Coumarin-glycoside and Ferulate from *Peucedanum decursivum*

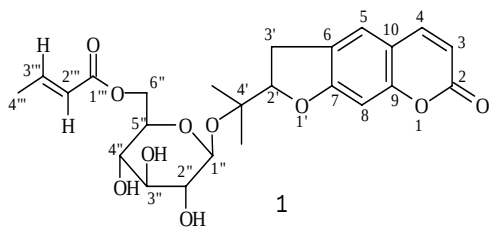
Ling Yi KONG*, Nian Huan YAO

Department of Natural Medicinal Chemistry, China Pharmaceutical University, Nanjing 210038

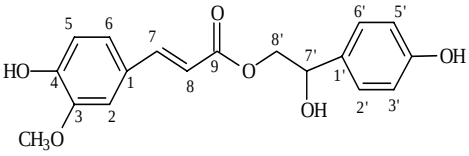
Abstract: Two new compounds named decuroside VI (**1**) and decursidate (**2**) were isolated from the roots of *Peucedanum decursivum* - a traditional Chinese medicine. Their structures were elucidated on the basis of chemical evidence and spectral analysis.

Keywords: *Peucedanum decursivum*, decuroside VI, decursidate.

The root of *Peucedanum decursivum* (Miq.) Maxim (umbelliferae) is known as a famous traditional Chinese medicine. In our studies on the chemical constituents, compounds **1** and **2** were isolated from the extract of the roots by combination of silica gel column chromatography and preparative HPLC.



1



2

Compound **1**, yellow powder, $C_{24}H_{28}O_{10}$ (HRFAB-MS (M-H)$^+$ *m/z*. calcd. 475.1604, obs. 475.1594), UV spectrum (λmax 334 and 203 nm), ^{1}H and ^{13}C NMR spectra were quite similar to those of furocoumarin glycoside such as nodakenin [1,2] (see **Table 1**). On acid hydrolysis, **1** afforded nodakenetin as an aglycone and a β-D-glucose on the basis of spectral analysis. ^{1}H NMR δ:1.72 (3H, dd, *J*=7.0, 2.0 Hz), 5.77 (1H, dd, *J*=15.5, 2.0 Hz), 6.88 (1H, dd, *J*=15.5, 7.0 Hz) and ^{13}C NMR δ 17.9, 123.1, 145.2, 166.6 showed the existence of 2-*trans*-butenoyloxy, which was linked to C-6" of β-D-glucose, because of a 3.3 ppm downfield shift at C-6" of β-D-glucose. Therefore, the structure of **1** was elucidated as 6′-[2-*trans*-butenoyloxy]-nodakenin, named

decuroside VI.

Table 1. ^{1}H and ^{13}C NMR spectral data comparison between compound **1** and nodakenin

Position	**1**		nodakenin	
	H[a)]	C[a)]	H[b)]	C[b)]
Aglycone				
2		161.5		160.3
3	6.14 (1H, d, *J*=9.5 Hz)	112.4	6.24 (1H, d, *J*=9.5 Hz)	111.2
4	7.84 (1H, d, *J*=9.5 Hz)	145.7	7.92 (1H, d, *J*=9.5 Hz)	144.4
5	7.40 (1H, s)	124.8	7.52 (1H, s)	123.8
6		126.4		125.4
7		164.3		162.9
8	6.65 (1H, s)	97.7	6.80 (1H, s)	96.7
9		156.4		154.9
10		113.5		112.2
2′	4.91 (1H, t, *J*=8.0 Hz)	90.9	4.97 (1H, t, *J*=8.0 Hz)	89.7
3′	overlap	29.7	overlap	29.0
4′		78.5		77.0
Gem$(CH_3)_2$	1.20 (3H, s)	21.3	1.17 (3H, s)	20.6
	1.37 (3H, s)	23.7	1.35 (3H, s)	23.2
Glucose				
1"	4.60 (1H, d, *J*=7.7 Hz)	98.2	4.50 (1H, d, *J*=7.5 Hz)	97.1
2"	overlap	74.5	overlap	73.4
3"	overlap	77.7	overlap	76.6
4"	overlap	71.6	overlap	70.3
5"	overlap	74.6	overlap	76.6
6"	overlap	64.5	overlap	61.2
1′′′		166.6		
2′′′	5.77 (1H, dd, *J*=15.5, 2.0 Hz)	123.1		
3′′′	6.88 (1H, dd, *J*=15.5, 7.0 Hz)	145.7		
4′′′	1.72 (3H, dd, *J*=7.0, 2.0 Hz)	17.9		

