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A New Picrotoxane Type Sesquiterpene from *Dendrobium densiflorum*

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Abstract： A new picrotoxane type sesquiterpene named dendrodensiflorol has been isolated from the stems of *Dendrobium densiflorum*. Its structure was identified on the basis of spectroscopic method.

Keywords: Orchidaceae, *Dendrobium densiflorum*, sesquiterpene, dendrodensiflorol.

Dendrobium densiflorum lindl. (Orchidaceae) is a plant of the *Dendrobium* genus used in the popular Chinese patent medicine Mai-Luo-Ning, which is used for treatment of cerebral thrombosis and obliterative thromboangitis[1, 2]. Some stilbenoids, coumarins and fluorenones have been isolated from *Dendrobium densiflorum* before[3, 4]. In our further investigation on chemical components of *Dendrobium densiflorum*, a new sesquiterpene named dendrodensiflorol has been isolated, and its structure was identified on the basis of spectroscopic methods.

Compound **1**, was obtained as white amorphous powder. The molecular formula of **1** was deduced to be $C_{15}H_{24}O_5$ according to HRESIMS and ^{13}C NMR data. In IR spectrum of **1**, absorption bands at 3415 and 1757 cm^{-1} revealed the existence of hydroxyl and γ-lactone groups, respectively. In ^{13}C NMR spectrum of **1** (**Table 1**), 15 carbon signals including three methyls, three methylenes, six methines and three quarterary carbons were found. The ^1H NMR spectrum of **1** (**Table 1**) demonstrated the presence of three methyls (δ 1.15, 1.37, 1.39), two oxygenated methylene protons (δ 3.50, 3.56) and two oxygenated methine protons (δ 4.39, 4.72). These spectral data and the presence of four degree of unsaturation in compound **1** suggested that it was a sesquiterpene with a γ-lactone and three hydroxyl groups. Analysis of ^1H-^1H COSY and HMQC spectra enabled deduction of structure fragment –C-2-C-3-C-4-C-5-C-6-C-7-C-8-C-9-C-11- in the structure of **1**. In HMBC spectrum of **1**, ^{13}C-^1H long range correlation signals were found between C-1 and H-2, H-3, H-5, H-6, H-7, H-9, H-10, H-11a; C-4 and H-3, H-13, H-14; and C-15 and H-3, H-4, H-5, which enabled establishment of the planar structure of **1**. Relative configuration of **1** was determined on the basis of its ROESY spectrum, in which, NOE correlation signals were observed between H-10 and H-2, H-6, H-11b；H-3 and H-5, H-13. Therefore, compound **1** was

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identified to be a sesquiterpene possessing a picrotoxane type skeleton as shown in **Scheme 1**. To our best knowledge, compound **1** is a new compound, and has been assigned the trivial name dendrodensiflorol.

Scheme 1

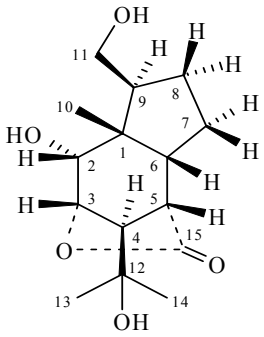

Table 1 ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of **1** ($CDCl_3$) (δ_{ppm}, J_{Hz})

No.	δ_H	δ_C	No.	δ_H	δ_C
1		50.6 (s)	8β	1.24, m	
2	4.39, brs	72.2 (d)	9	2.70, m	45.6 (d)
3	4.72, brd, 4.1	84.3 (d)	10	1.15, s	22.1 (q)
4	2.29, dd, 4.1, 3.6	53.3 (d)	11a	3.56, m	62.3 (t)
5	2.47, t, 3.6	46.2 (d)	11b	3.50, m	
6	2.90, ddd, 2.9, 3.6, 6.5	45.3 (d)	12		69.9 (s)
7α	1.83, m	25.6 (t)	13	1.37, s	30.7 (q)
7β	1.99, m		14	1.39, s	30.5 (q)
8α	1.94, m	26.8 (t)	15		179.4 (s)

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