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A New Sesquiterpenoid from *Magnolia delavayi*

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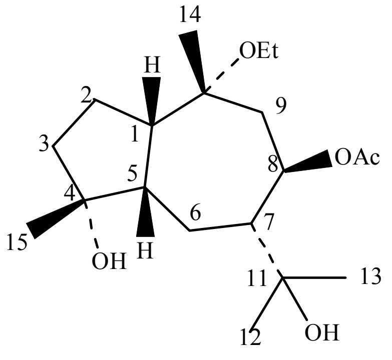
Abstract: A new sesquiterpenoid was obstained from the leaves of *Magnolia delavayi*. Its structure was determined as 8β-acetoxy-10α-ethyloxy-guaia-4α, 11-diol on the basis of spectral evidence.

Keywords: *Magnolia delavayi*, Magnoliaceae, sesquiterpenoid, 8β-acetoxyl -10α-oxyethyl-guaia - 4α, 11-diol.

Magnolia delavayi (Magnoliaceae) is distributed in the southwest of China. It is a traditional Chinese herb and has been used to treat gastric and abdominal distending pain, vomiting and cough[1]. Up to now, the chemical constituents of this plant have not been reported. In this paper, we report the structural elucidation of a new sesquiterpenoid from this plant.



Compound **1**, colorless viscous, $[\alpha]_{D}^{25}$ -55.0 (*c* 0.20, $CHCl_3$), showed a molecular ion peak at *m/z* 341 $[M-H]^-$ in the negative FAB mass spectrum. In combination with ^1H and ^{13}C NMR spectra (see **Table 1**), its molecular formula was deduced to be $C_{19}H_{34}O_5$

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(ESI^+ *m/z*: 343.2464 $[M+H]^+$, calcd. 343.2484). The ^1H and ^{13}C NMR showed the presence of six tertiary methyls (δ_H1.10, 1.13, 1.16, 1.23, 1.30, 1.94), in which one was attributed to acetate, five methylenes, one of which was oxygenated (δ_C57.6), four methines at δ_C48.1, 48.8, 50.9, 72.3, three quaternary carbons (δ_C73.8, 78.5, 83.4) and one carbonyl carbon (δ_C170.4).

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

Position	δ_C	δ_H
1	48.8 (d)	2.81 (m)
2	23.7 (t)	α: 1.78 (m); β: 1.45 (m)
3	36.2 (t)	β: 1.57 (m)
4	83.4 (s)	
5	48.1 (d)	2.36 (m)
6	25.3 (t)	α: 1.60 (m); β: 1.39 (m)
7	50.9 (d)	1.82 (m)
8	72.3 (d)	5.33 (m)
9	36.5 (t)	α: 1.86 (m); β: 2.03 (m)
10	78.5 (s)	
11	73.8 (s)	
12	28.6 (q)	1.23 (s)
13	30.7 (q)	1.13 (s)
14	26.8 (q)	1.10 (s)
15	25.4 (q)	1.30 (s)
$\underline{CH_3}COO$-	21.9 (q)	1.94 (s)
$CH_3\underline{C}OO$-	170.4 (s)	
$\underline{CH_3}CH_2O$-	15.8 (q)	1.16 (t, J=8.6)
$CH_3\underline{CH_2}O$-	57.6 (t)	3.55 (m)

Inspection of 1D and 2D-NMR spectra proposed that **1** possessed aguaiane skeleton bearing one acetyl and one oxyethyl[2]. The acetyl was attached to C-8 for the obvious correlations from δ_H2.36 (H-5) to δ_H1.39 (H-6), δ_H5.33 (H-8) to δ_H1.82 (H-7) and δ_H2.03 (H-9β) in the ^1H-^1H COSY of **1**. This was supported by the correlations from δ_C170.4 to δ_H5.33 (H-8) and δ_H1.94 (s) in the HMBC. The cross signals from δ_C73.8 (C-11) to δ_H1.39 (H-6), δ_H1.82 (H-7), δ_H5.33 (H-8), δ_H1.23 (H-12) and δ_H1.13 (H-13) in the HMBC indicated an isopropanol connected to C-7. This was supported by the strong correlation of δ_H1.13 (H-13) with δ_C28.6 (C-12) in the HMBC (see **Table 2**).

