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A New Binary Carbazole Alkaloid from *Murraya koenigii*

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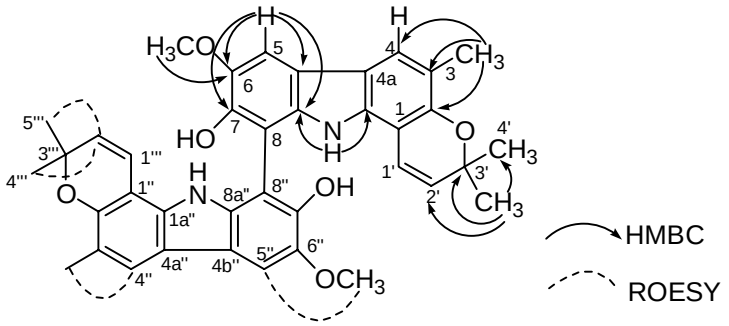
Abstract: A new binary carbazole alkaloid, 8, 8″-biskoenigine (**1**), along with its monomer, koenigine, was isolated from the dried leaves of *Murraya koenigii* collected in Xishuangbanna, Yunnan province. The structure of **1** was established by spectroscopic methods.

Keywords: *Murraya koenigii*, rusticate, 8, 8″-biskoenigine, carbazole alkaloid.

The plants from genus *Murraya*, being rich in bioactive carbazole alkaloids[1, 2], have been attracting much attention. The extract of *Murraya koenigii* displayed significant *in vitro* activity against cultured KB cells[1]. We report here the isolation and elucidation of a new binary carbazole alkaloid, 8, 8″-biskoenigine (**1**) and its monomer, koenigine[3, 4].

Figure 1 The structure, selected HMBC (H→C) and ROESY (H→H) of **1**



Compound **1**, $[\alpha]_D^{17}$ +139.6 (c 0.01, $CHCl_3$), was isolated as a brown gum. HREIMS gave the $[M]^+$ peak at *m/z* 616.2585 corresponding to the molecular formula $C_{38}H_{36}N_2O_6$ (calcd. 616.2573). The ^1H and ^{13}C NMR spectra of **1** disclosed that **1** was a carbazole alkaloid[2, 4]. The number of the proton and ^{13}C NMR signals was half of that expected, suggesting that **1** has a completely symmetrical structure[5]. The data of EIMS spectra in **1** [*m/z* (%): 616 (M^+, 100), 601(56), 308(10), 293(36)] suggested that koenigine[3] [(*m/z* (%): 309(M^+, 93), 294(100)) was the monomer of **1**. The UV (343, 301, 225 nm), ^1H and ^{13}C NMR spectra of **1** were similar to those of koenigine (**Table 1**), supporting that **1**

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was a dimer of koenigine[3, 4, 5]. The HMBC experiment revealed the presence of the correlations between H-5 (δ 7.61s, C-5 δ 102.3d) and C-6 (δ 143.5s), C-7 (δ 144.4s) and C-8 (δ 105.0s). The correlations between δ_H 4.05s (OMe) and δ_C 143.5s (C-6) proved that OMe group was linked to C-6 (**Figure 1**). This was also supported by the NOE correlation between δ_H 4.05s (OMe) and δ_H 7.61s (H-5) (**Figure 1**). The ^{1}H NMR signal at δ 7.43s for the H-8 of koenigine disappeared in **1**, and the ^{13}C NMR signal at δ 97.9d for the C-8 of koenigine was replaced by δ 105.0s in **1**, revealing that the C-8 and C-8" were connected. The linkage was further supported by 2.0 and 0.2 ppm of upfield shifts observed for C-7 and C-8a, respectively (**Table 1**). Thus, the structure of **1** named 8, 8″-biskoenigine, was elucidated to be as shown in **Figure 1**.

Table 1 The NMR data of compound **1** and koenigine[a] in CD_3COCD_3

1			koenigine		
Position	δ_H[b]	δ_C	Position	δ_H[b]	δ_C
1 (1″)	/	105.7s	1	/	105.4s
1a (1a″)		136.1s	1a		136.1s
2 (2″)	/	149.0s	2	/	149.1s
3 (3″)	/	117.5s	3	/	117.5s
Me-3 (Me-3″)	2.31(s, 3H)	16.3q	Me-3	2.28(s, 3H)	16.2q
4 (4″)	7.66 (s, 1H)	120.5d	4	7.58 (s, 1H)	120.7d
4a (4a″)		115.4s	4a		116.3s
4b (4b″)	/	118.8s	4b	/	118.3s
5 (5″)	7.61 (s, 1H)	102.3d	5	7.53 (s, 1H)	103.0d
6 (6″)		143.5s	6		143.4s
7 (7″)	/	144.4s	7	/	146.4s
8 (8″)	/	105.0s	8	7.43 (s, 1H)	97.9d
8a (8a″)	/	135.9s	8a	/	136.1s
1′ (1‴)	6.74 (d, 9.8,1H)	119.2d	1′	6.87 (d, 9.7,1H)	118.7d
2′ (2‴)	5.56 (d, 9.8,1H)	129.2d	2′	5.73 (d, 9.7,1H)	129.7d
3′ (3‴)	/	76.0s	3′	/	76.2s
4′ (4‴)	1.41 (s, 3H)	27.2q	4′	1.45 (s, 3H)	27.8q
5′ (5‴)	1.41 (s, 3H)	27.9q	5′	1.45 (s, 3H)	27.8q
OMe (OMe″)	4.05 (s, 3H)	57.1q	OMe	4.05 (s, 3H)	57.0q
NH (N″H)	9.56 (s, 1H)		NH	9.56 (s, 1H)	

[a] ^{1}H, ^{13}C NMR and HMBC spectra were obtained at 500 MHz, 125 MHz and 500 MHz. [b] J in Hz.

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