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A New Alkaloid from *Patrinia scabra*

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Abstract: A new alkaloid has been isolated from the root of *Patrinia scabra*. Its structure was elucidated as 2′-acetamido-3′-phenyl propyl 2-benzamido-3-phenyl propionate by extensive spectroscopic analysis.

Keywords: *Patrinia scabra*, patriscabratine.

Patrinia scabra Bunge is indigenous to the northeastern part of China. It has long been used as a traditional medicine for treating leukemia, cancer and for regulating host immune response. Some iridoids and iridoid glycosides have been found previously in this plant[1, 2]. We report here the isolation and structural elucidation of a new alkaloid, patriscabratine (**1**) from *P. scabra*.

The EtOAC-soluble fraction from the ethanolic extraction of the air-dried roots of *P. scabra* was further fractionated by silica gel and Sephadex LH-20 column chromatography to afford **1** as white needles, $[\alpha]_D^{25}$ -32.8 (c 1.0 in MeOH), mp. 182.0~184.0°C. The molecular formula of **1** was established as $C_{27}H_{28}O_4N_2$ by HR EI-MS (*m/z* 444.2041, calcd. 444.2049) and by FAB-MS (*m/z* 467, $[M+Na]^+$). EI-MS *m/z*: 444 $[M^+]$, 353, 311, 269, 252, 224, 172, 120, 105 (base), 91, 77. Its IR spectrum indicated the presence of amino group (3314 cm^{-1}), ester carbonyl (1726 cm^{-1}), amide carbonyl (1661 and 1632 cm^{-1}) and mono-substituted aromatic ring (1683 cm^{-1}). The ^{13}C NMR spectrum of **1** (See **Table 1**) gave rise to 27 carbon signals: one methyl group, three methylenes, sevent- een methines and six quaternary carbons identified *via* DEPT. Three quaternary signals at δ 170.2, 170.8 and 167.1 were assigned obviously as a ester and two amide carbonyls according to the molecular formula, which was further confirmed by IR spectrum. Three mono-substituted aromatic rings were confirmed by the other three quaternary carbons (δ 133.6, 136.5, 136.7) together with fifteen methylenes (126.7-131.9).

The ^1H NMR spectrum exhibited the proton signals at δ 4.81 (1H, m) and 4.36 (1H, m) assignable for the two methine protons respectively. The proton signals at δ 3.08 (dd, 1H, *J*=8.2 and 13.7 Hz) and 3.24 (dd, 1H, *J*=5.6 and 13.7 Hz) as well as at δ 3.84 (dd, 1H, *J*=6.0 and 11.4 Hz) and 3.94 (dd, 1H, *J*=4.2 and 11.4 Hz) corresponding to two AB methylenes respectively. It showed also another methylene at δ 2.77 (2H, m), a

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methyl group at δ 2.03 (3H, s), two amino signals at δ 6.10 (d, 1H, *J*=8.0) and δ 6.82 (d, 1H, *J*=6.8) together with fifteen aromatic protons at δ 7.73-7.08. The ^{1}H-^{13}C COSY spectral analysis of **1** assigned the correlations between each carbon and its directly attached protons. The ^{1}H-^{1}H COSY showed correlation peaks between H-2 with both H-3 and 5-NH, H-2′ with H-1′, H-3′ and 5′-NH. The HMBC spectral analysis displayed correlation peaks between H-3 with C-4, C-2 and C-1, H-3′ with C-4′, C-2′ and C-1′, H-7′ with C-6′. Consequently, the planar structure of **1** is identified as shown and named patriscabratine(See **Figure 1**). To our knowledge, **1** is the first alkaloid isolated from this plant.

Figure 1 Significant HMBC coorrelations of **1**

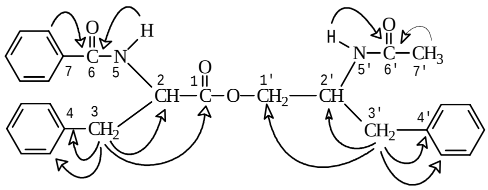

Table 1 ^{1}H, ^{13}C NMR spectral data of **1**

No	δ_C	δ_H (J_{Hz})	No	δ_C	δ_H (J_{Hz})
1	170.2		1’	64.5	3.84 (dd, 6.0, 11.4)
2	54.9	4.81 (m)			3.94 (dd, 4.2, 11.4)
3	38.4	3.08 (dd, 8.2, 13.7)	2’	49.4	4.36 (m)
		3.24 (dd, 5.6, 13.7)	3’	37.4	2.77 (m)
4	136.7		4’	136.5	
6	167.1		6’	170.8	
7	133.6		7’	20.8	2.03 (m)
5 (NH)		6.82 (d, 6.8)	5’(NH)		6.10 (d, 8.0)

References

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