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New α-glucosidase inhibitors and antioxidants in optimized Psychotria malayana Jack leaves extract identified by gC-MS-based metabolomics and in silico molecular docking
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Abstract
Our earlier research demonstrated α-glucosidase inhibitory (AGI) and antioxidant activities of the optimised extract of Psychotria malayana leaves. It was reported having numerous compounds, although it was unclear which compounds exhibit the bioactivities as well as their binding interaction to the enzyme. This study aimed to identify the compounds possessing AGI and antioxidant activities in the extract utilising GC-MS-based metabolomics, and to analyse the ligand-enzyme binding interactions via in-silico molecular docking. A partial least square was employed to correlate the metabolite profile and bioactivities. The loading plot reveals the bioactive compounds in this extract. The AGI activity of 1-cyclohexene-1-carboxylic, propanoic, butanedioic and D-gluconic acid together with the antioxidant activity of some compounds were reported for the first time through this study. The docking study reveals that all compounds, except for 1-cyclohexene-1-carboxylic acid, exhibit binding to the enzyme's catalytic site. This discovery demonstrates the potential of this plant for diabetes therapy. © 2024 Informa UK Limited, trading as Taylor & Francis Group.

Author Keywords
antioxidant; GC-MS; metabolomics; molecular docking; Psychotria malayana; α -glucosidase

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