New Flavonoid Glycoside from Thalictrum przewalskii

Shi Chun YU*, Qing Li WU, Li Wei WANG, Pei Gen XIAO

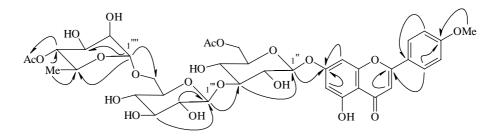
Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100094.

Abstract: A new flavonoid glycoside, 5, 7-dihydroxy-4'-methoxyflavonoid 7-O-[6-O-(4-O-acetyl- α -L-rhamnosyl)-3-O- β -D-glucosyl]-6-O-acetyl- β -D-glucoside was isolated from *Thalictrum przewalskii*. Its structure was determined on basis of spectroscopic evidences.

Keywords: *Thalictrum*; *Thalictrum* przewalskii; flavonoid glycoside, 5, 7-dihydroxy-4'-methoxyflavonoid; 7-O-[6-O-(4-O-acetyl- α -L-rhamnosyl)-3-O- β -D-glucosyl]-6-O-acetyl- β -D-glu-coside.

Compound 1, white powder, gave a molecular formula of $C_{38}H_{46}O_{21}$ based on its EI-MS (m/z 284 M⁺ of aglycone), positive MALDI-TOF-HRMS (M⁺ +1 m/z 839.2610, calcd. For $C_{38}H_{46}O_{21}$, 839.2604), ¹H NMR and ¹³C NMR spectra. The UV (MeOH) bands at 268, 328 nm suggested a flavonoid skeleton. Its IR (KBr) spectrum showed absorption at 3440 (OH), 2950 (saturated CH), 1735 (ester C=O), 1650 (α , β -unsaturated C=O), 1615 (C=C), 1590, 1515, 1500 cm⁻¹ (aromatic system).

Figure 1. Key interactions of 1 in its HMBC spectrum



In its ¹H NMR (500 MHz, DMSO-d₆), the aromatic protons at δ 8.02 (2H, brd, J=8.5 Hz), 7.12 (2H, brd, J=8.9 Hz), 6.92 (1H, s), 6.75, 6.48 (each 1H, brs) and the methoxyl singlet at δ 3.85 ppm suggested the presence of 5, 7-dihydroxy-4'-methoxyflavonoid as the aglycone of **1** and should be assigned to H-2', 6', H-3', 5', H-3, H-8, H-6 and 4'-OMe, respectively¹. In the ¹³C NMR (DMSO-d₆, 125MHz) of **1**, the characteristic glycosylation shift –2.0 ppm was observed for C-7, indicating the locations of the sugar

Shi Chun YU et al.

moiety to be in the C-7, while the chelated hydroxy signal at δ 12.89 (1H, br) was due to 5-OH. From the ¹H and ¹³C NMR spectra, this compound also contained the signals attributed to two β -D-glucoses, an α -L-rhamnose and two acetyl groups. The nature of these groups was also investigated by using HMBC (see Figure 1) spectroscopic technique. The anomaric proton signals at δ 5.25 (1H, d, J=6.8 Hz, H-1") correlated to C-7, 4.52 (1H, d, J=7.8 Hz, H-1"") to C-3" (82.9, glycosylation shift ca. +7.8 ppm) and 4.60 (1H, br, H-1"") to C-6" (65.8, glycosylation shift ca. +4.0 ppm) and the MALDI-TOF-HRMS also gave an ion peak at m/z 651.1903 (C₃₀H₃₅O₁₆, M⁺-acetylrhamnosyl). Whereas the acetylation shifts for C-6" (ca. + 2.5 ppm) and C-4"" (ca. +2.0 ppm) were also observed, respectively¹. Thus, the acetylated sugar moiety at C-7 determined was as 7-O-[6-O-(4-O-acetyl- α -L-rhamnosyl)-3-O- β -D-glucosyl]-6-O-acetyl- β -D-glucoside. Consequently, the whole structure of 1 was concluded 5, to be 7-dihydroxy-4'-methoxyflavonoid

7-O-[6-O-(4-O-acetyl- α -L-rhamnosyl)-3-O- β -D-glucosyl]-6-O-acetyl- β -D-glucoside which is in agreement with its ¹³C NMR spectral data².

References and notes

1. H. Ina and H. Iida, Phytochem., 1981, 20, 1176.

2. ¹H NMR of **1** in DMSO-d₆ (500 MHz, δ in ppm): 12.89 (1H, br, 5-OH), 8.02 (2H, brd, J=8.5 Hz, H-2', 6'), 7.12 (2H, brd, J=8.9 Hz, H-3', 5'), 6.92 (1H, s, H-3), 6.75, 6.48 (each 1H, brs, H-8, 6), 5.25 (1H, d, J=6.8 Hz, H-1"), 4.60 (1H, br, H-1""), 4.52 (1H, d, J=7.8 Hz, H-1""), 3.85 (3H, s, 4'-OMe), 1.97 (3H, s, 6"-COMe), 1.94 (3H, s, 4""-COMe), 0.92 (3H, d, J=6.8 Hz, H-6""); ¹³C NMR of **1** in DMSO-d₆ (125 MHz, δ in ppm): 181.9 (C-4), 170.2 (6"-MeC=O), 169.9 (4""-MeC=O), 163.9 (C-2), 162.7 (C-7), 162.4 (C-4'), 161.1 (C-5), 156.8 (C-9), 128.3 (C-2', 6'), 122.6 (C-1"), 114.6 (C-3', 5), 105.4 (C-10), 104.6 (C-1"), 103.8 (C-3), 100.0 (C-1""), 99.6 (C-6), 98.1 (C-1""), 94.9 (C-8), 82.9 (C-3""), 75.9 (C-5""), 75.6 (C-5"), 75.1 (C-3"), 74.5 (C-2""), 65.6 (C-5""), 63.5 (C-6"), 55.5 (4'-OMe), 20.8 (6"-MeC=O), 20.4 (4""-MeC=O), 17.2 (C-6"").

Received 16 November 1998