Chinese Chemical Letters Vol. 12, No. 4, pp. 337 – 338, 2001

A New Quinolizidine Alkaloid from *Boehmeria siamensis*

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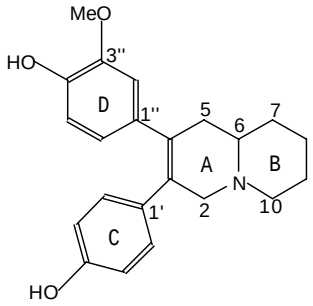
Abstract: A new quinolizidine alkaloid, 3-(4-hydroxyphenyl)-4-(3-methoxy-4-hydroxyphenyl)-3, 4-dehydroquinolizidine (**1**), was isolated from the ethanol extract of the whole plants of *Boehmeria siamensis* Craib. Its structure was elucidated on the analysis of 1D NMR and 2D NMR spectrum.

Keywords: *Boehmeria siamensis* Craib, Urticaceae, 3-(4-hydroxyphenyl)-4-(3-methoxy-4-hydroxyphenyl)-3, 4-dehydroquinolizidine.

Boehmeria siamensis Craib is distributed in China, Vietnam, Laos and Thailand[1]. The whole plants of *B. siamensis* were used in folk medicine[2,3]. Previous studies on the plants of this genus led to the isolation of different compounds such as alkaloids, flavones, lignans, triterpenoids and its glycosides[4-9]. Some antimicrobial alkaloids were obtained from *B. cylindrical*[4]. In the investigation of the whole plant of *B. siamensis*, a new alkaloid, 3-(4-hydroxyphenyl)-4-(3-methoxy -4-hydroxyphenyl)-3, 4-dehydroquinolizidine **1**, was isolated and its structure was elucidated based on spectral data.



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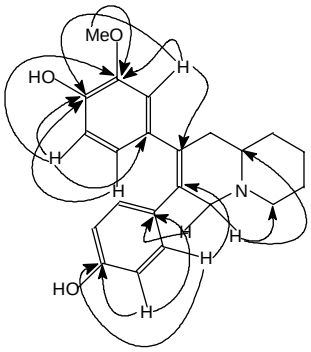

The important HMBC correlation of **1**

Compound **1**, colorless crystal, m. p. 123~125°C, gave positive reaction with Dragendorff's reagent. Its APIESMS gave quasi-molecular ion peak at *m/z* 352 ($[M+H]^+$). Its ion peak at *m/z* 351.1828 in HREIMS revealed the molecular formula $C_{22}H_{25}NO_3$ (calcd: 351.1834). The ^1H NMR signals (**Table 1**) of compound **1** at δ 7.25 and 7.07 (each 2 H, d, J = 8.0 Hz) suggested the presence of one *p*-substituted phenyl ring (ring C). A 1, 3, 4-substituted phenyl ring (ring D) was recognized from the signals at δ 7.12 (1 H, d, J = 8.4 Hz), 6.94 (1 H, dd, J = 8.4, 1.6 Hz) and 6.92 (1 H, d, J = 1.6 Hz). The hydroxy groups provided by the IR absorption at 3423 cm^{-1} could be

located to the aromatic rings considering the ^{13}C NMR signals at δ 157.4 and 146.5 for oxygenated C-atom (**Table 1**). The ^{1}H NMR signal at δ 3.59 (3 H, s) and the ^{13}C NMR signal at δ 55.6 (q) suggested the presence of a methoxy group, which could be located at C-3" in view of the HMBC cross signals -OMe/C-3", H-2''/C-3'' and H-5"/C-3" (**Table 1**). Besides the signals for the two phenyl rings and a methoxy group, in the ^{13}C NMR spectrum (DEPT, **Table 1**) six signals for methenes, two signals for double bond and one signal for methine at δ 61.2, 55.7, 40.1, 33.5, 26.2, 24.7, 131.8, 131.3 and 58.1 were observed. The ion peaks in EIMS at *m/z* 268 and 84 resulted from Retro Diels-Alder reaction of A/B rings suggested the presence of quinolizidine skeleton. The Bohlman adsorption at 2853 cm^{-1} in the IR spectrum of **1** suggested that A and B ring must be *trans* fused. According to ^{1}H, ^{1}H-COSY, HMQC and HMBC (**Table 1**) the connectivity of the phenyl rings and the quinolizidine backbone were confirmed. Thus, the structure of **1** was elucidated as 3-(4-hydroxyphenyl)-4-(3- methoxy-4-hydroxyphenyl)-3, 4-dehydroquinolizidine.

Table 1 NMR data of compound **1** in C_5D_5N (^{1}H: 400 MHz; ^{13}C: 100 MHz)

NO.	δ_C	δ_H (J in Hz)	^{1}H-^{1}H COSY	HMBC (observed)
2	61.2	3.76, 3.11 (d, 11.6)	2-Ha, 2-Hb	
3	131.8			2'-H, 6'-H
4	131.3			2''-H
5	40.1	2.65, 2.52 m	5-Ha, 5-Hb, 6-H	
6	58.1	2.21 m	5-Ha, 5-Hb, 7-H	2-H
7	26.2	1.31 m	6-H, 8-H	
8	24.7	1.31 m	7-H, 9-H	
9	33.5	1.69 m	8-H, 10-Ha, 10-Hb	
10	55.7	3.03, 2.00 (d, 11.6)	9-H	2-H
1'	132.8			2-H, 3'-H, 5'-H
2', 6'	130.8	7.25 d (8)	3'-H, 5'-H	
3', 5'	115.8	7.07 d (8)	2'-H, 6'-H	
4'	157.4			2', 6'-H, 3', 5'-H
1''	133.7			5''-H
2''	114.2	6.92 d (1.6)		
3''	147.9			2''-H, 5''-H, -OMe
4''	146.5			5''-H, 6''-H, -OMe
5''	122.0	7.12 d (8.4)	6''-H	
6''	115.8	6.94 dd (8.4, 1.6)	5''-H	
-OMe	55.6	3.59 s		

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Received 4 September, 2000