Chinese Chemical Letters Vol. 11, No. 12, pp. 1069–1072, 2000

Two New Abietane Diterpenoids from *Coleus xanthanthus*

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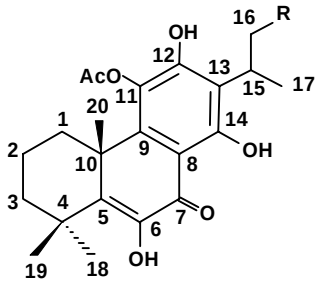
Abstract: From the petroleum part of the 70% acetone extract of *Coleus xanthanthus*, two new abietane diterpenoids have been isolated and identified as 11-acetoxy-coleon U(**1**) and 11,16-diacetoxy-coleon U(**2**).Their structures were elucidated with spectral methods.

Keywords: *Coleus xanthanthu*s, abietane diterpenoids, coleone, 11-acetoxy-coleon U, 11,16-diacetoxy-coleon U.

In our previous paper[1], we reported a novel sesquiterpenoid from the EtOAc part of *Coleus xanthanthus.* The continuous work for the investigation of the petroleum part of *C. xanthanthus* led to the isolation of two new abietane diterpenoids which were identified as 11-acetoxy-coleon U(**1**) and 11,16-diacetoxy-coleon U(**2**) by spectral methods.

Figure 1 The structures of **1** and **2**



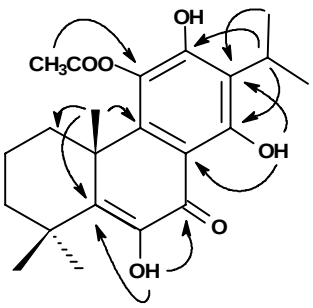
1 **2**

R= H OAc

Compound **1** was obtained as pale yellow cubic crystals, mp:190.5-192^{0}C; $[\alpha]_D^{13.5}$ +

20.50 (c=0.875, $CHCl_3$). Its molecular formula, $C_{22}H_{28}O_6$, was determined by its negative HRMS (found 387.1857, cacl. 387.1866) and NMR spectral data. UVλ_{max}:367.5, 283.5, 258 nm and IRν(KBr): 3416 (OH), 1747 (OAc), 1649 (conjugated C=O), 1620 and 1599 (C=C of aromatic ring) cm^{-1} spectra showed the presence of aromatic ring. Compound **1** exhibited signals of five methyl, three methylene, one methine, eight olefinic carbons, two quaternary carbons, one carbonyl and one acetoxyl group in its NMR spectra. Its ^{1}H NMR spectrum showed the presence of three hydroxyl groups at δ 13.19 (1H, s, 14-OH), 6.94 (1H, s, 6-OH), 5.64 (1H, s, 12-OH) and one isopropyl group (δ 1.34 ,6H, d, J=6.8 Hz; 1.45, 1H, m) . The above spectral data suggested that this compound was an abietane diterpenoid with an aromatic C-ring (coleone)[2]. Comparison of the ^{13}C NMR spectra (**Table 1**) between **1** and the known compound coleon U [2], showed that the signals of **1** were in agreeement with those of coleon U except for the signal of an acetoxyl. The carbon signals at C-8, C-9, C-12, C-13 and C-14 were downfield shifted, and the signal at C-11 was upfield shifted, indicating that the acetoxyl was at C-11 position. The peaks at *m/z* 388 $[M]^+$ and 346 [M-42] in EIMS spectrum and the correlation between C-11 and the H of the acetoxyl in HMBC spectrum of compound **1** (**Figure 2**) confirmed the conclusion. Thus, **1** was elucidated as 11-acetoxy-coleon U.

Figure 2 The key HMBC correlations of **1**



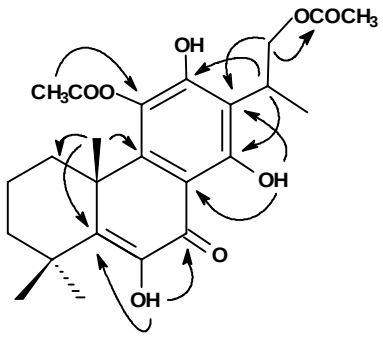
Compound **2**, pale yellow wax-solid, its molecular formula, $C_{22}H_{28}O_6$, was determined by its HREIMS (found 446.1920, cacl. 446.1941) and DEPT spectral data. UVλ_{max}:368.5, 284, 258.5 nm and IRν(KBr): 3403 (OH), 1776 and 1740 (OAc), 1713 (conjugated C=O), 1623 and 1598 (C=C of aromatic ring) cm^{-1} spectra showed the presence of aromatic ring.The difference of the NMR spectral data between **2** and **1**

suggested that another acetoxyl group was substituted at C-16 position in compound **2**. This was supported by the absence of one methyl signal of the isopropyl group and the presence of one methylene[δ_H 4.41 (1H, dd, J=6.0, 10.0 Hz), 4.30 (1H, dd, J=5.6, 10.0 Hz); δ_C 68.5 (t)] and an acetoxyl group [δ_H 2.05 (3H , s); δ_C 20.9 (q) and 169.2 (s)] in **2**. The fragments of *m/z* 404 [M-42], 386 [M-60] and 344 [M-42-60] in EIMS spectrum and the correlations between H-16 and the carbonyl C of an acetoxyl, H-16 and C-13 and H-16 and C-15 in HMBC spectrum (**Figure 3**) of **2** testified the deduction above. So, compound **2** was identified as 11,16-diacetoxy-coleon U.

Table 1 The ^{13}C (100.5 MHz) NMR Data of **1 , 2** and Coleon U in $CDCl_3$ (δ in ppm)

C	1	2	Coleon U	C	1	2	Coleon U
1	32.3 (t)	32.2 (t)	31.5 (t)	13	120.4 (s)	115.9 (s)	118.4 (s)
2	18.6 (t)	18.6 (t)	18.2 (t)	14	160.1 (s)	160.0 (s)	156.7 (s)
3	36.4 (t)	36.5 (t)	36.5 (t)	15	24.5 (d)	29.1 (d)	24.5 (d)
4	36.7 (s)	36.8 (s)	36.5 (s)	16	20.0 (q)	68.5 (t)	20.5 (q)
5	143.3 (s)	143.6 (s)	142.9 (s)	17	20.0 (q)	14.9 (q)	20.5 (q)
6	142.0 (s)	142.0 (s)	142.0 (s)	18	27.7 (q)	27.8 (q)	28.0 (q)
7	182.3 (s)	182.4 (s)	182.5 (s)	19	27.0 q)	27.0 (q)	27.1 (q)
8	106.0 (s)	105.9 (s)	105.5 (s)	20	30.4 (q)	30.3 (q)	29.6 (q)
9	143.8 (s)	144.9 (s)	137.1 (s)	11-OAc	169.7 (s)	170.9 (s)	
10	41.1 (s)	41.3 (s)	41.0 (s)		21.3 (q)	21.2 (q)	
11	129.4 (s)	129.9 (s)	133.1 (s)	16-OAc		169.2 (s)	
12	152.8 (s)	153.8 (s)	150.2 (s)			20.9 (q)	

Figure 3 The key HMBC correlations of **2**



Acknowledgment

This work was financially supported by the National Natural Science Foundation of China (No. 2973040).

References

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Received 23 May 2000