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Two New Acetylenic Compounds from *Asparagus gobicus*

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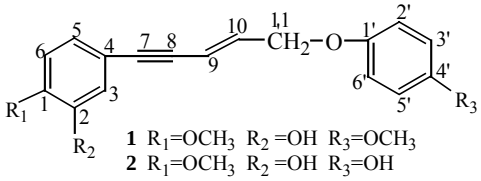
Abstract: Two new acetylenic compounds were isolated from the roots of *Asparagus gobicus*. Their structures were elucidated by spectroscopic methods including 2D NMR techniques.

Keywords: *Asparagus gobicus*, Asparagaceae, acetylenic compounds.

Asparagus gobicus N. Ivan ex. Grubov has been used as a Chinese folk medicine for the treatment of rheumatism, neuritis and sore[1]. Three acetylenic compounds (**1**, **2** and **3**) have been isolated from this plant, and here the structural elucidation of two new ones (**1** and **2**) was reported.



The molecular formula $C_{19}H_{18}O_4$ of **1** was deduced from HREIMS ($[M]^+$ at *m/z* 310.1205, calcd. 310.1200). Its IR (KBr) spectrum showed the presence of hydroxy group (3360 cm^{-1}), acetylene bond (2202 cm^{-1}) and aromatic ring (1610, 1511, 1450 cm^{-1}). The ^1H NMR data of **1** (Table **1**) gave signals of a *p*-substituted benzene ring at δ 6.85 (4H, overlapped, AA'BB' system) and a 1, 2, 4-trisubstituted benzene ring at δ 6.80 (d, 1H, 8.1 Hz), 6.99 (dd, 1H, 1.8, 8.1 Hz) and 6.95 (d, 1H, 1.8 Hz), except the signals of two methoxy groups at δ 3.90 and 3.77 (s, each 3H) and an AMX_2 system at δ 4.58 (dd, 2H, 1.8, 5.1 Hz), 6.03 (dt, 1H, 1.8, 15.9 Hz) and 6.34 (dt, 1H, 5.1, 15.9 Hz), confirmed by its ^{13}C NMR and DEPT spectra. Two partial structures of -CH=CH-CH_2-O- and -CH=CH-C≡C- were deduced from the HMBC correlations: H-9/C-7, 8, 10; H-10/C-9, 8, 11. Taken into account the other HMBC correlations: -OCH_3 (δ 3.90, s)/C-1, -OCH_3 (δ 3.77, s)/C-4', H-3/C-2, 4, H-5/C-1, 4, 7; H-9/C-7, 8, 11; H-10/C-8, 11; H-11/C-9, 10, 1', the skeleton of **1** was established. The large coupling constant (15.9 Hz) between H-9

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and H-10 disclosed the *trans* configuration of the double bond. Comparison of its NMR data with those of **3**[2] indicated **1** had two methoxy groups, but **3** had one at C-4'. The locations of two methoxy groups in **1** were assigned by its HMBC correlations, further supported by NOE results that the methoxy methyls at δ 3.90 and 3.77 showed effect with their neighboring aromatic proton signals at δ 6.99 (H-6) (11.5%) and 6.85 (H-3', 5') (10.1%), respectively. Thus, the structure of **1** was elucidated as 1-methoxy-2-hydroxy-4-[5-(4-methoxy-phenoxy)- 3-penten-1-ynyl] phenol.

From the EIMS (showed $[M]^+$ at *m/z* 296) and ^{13}C NMR (DEPT) spectral data, the molecular formula $C_{18}H_{16}O_4$ of **2** was assigned. The NMR spectral data (**Table 1**) of **2** were very similar to those of **1** except that **2** had only one methoxy group at δ 3.89 (s, 3H), which suggested they had a similar skeleton. The HMBC spectrum exhibited correlations of OCH_3 (δ 3.89) with C-1 (δ 147.7); H-3 (δ 7.00) with C-2 (δ 147.5), C-4 (δ 114.3); H-6 (δ 6.76) with C-1 (δ 147.1), C-5 (δ 125.3) and hydroxy protons at δ 8.01 and 8.12 with C-2 (δ147.5) and C-4' (δ 152.0), respectively. The structure of **2** was thus concluded as 1-methoxy-2- hydroxy-4-[5-(4-hydroxyphenoxy)-3-penten-1-ynyl] phenol.

Table 1 ^1H NMR, ^{13}C NMR and DEPT data of **1** and **2** (δ ppm, TMS, $CDCl_3$)

No.	δ_H		δ_C (DEPT)		
	1	**2**	**1**	**2**	**3**
1			147.2 s	147.7s	156.0s
2			145.5 s	147.5s	114.9d
3	6.95 (d, 1.8)	7.00 (d, 1.8)	117.7 d	114.7d	133.4d
4			116.0 s	114.3s	115.7s
5	6.80 (d, 8.1)	6.94 (dd, 8.4, 1.8)	124.5 d	125.3d	133.4d
6	6.99 (dd, 8.1, 1.8)	6.76 (d, 8.4)	110.7 d	115.4d	114.9d
7			90.7 s	91.0s	90.7s
8			85.9 s	85.3s	86.0s
9	6.03 (dt, 1.8, 15.9)	6.07 (dt, 1.8, 6.0)	112.7 d	112.0d	112.7d
10	6.34 (dt, 5.1, 15.9)	6.34 (dt, 4.8, 6.0)	137.5 d	138.1d	137.4d
11	4.58 (dd, 1.8, 5.1)	4.59 (dd, 1.8, 4.8)	68.7 t	68.3t	68.7t
1'			152.3 s	151.8s	152.7s
2', 6'	6.85 (overlapped)	6.82 (overlapped)	116.2 d	116.0d	116.0d
3', 5'	6.85 (overlapped)	6.82 (overlapped)	114.9 d	115.9d	114.9d
4'			154.3 s	152.0s	154.3s
OMe	3.90 (s)	3.89 (s)	56.1 q	55.6q	56.0q
OMe	3.77 (s)		56.0 q		

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