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A New Abietane Diterpenoid from the Barks of *Taxus yunnanensis*

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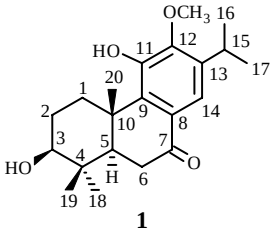
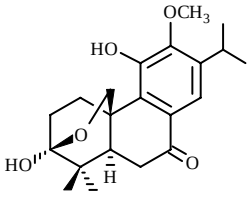
Abstract: The structure of a new abietane diterpenoid, taxayunnin (**1**), from the barks of *Taxus yunnanensis*, was determined by spectroscopic analysis. A known abietane diterpenoid, taxamairin C (**2**), was also isolated.

Keywords: *Taxus yunnanensis*, *Taxaceae*, abietane diterpenoid, Taxayunnin.

Along with the major constituents taxoids, some non-taxane diterpenoids have also been isolated[1]. During the course of our phytochemical investigation on the bark of *Taxus yunnanensis*. Cheng *et* L. K. Fu, a new abietane diterpenoid, taxayunnin (**1**), and the known taxamairin C (**2**)[2], were isolated. The structure elucidation of taxayunnin **1** was established by spectral analysis.



1



2

Taxayunnin **1**, pale yellow needles, mp 215ºC, showed a molecular ion peak at *m/z* 346 [M^+] in its EI mass spectrum, which was in combination with ^1H and ^{13}C NMR (including DEPT) spectra to suggest a molecular formula $C_{21}H_{30}O_4$. Its ^1H NMR spectrum displayed three methyls bound to quaternary carbon atoms, an isopropyl group, and a deshielded aromatic proton at δ 7.62. These evidences indicated **1** was an abietane diterpenoid. Analogy of ^1H and ^{13}C NMR spectra of **1** with those of **2** revealed that **1** was similar to **2** except for A-ring moiety[2]. The difference could be rationalized to an oxygen bridge, which occurred between C-3 and C-20 in **2**. Further comparison of the ^1H NMR data of **1** with those of 3β-hydroxy-demethyl cryptojaponol[3], an abietane diterpenoid isolated from *S. pubescens*, suggested that **1** was a mono-methylate of 3β-hydroxy-demethyl cryptojaponol. The methoxy group attached to C-12 was supported by the HMBC correlations of C-12 with both of 12-OCH_3 and H-15. Thus the structure of taxayunnin was determined as 3,11-dihydroxy-12-methoxy-8,11,13-abietatrien-7-one, and was given the trivial name taxayunnin.

Table 1 NMR data of **1** (500 MHz, $CDCl_3$, J in Hz, δ in ppm, * values may be interchanged)

Proton	δ_H	Carbon	δ_C	Carbon	δ_C
H-1a	3.30 (1H, dt, J = 3.6, 13.9)	C-1	34.7 t	CH_3-17	*23.5 q
H-1b	1.58 (1H, m)	C-2	27.9 t	CH_3-18	28.0 q
H-2	1.81 (2H, m)	C-3	78.0 d	CH_3-19	15.3 q
H-3	3.35 (1H, dd, J = 5.2, 6.9)	C-4	39.2 s	CH_3-20	18.0 q
H-5	1.83 (1H, dd, J = 3.1, 13.9)	C-5	49.7 d	12-OCH_3	61.8 q
H-6a	2.68(1H, dd, J = 3.1, 16.9)	C-6	35.3 t		
H-6b	2.60 (1H, dd, J = 14.2, 16.9)	C-7	198.5 s		
H-14	7.62 (1H,s)	C-8	128.6 s		
H-15	3.20 (1H, spt, J = 6.9)	C-9	137.3s		
CH_3-16	1.24 (3H,d, J = 6.9) *	C-10	39.9 s		
CH_3-17	1.26 (3H,d, J = 6.9) *	C-11	146.5 s		
CH_3-18	1.07 (3H, s)	C-12	149.3 s		
CH_3-19	0.95 (3H, s)	C-13	139.4 s		
CH_3-20	1.39 (3H, s)	C-14	117.5 d		
11-OH	6.12 (1H, s)	C-15	26.8 d		
12-OCH_3	3.81 (3H, s)	CH_3-16	*23.4 q		

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