

A New 6,7-Seco-Ent-Kaurane Diterpenoid from *Isodon eriocalyx* Var. *laxiflora*

Xue Mei NIU, Sheng Hong LI, Shuang Xi MEI, Zhong Wen LIN, Han Dong SUN*

Laboratory of Phytochemistry, Kunming Institute of Botany, Academia Sinica, Kunming 650204

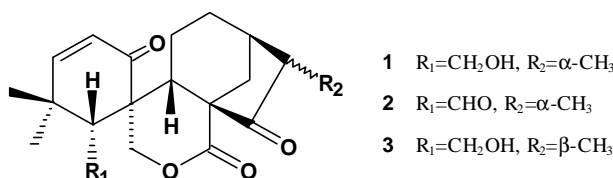
Abstract: A new 6,7-seco-ent-kaurane diterpenoid, together with two known ones, was isolated from the leaves of *Isodon eriocalyx* var. *laxiflora* C. Y. Wu & H. W. Li. Their structures were established by spectroscopic methods.

Keywords: *Isodon eriocalyx* var. *laxiflora*, 6,7-seco-ent-kaurane diterpenoid, laxiflorin E.

Isodon eriocalyx var. *laxiflora* C. Y. Wu & H. W. Li, is a perennial herb naturally growing in the southern area of Yunnan province. In our continuing studies¹ on its leaves collected from Xishuanbana prefecture, a new 6,7-seco-ent-kaurane diterpenoid, named laxiflorin E (**1**), together with two known 6,7-seco-ent-kaurane diterpenoids², eriocalyxin A (**2**) and laxiflorin C (**3**), was isolated. Their structures were established by spectroscopic analysis.

Compound **1**, obtained as colorless rhombus crystal (from Me₂CO), mp: 214.0–216.5°C, [α]_D^{15.3} +121.18 (c=0.85, CH₃OH), showed a molecular formula peak at *m/z* 346 for C₂₀H₂₆O₅ in the EIMS spectrum, which was confirmed by HREIMS (found 346.1750, calc. 346.1780). The analysis of ¹H and ¹³C NMR (DEPT) data revealed that compound **1** closely resembled compound **2** except for A-ring. The methine carbon signal at δ_C 199.82 assigned to CHO group in **2** was replaced by an oxy-methylene carbon signal at δ_C 58.3 arising from CH₂OH group in **1**. In the ¹H NMR spectrum³, the doublet signal at δ_H 9.90 in **2** was substituted by the proton signal at δ_H 4.29 (2H, brs) in **1**. Therefore, compound **1** was identified as 16(S)-methyl-6-hydroxyl-1, 15-dioxo-6,7-seco-ent-kaur-2-en-7, 20-olide (**Figure 1**), named laxiflorin E.

Figure 1 The structures of **1-3**



* E-mail: hdsun@mail.kib.ac.cn

Table 1 The ^{13}C NMR data of **1-3** (125 MHz, δ in ppm, $\text{C}_5\text{D}_5\text{N}$)

Carbon	1	2*	3
1	200.9 (s)	197.1 (s)	200.9 (s)
2	124.6 (d)	125.1 (d)	124.5 (d)
3	158.9 (d)	156.4 (d)	158.9 (d)
4	36.8 (s)	36.1 (s)	36.7 (s)
5	47.6 (d)	57.5 (d)	47.6 (d)
6	58.3 (t)	199.8 (d)	58.3 (t)
7	170.4 (s)	168.9 (s)	170.4 (s)
8	60.0 (s)	59.1 (s)	60.0 (s)
9	41.9 (d)	42.6 (d)	41.9 (d)
10	52.7 (s)	49.9 (s)	52.3 (s)
11	18.6 (t)	17.8 (t)	20.3 (t)
12	30.6 (t)	29.6 (t)	18.1 (t)
13	36.0 (d)	35.3 (d)	32.7 (d)
14	30.1 (t)	29.4 (t)	32.8 (t)
15	217.1 (s)	216.0 (s)	217.4 (s)
16	51.3 (d)	51.0 (d)	48.8 (d)
17	16.9 (q)	16.7 (q)	11.8 (q)
18	31.9 (q)	31.5 (q)	31.8 (q)
19	23.8 (q)	24.3 (q)	23.8 (q)
20	70.8 (t)	68.5 (t)	70.8 (t)

*The data were measured in CDCl_3 with reference to the signal of CDCl_3

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References and notes

1. H. D. Sun, Z. W. Lin, F. D. Niu, P. Q. Shen, L. T. Pan, L. Z. Lin and G. A. Coedell, *Phytochemistry*, **1995**, *38*, 1451.
2. J. Wang, Z. W. Lin, H. D. Sun, *Chinese Chemical Letters*, **1997**, *8*, 421.
3. The ^1H NMR data of **1** ($\text{C}_5\text{D}_5\text{N}$, 500 MHz, δ in ppm, J in Hz): 5.90 (d, 1H, $J=10.2$ Hz, H-2), 6.48 (d, 1H, $J=10.2$ Hz, H-3), 2.25 (brs, 1H, H-5), 4.29 (brs, 2H, H-6), 2.91 (dd, 1H, $J=4.3$, 3.0 Hz, H-9), 1.80 (m, 1H, H-11a), 1.64 (m, 1H, H-11b), 2.02 (m, 1H, H-12a), 1.29 (m, 1H, H-12b), 1.99 (brs, 1H, H-13), 2.81 (m, 2H, H-14), 2.08 (brd, 1H, $J=7.6$ Hz, H-16), 1.06 (d, 3H, $J=7.6$ Hz, H-17), 1.17 (s, 3H, H-18), 1.22 (s, 3H, H-19), 5.27 (d, 1H, $J=11.1$ Hz, H-20a), 4.82 (d, 1H, $J=11.1$ Hz, H-20b).

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