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Identification of alpha-glucosidase inhibitors from Clinacanthus nutans leaf extract using liquid chromatography-mass spectrometry-based metabolomics and protein-ligand interaction with molecular docking

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JOURNAL OF PHARMACEUTICAL ANALYSIS

Volume: 9 Issue: 2 Pages: 91-99

DOI: 10.1016/j.jpba.2018.11.001

Published: APR 2019

Document Type: Article

[View Journal Impact](#)

Abstract

The present study used in vitro and in silico techniques, as well as the metabolomics approach to characterise oc-glucosidase inhibitors from different fractions of Clinacanthus nutans. C. nutans is a medicinal plant belonging to the Acanthaceae family, and is traditionally used to treat diabetes in Malaysia. n-Hexane, n-hexane: ethyl acetate (1:1, v/v), ethyl acetate, ethyl acetate: methanol (1:1, v/v), and methanol fractions were obtained via partitioning of the 80% methanolic crude extract. The in vitro alpha-glucosidase inhibitory activity was analyzed using all the fractions collected, followed by profiling of the metabolites using liquid chromatography combined with mass spectrometry. The partial least square (PLS) statistical model was developed using the SIMCA P+ 14.0 software and the following four inhibitors were obtained: (1) 4,6,8-Megastigmatrien-3-one; (2) N-Isobutyl-2-nonen-6,8-diynamide; (3) 1',2'-bis(acetyloxy)-3',4'didehydro-2'-hydro-beta, psi-carotene; and (4) 22-acetate-3-hydroxy-21-(6-methyl-2,4-octadienoate)olean-12-en-28-oic acid. The in silico study performed via molecular docking with the crystal structure of yeast isomaltase (PDB code: 3A4A) involved a hydrogen bond and some hydrophobic interactions between the inhibitors and protein. The residues that interacted include ASN259, HID295, LYS156, ARG335, and GLY209 with a hydrogen bond, while TRP15, TYR158, VAL232, HIE280, ALA292, PRO312, LEU313, VAL313, PHE314, ARG315, TYR316, VAL319, and TRP343 with other forms of bonding. (C) 2019 Xi'an Jiaotong University. Production and hosting by Elsevier B.V.

Keywords

Author Keywords: [Clinacanthus nutans](#); [LC-MS-QTOF](#); [Metabolomics](#); [alpha-Glucosidase inhibitors](#); [Diabetes](#); [Molecular docking](#)

KeyWords Plus: [GAS-CHROMATOGRAPHY](#)

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Funding

Funding Agency	Grant Number
Ministry of Agriculture of Malaysia	NRGS SP15-060-0182
International Islamic University Malaysia	PRIGS18-027-0027

[View funding text](#)

Publisher

ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS

Journal Information

Impact Factor: [Journal Citation Reports](#)

Categories / Classification

Research Areas: Pharmacology & Pharmacy

Web of Science Categories: Pharmacology & Pharmacy

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