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A New Taxoid from Leaves and Branches of *Taxus chinensis*

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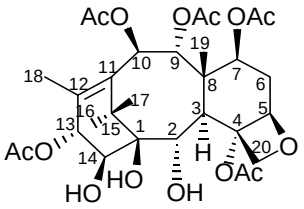
Abstract: A new taxoid, 2-deacetyl-2α, 14β-dihydroxybaccatin IV (**1**), was isolated from the leaves and branches of *Taxus chinensis* together with the known compound baccatin IV (**2**). The structure of the new compound was elucidated by spectroscopic techniques. The detailed ^{13}C NMR assignments of baccatin IV are reported for the first time.

Keywords: Taxoids, *Taxus chinensis*, 2-deacetyl-2α, 14β-dihydroxy-baccatin IV.

Ongoing study of the ethanolic extracts of the leaves and branches of *Taxus chinensis* collected in Sichuan Province, a new taxoid, 2-deacetyl-2α, 14β-dihydroxybaccatin IV (**1**) along with the known compound baccatin IV were isolated. Their structures were determined by means of spectral methods including 1D and 2D NMR spectroscopy.



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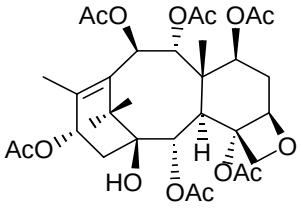

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2-Deacetyl-2α, 14β-dihydroxybaccatin IV (**1**)[1], has the molecular formula $C_{30}H_{42}O_{14}$ deduced from positive FABMS *m/z* 627 $[M + H]^+$, ^1H, ^{13}C and DEPT NMR spectral data. The molecular formula was finally determined by HRFABMS (*m/z* 627.2646 $[M+H]^+$, calc. 627.2653). The 1D NMR data (**Table 1**) indicated that **1** was very similar to baccatin IV (**2**)[2]. Compound **1** differed from **2** by the presence of the hydroxy group at C-14 and the acetyl group at C-2 in **2** was changed to hydroxy group. The chemical shifts of C-14 in compound **1** and **2** are different: δ_C 69.9 ppm in **1** and δ_C 36.9 ppm in **2.** Meanwhile, the upfield shift of H-2β from 5.65 (d, 5.8) in **2** to 4.23 (dd, 5.8,

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1.6) in **1** indicated that the hydroxy group at C-2 in **1** was replaced by the acetyl group at C-2 in **2**[3]. The relative upfield signal at δ 4.23 for H-2 and the signal at δ 3.98 for H-14 in **1** indicated that the hydroxy groups attached at C-2, C-14. Moreover, the HMBC correlations between H-14 and C-1, C-2, C-13, C-15; H-2 and C-1, C-8, C-14 in **1** also confirmed that the hydroxy groups attached at C-2, C-14. Finally, in its NOESY spectrum of **1**, the protons H-14/H-3, H-13/Me-16, H-2/H-9, Me-17 and H-9 showed correlations with each other, which indicated that H-2, H-14 possessed β, α orientation, respectively. Therefore, **1** was elucidated as 2-deacetyl-2α,14β-dihydroxybaccatin IV.

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

Position	δ_C	δ_H	Position	δ_C	δ_H
1	76.8 s		16	28.5 q	1.20 (3H, s)
2	71.7 d	4.23 (1H, dd, 5.8, 1.6)	17	24.0 q	1.65 (3H, s)
3	47.0 d	2.88 (1H, d, 5.8)	18	14.2 q	1.94 (3H, s)
4	82.7 s		19	12.9 q	1.59 (3H, s)
5	84.1 d	4.87 (1H, d, 8.7)	20	78.2 t	4.45 (1H, d, 8.7)
6	35.6 t	2.40 (1H, m)			4.60 (1H, d, 8.7)
		1.80 (1H, m)	OAc	169.3 s	
7	72.8 d	5.54 (1H, dd, 9.8, 7.5)		170.2 s	
8	46.4 s			170.7 s	
9	75.6 d	5.93 (1H, d, 11.3)		170.9 s	
10	71.4 d	6.11 (1H, d, 11.3)		171.4 s	
11	136.3 s		OAc	22.9 q	2.21 (3H, s)
12	138.5 s			21.5 q	2.19 (3H, s)
13	79.4 d	6.07 (1H, brd, 6.6)		21.1 q	2.11 (3H, s)
14	69.9 d	3.98 (1H, brd, 6.6)		20.8 q	2.10 (3H, s)
15	43.2 s			20.8 q	1.96 (3H, s)

^{13}C NMR data were recorded in acetone-d_6 (100 MHz, δc in ppm), ^{1}H NMR data were recorded in acetone-d_6 (400 MHz, δ_H in ppm and *J* in Hz).

Acknowledgment

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References and Notes

1. Compound **1,** colorless lamellar crystals, mp. 242-245°C, $[\alpha]_D^{19.3}$ +26.19 (*c* 0.42, $CHCl_3$). UV ($CHCl_3$) λ_{max} nm (log ε): 239 (3.14), 212 (2.88). IR (KBr) ν (cm^{-1}): 3473, 3419, 2927, 2856, 2362, 2338, 1707, 1635, 1437, 1374, 1271, 1231, 1093, 1020, 911, 744. Positive FABMS *m/z* (rel. int. %): 627 ($[M+H]^+$, 57), 567 (100), 507 (15), 489 (3), 465 (6), 447 (19), 419 (9), 387 (8), 327 (4), 279 (64), 205 (6), 149 (53).
2. D. P. Della Casa de Marcano, T. G. Halsall, *J. Chem. Soc., Chem. Commun.*, **1975**, 365.
3. ^{13}C NMR data (100 MHz, acetone-d_6, δ_C in ppm) of **2:** 77.7 (s, C-1), 70.2 (d, C-2), 47.9 (d, C-3), 81.8 (s, C-4), 84.3 (d, C-5), 35.3 (t, C-6), 72.5 (d, C-7), 46.4 (s, C-8), 73.3 (d, C-9), 71.3 (d, C-10), 135.0 (s, C-11), 141.3 (s, C-12), 75.6 (d, C-13), 36.9 (t, C-14), 43.7 (s, C-15), 28.4 (q, C-16), 23.2 (q, C-17), 15.1 (q, C-18), 13.1 (q, C-19), 76.6 (t, C-20), 169.4 (s, OAc), 170.2 (s, OAc), 170.4 (s, OAc), 170.8 (s, OAc), 171.1 (s, OAc), 171.1 (s, OAc), 23.0 (q, OAc), 21.4 (q, OAc), 21.2 (q, OAc), 20.8 (q, OAc), 20.8 (q, OAc), 20.8 (q, OAc).

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