A NEW DITERPENOID FROM COLEUS SCUTELLARIOIDES

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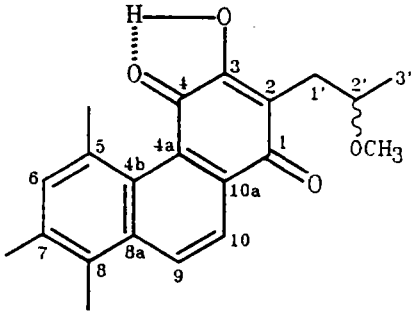
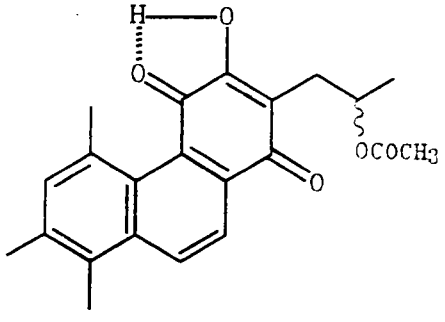
Abstract From the herbs of *Coleus scutellarioides*, a new diterpenoid was isolated and identified as 2-(2′ξ-methoxypropyl)-3-hydroxy-5,7,8-trimethylphenanthrene-1, 4-dione, named as scutequinone (**1**).

Coleus scutellarioides is an ornamantal plant cultivated all over the country. Pharmacological test shows that the plant possesses the capability to increase the contents of cAMP in cells. In this paper, we report scutequinone (**1**), a new phenanthraquione isolated from *Coleus scutellarioides* collected from Xishuangbanna in Yunnan province.

Scutequinone (**1**) was obtained as needles, mp 155~ 156℃ , $[\alpha]_D^{26}$ +11.11° ($CHCl_3$), $[M]^+$338, and the molecular formula was determined as $C_{21}H_{22}O_4$ on the basis of the ^{13}C NMR and MS spectra. IR and ^1H NMR of compound **1** show that scutequinone (**1**) is very similar to planctranthon B (**2**) [1] , whose skeleton was established by X-ray method [2] . The only difference between **1** and **2** entails the substituent groups at C-2′ in the side chain. Comparing with the ^1H NMR(see Table 1) spectra of **2**, the upfield shift of 2′-H showed the replacement of an acetyl group by a methoxy group(δ_H3.74, 1H, sext., J=6.2Hz) at C-2′(δ_C77.2 d) which was confirmed by the observation of the long-range correlation between the proton signal of $-OCH_3$ and C-2′. In addition, the assignments of three methyls and side chain in compound **1** was supported by ^{13}C-^1H XHCO, ^{13}C-^1H COLOC and ^1H-^1H COSY spectra. Thus, the compound **1** was identified as 2-(2′ξ-methoxypropyl)-3-hydroxy-5, 7, 8-trimethyl phenanthrene-1, 4-dione, named as scutequinone.



scutequinone (1)



plectranthon B (2)

Table 1. ^{13}C NMR Data of Compound **1** (in $CDCl_3$)

DC	δc	C	δc
1	182.9	4a	136.2
2	133.0	4b	133.6
3	156.7	8a	130.2
4	185.4	10a	117.2
5	128.6	5–CH_3	24.6
6	136.0	7–CH_3	20.5
7	136.5	8–CH_3	14.7
8	129.7	1′	29.9
9	121.4	2′	77.2
10	131.1	3′	18.7
–OCH_3	56.2		

Table 2. ^1H NMR Data of Compounds **1** and **2** (in $CDCl_3$)

H	1	2
1′–H	2.84, 2H, AA′X, J=6.2, 13.2Hz	2.89, 2H, AA′X, J=6.3, 13.4Hz
2′–H	3.74, 1H, sext., J=6.2Hz	5.25, 1H, sext., J=6.3Hz
3′–CH_3	1.24, 3H, d, J=6.2Hz	1.32, 3H, d, J=6.3Hz
5–CH_3	2.43, 3H, s	2.44, 3H, s
7–CH_3	2.45, 3H, s	2.48, 3H, s
8–CH_3	2.57, 3H, s	2.60, 3H, s
H–6	7.32, 1H, s	7.36, 1H, s
H–9, H–10	8.10, 8.32, ABd, J=8.8Hz	8.14, 8.39, ABd, J=8.8Hz
3–OH	9.42, s	
–OCH_3	3.42, 3H, s	
–$OCOCH_3$		1.99, 3H, s

References

[1] A. C. Alder, P. Ruedi and C. H. Eugster, *Helv. Chim. Acta*, 1984, 67, 1003.
[2] P. Buss, R. Prewo, J. H. Bieri, *Helv. Chim. Acta*, 1986, 69, 1395.

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