Metabolomics-based profiling with chemometric approach to identify bioactive compounds in Salacca zalacca fruits extracts and in silico molecular docking

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Abstract

Salak (Salacca zalacca) is well-known as snake fruit and it is immensely studied for its antioxidative and antidiabetic active metabolites throughout the southeast Asian countries. However, there are many remaining unidentified metabolites due to very low abundance and natural variation, which need to be further explored. Nowadays mass spectrometry (MS/MS) facilitates the tentative identification of unknown compounds in the crude herbal extracts. This study described the metabolite profiling of hydroalcoholic extracts of S. zalacca analysed by LC-QTOF-MS/MS. The 60% ethanolic extract exhibited the highest alpha-glucosidase inhibition and ferric reducing antioxidant power activities with IC50 of 15.94 mg/mL and 78.13 mu g AAE/g, respectively. Multivariate data analysis (MVDA) by an orthogonal partial least-squares (OPLS) algorithm was conducted to correlate the alpha-glucosidase inhibition activity with the LC-QTOF-MS data. A total of 4 compounds were reported for first time in this fruit and identified based on the molecular mass and fragment ions. LC-QTOF-MS analysis indicated the presence of carexane I, 5-phenoxytetra zol-1-yl)-2,3,5,6-hexahydrofurofuran-3-ethylurea, 3-acetylphenoxy)-N-[(2)-1-amino-4-methyl-1-oxo pentan-2-yl]-4,5-dihydroxycyclohexene-1-carboxamide and Ethyl 4-[5-methyl-2-oxo-1',2',5',6',7',7' alpha-hexahydro-1H-spiro[indole-3,3'-pyrrolizine]-20-ylamido] benzoate. Molecular docking of those compounds with the alpha-glucosidase enzyme was performed to confirm their antidiabetic potential. These bioactive compounds could be suggested as alpha-glucosidase inhibitors and functional food additives. (C) 2021 The Author(s). Published by Elsevier B.V. on behalf of King Saud University.

Keywords

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