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Two New Benzofuran Derivatives from *Ligularia stenocephala*

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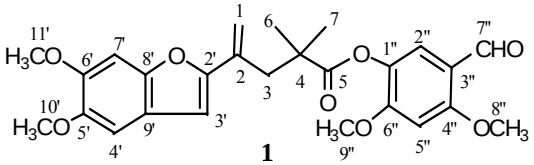
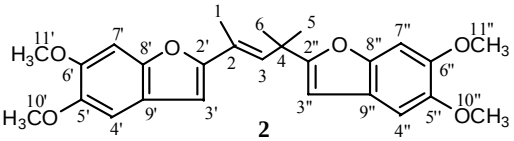
Abstract: Two new benzofuran derivatives were isolated from the roots of *Ligularia stenocephala*. Their structures were established by spectroscopic methods and 2D NMR experiments.

Keywords: *Ligularia stenocephala*, Compositae, benzofuran derivative.

Previously, we reported the structures of three new isopropenyl benzofuran-type polymers from Ligularia stenocephala1. Here, we report the structures of two new benzofuran derivatives isolated from this plant and named as stenocephalain D (1) and E (2).



1



2

Compound **1**, colorless crystals, mp 66-68℃. Its HREIMS showed $[M+H]^+$ at *m/z* 469.1837 (calcd. 469.1857), corresponding to the molecular formula $C_{26}H_{28}O_8$. The IR bands (1752, 1710, 1681, 1605, 1511, 1488 cm^{-1}) and UV absorptions (241.6, 281.0, 320.0 nm), exhibited the presence of benzofuran ring and carbonyl group. The ^1H and ^{13}CNMR data of compound **1** showed four methoxyl groups (δ_H 3.67, 3.90, 3.91, 3.93), one aldehyde group (δ_H 10.03), two geminal methyl groups (δ_H 1.47) and a terminal double bond (δ_H 5.21, 5.92). Four single peaks of proton (δ_H 7.01, 6.94, 7.32, 6.38) exhibited that they were in 1,4-relationship of benzene rings respectively. In the HMBC spectrum of compound **1**, the long-range correlations of H-1, H-3 and H-3' with C-2'; H-3, H-6 and H-7 with C-4 were shown respectively. Thus, the structure of compound **1** was confirm- ed and named as stenocephalain D.

Compound **2,** yellow crystals, mp 70-72℃. The molecular formula was deduced as $C_{26}H_{28}O_6$ from its HREIMS $[M+NH_4]^+$ at *m/z* 454.2232 (calcd. 454.2224). The IR

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spectrum (1621, 1486 and 1456 cm^{-1}) and UV (328.2 nm) verified the presence of benzofuran ring. The ^{1}H and $^{13}CNMR$ data of compound **2** showed three methyl groups (δ_H 1.70, 1.61 and 1.61), four methoxyl groups (δ_H 3.87, 3.90, 3.91, 3.92) and a double bond proton (δ_H 6.50). In the HMBC spectrum of **2**, the long-range correlations of H-1, H-3 and H-3' with C-2'; H-3, H-5, H-6 and H-3" with C-2" were obviously shown respectively. Therefore, the structure of compound **2** was determined and named as stenocephalain E.

Table 1 $^{1}HNMR$ (300 MHz) , $^{13}CNMR$ (75 MHz) , DEPT and HMBC data of **1** and **2**

	1				**2**		
No.	δ_H	δ_C	HMBC	No.	δ_H	δ_C	HMBC
1	5.20 s 5.92 s	115.4 t	C-2,3,2'	1	1.70 s	13.2 q	C-2,3,2'
2		133.6 s		2		126.1 s	
3	2.90 s	42.7 t	C-1,2,4,5,6,7,2'	3	6.50 s	133.2 d	C-1,2,4,5 6,2',2"
4		43.6 s		4		37.4 s	
5		175.8 s		5	1.61 s	29.2 s	C-3,4,6,2"
6	1.47 s	25.6 q	C-3,4,5,7	6	1.61 s	29.2 s	C-3,4,5,2"
7	1.47 s	25.6 q	C-3,4,5,6	2'		157.4 s	
2'		155.8 s		3'	6.46 s	102.2 d	C-2',4',8',9'
3'	6.66 s	103.8 d	C-2,2',4',8',9'	4'	6.95 s	101.1 d	C-3',5',6' 7',8',9'
4'	6.94 s	102.4 d	C-3',5',6',8',9'	5'		146.3[a] s	
5'		146.7 s		6'		146.3[a] s	
6'		148.5 s		7'	7.04 s	95.1 d	C-5',6',8',9'
7'	7.01 s	95.1 d	C-5',6',8',9'	8'		149.3 s	
8'		149.6 s		9'		121.0 s	
9'		120.7 s		10'	3.87 s	56.2[b] q	C-5'
10'	3.90[a] s	56.0[a] s	C-5'	11'	3.90[a] s	56.3[b] q	C-6'
11'	3.93[a] s	56.4[a] s	C-6'	2"		164.2 s	
1"		154.7 s		3"	6.42 s	100.7 d	C-2",4",8",9"
2"	7.32 s	109.0 d	C-1",3"	4"	6.98 s	101.9 d	C-3",5",6",7"8",9"
3"		120.6 s		5"		147.2[a] s	
4"		147.2 s		6"		147.9[a] s	
5"	6.38 s	105.8 d	C-4",6"	7"	7.04 s	95.5 d	C-5",6",8",9"
6"		148.5 s		8"		149.3 s	
7"	10.03 s	186.6 d	C-2",3"	9"		120.4 s	
8"	3.91[a] s	56.2[a] s	C-4"	10"	3.91[a] s	56.3[b] q	C-5"
9"	3.67 s	56.3[a] s	C-1",6"	11"	3.92[a] s	56.5[b] q	C-6"

[a,b]. Assignments in the vertical column with the same sign may be alternated although those given here are preferred

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References

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