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A New Bibenzyl Glycoside from *Dendrobium moniliforme*

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Abstract: A new bibenzyl glycoside has been isolated from the stems of *Dendrobium moniliforme* (L.) Sw. (Orchidaceae). Its structure has been identified on the basis of spectroscopic and chemical methods.

Keywords: *Dendrobium moniliforme*, Orchidaceae, bibenzyl glycoside, dendromoniliside E.

Several species of *Dendrobium* plants (Orchidaceae) are used in traditional Chinese medicine as a Yin tonic to nourish stomach, reduce fever and promote secretion of saliva[1]. Chemical components of several *Dendrobium* species have been widely investigated[2]. *D. moniliforme* is one species of *Dendrobium* plants distributed widely in the south of China, Korea peninsula, Japan and northeast of India. The lipophilic components of *D. moniliforme* have been studied recently[3, 4]. As a result of our systematically chemical investigation of *Dendrobium* plants[5-7], we herein report the identification of one new bibenzyl glycoside **1** obtained from the polar fraction of 95% ethanol extract of the stems of *D. moniliforme.*

Compound **1** was obtained as white amorphous powder, $[\alpha]_D^{20}$ 0 (*c* 0.3, H_2O), mp 202~204°C. The molecular formular of **1** was established as $C_{28}H_{38}O_{14}$ by HRESIMS at *m/z* $[M+Na]^+$ 621.2155 (calcd 621.2159 $C_{28}H_{38}O_{14}Na$). Hydrolysis of **1** yielded glucose as its sugar component. In ^{13}C NMR spectrum of **1**, 28 carbon signals were observed, among which there were twelve aromatic carbon signals, a pair of glucose units signals, two methoxyls and two methylenes. One 1, 4-bissubstituted benzene ring and one 1, 3, 4, 5-tetrasubstituted benzene ring were deduced according to proton signals at δ 7.22 (2H, d, 8.4), 7.01 (2H, d, 8.4) and at δ 6.75 (1H, d, 1.4), 7.36 (1H, d, 1.4) in its ^1H NMR spectrum and also according to its ^1H-^1H COSY spectrum (**Table 1**). A bibenzyl skeleton was assigned to the aglycon of **1** on the basis of above information. Furthermore, the two glucose units should link to the aglycon with β glycosidic linkages according to the two anomeric proton signals at δ 5.50 (1H, d, 7.2) and 5.89 (1H, d, 7.4) in its ^1H NMR spectrum.

The substitution positions of the two methoxyls and the two sugar moieties were

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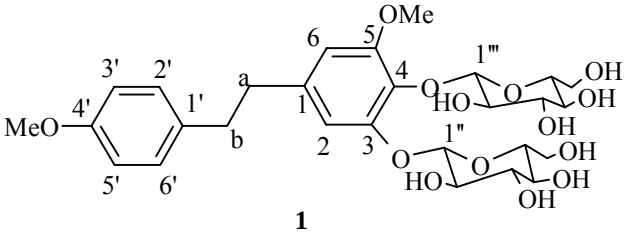
established on the basis of ROESY and HMBC experiments. In ROESY spectrum of **1**, correlations were found between H-4′-OCH_3 and H-3′, H-5′; H-5-OCH_3 and H-6; H-a, b and H-2, H-2′, H-6, H-6′; H-glc-1″ and H-2. In HMBC spectrum of **1**, ^{13}C-^{1}H long range correlations were observed between C-3 and H-glc-1″; C-4 and H-glc-1‴; C-a and H-2, H-6; C-b and H-2′, H-6′; C-4′ and H-4′-OCH_3; C-5 and H-5-OCH_3. On the basis of the above evidence, the two methoxyl groups should be connected to C-4′ and C-5, while the two glucose units should be linked to C-3 and C-4. Thus, **1** was identified to be 3, 4-dihydroxy-4′, 5-dimethoxybibenzyl-3, 4-*di*-O-β-D-glucopyranoside, and named den- dromoniliside E.



1

Table 1 ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of **1** (C_5D_5N) (δ ppm, *J* Hz)

No.	^{1}H	^{13}C	No.	^{1}H	^{13}C
a	2.81, m	38.5 (t)	5- OCH_3	3.82	56.7 (q)
b	2.83, m	37.0 (t)	4'-OCH_3	3.75, s	55.2 (q)
1		138.9 (s)	Glc-1″	5.50, d, 7.2	104.6 (d)
2	6.75, d, 1.4	117.7 (d)	Glc-2″	4.42, m	75.4 (d)
3		152.4 (s)	Glc-3″	4.41, m	77.9 (d)
4		134.9 (s)	Glc-4″	4.38, m	71.5 (d)
5		153.8 (s)	Glc-5″	4.15, m	79.1 (d)
6	7.36, d, 1.4	108.8 (d)	Glc-6″	4.66, dd, 12.2, 2.4; 4.44, m	62.6 (t)
1'		134.2 (s)	Glc-1‴	5.89, d, 7.4	105.7 (d)
2'	7.22, d, 8.4	130.0 (d)	Glc-2‴	4.38, m	75.9 (d)
3'	7.01, d, 8.4	114.3 (d)	Glc-3‴	4.35, m	78.5 (d)
4'		158.5 (s)	Glc-4‴	4.38, m	71.5 (d)
5'	7.01, d, 8.4	114.3 (d)	Glc-5‴	3.95, m	78.7 (d)
6'	7.22, d, 8.4	130.0 (d)	Glc-6‴	4.44, m; 4.44, m	62.6 (t)

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