a) in $(CD_3)_2CO$
b) in DMSO-d_6

Compound **2**, yellow powder, $C_{18}H_{18}O_{16}$ (HREI-MS: *m/z* calcd. 330.1108, obs. 330.1106), UV λ_{max}^{MeOH} : 325 nm. In ^{1}H NMR and ^{1}H -^{1}H COSY spectra δ 6.87 (1H, d, *J*=8.3 Hz), 7.13 (1H, dd, *J*=8.3, 2.0 Hz) and 7.30 (1H, d, *J*=2.0 Hz) showed the existence of 1,3,4-trisubstituded aromatic ring, δ 7.25 (2H, d, *J*=8.0 Hz) and 6.81 (2H, d, *J*=8.0 Hz) showed the existence of para-disubstituded aromatic ring, δ 4.91 (1H, dd, *J*=7.0, 5.0 Hz) and 4.21 (2H, m) showed the existence of a -CH(OH)CH_2O- subunit. The HMBC spectrum showed that the olefinic proton at δ 7.63 (1H, d, *J*=16 Hz) correlated with the trisubstituded aromatic carbons (C-2 and C-6), indicating the presence of *trans*-feruloyl, and the correlation between the methine proton at δ 4.91 and the para-disubstituded aromatic carbons (C-1',C-2' and C-6') suggested the presence of a 4'-hydroxy-phenyl glycol, which was esterified with *trans* feruloyl (see **Table 2** and **Figures 1** and **2**). Therefore, the structure of **2** was finally elucidated as 2-[4'-hydroxyphenyl]- glycol mono t*rans*-ferulate. The stereochemistry of C-7' remains

to be clarified.

Table 2. ^{1}H and ^{13}C NMR spectral data of compound **2**

position	δ H	δ C
1		127.2
2	7.30(1H, d, *J*=2.0 Hz)	111.4
3		148.8
4		150.1
5	6.87(1H, d, *J*=8.3 Hz)	116.1
6	7.13(1H, dd, *J*=8.3, 2.0Hz)	123.9
7	7.63(1H, d, *J*=16 Hz)	146.0
8	6.40(1H, d, *J*=16 Hz)	115.5
9		167.7
1′		133.2
2′ and 6′	7.25(2H, d, *J*=8.0 Hz)	128.3
3′ and 5′	6.81(2H, d, *J*=8.0 Hz)	115.8
4′		157.7
7′	4.91(1H, dd, *J*=7.0, 5.0Hz)	71.8
8′	4.21(2H, m)	69.9
CH_3O	3.90(3H, s)	56.3

Figure 1 Major correlations in HMBC spectrum of 2

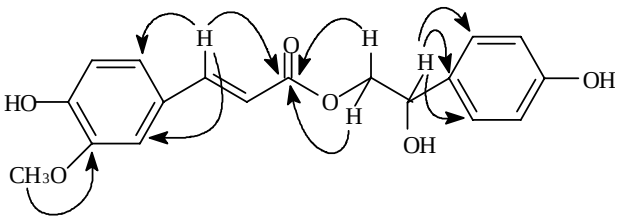
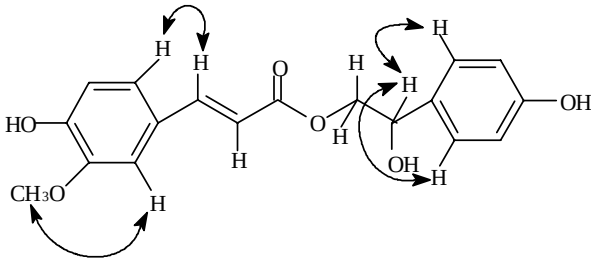


Figure 2 Major corelations in NOESY spectrum of 2

Acknowledgment



The work was supported by youth science and technology foundation of Jiangsu Province, China.

References

1. Y. Matano, T. Okuyma , S. Shibata, *Planta,Medica.*, **1986**, *52*,135.
2. T. Asahara, I. Sakakibara, T. Okuyma, S. Shibata. *Planta Medica* **1984**, *50*, 488.

Received 27 October 1999
Revised 24 January 2000