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Sesquiterpene Lactones from *Elephantopus scaber*

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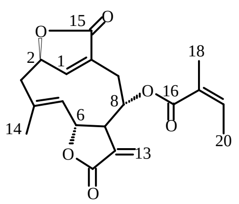
Abstract: A new germacranolide sesquiterpene lactone, isoscabertopin, was isolated from *Elephantopus scaber* together with the known scabertopin. Their structures were determined by spectroscopic methods.

Keywords: *Elephantopus scaber*, Compositae, germacranolide sesquiterpene lactone, isoscabertopin.

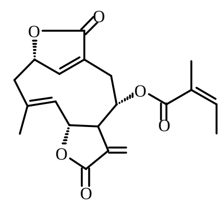
The sesquiterpene lactones were isolated from *Elephantopus scaber* Linn.[1]. It has recently reported these type compounds have nerve system effect[2]. We further investigated the plant and isolated a new germacranolide sesquiterpene lactone, isoscabertopin (**1**), and the known scabertopin (**2**)[1]. This paper deals with the structural elucidation of the new compound.

Isoscabertopin (**1**), $C_{20}H_{22}O_6$ [HRESIMS (pos.) *m/z*: 359.1410 $[M+H]^+$, calcd. 359.1417], colorless needles. Its IR (KBr, ν) 1762, 1656 and 1646 cm^{-1} and the characteristic pair of low-field signals at δ 6.24 (*d*, 1H, *J*=3.2 Hz, H-13a) and δ 5.61 (*d*,1H, *J*=3.2 Hz, H-13b) in ^1H NMR spectrum indicated the presence of α-methylene-γ-lactone. In addition, its IR (KBr, ν) 1746 cm^{-1} and ^1H NMR signal at δ 7.07 (*s*, 1H, H-1) and ^{13}C NMR signals at δ 153.2 (C-1), 128.9 (C-10), 172.5 (C-15) (assigned by HMQC) showed the presence of α,β-unsaturated lactone in **1**. Furthermore, the IR (KBr, ν) 1711cm^{-1} showed an ester group in **1**. These assignment were also supported by the presence of three carbonyl carbon signals at δ 172.5, 169.5 and 166.8, respectively, in the ^{13}C NMR spectrum of **1** (**Table 1**).

Figure 1 The structure of compound **1** and **2**



1 Isoscabertopin



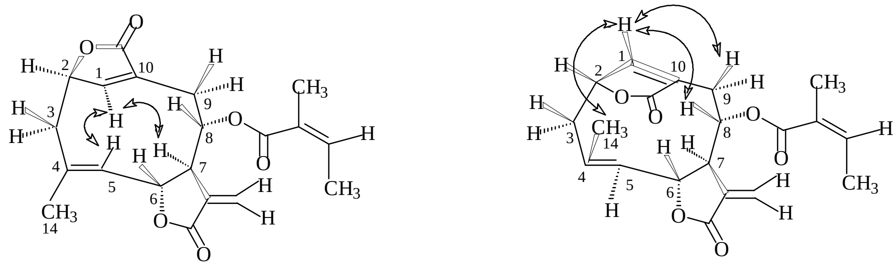
2 Scabertopin

In the ^{1}H NMR spectrum, a doublet signal at δ 4.78 (J = 10.4Hz) was attributed to H-5 which coupled with H-6. The signal at δ 5.17 ($J_{5,6}$ = 10.4 Hz, $J_{6,7}$ = 8.0 Hz) was assigned as H-6. The H-7 (δ 2.92) was shown as a complex signal (*ddd*) with large coupling constants ($J_{7,8}$ = 11.5, $J_{6,7}$ = 7.3, $J_{7,13}$ = 3.4 Hz). This indicated *trans*-axial relationships between H-6, H-7 and H-8, *i.e.* H-6β, H-7α and H-8β-oriented. These assignments were based on the assumption that H-7 is α-oriented as in all other naturally occurring germacranolides[1].

A comparison between the ^{1}H NMR spectrum of **1** and **2** showed that the signals of H-5 and H-7 in **1** were shifted upfield (H-5: δ 4.78 in **1** cf. 5.13 in **2**; and H-7: δ 2.92 in **1** cf. 3.13 in **2**). It is evident that the carboxyl group of the α,β-unsaturated lactone in **1** is in rather long distance from both H-5 and H-7. In agreement with this notion, the oxygen atom at C-2 should be β-oriented in **1**. This assignment was supported by NOEs experiments. In the NOESY spectrum of **1**, the correlations between H-1 and H-5, H-1 and H-7 were observed. Whereas, the correlations were observed between H-1 and H-8, H-1 and H-9a, as well as H-1 and CH_3-14 in **2** of which C-2 is α-oriented (**Figure 2**).

Thus the above data allowed the assignment of structure **1** to isoscabertopin.

Figure 2 Key NOESY correlations of compound **1** and **2**



1 Isoscabertopin **2** Scabertopin

Table 1 ^{13}C NMR data for **1** and **2** in $CDCl_3$ (δ ppm)

C	**1**	**2**	C	**1**	**2**	C	**1**	**2**	C	**1**	**2**
1	153.2	149.3	6	78.1	78.9	11	134.4	134.3	16	166.8	167.0
2	81.4	79.5	7	52.4	49.8	12	169.5	169.6	17	126.8	126.8
3	41.5	40.2	8	71.2	73.7	13	123.7	123.2	18	20.2	20.4
4	136.0	135.4	9	33.7	30.3	14	20.4	21.7	19	140.8	140.7
5	133.9	125.6	10	128.9	131.7	15	172.5	174.4	20	15.9	15.9

References

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