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Original Article

A New Flavonoid Glycoside from *Thlaspi arvense*

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A new flavonoid glycoside (1) together with four known compounds (2–5) were isolated and characterized from the 80% MeOH extract of *Thlaspi arvens* Linn.. The structure of 1 was determined to be isovitexin-4'-*O*-maltoside that was elucidated by detailed NMR and HR-ESI-MS spectroscopic analysis.

Key words: *Thlaspi arvens*, isovitexin-4'-*O*-maltoside, isovitexin

Introduction

Thlaspi arvense Linn. is a traditional Chinese medicine used to brighten the eye, and relieve pain in the eye with shedding of tears. It is good for treating arthralgia, epigastric and abdominal pain as well as lumbago [1]. Flavonoids are the major components found in *T*. arvense [2-4]. Naturally occurring and synthetized flavonoids were reported to possess anti-oxidant, anti-bacterial, anti-inflammatory, anti-diabetic, and neuroprotective effects [5-10]. In this paper, we report the isolation and characterization of a new flavonoid glycoside (1) from the 80% MeOH extract of *T. arvense*. In addition, four known compounds were also isolated from this plant including isosaponarin (2) [11,12], isoorientin (3) [13], isovitexin (4) [13,14], and swertisin (5) [15,16]. The structure of **1** was elucidated on the basis of spectroscopic analysis. Components **2–5** were identified by comparing the data with those in the literature (Fig. 1).

Results and Discussion

The concentrated 80% MeOH extract of *T. arvense* was repeatedly subjected to Sephadex LH-20 and reversed phase C-18 column chromatography to obtain a new compound **1** and four known compounds **2–5**.

Compound **1** was obtained as a pale yellow solid with a molecular formula of $C_{33}H_{40}O_{20}$ determined by HR-ESI-MS spectrum ([M-H]-, *m/z* 755.2024). The ^{13}C and DEPT spectra of **1** indicated the presence of 33 carbon resonances including three sugar moieties, and the rest are methines and quaternary carbons. The

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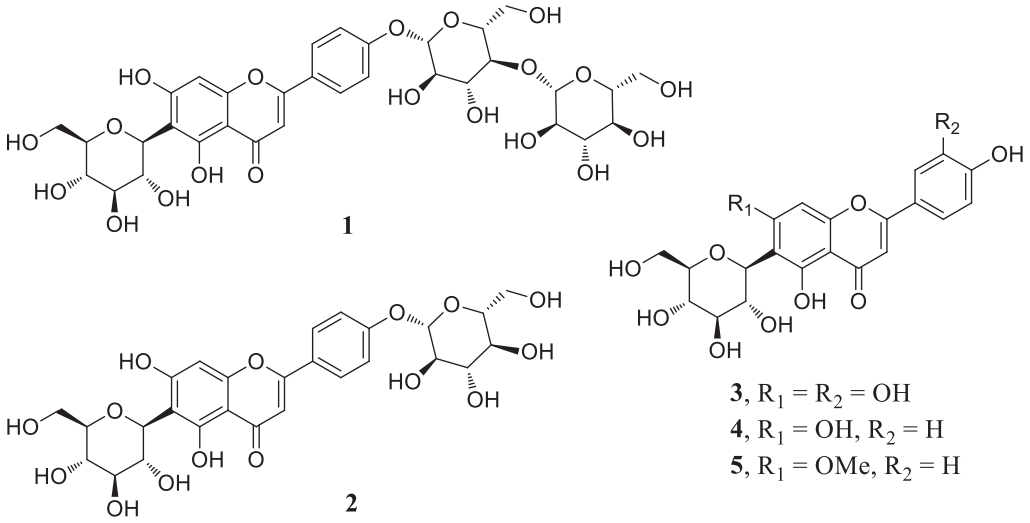

Figure 1. The structures of 1–5.

