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A New Highly Oxygenated Eremophilenolide from *Ligulariopsis shichuana*

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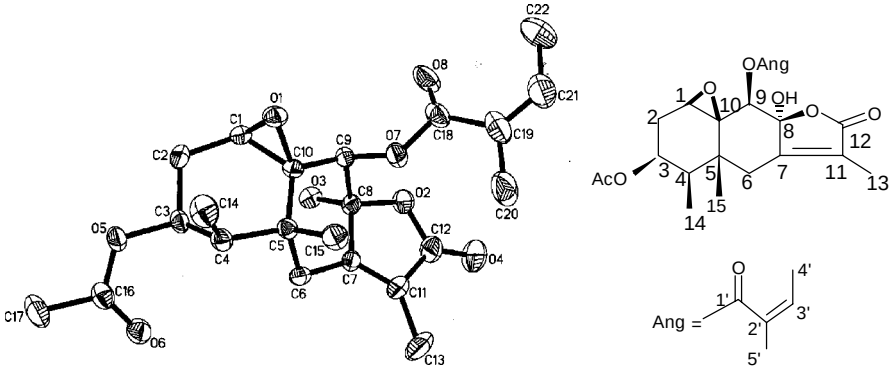
Abstract: a new highly oxygenated eremophilenolide was isolated from *Ligulariopsis shichuana*. Its structure was elucidated by NMR spectroscopic and X-ray diffraction methods.

Keyword: *Ligulariopsis shichuana*, compositae, sesquiterpene, eremophilenolide.

From the acetone extracts of *Ligulariopsis shichuana* Y. L. Chen, gen. nov.[1], a sesquiterpene **1** was afforded as white column crystals mp 212-214°C. HRESIMS gave a molecular formula $C_{22}H_{28}O_8$ ($[M+Na]^+$=443.1671, calcd. $[M+Na]^+$ =443.1676). The NMR spectrum (**Table 1**) was similar to those of known 8–hydroxyeremophil -7(11)en-8(12)-olides[2].

Figure 1 Structure of compound **1**



^{1}H NMR showed signals of angeloyloxy δ 1.74 (dq, 3H, J=1.5, 1.5Hz), δ 1.95 (dq, 3H, J=7.2, 1.5Hz), δ 6.09 (qq, 1H, J=7.2, 1.5Hz) and acetoxy δ 2.07 (s, 3H), corresponding to the oxygenated protons δ 5.41 (s, 1H) and δ 5.17 (ddd, 1H, J= 10.8, 6.4, 4.4Hz). ^{13}C NMR showed two epoxy signals δ 61.5(C), 60.3 (CH). Fortunately, the single crystal was obtained. Compound **1** was deduced as 1β, 10βepoxy-3β-acetoxy-9β-angeloyloxy

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-8α-hydroxyeremophil-7(11)-en-8β(12)-olide by X- ray diffraction analysis.

Table 1 ^{1}H NMR and ^{13}C NMR data of **1** (400, 100MHz, $CDCl_3$, TMS, δ, ppm)

H	**1** δ_H (α / β), J (Hz)	C	**1** δ_C	DEPT	C	**1** δ_C	DEPT
1	3.37d (J=5.8)	1	60.3	CH	12	171.3	C
2	2.16dd / 2.27ddd (J=12.0, 6.4 / 12.0, 10.8, 5.8)	2	24.4	CH_2	13	8.2	CH_3
3	5.17ddd (J=10.8, 6.4, 4.4)	3	68.8	CH	14	9.5	CH_3
4	1.75qd (J=5.4, 4.4)	4	40.8	CH	15	22.5	CH_3
6	2.99brd / 2.40d (J=14.0, 1.2 / 14.0)	5	39.3	C	OAng		
9	5.41s	6	34.7	CH_2	1’	165.7	C
13	1.87d (J=1.2)	7	154.7	C	2’	126.6	C
14	0.98d (J=5.4)	8	101.6	C	3’	140.7	CH
15	1.17s	9	77.0	CH	4’	20.3	CH_3
3’	6.09qq (J=7.2, 1.5)	10	61.5	C	5’	15.8	CH_3
4’	1.95dq (J=7.2, 1.5)	11	126.4	C	OAc	171.8	C
5’	1.74dq (J=1.5, 1.5)					21.3	CH_3
OAc	2.07s						

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