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2-PHENOXYCHROMONE FLAVONOID GLYCOSIDE FROM *Artemisia rupestris*

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A new 2-phenoxychromone glycoside was isolated from the n-*butanol extract of* Artemisia rupestris. *Its structure was established as 6-demethoxy-4′-*O-*methylcapillarisin-7-*O-β-*glucoside based on spectral data.*

Key words: *Artemisia rupestris*, Asteraceae, 2-phenoxychromone glycoside.

Artemisia rupestris L. (Asteraceae) is a perennial flowering plant that is used traditionally in Uygur folk medicine to treat dyspepsia, upset stomach, hepatitis, rashes, and snake bites. Modern pharmacological research found that extracts of this plant have anti-inflammatory, antioxidant, and anticancer activity [1]. Common components isolated from *A. rupestris* are sesquiterpenoids and flavonoids [1-6].

Herein we report the isolation and structure elucidation of a new 2-phenoxychromone derivative, 6-demethoxy-4′-*O*-methylcapillarisin-7-*O*-*β*-glucoside (**1**), which was isolated from the *n*-butanol extract of *A. rupestris*.

The structure of **1** was fully elucidated by studying chemical shifts and spin—spin coupling constants in PMR and ^{13}C NMR spectra and by analyzing in detail HMQC and HMBC spectra.

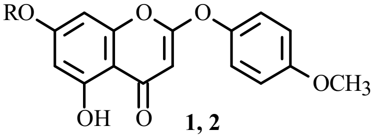
The mass spectrum of **1** shows a pseudomolecular peak for the $[M + H]^+$ ion at *m/z* 463 that corresponds to the molecular formula $C_{22}H_{22}O_{11}$, which was also confirmed by PMR and ^{13}C NMR spectra.

The ^{13}C NMR spectrum (DEPT experiment) of **1** showed 22 resonances for C atoms, 6 of which were assigned to the hexose part. The remaining 16 resonances of C atoms in addition to the corresponding proton resonances in the PMR spectrum were consistent with a 2-phenoxychromone skeleton or 6-demethoxy-4′-*O*-methylcapillarisin (**2**), which we isolated earlier from the ethylacetate extract of *A. rupestris* [7].

Proton spectra of **1** were identical to those of 6-demethoxy-4′-*O*-methylcapillarisin with the exception of additional resonances due to the presence in **1** of the glucose. A resonance for the anomeric sugar proton at δ 5.05 (d, J = 7.2 Hz) and SSCC for protons H-3″ (t, J = 9.0) and H-4″ (t, J = 9.5) in addition to the corresponding resonances in the ^{13}C NMR spectrum confirmed that the glucose was present. A comparison of resonances for C-7, C-6, C-8, and C-10 of **1** with the corresponding resonances of 6-demethoxy-4′-*O*-methylcapillarisin showed that C-7 experienced a strong-field shift by 1.2 ppm whereas C-6, C-8, and C-10 underwent weak-field shifts by 0.7, 0.8, and 1.7 ppm (Table 1).

These data indicate that C-7 of the aglycon is glycosylated by *β*-glucose. The location of the *β*-glucose was also confirmed by HMBC spectra in which through-space coupling between anomeric proton H-1″ (δ_H 5.05) of glucose and C-7 (δ_C 162.7) of the aglycon was observed. Figure 1 shows the main correlations in **1**.

Thus, the structure of **1** was determined as 6-demethoxy-4′-*O*-methylcapillarisin-7-*O*-*β*-glucoside based on these data.



1, 2

1: R = Glc
2: R = H

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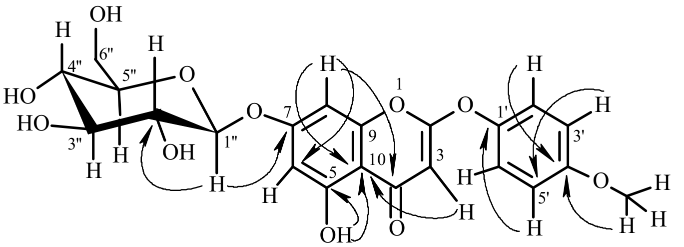
TABLE 1. Chemical Shifts of C Atom Resonances of **1** and **2** (100 MHz, DMSO-d_6, δ, ppm)

C atom	**1**	**2**	C atom	**1**	**2**
2	168.1	167.8	1′	144.3	144.4
3	87.5	87.1	2′/6′	121.9	122.0
4	183.2	183.1	3′/5′	115.4	115.4
5	160.7	161.4	4′	157.8	157.8
6	100.0	99.3	OCH_3	55.9	55.5
7	162.7	163.9	Glc-1	99.9	
8	94.8	94.0	2	73.0	
9	154.5	155.0	3	76.2	
10	103.7	102.0	4	69.5	
			5	77.1	
			6	60.6	



1

Fig. 1. Main HMBC correlations of **1**.

EXPERIMENTAL

Air-dried whole plant (15 kg) was extracted with ethanol (70%). The condensed extracts were suspended in water and extracted successively with petroleum ether, ethylacetate, and *n*-butanol. The *n*-butanol fraction (200 g) was chromatographed over a column of silica gel (100-200 mesh) with gradient elution by a EtOAc:EtOH mixture to afford **1** (0.9 g).

6-Demethoxy-4′-*O*-methylcapillarisin-7-*O*-*β*-glucoside. $C_{22}H_{22}O_{11}$, colorless needle-like crystals, mp 128-130°C. Mass spectrum (*m*/*z*): 463.0 $[M + H]^+$ (ESI-MS).

IR spectrum (KBr, ν, cm^{-1}): 3428 (OH), 1664 (*α*,*β*-unsaturated ketone), 1604, 1497, 824 (aromatic ring), 1179, 1080 (ether).

PMR spectrum (400 MHz, DMSO-d_6, δ, ppm, J/Hz): 12.81 (1H, br.s, 5-OH), 7.36 (2H, d, J = 9.2, H-2′, H-6′), 7.08 (2H, d, J = 9.2, H-3′, H-5′), 6.72 (1H, d, J = 2.0, H-8), 6.47 (1H, d, J = 2.0, H-6), 5.09 (1H, s, H-3), 5.05 (1H, d, J = 7.2, H-1″), 3.80 (3H, s, 4′-OMe), 3.71 (1H, br.d, J = 11.6, H-6″), 3.47 (1H, m, H-6″), 3.44 (1H, m, H-5″), 3.31 (1H, t, J = 9.0, H-3″), 3.24 (1H, dd, J = 9.0, 8.4, H-2″), 3.17 (1H, t, J = 9.5, H-4″).

Table 1 gives the ^{13}C NMR spectrum (100 MHz, DMSO-d_6, δ, ppm).

It is noteworthy that chemical shifts of protons on C-3, C-6, and C-8 in the previous publication [7] should be corrected to 87.1, 99.3, and 94.0 ppm, respectively.

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