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A New Eudesmanoilde from *Carpesium macrocephalum*

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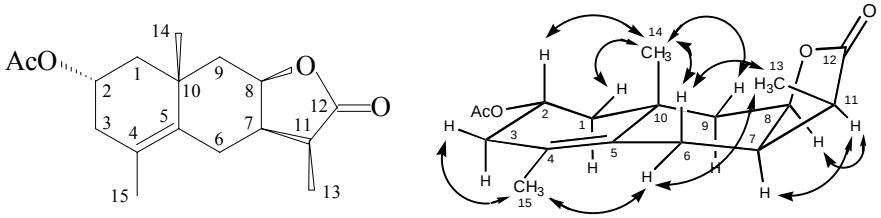
Abstract: A new eudesmanoilde was isolated from the aerial parts of *Carpesium macrocephalum*. Its structure was elucidated as 2α-acetoxy-11αH-eudesma-4-en-12, 8β-olide by spectral methods.

Keywords: *Carpesium macrocephalum*, Compositae, eudesmanolide.

The investigation of the aerial parts of *Carpesium macrocephalum* F. *et* S. a cinese folk medicine for hemostatic and antipyretic properties[1] led to the isolation of a new eudesmanoilde **1**. Here we report the structure elucidation of it.

Figure 1 Key NOESY correlation of compound **1**



1

Compound **1** was obtained as colorless crystal, mp: 128°C, $[\alpha]_D^{20}$ +68.8 (c 0.46, $CHCl_3$), had the molecular formula $C_{17}H_{24}O_4$ indicated by the quasi-molecular ion at *m/z* 293.1743 $[M+H]^+$, calc 293.1747, in HR-positive-SIMS. Its IR spectrum exhibited strong absorptions at 1768, 1732, 1642cm^{-1}. The ^{1}H NMR data of **1** (**Table 1**) were in part similar to those of 2α-hydroxy-eudesma-4, 11(13)-dien-12, 8β-olide[2], but the characteristic exocyclic methylene of the lactone ring at C-11 was replaced by methyl doublet at δ_H 1.25 (3H, d, J= 7Hz), and an additional acetyl side chain singlet was observed at δ_H 2.05 (3H, s) as well as H-2β was shifted downfield at δ_H 4.99 (1H, dddd, J= 12, 10, 5.5, 3.5Hz), which explicated that a corresponding 2α-acetoxy was present. Moreover, together with ^{1}H-^{13}C long-range correlations (**Table 1**): such as C-1 / H-14; C-2 / H-1, H-3; C-3 / H-1, H-15; C-5 / H-3, H-9, H-14, H-15; C-6 / H-11; C-7 / H-9, H-13; C-9 / H-14 and C-12 / H-13 in HMBC experiment, structural elucidation of compound **1**

was confirmed. Finally, the stereochemistry was established by ^{1}H-^{1}H NOESY spectrum. Clear NOE correlations (**Figure 1**) between H-2β and H-14, H-8 and H-11, H-6β and H-14, H-13, and H-15 and H-6α indicated that 14-CH_3, 13-CH_3 and H-2 were β-configuration, as well as H-7, H-8 and H-11 were in α-orientation. Consequently, compound **1** was characterized as 2α-acetoxy-11αH-eudesma-4-en-12, 8β-olide.

Table 1 NMR and HMBC data of **1** ($CDCl_3$, δ in ppm, J in Hz)

NO.	δ_H (α / β)	δ_C (DEPT)	HMBC (C / H)
	1	**1**	**1**
1α	1.40 (dd, 12, 12) /	45.1 (CH_2)	C-1 / H-3, 9, 14
1β	1.99 (ddd, 12, 3.5, 2)		
2β	4.99 (dddd, 12, 10, 5.5, 3.5)	67.6 (CH)	C-2 / H-1, 3
3α	2.08* (dd, 16.5, 10) /	38.4 (CH_2)	C-3 / H-1, 15
3β	2.38* (ddd, 16.5, 5.5, 2)		
4	-	124.0 (C)	C-4 / H-3, 6, 15
5	-	131.1 (C)	C-5 / H-3, 6, 9, 14, 15
6α	2.50 (dd, 14, 6) /	21.8 (CH_2)	C-6 / H-11
6β	1.70* (dd, 14, 11.5)		
7α	2.34* (m, 11.5, 7, 6, 6)	40.7 (CH)	C-7 / H-6, 9, 11, 13
8α	4.44 (ddd, 6, 4, 2)	77.5 (CH)	C-8 / H-6, 9
9α	1.54 (dd, 15.5, 4) /	42.6 (CH_2)	C-9 / H-1, 14
9β	2.28 (dd, 15.5, 2)		
10	-	36.0 (C)	C-10 / H-1, 6, 9, 14
11α	2.81 (dq, 7, 7)	42.0 (CH)	C-11 / H-13
12	-	179.5 (C)	C-12 / H-11, 13
13	1.25* (d, 7)	9.3 (CH_3)	C-13 / H-11
14	1.23* (s)	27.1 (CH_3)	C-14 / H-1, 9
15	1.68 (s)	19.2 (CH_3)	C-15 / H-3
1′	-	170.6 (C)	C-1′ / H-2′
2′	2.05 (s)	21.4 (CH_3)	-

a. Signal multiplicity and coupling constants (Hz) are in parentheses;
b. *Overlapping signals.

Acknowledgment

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