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New Bibenzyl and Phenanthrenedione from *Dendrobium densiflorum*

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Abstract: A new bibenzyl **1** and a new phenanthrenedione **2** were identified from the stems of *Dendrobium densiflorum* (Orchidaceae).

Keywords: *Dendrobium densiflorum*, Orchidaceae, phenanthrenedione, bibenzyl.

Several species of *Dendrobium* plants (Orchidaceae) are used in traditional Chinese medicine as a Yin tonic to nourish the stomach, promote the production of body fluid, and reduce fever[1]. Chemical components of several *Dendrobium* plants have been widely investigated[2, 3]. *D. densiflorum* Lindl. ex Wall. is one species of *Dendrobium* plants, several components of this species have been reported before[4, 5]. We herein report structural elucidation of a new bibenzyl named densiflorol A **1** and a new phenanthrenedione named densiflorol B **2** obtained from *D. densiflorum.*

Compound **1** was obtained as a white amorphous powder. HREI mass spectrum of **1** exhibited a molecular ion peak at *m/z* 272.1031 [M^+], calculated for $C_{16}H_{16}O_4$. In the ^{13}C NMR spectrum of **1**, 16 carbon signals were observed as one methyl, three methylenes, six methines and six quaternary carbons (**Table 1**). A bibenzyl skeleton with one methoxy, one hydroxyl and one methylenedioxy group were deduced to the structure of **1** according to ^{13}C NMR data. Proton signal splitting manner in ^1H NMR spectrum of **1** revealed a 1,3,4-substituted benzene ring [δ 6.60 (1H, d, 1.5), 6.55 (1H, dd, 1.5, 7.9), 6.65 (1H, d, 7.9)] and a 1,3,5-substituted benzene ring [δ 6.15(2H, d, 1.6) and 6.25(1H, d, 1.6)]. On the basis of above evidence and information from HMQC and HMBC spectra, the structure of **1** was identified to be 5-[2′-(3″-hydroxy-5″-methoxyphenyl) ethyl]-1,3-benzodioxole (**Figure 1**). Compound **1** is a new compound named densiflorol A.

Compound **2** was obtained as a red amorphous powder. HREI mass spectrum of **2** exhibited a molecular ion peak at *m/z* 254.0584 [M^+], calculated for $C_{15}H_{10}O_4$. In the ^{13}C NMR spectrum of **2**, 15 carbon signals were observed as one methyl, six methines and eight quaternary carbons, and two of them belong to carbonyl carbons (**Table 1**). One hydroxyl and one methoxy group should exist in the structure of **2** according to proton signals at δ10.45 (1H, s) and δ3.90 (3H, s) and downfield carbon signals at δ158.3 and δ157.5. Compound **2** was suggested to be an anthrenedione or phenanthrenedione from above NMR spectra data.

Three aromatic proton signals at δ7.25 (d, 2.2), 7.30 (dd, 2.2, 9.5) and 9.35 (d, 9.5) in ^{1}H NMR spectrum of **2** enabled the deduction of one aromatic ring of 1,3,4-substitution pattern. Another aromatic ring was suggested to be of 1,2,3,4-substitution pattern according to two coupled aromatic protons at δ 7.95 (d, 8.6) and 8.10 (d, 8.6). NOE correlation signals were observed between protons at δ 7.25 and 8.10, and between the methoxy proton and a proton at δ 6.30 (s) in NOESY spectrum. The skeleton of **2** was thus revealed to be phenanthrenedione. According to ^{1}H-^{13}C long range correlation signals in HMBC spectrum of **2**, and especially to those between C-4a and H-5, and between C-4a and H-3, the structure was established to be 7-hydroxy-2-methoxy-1, 4-phenanthrenedione (**Figure 1**). Compound **2** is a new compound named densiflorol B.

Figure 1. Structures of Compounds **1** and **2.**

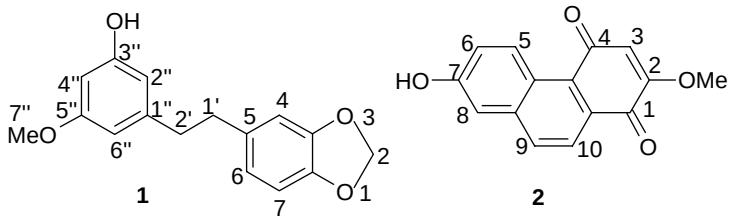

Table 1. ^{1}H (400MHz) and ^{13}C (75MHz) NMR Data of Compounds **1** and **2**.

	1 ($CDCl_3$)			**2** (d_6-DMSO)	
No.	^{1}H	^{13}C	No.	^{1}H	^{13}C
2	5.85, s	100.8	1		180.2
3a		147.6	2		158.3
4	6.60, d, 1.5	109.0	3	6.30, s	111.1
5		135.6	4		188.4
6	6.55, dd, 1.5, 7.9	121.3	4a		126.8
7	6.65, d, 7.9	108.2	4b		123.3
7a		145.7	5	9.35, d, 9.5	121.8
1′	2.70, m	37.3	6	7.35, dd, 2.2, 9.5	122.4
2′	2.70, m	38.3	7		157.5
1″		144.5	8	7.25, d, 2.2	109.7
2″	6.15, d, 1.6	108.1	8a		138.9
3″		156.7	9	8.10, d, 8.6	132.3
4″	6.15, d, 1.6	99.2	10	7.95, d, 8.6	129.7
5″		160.9	10a		128.3
6″	6.25, d, 1.6	106.8	OMe	3.90, s	56.4
7″	3.70, s	55.3	OH	10.45, s	

References

1. Jiangsu New Medical College. *Dictionary of Chinese Medicines*, Shanghai Scientific and Technologic Press, Shanghai, **1986**, p586.
2. X. K. Wang, T. F. Zhao, *Yaoxue Tongbao*, **1986**, *21*(11), 666.
3. K. Z. Wang, W. Y. Gao, *Zhongcaoyao*, **1997**, *28*(10), 633.
4. S. K. Talapatra, S. Bose, A. K. Mallik, *J. Indian Chem. Soc.*, **1984**, *61*(11-12), 1010.
5. D. Jan, L. Kurt, R. Jan, *Acta. Chem. Scand.*, **1975**, *B29*(5), 627.

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