A New Dendrobine-Type Alkaloid from Dendrobium nobile

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Abstract: A new dendrobine-type alkaloid has been isolated from stems of *Dendrobium nobile* lindl. Its structure has been identified on the basis of spectroscopic method.

Keywords: Dendrobium nobile, Orchidaceae, alkaloid, dendronobiline A.

Several species of *Dendrobium* plants (Orchidaceae) are used in traditional Chinese medicine as a Yin tonic to nourish stomach, promote production of body fluid, and reduce fever¹. *D. nobile* lindl. (Chinese name "Jin-Chai-Shi-Hu") is an abundant medicinal *Dendrobium* species distributed in China. Several sesquiterpene alkaloids², phenanthrenoids³, bibenzyls⁴ coumarins⁵ and sesquiterpenoids⁶ have been reported from *D. nobile* lindl. up to now. As a result of our systematical investigation in chemical components of *Dendrobium* plants⁶⁻⁸, we herein report the identification of a new dendrobine-type alkaloid (1) isolated from the stems of *D. nobile*.

Compound 1 was obtained as colorless crystals, mp 85-87°C, $[\alpha]_p^{20}$ -69.0 (c 0.1, CH₃OH). HREIMS of **1** exhibited molecular ion peak at m/z 319.2163 [M⁺] (calculated for $C_{19}H_{29}NO_3$). In ¹³C NMR spectrum of 1, 19 carbon signals were observed as five methyls, three methylenes, eight methines and three quaternary carbons (Table 1). Among them, two signals at δ 178.9 and 208.0 ppm should belong to carbonyl carbons. ¹H NMR spectrum of **1** showed five methyls at δ 0.98 (d, 6H, 6.5), 1.39 (s, 3H), 2.15 (s, 3H) and 2.45 (s, 3H). In ¹H-¹H COSY spectrum of 1, correlation signals were observed between H₃ and H₂, H₄; between H₅ and H₄, H₆; between H₆ and H_{7a}, H_{7β}; between H_{8a} and H_{7a} , $H_{7\beta}$, H_9 ; between H_{11} and H_9 , H_{12a} , H_{12b} ; between H_{12a} and H_{12b} ; between H_{15} and H₁₆, H₁₇. Further analysis of TOCSY and HMQC spectra of 1 led to deduction of fragments $-C_2 \cdot C_3 - C_4 \left[-C_{15}(-C_{16}) - C_{17} \right] - C_5 - C_6 - C_7 - C_8 - C_9 - C_{11} - C_{12}$ in the structure. ¹³C-¹H long-range correlation signals were observed at H_{10} / C_2 , H_{19} / C_2 , H_2 / C_4 , H_3 / C_{18} , H_4 / C_{18} , H_{16} / C_4 , H_{17} / C_4 , H_4 / C_6 , H_{11} / C_8 , H_{10} / C_9 , H_{12} / C_9 , H_{14} / C_{12} and H_{19} / C_{11} , which enabled linkage of above fragments with other two methyls and three quaternary carbons. Relative configuration of 1 was established according to NOE correlations between H₂ and H_3 , H_{10} , H_{11} , H_{19} ; between H_6 and H_5 , H_{10} ; and between H_{11} and $H_{8\alpha}$, H_9 , H_{12a} . Compound 1 is a new compound named dendronobiline A.

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Table 1 1 H NMR (400 MHz) and 13 C NMR (100 MHz) data of 1 (CDCl₃)

No.	¹ H	¹³ C	No.	¹ H	¹³ C
1		50.5, s	10	1.36, m	32.8, q
2	2.86, m	67.6, d	11	3.19, m	68.7, d
3	4.89, dd, 2.6, 5.6	78.9, d	12a	2.82, m	49.8, t
4	2.12, m	51.4, d	12b	2.31, dd, 8.5, 13.1	
5	2.43, dd, 4.5, 5.4	44.0, d	13		208.0, s
6	1.98, m	43.0, d	14	2.15, s	30.8, q
7α	2.04, m	30.9, t	15	1.75, m	24.6, d
7β	2.04, m		16	0.98, d, 6.5	20.4, q
8α	1.60, m	32.6, t	17	0.98, d, 6.5	21.1, q
8β	1.82, m		18		178.9, s
9	2.01, m	60.6, d	19	2.47, s	34.0, q

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