Minutaside A, new a-amylase inhibitor flavonol glucoside from Tagetes minuta: Antidiabetic, antioxidant, and molecular modeling studies

Sabrin RM Ibrahim, Gamal A Mohamed, Mohamed MM Abdel-Latif, Shahenda M El-Messery, Nawal M Al Musayeib, Ibrahim A Shehata.

Abstract:

Investigation of the EtOAc fraction of Tagetes minuta L. (Asteraceae) aerial parts has afforded a new flavonol glucoside, minutaside A (quercetagetin 6-O-(6-O-hexanoyl)-b-D-glucopyranoside) (1), together with four known flavonoids: axillarin 7-O-b-D-glucopyranoside (2), quercetagetin 3,7-dimethoxy-6-O-b-D-glucopyranoside (3), quercetagetin 7-methoxy-6-O-b-D-glucopyranoside (4), and quercetagetin 6-O-b-D-glucopyranoside (5). Their structures were established by multiple spectroscopic methods in addition to HRESIMS (high-resolution electrospray ionisation mass spectra) and comparison with literature data. The antioxidant and anti-diabetic activities of the isolated flavonoids were evaluated using 2,2-diphenyl-1-picrylhydrazyl (DPPH) and a-amylase inhibition assays. Compounds 1 and 5 showed significant antioxidant activity (84.1 and 83.0% at a 20 mM dose, respectively). Compounds 1, 4, and 5 exhibited strong aamylase inhibitory activity compared with acarbose (a reference a-amylase inhibitor). However, 2 and 3 showed moderate activity. Molecular modeling studies of 1–5 that included docking, flexible alignment, and surface mapping were performed to evaluate their recognition profile aamylase receptor. In docking simulations, 5 displayed a binding mode similar to that of acarbose in the active site of a-amylase enzyme.

Keywords:

a-Amylase inhibitor and antioxidant / Flavonol / Molecular modeling / Tagetes minuta (Asteraceae)

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