

# **<sup>1</sup>H NMR-based metabolomics approach in investigating the chemical profile, antioxidant and anti-inflammatory activities of *Gynura procumbens* and *Cleome gynandra***

## **ABSTRACT**

*Gynura procumbens* and *Cleome gynandra* are two herbs commonly used in Malaysia to treat various ailments and are also consumed as salads (ulam) and vegetables. The present study aims to evaluate the relationship between the chemical compositions of both herbs and their antioxidant and anti-inflammatory properties using nuclear magnetic resonance (NMR) metabolomics approach, which is being reported for the first time. Different ethanolic extracts of both herbs were tested for DPPH scavenging and inhibition of nitric oxide (NO) via RAW 264.7 macrophage cell induction. Principal component analysis (PCA) revealed a good separation between the extracts and the corresponding metabolites identified via <sup>1</sup>H NMR spectroscopy. The 100% ethanolic extract from both herbs and 20% ethanolic extract of *C. gynandra* were found to have the best antioxidant and anti-inflammatory activities. Kaempferol, quercetin, caffeoylquinic, dicaffeoylquinic acids, gallic acid, mallic acid, citric acid, phenylalanine, and choline are among the metabolites that contributed to bioactivities. The partial least square (PLS) model for both herbs have an overall acceptable goodness of fit and predictive power, which further strengthens the validity of this study. The present study provides a preliminary reference for the selection of optimum extract and will shed some light on the potential use of *G. procumbens* and *C. gynandra* as a phytomedicinal preparation.

**Keyword:** <sup>1</sup>H NMR; *C. gynandra*; *G. procumbens*; Metabolomics; PCA; PLS