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A New Monoterpene Glycoside from *Paeonia veitchii*

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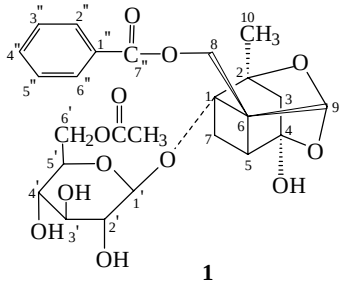
Abstract: A new monoterpene glycoside, acetoxypaeoniflorin, was isolated from the root cortex of *Paeonia veitchii* Lynch.. The structure was elucidated by spectral methods.

Keywords: *Paeonia veitchii* Lynch., Paeoniaceae, monoterpene glycoside, acetoxypaeoniflorin.

The root cortex of *Paeonia veitchii* Lynch. is one of the most important crude drugs in Chinese traditional medicine. It is used as an analgesic, sedative, anti-inflammatory agent and a remedy for cardiovascular, extravasated blood[1]. The present paper deals with the structural elucidation of a new compound from this material.



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Compound **1**, obtained as viscous oil, gave a quasi-molecular ion peak at *m/z* 521 $[M-1]^-$ in the negative FAB-MS, which was 42 amu greater than that of paeoniflorin. Its ^1H and ^{13}C NMR spectra were analogous to those of paeoniflorin[2, 3], except for the additional methyl protons at δ_H 1.99 (3H, *s*) in the ^1H NMR spectrum, corresponding to the signal at δ_C 20.9 (CH_3), and the additional carboxylic carbon at δ_C 170.8 in the ^{13}C NMR spectrum. The HMBC spectrum showed the cross-peaks from the methyl protons (δ_H 1.99) to the carboxylic carbon (δ_C 170.8), indicating the presence of an acetoxyl group in **1**, which was different from paeoniflorin. The long-range couplings were also observed for H-6' [δ_H 4.63 (1H, *dd*, *J* = 10.8, 6.5 Hz), 4.92 (1H, *d*, *J* = 10.8 Hz)] to the carboxylic carbon (δ_C 170.8), and for H-8 [δ_H 5.06 (1H, *d*, *J* = 12.4 Hz), 5.20 (1H, *d*, *J* = 12.4 Hz)] to C-1 [δ_C 89.1 (quaternary carbon)], C-5 [δ_C 44.1 (CH)], C-6 [δ_C 71.6 (quaternary carbon)], C-9 [δ_C 101.8 (CH)], and C-7" [δ_C 166.8 (quaternary carbon)]. Thus, the acetoxyl group was attached to the C-6' of the glucose, and the structure of

compound **1** was accordingly determined as acetoxypaeoniflorin.

Table 1 The ^{1}H-^{1}H COSY, HMQC, HMBC correlations of compound **1** (400 MHz, in pyridine-d_5)

position	δ_H	δ_C	^{1}H-^{1}H COSY	HMBC
1		89.1 s		H-7, 8, 10, 1'
2		86.2 s		H-3, 7, 9, 10
3	2.37 (1H, d, 12.3)	45.0 t		H-5, 10
	2.58 (1H, d, 12.3)			
4		106.1 s		H-3, 5, 7, 9
5	3.10 (1H, d, 6.6)	44.1 d	H-7	H-7, 8
6		71.6 s		H-5, 7, 8, 9
7	2.26 (1H, d, 10.8)	23.3 t	H-5, H-7α/7β	
	2.85 (1H, dd, 10.8, 6.9)			
8	5.06 (1H, d, 12.4)	61.5 t	H-8a/8b	H-5, 9
	5.20 (1H, d, 12.4)			
9	5.93 (1H, s)	101.8 d		H-8
10	1.66 (3H, s)	19.9 q		H-3
1'	5.08 (1H, d, 8.4)	100.4 d	H-2'	H-2', 5'
2'	3.98 (1H, t, 8.4)	75.0 d	H-1', 3'	H-1', 3'
3'	4.15 (1H, t, 8.4)	78.3 d	H-2', 4'	H-2', 4'
4'	3.95 (1H, overlap)	71.7 d	H-3', 5'	H-3', 5'
5'	3.93 (1H, overlap)	75.2 d	H-4', 6'	H-4', 6'
6'	4.63 (1H, dd, 10.8, 6.5)	64.7 t	H-5'	H-4',5', C<u>H</u>$_3$COO
	4.92 (1H, d, 10.8)			
1"		130.8 s		H-2", 6"
2", 6"	8.10 (2H, d, 7.8)	130.0 d	H-3", 5"	H-3", 4", 5"
3", 5"	7.30 (2H, t, 7.8)	128.9 d	H-2", 4", 6"	H-2", 4", 6"
4"	7.47 (1H, t, 7.8)	133.5 d	H-3", 5"	H-2", 3", 5", 6"
7"		166.8 s		H-8, 2", 6"
CH$_3$<u>C</u>OO		170.8 s		H-6', C<u>H</u>$_3$COO
<u>C</u>H$_3$COO	1.99 (3H, s)	20.9 q		

Compound **1**, $[\alpha]_D^{22}$ -9.78 (*c* 0.46, CH_3OH); UV (MeOH) λ_{max} (logε) 202.0 (4.15), 228.5 (4.04), 273.0 (2.54) nm; IR (KBr) *v* 3425, 2923, 1718, 1599, 1450, 1345, 1314, 1277, 1178, 1075, 1008, 943, 823, 754, 713 cm^{-1}; ^{1}H and ^{13}C NMR spectral data, see **Table 1**; negative FAB-MS *m/z* (%): 521 $[M-1]^-$ (20), 491 (5), 387 (5), 121 (100), 77 (6).

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