A New Eremophilanoid Sesquiterpene from Senecio oldhamianus

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Abstract: A new Eremophilanoid sesquiterpene (1) was isolated from the whole plant of *Senecio oldhamianus*. Its structure was elucidated as 7, 11-epoxy-9, 10 -epoxy-8-oxoeremophilane using spectroscopic methods and X-ray analysis.

Keywords: Senecio oldhamianus, Compositae, sesquiterpene, eremophilanoid.

Senecio oldhamianus, a traditional Chinese herb, is mainly distributed in eastern, midsouthern and southwest China¹. No phytochemical examination on the plant has been reported up to now. A new eremophilanoid sesquiterpene was obtained from this plant.





Compound **1** was obtained as colorless needle crystals, mp 165-166°C, $[]_{D}^{20} - 14.6$ (*c* 0.49, acetone). Its HREIMS exhibited $[M]^+$ at *m/z* 250.15931 (calc 250.15689) corresponding to the molecular formula $C_{15}H_{22}O_3$ (U = 5) and its IR (KBr) revealed the presence of ketone carbonyl group (1711 cm⁻¹). ¹³CNMR showed it should contain two epoxy rings (δ 62.7, 64.2, 64.8, 71.4). ¹HNMR featured it as a eremophilanoid compound² (**Table**): Me-14 (δ 1.00, s, 3H), Me-15 (δ 0.89, d, 3H, J = 6.8Hz), Me-12 and Me-13 (δ 1.38, 1.28, s, each 3H). Because the chemical shifts of Me-12 and Me-13 were in relatively lower field in ¹HNMR, one epoxy should be on C-7 and C-11. The other epoxy should be on C-9 and C-10 and the ketone carbonyl located on C-8, since the

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epoxy proton (δ 3.29, s, 1H) showed no splitting. The cross peaks in ${}^{1}H^{-1}HCOSY/HMQC$ spectra indicated two main structural fragments ($-CH_2-CH_2-CH_2-CH_2-CH_3$ and $-CH_2-$) of **1**. HMBC also revealed that the ketone carbonyl was on C-8 and two epoxy rings were on C9, C-10 and C7, C-11 respectively. According to the biogenesis, Me-14 and Me-15 were β-oriented³, and which were finally confirmed by X-ray analysis. Furthermore, the X-ray analysis suggested the epoxy on C-9, C-10 was -oriented and the epoxy on C-7, C-11 was β-oriented (**Figure 1**).

Table ¹HNMR(400mHz), ¹³CNMR(100 mHz) and DEPT data of 1 (CDCl₃, TMS, δ ppm)

No.	¹ H (/) J (Hz)	¹³ C	DEPT	No.	¹ Η (α/β) J (Hz.)	¹³ C	DEPT
1	1.22 (m)/2.25 (ddd, 14.2, 14.2, 4.9)	30.5	CH_2	9	3.29 (s)	62.7	CH
2	1.64 (m)/1.79 (m)	23.8	CH_2	10	-	71.4	С
3	1.35 (m)/1.59 (m)	29.7	CH_2	11	-	64.2	С
4	1.70 (m)	40.4	CH	12	1.38 (s)	21.1	CH_3
5	-	38.2	С	13	1.28 (s)	16.5	CH_3
6	2.39 (d, 14.6)/1.58 (d, 14.6)	40.7	CH_2	14	1.00 (s)	16.1	CH_3
7	-	64.8	С	15	0.89 (d, 6.8)	15.7	CH_3
8	-	204.3	С				

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