^{1}H NMR spectrum of **1** displayed a pair of coupled doublets at δ_H 7.19 (2H, *J* = 9.0 Hz) and 8.04 (2H, *J* = 9.0 Hz) assigned to H-3',.5' and H-2',6', respectively; which were attributed to the protons of an AA'BB'-type benzene ring. A singlet signal at δ_H 13.5 was attributed to a hydrogen-bonded hydroxy group (5-OH). Another two singlet signals at δ_H 6.54 (1H, H-8) and 6.90 (1H, H-3) were also observed. In the HMBC spectrum of **1**, a hydroxy group (5-OH) showed correlations with C-4a (δ_C 103.5), C-5 (δ_C 160.6), and C-6 (δ_C 109.0). An anomeric proton signal at δ_H 4.58 (H-1") showed ^{2}J and ^{3}J correlations with C-5, C-6, and C-7 (δ_C 163.4), which indicated a glucose moiety was connected to C-6 and in carbon linkage type in compound **1**, similar to the isovitexin (4) structure [13,14]. In addition, the high-resolution mass spectrum of **1** showed the presence of an ion fragment at *m/z* 431.0968 indicated isovitexin aglycone in compound **1**. In the HMBC spectrum of **1**, an anomeric proton signal at δ_H 5.13 (H-1'") showed ^{3}J correlations with C-4' (δ_C 160.1), which

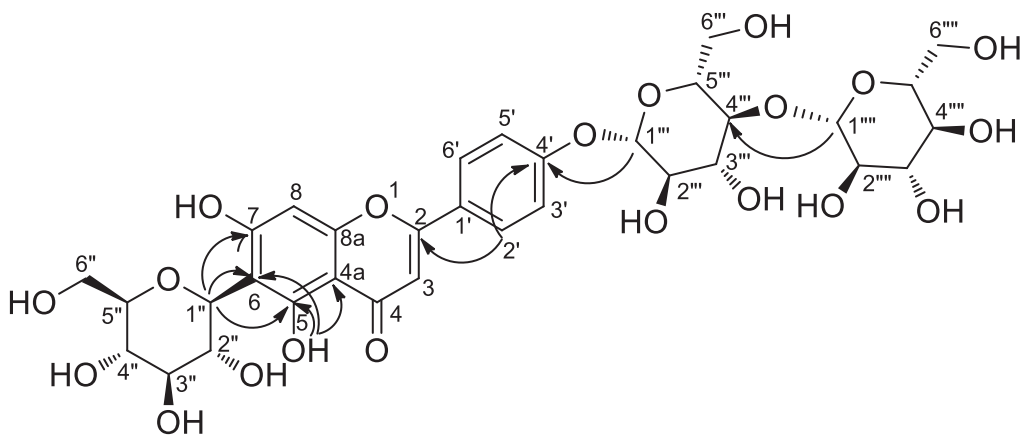

Figure 2. Partial HMBC corrections of 1.

indicated the second glucose moiety was connected to C-4' and in oxygen linkage type in compound **1**, similar to the isosaponarin (**2**) structure [11,12]. The peak for appeared at 3.06 ppm (H-4'''') as triplets with a vicinal axial-axial coupling constant of 9.0 Hz is due to vicinal protons at H-3'''' and H-5'''' coupling, which indicated that the third sugar is a glucose moiety. Furthermore, an anomeric proton signal at δ_H 4.29 (H-1'''', J = 7.8 Hz) showed ^3J correlations with C-4''' (δ_C 79.8) which indicated that β (1→4) glucosidic linkage was presented in a disaccharide moiety [17,18].

The partial correlations in HMBC spectrum are shown in Fig. 2. Based on the extensive 1D-TOCSY, COSY, HMQC, and HMBC spectral data, the structure of compound **1** was established and it was named isovitexin-4'-*O*-maltoside.

In summary, one novel flavonoid glycoside (isovitexin-4'-*O*-β--D-glucopyranosyl-(1→4)-β-D-glucopyranoside, **1**) and four known compounds (**2**–**5**) were isolated and identified from the 80% MeOH extract of *T. arvense*.

Experimental

General. Melting points were determined on a Yanaco MP-S9 micro-melting point apparatus and are uncorrected. IR spectra were obtained on a Nicolet Avatar 320 FTIR spectrophotometer. Nuclear magnetic resonance spectra were recorded on a Varian VNMRS 600 MHz FT-NMR spectrometers. Chemical shifts are reported in parts per million (δ) units relative to internal tetramethylsilane. The high resolution ESI-MS spectra were measured on a Thermo Scinetific Q Exactive Focus Orbitrap mass spectrometer. Column chromatography was performed with Sephadex LH-20 and reversed phase C-18.

