

## A New Nitro Alkaloid from *Corydalis saxicola* Bunting

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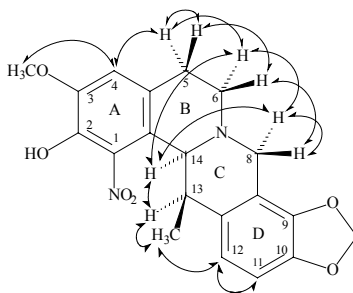
**Abstract:** A new nitro tetrahydropprotoberberins alkaloid, 1-nitro-apocavidine was isolated from *Corydalis saxicola* Bunting. The structure was established by spectroscopic methods.

**Keywords:** *Corydalis saxicola*, nitro alkaloid.

The herb of *Corydalis saxicola* Bunting has been used as a kind of Chinese traditional medicine. Our investigation on chloroform extract of this plant resulted in the isolation of a new tetrahydropprotoberberins alkaloid, to our knowledge, which is the first nitro alkaloid isolated from natural products.

Compound **1** was isolated as yellow amorphous powder; mp 229~231 °C, UV  $\lambda_{\max}$  (MeOH): 280 nm; The ESI-MS afforded the positive ion at  $m/z$  385  $[M+H]^+$ , implying a molecular formula of  $C_{20}H_{20}O_6N_2$ , which was confirmed by the HRESI-MS ( $[M+H]^+$  found 385.1394, calcd. 385.1400). The fragments with  $m/z$  223 (2.1%) and 162 (100%) in the EI-MS suggested the substitution pattern of 9, 10-methylenedioxy-13-methyl at ring C and D. The IR spectrum of **1** indicated the presence of nitril ( $1534\text{ cm}^{-1}$ ) and a phenolic hydroxy groups ( $3509\text{ cm}^{-1}$ ). The  $^1\text{H-NMR}$  spectrum shows one methoxy at  $\delta$  3.92 (s), one methyl at  $\delta$  0.89 (d) and one methylenedioxy at  $\delta$  5.91 (d) and 5.94 (d), four mutually coupling aliphatic protons at  $\delta$  2.52-3.21 (m, 4H, H-5, H-6), and other two mutually coupling aliphatic protons at  $\delta$  2.83 (qd, 1H,  $J=7.3\text{ Hz}$ , H-13),  $\delta$  4.29 (d, 1H,

**Figure 1** NOESY interactions observed for **1**



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**Table 1**  $^1\text{H}$  NMR (500MHz) and  $^{13}\text{C}$  NMR (125MHz) spectral data of **1** ( $\text{CDCl}_3$ )

	$\delta_{\text{C}}$	HMQC ( $\delta_{\text{H}}$ , $J$ Hz)	HMBC
1	136.59	--	
2	146.39	--	
3	140.16	--	
4	114.00	H-4 (6.74, s)	C-2, C-3, C-5, C-4a, C-14a
4a	129.67	--	
5	30.67	H-5 $\alpha$ (3.12, m) H-5 $\beta$ (2.62, m)	C-6, C-4a C-4, C-4a, C-14, C-14a
6	49.74	H-6 $\alpha$ (2.67, m) H-6 $\beta$ (3.09, m)	C-4, C-4a C-4a, C-5, C-8, C-14
8	53.22	H-8 $\alpha$ (3.63, d, $J = 15\text{Hz}$ ) H-8 $\beta$ (4.03, d, $J = 15\text{Hz}$ )	C-8a, C-9, C-12a, C-14 C-8a, C-9, C-12a, C-14, C-6
8a	116.40	--	
9	142.88	--	
10	144.76	--	
11	106.85	H-11 (6.67, d, $J = 8\text{ Hz}$ )	C-9, C-10, C-12a
12	121.52	H-12 (6.57, d, $J = 8\text{ Hz}$ )	C-8a, C-10, C-13
12a	135.29	--	
13	37.28	H-13 (2.83, qd, $J = 7, 3\text{ Hz}$ )	C-8a, C-12, C-12a, C-13-Me
13-Me	18.74	H-Me-13 (0.89, d, $J = 7\text{ Hz}$ )	C12a, C-13, C-14
14	60.41	H-14 (4.29, d, $J = 3\text{ Hz}$ )	C-4a, C-6, C-14a, C-13-Me
14a	122.27	--	
-OCH <sub>3</sub>	56.50	3.92, s	C-2
-O-CH <sub>2</sub> -O-	101.03	5.94, d, $J = 2\text{ Hz}$ 5.91, d, $J = 2\text{ Hz}$	C-9, C-10 C-9, C-10

$J = 3\text{ Hz}$ , H-14). In addition, the chemical shifts of aliphatic protons of ring B and C, including the signals at  $\delta$  3.63 and 4.03 (d, each 1H,  $J = 15\text{ Hz}$ , H-8 $\alpha$  and H-8 $\beta$ ) were similar to those of apocavidine<sup>1</sup>. The aromatic region of the spectrum showed three protons: one at  $\delta$  6.74 (s, 1H), and the other two *ortho*-coupled protons at  $\delta$  6.57 and 6.67 (d, each 1H,  $J = 8\text{ Hz}$ ), due to H-12 and H-11. The  $^{13}\text{C}$ -NMR spectrum gave twenty carbon signals. The signal of  $\delta_{\text{C}}$  136.59 indicated that compound **1** has the nitril substituted pattern at ring A compared with those of apocavidine<sup>1</sup>. A NOESY spectrum was run to establish the nitro-substituted location. From the spectrum, the proton signal at  $\delta$  6.74 (s, 1H) was related to H-5 and H-OMe, which suggested a proton at C-4. So the 1-nitro substituted pattern was determined (**Figure 1**).  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR are listed in **Table 1**.

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### References

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