embryonic kidney cancer cells. One of the compounds showed significant cytotoxicity breast cancer cell line and induces apoptotic cell death.

Keywords: Dereplication, LC-MS, triterpenoids, Bioassay-guided isolation Dysoxylum malabaricum

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