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A New Nor-neolignan from *Cremanthodium ellisii*

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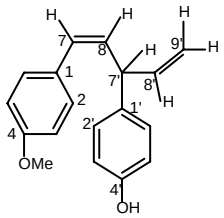
Abstract: A new nor-neolignan, named ellisinin A (**1**), has been isolated from the traditional Tibetan medicinal plants of *Cremanthodium ellisii*. Its structure has been determined on the basis of spectroscopic evidence, especially by 2DNMR (^{1}H-^{1}HCOSY, HMQC, HMBC).

Keywords: *Cremanthodium ellisii;* compositae; nor-neolignan; ellisinin A.

The genus *Cremanthodium* (Compositae) consists of about 55 species distributed in many countries. Among them, about 47 species grow in China, especially in the northwest and southwest regions[1]. *Cremanthodium ellisii* Kitam. has been used as traditional Tibetan medicine for anti-inflammation, detoxication and relief of pain since ancient times[2]. Now, we report a new nor-neolignan **1** isolated from the whole medicinal plant of *Cremanthodium ellisii* Kitam. collected in Huzhu county, Qinghai province of China.



1

Compound **1** was obtained as a yellowish gum, $[\alpha]_D^{20}$-34.5 (c 0.45, $CHCl_3$). Its EI mass spectrum gave the molecular ion peak at m/z 266 $[M]^+$, suggesting the molecular formula to be $C_{18}H_{18}O_2$, which was confirmed by ^{1}H, ^{13}CNMR and DEPT data (see **Table 1**). ^{1}HNMR spectrum of compound **1** showed the presence of two p-substituted aromatic rings at δ 6.76 (2H, d, J=8.4Hz, H-3', H-5'), 6.89 (2H, d, J=8.5Hz, H-3, H-5), 7.04 (2H, d, J=8.5Hz, H-2', H-6'), 7.23 (2H, d, J=8.5Hz, H-2, H-6), two pairs of double bonds at δ 6.50 (1H, d, J=11.4Hz, H-7), 5.70 (1H, t, J=11, 4Hz, H-8), 6.00 (1H, ddd, J=17.6, 11.4, 6, 0Hz, H-8'), 5.15-5.19 (2H, m, H-9'), a methine proton signal at δ 4.48 (1H, m, H-7') and a methoxy group at δ 3.77 (3H, s, MeO). The above results were confirmed by ^{13}CNMR and DEPT spectral data: two p-substituted aromatic rings (δ 129.8, C-1, 129.8, C-2, C-6, 113.6, C-3, C-5, 158.5, C-4; 135.6, C-1', 128.8, C-2', C-6', 115.3, C-3', C-5', 154.0, C-4'), two pairs of double bonds (δ 128.6, C-7, 131.6, C-8; 140.7, C-

8', 115.0, C-9'), a methoxy at δ 55.2 and a methine signal at δ 46.8, DEPT spectrum indicated that C-9' was a methylene carbon, suggesting C-8' and C-9' was a terminal double bond. The ^{1}HNMR signal of H-7 was a doublet, indicated that C-7 was connected with aromatic carbon. From above results, the skeleton of **1** was as given, confirmed by 2D^{1}H-^{1}HCOSY.

The ^{13}CNMR signal of C-1 was overlapped by other carbon signals when used $CDCl_3$ as solvent (δ 129.8, C-1, C-2, C-6). However, it was separated just as expected when used CD_3COCD_3 as solvent (δ 130.3, C-1, 130.6, C-2, C-6). For determining the positions of methoxy and hydroxy, HMQC and HMBC spectra have been done. The HMBC correlations of δ_H3.77 (OMe) with δ_C159.6 (C-4), δ_H7.23 (H-2, H-6) with δ_C159.6 (C-4) and 130.3 (C-1), δ_H6.50 (H-7) with δ_C130.3 (C-1); δ_H4.41 (H-7') with δ_C134.7 (C-1'), 142.2 (C-8') and 132.5 (C-8), δ_H7.04 (H-2', H-6') with δ_C156.8 (C-4'), suggested that methoxy and hydroxy were connected with C-4 and C-4', respectivelly. H-7 and H-8 must to be cis-relationship according to their coupling constant ($J_{7/8}$=11.4Hz). Thus, the structure of **1** has been determined, named ellisinin A. It was a nor-neolignan compound.

Table1. ^{1}H, ^{13}CNMR and DEPT spectral data of 1
(δ, ppm, TMS, 400MHz for ^{1}HNMR, 100MHz for ^{13}CNMR)

	CD_3COCD_3			$CDCl_3$		
No.	δ_C	DEPT	δ_H	δ_C	DEPT	δ_H
1	130.3	C		129.8	C	
2,6	130.6	CH	7.23 (d, 8.5)	129.8	CH	7.22 (d, 8.5)
3,5	114.4	CH	6.89 (d, 8.5)	113.6	CH	6.86 (d, 8.5)
4	159.6	C		158.5	C	
7	128.9	CH	6.50 (d, 11.4)	128.6	CH	6.53 (d, 11.4)
8	132.5	CH	5.70 (t, 11.4)	131.6	CH	5.67 (t, 11.4)
1'	134.7	C		135.6	C	
2',6'	129.3	CH	7.04 (d, 8.5)	128.8	CH	7.10 (d, 8.5)
3',5'	116.1	CH	6.76 (d, 8.5)	115.3	CH	6.77 (d, 8.5)
4'	156.8	C		154.0	C	
7'	47.8	CH	4.41m (m)	46.8	CH	4.51 (m)
8'	142.2	CH	6.00 (ddd, 17.6, 11.4, 6.0)	140.7	CH	6.01 (ddd, 17.6, 11.4, 6.0)
9'	114.6	CH_2	5.15-5.19 (m)	115.0	CH	5.65-5.70 (m)
MeO	55.4	CH_3	3.77 (s)	55.2	CH_3	3.81 (s)

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