Plant Material. *Thlaspi arvense* was purchased from local market in Taiwan, and identified by Dr. Chia-Ching Liaw. A voucher specimen (NRICM 020701) was deposited in the Herbarium of the National Research Institute of Chinese Medicine.

Extraction and isolation. The powder of dried *Thlaspi arvense* (3.6 Kg) were extracted with 80 % MeOH (10 L) under reflux for 1 hour and the filtrate was collected. The residue was repeatedly extracted for two times. The combined filtrate was concentrated under reduced pressure to give a dark brown syrup (77.5 g). The 80% MeOH extract was subjected to Sephadex LH-20 column chromatography eluting with 100% MeOH to give four fractions (TA-1~TA-4). A fraction of TA-2 was further subjected to reversed phase C-18 column chromatography eluting successive with 5% MeOH, 10% MeOH, and 20% MeOH to give three fractions (TA-2-1~TA-2-3). A fraction of TA-2-1 was further subjected to Sephadex LH-20 column chromatography eluting with 80% MeOH to give compound **1** (10 mg) and **2** (33 mg). A fraction of TA-2-2 was further subjected to Sephadex LH-20 column chromatography eluting with 80% MeOH to give compound **3** (67 mg). A fraction of TA-2-3 was further subjected to Sephadex LH-20 column chromatography eluting with 80% MeOH to give compound **4** (6.9 mg). A fraction of TA-3 was further subjected to Sephadex LH-20 column chromatography eluting with 80% MeOH to give compound **5** (3.1 mg).

Isovitexin-4'-*O*-maltoside (1). pale yellow solid; mp 237–239 ºC; $[\alpha]^{25}_D$ -41° (*c* 0.3, MeOH); IR (KBr) ν_{max} 3360, 2919, 1658, 1626, 1491, 1429, 1242, 1195, 1163, 1089, 836 cm^{-1}; ^1H NMR (DMSO-d_6, 600 MHz) and ^{13}C NMR (DMSO-d_6, 150 MHz) data see Table 1; HR-ESI-MS *m/z* 755.2024 [M-H]- (calcd for $C_{33}H_{39}O_{20}$, 755.2029).

Table 1. ^{1}H and ^{13}C NMR data of compound 1 in DMSO-d_6.

position	δ_H[a]	δ_C	position	δ_H[a]	δ_C
2	-	162.8	3”	3.19 (m)	78.9
3	6.90 (s)	103.8	4”	3.12 (dd, 9.0, 4.2)	70.6
4	-	182.0	5”	3.16 (m)	81.6
4a	-	103.5	6”	3.40 (m), 3.68 (m)	61.5
5	-	160.6	1”’	5.13 (d, 7.8)	99.3
6	-	109.0	2”’	3.33 (t, 8.4)	72.9
7	-	163.4	3”’	3.48 (dd, 9.0, 1.8)	74.8
8	6.54 (s)	93.7	4”’	3.44 (t, 9.0)	79.8
8a	-	156.3	5”’	3.61 (m)	75.1
1’	-	124.0	6”’	3.47 (m), 3.68 (m)	59.9
2’,6’	8.04 (d, 9.0)	128.2	1””	4.29 (d, 7.8)	103.1
3’,5’	7.19 (d, 9.0)	116.6	2””	3.01 (dt, 4.2, 8.4)	73.3
4’	-	160.1	3””	3.19 (m)	76.5
5-OH	13.5 (s)		4””	3.06 (dt, 4.2, 9.0)	70.0
1”	4.58 (d, 10.2)	73.0	5””	3.21 (m)	76.8
2”	4.03 (brs)	70.2	6””	3.41 (m), 3.71 (m)	61.1

[a](Multiplicity, *J* in Hz) in ppm.

Supporting Information

Original NMR and HR-ESI-MS spectra of compounds **1–5**. (PDF)

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原始論文

從莕菜分離一個新黃酮苷化合物

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從中藥莕菜的 80% 甲醇萃取物中分離與確定了一個新黃酮苷 (1) 及四個已知化合物 (2–5)。化合物 1 的結構是經由詳細的核磁共振光譜與高解析質譜分析確定其為異牡荊素 -4'-*O*-β- 麥芽糖苷。

關鍵字：莕菜、異牡荊素 -4'-*O*-β- 麥芽糖苷、異牡荊素

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