A Novel Sesquiterpenoid from *Coleus xanthanthus*

Shuang Xi MEI[1], Chao Ming LI[1], Hui Lan ZHENG[1], Qi Tai ZHENG[2], Yang LU[2], Han Dong SUN[1*]

[1]Laboratory of Phytochemistry, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204
[2]Institute of Meteria Medica, Chinese Academy of Medical Sciences, Beijing 100050

Abstract: Phytochemical re-investigation of *Coleus xanthanthus* led to the isolation and identification of a novel sesquiterpenoid **1**, named as 4,5,11-trimethyl-8,9-seco-1(10),7(11)-eremophiladien-8,12-olid-9-oic acid. The structure of **1** was elucidated by modern spectroscopic methods, especially by X-ray diffraction.

Keywords: *Coleus xanthanthus*, sesquiterpenoid, 4,5,11-trimethyl-8,9-seco-1(10),7(11)-eremophila -dien-8,12-olid 9-oic acid.

Coleus xanthanthus C.Y.Wu et Y.C.Huang is an endemic plant in Xishuangbanna of Yunnan province[1]. Its chemical constituents were studied by Prof. Chao Ming LI and five diterpenoid quinones had been obtained[2-4]. It was reported that some diterpenoid quinones had insect anti-feeding and anti-tumor activity[5]. In order to search for more significant compounds of the plant, we did a careful phytochemical investigation. From 70% acetone extract of the aerial part of this plant, a novel sesquiterpenoid **1**, named as 4,5,11-trimethyl-8,9-seco-1(10),7(11)-eremophiladien-8,12-olid-9-oic acid, was isolated by repeated chromatography of silica gel columns. Its structure and relative configuration were elucidated by spectral methods, especially by the X-ray technique.

Figure 1 The Structure of **1**

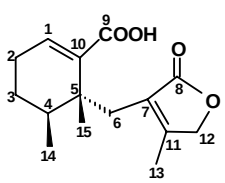
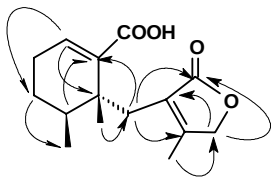


Figure 2 The Key HMBC Correlations of **1**



Compound **1** was obtained as colorless crystals (from $CHCl_3$), mp: 149.5~151.5°C; $[\alpha]_D^{25}$ +11.73 (c=0.0055, $CHCl_3$). IR spectrum showed the following characteristic signals, a conjugated carboxy (3092, 1654, 1633 cm^{-1}) and an α,β-unsaturated lactone (1727, 1559, 1200 cm^{-1}), which was supported by the UV spectrum (239 nm). Its ^{13}C NMR spectrum indicated fifteen carbon signals; DEPT experiments differentiated them as

3×CH_3, 4×CH_2, 2×CH, 6×C (**Table 1**). The above evidence and HRFAB$^+$MS (found 265.1428, cacld. 265.1440) suggested that the molecular formula of **1** was $C_{15}H_{20}O_4$. ^{1}H NMR spectrum indicated an olefinic proton [δ7.19 (1H, brs, 1-H)], two methylene protons that linked with oxygen [δ4.63 (2H, brs, 12-H)], a pair of AB system protons [δ2.74 (1H, d J=13.7Hz, 6α-H) and δ2.84 (1H, d J=13.7Hz, 6β-H)], a methine proton [δ1.80 (1H, m, 4-H)], four methylene protons [δ2.18 (2H, m, 2-H); δ1.43 (1H, m, 3α-H) and δ1.90 (1H, m, 3β-H)] ; nine methyl protons [δ2.06 (3H, s, 13-H); δ0.94 (3H, s, 15-H); δ0.93 (3H, d J=6.8Hz, 14-H)]. From ^{1}H NMR, ^{13}C NMR, H-^{1}H COSY and HMBC (**Figure 2**) spectra, two partial structures [$C_9H_{13}O_2$ (**A**) and $C_5H_5O_2$ (**B**)] that connected to a methylene carbon (C-6) were determined. The conclusion was supported by the EIMS m/z 264[M]$^+$, 246[M-H_2O] (13), 153[M-($C_5H_5O_2$+CH_2)] (56), 135[M-$C_6H_7O_2$-H_2O] (99) and 112[M-$C_9H_{13}O_2$+H] (100). The partial structures **A** and **B** were shown in **Figure 3**. The remaining problem was whether C_6 linked with C_7 or C_{11}. The X-ray diffraction solved the problem, and the relative configuration of **1** was identified by the X-ray diffraction (**Figure 1**).

Figure 3 The Structures of **A** and **B**

A **B**

Table 1 The ^{1}H(500MHz) and ^{13}C(125MHz) NMR Data of **1** in $CDCl_3$ (δ in ppm; J in Hz)

No	C	H	No	C	H
1	144.14(d)	7.19(br s)	**9**	175.51(s)	
2	24.19(t)	2.18(br s)	**10**	135.37(s)	
3	25.32(t)		**11**	159.54(s)	
3α		1.43(m)			
3β		1.90(m)			
4	35.07(d)	1.80(m)	**12**	72.50(t)	4.63(br s)
5	40.76(s)		**13**	13.17(q)	2.06(s)
6	31.74(t)		**14**	15.67(q)	0.93(d,J=6.8)
6α		2.74(d,J=13.7)			
6β		2.84(d,J=13.7)			
7	125.41(s)		**15**	21.29(q)	0.94(s)
8	175.51(s)				

References

1. Kunming Institute of Botany, Chinese Academy of Sciences, ″ *Flora Yunnanica*", Vol. 1, Science Press, **1977**, P 808.
2. C. M. Li, H. D. Sun *etc.*, *Acta Botanica Yunnanica*, **1991**, *13*(3), 327.
3. C. M. Li, H. D. Sun *etc.*, *Acta Botanica Yunnanica*, **1993**, *15*(4), 403.
4. Xishuangbanna Tropical Garden, Chinese Academy of Sciences, ″ *Collected Research Papers on the Tropical Botany (IV)* ", Yunnan University Press, **1996**, P 125.
5. T. Miyase, P. Rüed, C. H. Eugster *et al*., *Helv Chem Acta* **1977**, *60*, 2770.

Received 8 July 1999