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A New Sesquiterpene and a New Norsesquiterpene from *Cacalia deltophylla*

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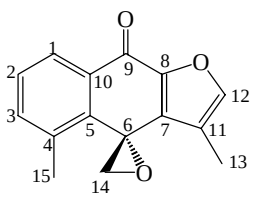
Abstract: A new sesquiterpene and a new norsesquiterpene were isolated from the whole plant of *Cacalia deltophylla* (Maxim) Mattf. Their structures were elucidated as deltocacalone (**1**) and deltonorcacalol (**2**) by spectroscopic methods including 2D NMR.

Keywords: *Cacalia deltophylla*, Compositae, cacalone, cacalol.

Several species of genus *Cacalia* are efficacious in invigorating circulation of blood, relieving coughs and phlegm[1]. Up to now, no phytochemical investigations of *Cacalia deltophylla* (Maxim) Mattf have been carried out. Here we report the structure elucidation of a new sesquiterpene deltocacalone (**1**) and a new norsesquiterpene deltonorcacalol (**2**) from this plant.

Compound **1** was obtained as yellow crystals from acetone, mp: 183-185°C, $[\alpha]_D^{20}$ – 5.4 (*c* 0.35, acetone). Its molecular formula was deduced to be $C_{15}H_{12}O_3$ from the EIMS ($[M]^+$ *m/z* 240) together with ^{13}C NMR and DEPT spectra (2×CH_3, 1×CH_2, 4×CH and 8×C). The IR spectrum displayed a conjugated carbonyl group (1652 cm^{-1}). The ^1H NMR spectrum showed the presence of a methyl substituted furan ring, a 1,2,3-trisubstituted benzene, a methyl group on benzene ring and a pair of protons (δ 3.50, 3.78) belong to an oxygen-bearing methylene. In its ^{13}C NMR spectrum, the signal of methylene (δ 52.0) appeared at relative high field implying a tri-member epoxy ring. The supposed structure was proved by ^3J cross peaks in HMBC experiment: C-5/H-1, 3, 14, 15; C-7/H-12, 13, 14; C-8/H-12; C-9/H-1. The configuration of the methylene at C-6 could be assigned as β [2-4] in the biogenetic consideration of cacalone (a common component of *Cacalia*). Thus, compound **1** was established as deltocacalone.



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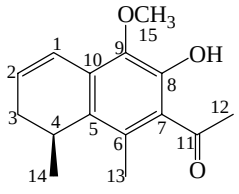

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Compound **2** was obtained as colorless needles from acetone, mp: 150-152 °C, $[\alpha]_D^{20}$ +84.6 (*c* 0.39, $CHCl_3$). The molecular formula $C_{15}H_{18}O_3$ was deduced from EIMS ($[M]^+$ *m/z* 246) and NMR spectra (4×CH_3, 1×CH_2, 3×CH and 7×C). The IR spectrum indicated a hydroxyl group (3282 cm^{-1}) and a conjugated carbonyl group (1670 cm^{-1}). The ^1H NMR spectrum showed the presence of a secondary methyl group, a methyl group on benzene ring, an acetyl group, a methoxyl group and a double bond. These groups was combined by the ^1H-^{13}C cross peaks (^3J) in HMBC experiment: C-1/H-3; C-2/H-4; C-3/H-1, 14; C-5/H-1, 3, 13, 14; C-7/H-12, 13, -OH; C-9/H-1, -OH, -O<u>C</u>H$_3$; C-10/H-2, 4. The configuration of 14-methyl group was assigned as β based on the strong correlation between 13-methyl group and H-4α in its NOESY experiment. Thus, compound **2** was described as deltonorcacalol.

Table 1 ^1H NMR (400 MHz), ^{13}C NMR (100 MHz) and DEPT data of **1-2** ($CDCl_3$, TMS)

No.	**1** δ_H	**2** δ_H	No.	**1** δ_C	DEPT	**2** δ_C	DEPT
1	8.31 (dd, 7.5, 1.6)	6.76 (dd, 9.8, 3.0)	1	126.4	CH	120.8	CH
2	7.40 (t, 7.5)	6.08 (ddd, 9.8, 6.4, 2.6)	2	128.0	CH	129.1	CH
3 (α)	7.35 (dd, 7.5, 1.6)	2.25 (ddd, 17.2, 2.6, 1.0)	3	137.1	CH	30.8	CH_2
3β	-	2.49 (dddd, 17.2, 7.0, 6.4, 3.0)	4	135.3	C	27.4	CH
4α	-	3.10 (ddq, 1.0, 7.0, 7.0)	5	135.9	C	131.4	C
12	7.50 (brs)	2.59 (s)	6	56.8	C	128.2	C
13	2.16 (brs)	2.30 (s)	7	136.1	C	125.9	C
14	3.50 (d, 5.8)	1.04 (d, 7.0)	8	149.0	C	148.2	C
14	3.78 (d, 5.8)	-	9	172.6	C	141.5	C
15	2.63 (s)	3.80 (s)	10	136.7	C	128.6	C
OH	-	8.67 (brs)	11	119.4	C	205.6	C
			12	146.0	CH	32.6	CH_3
			13	7.8	CH_3	16.3	CH_3
			14	52.0	CH_2	18.7	CH_3
			15	19.7	CH_3	61.4	OCH_3

Signals assigned on the basis of HMQC and HMBC spectra.

Acknowledgments

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References

1. Z. W. Xue, Y. Q. Yu, *ZhongGuo ZhongCaoYao MingJian* (in Chinese), People's Health Press, Beijing, **1996**, p.754.
2. A. Casares, L. A. Maldonado, *Tetrahedron Lett.*, **1976**, *29*, 2485.
3. F. Yuste, E. Diaz, F. Walls, *J. Org. Chem.*, **1976**, *41* (26), 4103.
4. M. Soriano-Garcia, F. Walls, H. Barrios, R. Sanchez-Obregon, B. Ortiz, E. Diaz, R. A. Toscano, F. Yuste, *Acta Cryst.*, **1988**, *C44* (6), 1092.

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