A New Benzylisoquinoline Alkaloid from Sabia parviflora

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Abstract: A new benzylisoquinoline alkaloid, 1, 2, 3, 4-tetrahydro-5-hydroxyl-8-methoxyl-2-methyl-4'-methoxyl-benzylisoquinoline, was isolated from the arial parts of *Sabia parviflora*. Its structure was established on the basis of spectral analysis.

Keywords: *Sabia parviflora*, benzylisoquinoline alkaloid, 1, 2, 3, 4-tetrahydro-5-hydroxyl-8-methoxyl-2-methyl-4'-methoxyl-benzylisoquinoline.

Sabia parviflora Wall. Ex Roxb is widely distributed in Yunnan, Guizhou province and Guangxi Zhuang Autonomous Region, China¹. Its arial parts is used as traditional medicine for the treatment of hepatitis A and B. This species have not been studied chemically before. The present paper reports the structure of a new benzylisoquinoline alkaloid 1, 2, 3, 4-tetrahydro-5-hydroxyl-8-methoxyl-2-methyl-4'-methoxyl-benzyl isoquinoline (1) from *Sabia parviflora*.



Compound 1, colorless needles, mp 87-89°C, showed positive reaction to Dragendorff's test on TLC. The MS showed the molecular formula of $C_{19}H_{23}NO_3$ (found 313.1668, req. 313.1685), which was consistent with the ¹³C and ¹H-NMR spectral data. Its NMR data showed the presence of two methoxyl groups, a four-substituted aromatic ring with two *ortho* coupled protons, a 1, 4-substituted aromatic ring, a methyl group connected with nitrogen atom, a methene and three methine groups. The UV absorption at 275 nm, together with -OH (3320cm⁻¹) and phenyl (1610, 820cm⁻¹) absorptions in the IR spectrum showed characteristics of a

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1-benzylisoquinoline derivative. The ¹H-NMR spectrum was very informative with two *ortho* coupled aromatic protons at δ 6.73 and 6.60 (J = 8.1 Hz), a pair of two *ortho* coupled aromatic protons at δ 7.19 and 6.76 (J = 8.4 Hz), methoxyl singlets at δ 3.87 (3H), 3.76 (3H) and methyl singlet at 2.47 (3H) which was attached to nitrogen atom. The HMBC experiment indicated the relations between H-4 and C-5, H-6 and C-5, 7, 10, H-7 and C-6, 8, OMe and C-8 respectively, suggesting one methoxyl group and one OH group were attached to C-8 and C-5, respectively. So compound **1** was elucidated to be 1, 2, 3, 4-tetrahydro-5-hydroxyl-8-methoxyl-2-methyl-4'-methoxyl-benzylisoquinoline, and its ¹H- and ¹³C-NMR spectra (**Table 1**) were completely assigned by detailed 2D-NMR experiments.

 Table 1
 ¹H-(500MHz) and ¹³C-(125MHz) NMR spectral data for compound 1 (CDCl₃, TMS)

Proton	δ ppm, J (Hz)	Carbon	δppm	Carbon	δ ppm	_
H-1	4.30, dd, (2.8, 7.2), 1H	C-1	60.7	C-4'	158.1	_
H-3a	3.32, m, 1H	C-3	45.8	OMe	55.4	
H-3b	2.90, m, 1H	C-4	23.3	OMe	56.3	
H-4a	2.59, m, 1H	C-5	142.7	NMe	42.7	
H-4b	2.88, m, 1H	C-6	109.4			
H-6	6.73, d, (8.1), 1H	C-7	119.5			
H-7	6.60, d, (8.1), 1H	C-8	144.6			
H-7'	3.09, m, 2H	C-9	123.3			
H-2', 6'	7.19, d, (8.4), 2H	C-10	127.0			
H-3', 5'	6.76, d, (8.4), 2H	C-7'	38.4			
OMe	3.87, s, 3H	C-1'	132.5			
OMe	3.76, s, 3H	C-2', 6'	130.6			
NMe	2.47, s, 3H	C-3', 5'	113.7			

Signal assignments are based on 2D-NMR (¹H-¹H COSY, HMQC and HMBC) spectra.

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