Complementary NMR- and MS-based metabolomics approaches reveal the correlations of phytochemicals and biological activities in Phyllanthus acidus leaf extracts

ABSTRACT

Proton nuclear magnetic resonance (1H NMR)- and ultra-high performance liquid chromatography-mass spectrometry (UHPLC-MS)-based analytical tools are frequently used in metabolomics studies. These complementary metabolomics platforms were applied to identify and quantify the metabolites in Phyllanthus acidus extracted with different ethanol concentrations. In total, 38 metabolites were tentatively identified by 1H NMR and 39 via UHPLC-MS, including 30 compounds are reported for the first time from this plant. The partial least square analysis (PLS) revealed the metabolites that contributed to α-glucosidase and nitric oxide (NO) inhibitory activities, including kaempferol, quercetin, myricetin, phyllanthusol A, phyllanthusol B, chlorogenic, catechin, cinnamic coumaric, caffeic, quinic, citric, ellagic and malic acids. This study shows the significance of combining 1H NMR- and UHPLC-MS-based metabolomics as the best strategies in identifying metabolites in P. acidus extracts and establishing an extract with potent antioxidant, anti-diabetic, and anti-inflammatory properties.

Keyword: NMR; Metabolomics; Multivariate data analysis; Phyllanthus acidus; UHPLC-MS