Identification of putative α-glucosidase inhibitors and antioxidants in Zingiber officinale rhizome using LCMS-based metabolomics and in silico molecular docking

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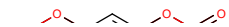
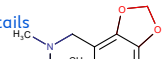
Abstract

Metabolite profiling is required to reveal bioactive chemicals in ginger rhizome for supporting its traditional claim as anti-diabetic agent. This study aimed to evaluate α-glucosidase inhibitory (AGI) and antioxidant activities of the rhizome, to identify its putative α-glucosidase inhibitors, and to analyse the protein-ligand interaction of the inhibitors. The ginger extracts were tested to in vitro AGI assay and analysed using LCMS-based metabolomics to pinpoint the putative α-glucosidase inhibitors. The methanol extract exhibited the highest AGI activity (IC_{50} = 185.2 µg/mL) compared to the other extracts. This extract showed antioxidant activities with DPPH-IC_{50} and FRAP value of 125.0 µg/mL and 16.95 mmol TE/mgDW, respectively. The LCMS-based metabolomics revealed α-glucosidase inhibitors in the extract, namely 7-methoxycoumarin, supinine and 12-hydroxycorynoline. The presence of these compounds in ginger is being reported for the first time in this study. The activity of these compounds was supported by computational study using in silico molecular docking. © 2024 Informa UK Limited, trading as Taylor & Francis Group.

Author keywords

diabetes; LCMS-QTOF; metabolomics; molecular docking; Zingiber officinale; α-glucosidase

View details  View details  View details  View details  View details

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Abstract

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