









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Volume 10, Issue 2, February 2020, Article number 287

Investigation of α -glucosidase inhibitory metabolites from *Tetracera scandens* leaves by GC–MS metabolite profiling and docking studies(Article) [Open Access](#)Nokhala, A.^a , Siddiqui, M.J.^{a,b} , Ahmed, Q.U.^{a,b} , Bustamam, M.S.A.^c , Zakaria, Z.A.^{d,e}  ^aDepartment of Pharmaceutical Chemistry, Kulliyah of Pharmacy, International Islamic University Malaysia, Indera Mahkota, Kuantan, Pahang 25200, Malaysia^bPharmacognosy Research Group, Kulliyah of Pharmacy, International Islamic University Malaysia, Indera Mahkota, Kuantan, Pahang 25200, Malaysia^cLaboratory of Natural Products, Institute of Bioscience, Universiti Putra Malaysia, Serdang, Selangor 43400, Malaysia[View additional affiliations](#) ∨

Abstract

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Stone leaf (*Tetracera scandens*) is a Southeast Asian medicinal plant that has been traditionally used for the management of diabetes mellitus. The underlying mechanisms of the antidiabetic activity have not been fully explored yet. Hence, this study aimed to evaluate the α -glucosidase inhibitory potential of the hydromethanolic extracts of *T. scandens* leaves and to characterize the metabolites responsible for such activity through gas chromatography–mass spectrometry (GC–MS) metabolomics. Crude hydromethanolic extracts of different strengths were prepared and in vitro assayed for α -glucosidase inhibition. GC–MS analysis was further carried out and the mass spectral data were correlated to the corresponding α -glucosidase inhibitory IC₅₀ values via an orthogonal partial least squares (OPLS) model. The 100%, 80%, 60% and 40% methanol extracts displayed potent α -glucosidase inhibitory potentials. Moreover, the established model identified 16 metabolites to be responsible for the α -glucosidase inhibitory activity of *T. scandens*. The putative α -glucosidase inhibitory metabolites showed moderate to high affinities (binding energies of -5.9 to -9.8 kcal/mol) upon docking into the active site of *Saccharomyces cerevisiae* isomaltase. To sum up, an OPLS model was developed as a rapid method to characterize the α -glucosidase inhibitory metabolites existing in the hydromethanolic extracts of *T. scandens* leaves based on GC–MS metabolite profiling. © 2020 by the authors. Licensee MDPI, Basel, Switzerland.

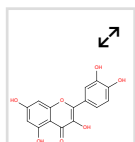
SciVal Topic Prominence ⓘ

Topic: Xanthine Oxidase | Antigout Agent | Hyperuricemia

Prominence percentile: 90.131

Chemistry database information ⓘ

Substances



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water extract of *Tetracera scandens*, leaves, dry, Malaysia, Pahang, Tasik Chini,

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		↗	↗	↗	↗
		60percent methanol-water extract of Tetracera scandens, leaves, dry, Malaysia, Pahang, forest at Tasik Chini	60percent methanol-water extract of Tetracera scandens, leaves, dry, Malaysia, Pahang, forest at Tasik Chini,	40percent methanol-water extract of Tetracera scandens, leaves, dry, Malaysia, Pahang, forest at Tasik Chini,	20percent methanol-water extract of Tetracera scandens, leaves, dry, Malaysia, Pahang, forest at Tasik Chini,

Author keywords

- GC
- Metabolite profiling
- Molecular docking
- MS metabolomics
- Orthogonal partial least squares
- Tetracera scandens
- α-glucosidase inhibition

Indexed keywords

- EMTREE drug terms:
- 1 monopalmitin
 - 24 methylenecycloartenol acetate
 - 5 methoxy 8,8 dimethyl 10 (3 methyl 2 butenyl) 2h,8h pyrano [3,2 g]chromen 2 one
 - alpha glucosidase
 - alpha tocopherol
 - catechin
 - cycloartenol
 - drug metabolite
 - emodin
 - herbaceous agent
 - linoleic acid
 - oligo 1,6 glucosidase
 - palmitic acid
 - phytol
 - plant extract
 - quercetin
 - questin
 - sitosterol
 - stigmasterol
 - Tetracera scandens extract
 - unclassified drug

- EMTREE medical terms:
- Article
 - binding affinity
 - controlled study
 - drug identification
 - drug potency
 - drug screening
 - drug synthesis
 - enzyme active site
 - enzyme inhibition
 - IC50
 - in vitro study
 - mass fragmentography
 - medicinal plant
 - metabolic fingerprinting
 - molecular docking
 - nonhuman
 - plant leaf
 - Tetracera scandens

Chemicals and CAS Registry Numbers:

alpha glucosidase, 9001-42-7; alpha tocopherol, 1406-18-4, 1406-70-8, 52225-20-4, 58-95-7, 59-02-9; catechin, 13392-26-2, 154-23-4; cycloartenol, 469-38-5; emodin, 518-82-1, 57828-45-2; linoleic acid, 1509-85-9, 2197-37-7, 60-33-3, 822-17-3; oligo 1,6 glucosidase, 9032-15-9; palmitic acid, 57-10-3; phytol, 150-86-7; quercetin, 117-39-5; sitosterol, 19044-06-5, 83-46-5; stigmasterol, 83-48-7

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