An Integrated Metabolomics Study on Antidiabetic Activity of *Christia vespertilionis* Leaves Extract Using Chemometric and Molecular Docking Analysis

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Aims and scope

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Abstract

In disease treatment, the utilisation of medicinal plants has witnessed a discernible rise, driven by concerns over the adverse effects associated with synthetic drugs available in the market. Analyses of the plant *Christia vespertilionis* (L.f.) Bakh. F., indigenous to Malaysia, has suggested its antidiabetic property linked to α-glucosidase inhibition, but

metabolites responsible for antidiabetic are unexplored. The metabolomics approaches and molecular docking simulations were integrated to identify the putative α-glucosidase inhibitors and their enzyme interaction. In this study, the crude leaves extracted from this plant were extracted using solvents of varying polarity, followed by gas and liquid chromatography coupled with mass spectrometry metabolomics. The highest inhibition activity in a mixture of n-hexane and ethyl acetate (1:1, v/v)) was observed. Six putative metabolites corresponding to antidiabetic activity were identified: palmitic acid (**2**), linolenic acid (**4**), 7-tetradecenal (**5**), aloeemodin-8-monoglucoside (**14**), bruceine I (**15**), and sanjidin B (**16**). The mechanism of action of all the identified compounds is competitive, mainly involving hydrophobic and hydrogen bonding interactions with the protein residues. Compounds **14**, **15**, and **16** exhibited strong binding capabilities with both enzyme crystal structures compared to the positive control, quercetin. The metabolites extracted from *C. vespertilionis* leaves have demonstrated promising antidiabetic effects. These antidiabetic compounds can potentially commercialise new drug candidates in managing diabetes conditions.