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A New β-Carboline Alkaloid and a New Derivate of Isoferulic Acid from *Anemone altaica*

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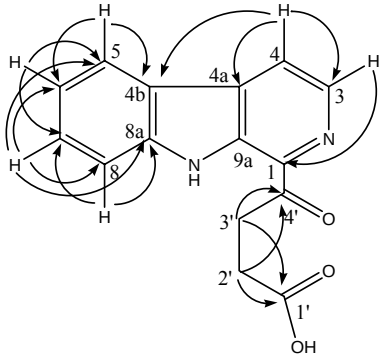
Abstract: A new β-carboline alkaloid, 4-(9H-β-carbolin-1-yl)-4-oxobutyric acid and a new derivate of isoferulic acid, (E)-3-(3-hydroxy-4-methoxyphenyl)acrylic acid carboxymethyl ester, were isolated from the roots of *Anemone altaica*. Their structures were determined on the basis of spectral data.

Keywords: *Anemone altaica*, β-carboline alkaloid, isoferulic acid derivate.

The roots of *Anemone altaica* are believed to have anti-inflammatory and analgesic properties and have been used for the treatment of epilepsia, neurasthenia and arthritis in chinese folk medicine for a long time[1]. In our chemical investigation of this plant, a new β-carboline alkaloid (**1**) and a new derivate of isoferulic acid (**2**) were isolated from its $CHCl_3$ extract. Here we report the structural elucidation of the two compounds.

Compound **1** was obtained as a yellow powder, m. p. 234-236℃. The EIMS of **1** showed the molecular ion peak at *m/z* 268, and the molecular formula was determined to be $C_{15}H_{12}N_2O_3$ from its HREIMS (calcd. 268.0848; found 268.0863). The UV spectrum

Figure 1 The key correlations in HMBC spectrum of compound **1** and **2**



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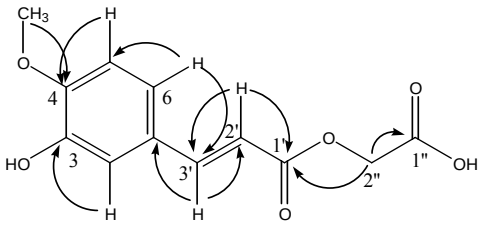

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Table 1 ^{1}H-NMR and ^{13}C-NMR data of **1** and **2** (DMSO-d_6, δ ppm)

No.	1		2	
	δ_H	δ_C	δ_H	δ_C
1	-	135.5	-	126.7
2	-	-	7.12 (s)	114.2
3	8.49 (d, *J*=4.5 Hz)	137.5	-	146.6
4	8.43 (d, *J*=4.5 Hz)	119.5	-	150.3
4a	-	133.8		
4b	-	119.8		
5	8.28 (d, *J*=8.0 Hz)	121.8	6.95 (d, *J*=8.0 Hz)	112.0
6	7.28 (t, *J*=8.0 Hz)	120.2	7.14 (d, *J*=8.0 Hz)	121.6
7	7.57 (t, *J*=8.0 Hz)	129.0		
8	7.76 (d, *J*=8.0 Hz)	113.0		
8a	-	141.7		
9a	-	131.0		
1′	-	174.0	-	165.9
2′	2.68 (d, *J*=6.5 Hz)	27.8	6.39 (d, *J*=15.5 Hz)	114.2
3′	3.56 (d,*J*=6.5 Hz)	32.6	7.56 (d, *J*=15.5 Hz)	145.8
4′	-	201.5		
1″			-	169.3
2″			4.64 (s)	60.5

of **1** exhibited maxima at 220, 283, 310 and 380 nm, resembling β-carboline containing a carbonyl function at C-1 position[2, 3]. The IR spectrum showed absorptions at 1700 and 1664 cm^{-1}, suggesting a carboxyl and a conjugated carbonyl group, respectively. The presence of the two groups was also indicated by the signals at δ 174.0 and 201.5 in ^{13}C-NMR spectrum. The signals in ^{1}H-NMR and ^{13}C-NMR spectra arising from β-carboline nucleus were almost same to those of 1-acetyl-β-carboline[4]. The ^{1}H-NMR spectrum indicated the signals of two sets of triplets at δ 2.68 (t, 2H, 6.5 Hz) and 3.56 (t, 2H, 6.5 Hz), due to protons H-2′ and H-3′ [2,5]. In the HMBC spectrum, the cross peaks H-2′/C-1′, H-2′/C-4′, H-3′/C-1′ and H-3′/C-4′ were observed, leading to the assumption of existing 4-oxobutyric acid group. This was supported by the rearrangement fragment ion peak at *m/z* 168 due to the 4-oxobutyric acid group in the EIMS. The full assignments of all the proton and carbon signals were made by means of ^{1}H-NMR, ^{13}C-NMR, HMQC, HMBC (**Figure 1**) and comparison with the data in the literatures[2,4,5]. On the basis of the above evidence, the structure of **1** was established as 4-(9H-β-carbolin- 1-yl)-4-oxobutyric acid.

Compound **2**, a yellow powder, m. p. 170-171℃, had the molecular formula of $C_{12}H_{12}O_6$, deduced from its HREIMS (calcd. 252.0633; found 252.0630). It showed IR absorptions at 3428 (hydroxyl), 2950 (broad band), 1725 cm^{-1} (conjugated ester carbonyl group) and 1680 (carboxyl). Analysis of the ^{1}H-NMR spectrum of **2** suggested the presence of a 1,3,4-trisubstituted aromatic ring [δ 7.12 (s, 1H), 6.95 (d, 1H, 8.0 Hz), 7.14 (d, 1H, 8.0 Hz)], a *trans* double bond [δ 6.39 (d, 1H, 15.5 Hz), 7.56 (d, 1H, 15.5 Hz)], an isolated methylene [δ 4.64 (s, 2H)] and a methoxyl group [δ 3.80 (s, 3H)]. An isoferuloyl moiety could be deduced, when carefully comparing the ^{1}H-NMR and ^{13}C-NMR data of chemical shift of **2** to those of cimicifugic acid B[6]. Furthermore, the location of methoxyl and hydroxyl group was confirmed by the HMBC experiment

(**Figure 1**). In the HMBC spectrum, signal of the isolated methylene correlated with the carbonyl (C-1′, δ 165.9) and the carboxyl group (C-1″, δ 169.3). Based on the above evidence, the structure of **2** was established as (E)-3-(3-hydroxy-4-methoxy-phenyl)acrylic acid carboxymethyl ester.

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