The other two upfield methyls (δ_H1.10, 1.30) appeared as singlet signals in the ^1H NMR spectrum, and it was assumed that two oxygenated groups were attached to C-4 and C-10, respectively. The assumption was confirmed by the presence of cross peaks from δ_H1.10 (H-14) to δ_C78.5 (C-10), and δ_H1.30 (H-15) to δ_C83.4 (C-4) in the HMBC spectrum. The crossing signals from oxymethylene proton (δ_H3.55) to δ_C78.5 (C-10) and δ_C15.8 (q) in the HMBC indicated that the oxyethyl was attached to C-10. This was supported by the cross signal between δ_H3.55 ($CH_3\underline{CH_2}O$-) to δ_H1.16 ($\underline{CH_3}CH_2O$-, t, J=8.6) in the ^1H-^1H COSY.

The stereochemistry at the chiral centers in compound **1** was supported by the ROESY spectrum (see **Table 2**). The NOE interactions from H-1 to H-14 and H-5 showed H-1, H-14 and H-5 at the same side. When they took β configurations, H-15 and

H-7 was at β positions too. The NOE interactions of H-5 with H-15 and H-7, H-7 with H-14 further comfirmed above assignment. H-8 was assumed to be α position because of the correlation between H-8 and the oxymethylene proton (δ_H3.55).

Therefore, the structure of **1** was elucidated as 8β-acetoxy-10α-oxyethyl-guaia-4α, 11-diol (see **Figure 1**).

Table 2 HMBC and ROESY of compound **1**

HMBC		ROESY	
H	Correlative C	H	Correlative H
1-H	C-2, C-3, C-5, C-6, C-9, C-10, C-14	1-H	2β-H, 3β-H, 5-H, 14-H, $CH_3\underline{CH_2}O$-
2α-H	C-1, C-3, C-4, C-10	2α-H	2β-H, 8-H
2β-H	C-1, C-3, C-4	2β-H	1-H, 2α-H
3β-H	C-1, C-2, C-4, C-5, C-15	3β-H	1-H, 15-H
5-H	C-1, C-3, C-4, C-6, C-7, C-15	5-H	1-H, 3β-H, 7-H, 12-H, 15-H
6α-H	C-1, C-4, C-5, C-7	6α-H	
6β-H	C-1, C-4, C-5, C-7, C-11	6β-H	5-H, 7-H
7-H	C-5, C-6, C-8, C-11	7-H	5-H, 6β-H, 8-H, 12-H
8-H	C-9, C-11, $CH_3\underline{C}OO$-	8-H	7-H, 9α-H, 9β-H, 13-H, $CH_3\underline{CH_2}O$-
9α-H	C-1, C-7, C-8, C-10, C-14	9α-H	8-H, $CH_3\underline{CH_2}O$-, 14-H
9β-H	C-1, C-7, C-8, C-10	9β-H	8-H, 14-H
12-H	C-7, C-11, C-13	12-H	5-H, 7-H, 13-H
13-H	C-7, C-11, C-12	13-H	7-H, 12-H
14-H	C-1, C-9, C-10	14-H	1-H, 2α-H, 9β-H
15-H	C-2, C-3, C-4, C-5	15-H	3β-H, 5-H, 7-H
$\underline{CH_3}COO$-	$CH_3\underline{C}OO$-	$\underline{CH_3}COO$-	
$\underline{CH_3}CH_2O$-	$CH_3\underline{CH_2}O$-	$\underline{CH_3}CH_2O$-	$CH_3\underline{CH_2}O$-
$CH_3\underline{CH_2}O$-	$\underline{CH_3}CH_2O$-, C-10	$CH_3\underline{CH_2}O$-	$\underline{CH_3}CH_2O$-, 1-H, 8-H, 9α-H, 14-H

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