Chinese Chemical Letters Vol. 9, No. 10, pp. 939–940

A New Sesquiterpene from *Michelia yunnanensis*

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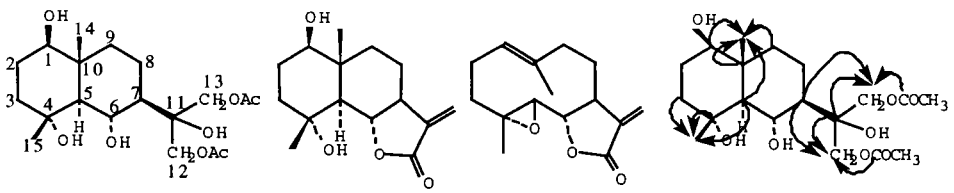
Abstract: A new sesquiterpene, 12,13-di-acetoxyl-1,4,6,11-eudesmanetetrol **1**, was isolated from *Michelia yunnanensis*. The structure was elucidated on the basis of spectral data.

Keywords: sesquiterpene; 12,13-di-acetoxyl -1,4,6,11-eudesmanetetrol; *Michelia yunnanensis*.

Michelia yunnanensis Fr. ex Fin. et Gagn is a Chinese traditional medicine for treatment of inflammation. We obtained a new sesquiterpene **1**, through investigation of the plant, together with two known compounds 1β-hydroxyarbusculin A **2**[1] and parthenolide **3**[2].

Compound **1**, needle crystal, mp 146°C, $[\alpha]_D^{22}$ -2.56 (c 0.391, $CHCl_3$), displayed strong absorptions for hydroxyl and ester groups (3339 cm^{-1}, 3298 cm^{-1}, 1750 cm^{-1}, 1742 cm^{-1}) in IR. HRFAB$^+$MS m/z: 389.2168 [$(M+1)^+$, Calc. for $C_{19}H_{33}O_8$: 389.2175] agreed with molecular formula $C_{19}H_{32}O_8$. Four unsaturations, two of which were attributed to two ester groups, implied presences of bicyclic carbon skeleton and four hydroxyl groups. An angular methyl (δ_H 0.86, s; δ_C 13.78) and a quaternary carbon atom (δ_C 40.04) suggested that **1** belonged to a structure of eudesmanes.



1 **2** **3**

Figure 1. Compounds 1,2,3 and selected HMBC of 1 (→ from C to H)

Comparison of ^{13}C, ^1H NMR spectral of **1** with those of **2** revealed four hydroxyl groups at C-1, C-4, C-6, C-11. In ^1H NMR of **1**, H-1 indicated a quartet at δ_H 3.32 (J=11Hz, 4Hz). H-5 gave a doublet (J=10.4 Hz) at δ_H 1.46. So the hydroxyl groups at C-1, C-6 should be β and α orientation respectively. The configuration of the hydroxyl group at C-4 was deduced from a positive NOE between H-14 and H-15. The differences between **1** and **2** were the appearance of two methylene groups and the absence of lactone ring in **1**. Because of low-field shifts of the two methylene groups that were observed in ^1H NMR and ^{13}C NMR, they might attach to two ester groups. So the moiety

at C-7 is assumed as shown in **Figure 1**. Thus the structure of **1** was assigned as 12,13-di-acetoxyl-1,4,6,11-eudesmanetetrol, which was further supported by HMBC and HMQC.

Table 1. ^{1}H NMR, ^{13}C NMR data of **1** and **2** (400MHz, $CDCl_3$)

(1)		(2)	
^{1}H NMR[a]	^{13}C NMR	^{1}H NMR[b]	^{13}C NMR
H-1α 3.32 dd	C-1 78.43 (d)	H-1α 3.37 dd	C-1 78.12 (d)
H-2α 1.59	C-2 28.07 (t)	H-2α 1.75-1.50 m	C-2 28.18 (t)
H-2β 1.71	C-3 40.66 (t)	H-2β 1.75-1.50 m	C-3 38.07 (t)
H-3α 1.78 dd	C-4 74.02 (s)	H-3α 1.75-1.50 m	C-4 71.26 (s)
H-3β 1.59	C-5 55.89 (d)	H-3β 1.75-1.50 m	C-5 56.47 (d)
H-5 1.46 d	C-6 71.02 (d)	H-5 1.79 d	C-6 80.93 (d)
H-6 4.30	C-7 50.12 (d)	H-6 4.07 t	C-7 50.39 (d)
H-7 1.94 ddd	C-8 21.60 (t)	H-7 2.54 ddd	C-8 21.69 (t)
H-8α 1.61	C-9 39.40 (t)	H-8α 2.03 dd	C-9 38.92 (t)
H-8β 1.38	C-10 40.04 (s)	H-8β 1.45	C-10 41.85 (s)
H-9α 1.13 ddd	C-11 75.44 (s)	H-9α 1.24	C-11 138.07 (s)
H-9β 1.86 dt	C-12 66.98 (t)	H-9β 1.97 dt	C-12 171.00 (s)
H-12 4.20 d	C-13 65.31 (t)		C-13 117.97 (t)
H-12' 4.10 d	C-14 13.78 (q)		C-14 13.54 (q)
H-13 4.31	C-15 23.39 (q)	H-13 6.07 d	C-15 24.20 (q)
H-13' 4.31	CH_3COO 171.25 (s)	H-13' 5.42 d	
H-14 0.88 s	CH_3 20.86 (q)	H-14 0.92 s	
H-15 1.39 s	CH_3COO 170.84 (s)	H-15 1.30 s	
2 CH3 2.12s, 2.11s	CH_3 20.86 (q)		

[a]Coupling constants in Hz: $J_{1\text{-}2\alpha}$= 4.1, $J_{1\text{-}2\beta}$=10.8, $J_{5\text{-}6}$=10.4, $J_{6\text{-}7}$=13.0, $J_{7\text{-}8\alpha}$=3.2, $J_{7\text{-}8\beta}$=13.0, $J_{8\alpha\text{-}9\alpha}$=4.6, $J_{8\alpha\text{-}9\beta}$=3.2, $J_{8\beta\text{-}9\alpha}$=14, $J_{8\beta\text{-}9\beta}$=3.4, $J_{9\alpha\text{-}9\beta}$=14.0, $J_{12\text{-}12'}$=11.7.

[b]Coupling constants in Hz: $J_{1\text{-}2\alpha}$=4.9, $J_{1\text{-}2\beta}$=10.6; $J_{5\text{-}6}$=11.2, $J_{6\text{-}7}$=11.2; $J_{13\text{-}13'}$=3.2.

Acknowledgments

This work was supported by the National Foundation for Outstanding Young Scientists (39525025) to Prof. Xiao-Jiang Hao.

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Received 15 April 1998