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Rapid investigation of α -glucosidase inhibitory activity of *Phaleria macrocarpa* extracts using FTIR-ATR based fingerprinting (Article)

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Abstract

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Phaleria macrocarpa, known as "Mahkota Dewa", is a widely used medicinal plant in Malaysia. This study focused on the characterization of α -glucosidase inhibitory activity of *P. macrocarpa* extracts using Fourier transform infrared spectroscopy (FTIR)-based metabolomics. *P. macrocarpa* and its extracts contain thousands of compounds having synergistic effect. Generally, their variability exists, and there are many active components in meager amounts. Thus, the conventional measurement methods of a single component for the quality control are time consuming, laborious, expensive, and unreliable. It is of great interest to develop a rapid prediction method for herbal quality control to investigate the α -glucosidase inhibitory activity of *P. macrocarpa* by multicomponent analyses. In this study, a rapid and simple analytical method was developed using FTIR spectroscopy-based fingerprinting. A total of 36 extracts of different ethanol concentrations were prepared and tested on inhibitory potential and fingerprinted using FTIR spectroscopy, coupled with chemometrics of orthogonal partial least square (OPLS) at the 4000–400 cm^{-1} frequency region and resolution of 4 cm^{-1} . The OPLS model generated the highest regression coefficient with $R^2Y = 0.98$ and $Q^2Y = 0.70$, lowest root mean square error estimation = 17.17, and root mean square error of cross validation = 57.29. A five-component (1+4+0) predictive model was build up to correlate FTIR spectra with activity, and the responsible functional groups, such as –CH, –NH, –COOH, and –OH, were identified for the bioactivity. A successful multivariate model was constructed using FTIR-attenuated total reflection as a simple and rapid technique to predict the inhibitory activity. © 2016

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