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A New Isopropenyl Benzofuran-type Tetramer from *Ligularia stenocephala*

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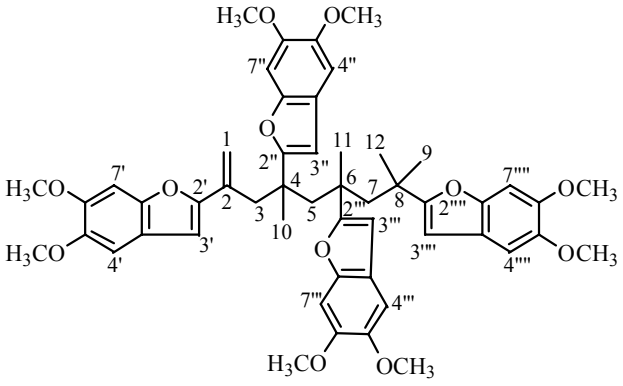
Abstract: A new isopropenyl benzofuran-type tetramer was isolated from the roots of *ligularia stenocephala* and its structure was established by spectroscopic methods.

Keywords: *Compositae, Ligularia stenocephala,* isopropenyl benzofuran-type tetramer.

Ligularia stenocephala has been used in traditional Chinese medicine [1]. From the roots of this plant, a new isopropenyl benzofuran-type tetramer was isolated and named as stenocephalain **1**. This paper describes the structure elucidation of **1.**



1

Compound **1** , white powder, mp 174-175℃, $[\alpha]_D^{23}$ -7 (*c* 1.0, $CHCl_3$). Its HREIMS showed $[M+Na]^+$ at *m/z* 895.3631 (calcd. 895.3664), corresponding to the molecular formula $C_{52}H_{56}O_{12}$. The IR (KBr) bands (1622, 1548, 1487 cm^{-1}) and UV absorptions (249 nm, 303 nm), displayed the typical of benzofuran ring. In the ^1H and ^{13}CNMR data of compound **1** showed 8 methoxy groups (δ_H 3.80∼3.90) at aromatic rings, two kinds of Ar-H (δ_H 6.64-6.70 and δ_H 6.78-6.96) in 1,4-relationship, 4 methyl groups (δ_H 0.75, 0.82, 1.04, 1.27) and a terminal double bond (δ_H 4.52, 5.57). EIMS

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gave a strong peak at *m/z* 219 (100) implied presence of a fragment of isopropyl dimethoxybenzofuran. In the HMBC spectrum of **1**, the correlations of C-2' with H-1，H-3 and H-3'; C-2'' with H-3, H-5, H-10 and H-3''; C-2''' with H-5, H-7, H-11 and H-3'''; C-2'''' with H-7, H-9, H-12 and H-3'''' were showed. All of these correlations showed a partial structure of 4, 6, 8-trimethyl-1-nonene, in which the C-2, C-4, C-6 and C-8 attached with C-2', C-2'', C-2''', C-2'''' respectively. Therefore, the planar structure of compound **1** was confirmed.

Table 1 ^{1}HNMR (400MHz) ,^{13}CNMR (100MHz) and DEPT data of **1***

No.	δ_C	HMQC (δ_H)	HMBC	No.	δ_C	HMQC	HMBC
1	115.3 t	H-1a (4.52) H-1b (5.57)	H-3	8'	149.1 s	--	H-3',4',7'
2	133.3 s	--	H-3',1,3	9'	120.6 s	--	H-3',4',7'
3	46.9 t	H-3a(2.49 J=13.6Hz) H-3b(2.90 J=13.6Hz)	H-1,5,10	2''	161.7 s	--	H-3,5,10,3''
4	40.1 s	--	H-3,5,10	3''	103.0 d	H-3'' (5.93)	H-4''
5	52.0 t	H-5a (2.29 J=14.0Hz) H-5b (2.42 J=13.6Hz)	H-3,7,10, 11	8''	148.4 s	--	H-3'',4'',7''
6	39.6 s	--	H-5,7,11	9''	120.6 s	--	H-3'',4'',7''
7	53.7 t	H-7a (2.03 J=14.4Hz) H-7b (2.42 J=13.6Hz)	H-5,9,11, 12	2'''	162.1 s	--	H-5,7,113''
8	36.0 s	--	H-7,9,12	3'''	102.7 d	H-3''' (5.86)	H-4'''
9	29.7 q	H-9 (1.27)	H-7,12	8'''	148.3 s	--	H-3''',4''',7'''
10	20.2 q	H-10 (0.75)	H-3,5	9'''	120.6 s	--	H-3''',4''',7'''
11	20.5 q	H-11 (0.82)	H-5,7	2''''	163.9 s	--	H-7,9,123'''
12	27.9 q	H-12 (1.04)	H-7,9	3''''	100.3 d	H-3'''' (5.82)	H-4''''
2'	156.4 s	--	H-1,3,3'	8''''	148.6 s	--	H-3'''',4'''',7''''
3'	102.5 d	H-3' (6.20)	H-4'	9''''	120.6 s	--	H-3'''',4'''',7''''

δ_H 6.64 -6.70 (H-4'~H-4''''), δ_C 101.7-102.1 (C-4'~C-4'''') ; δ_H 6.78-6.96 (H-7'~H-7'''') , δ_C 94.8- 95.2 (C-7'~C-7''''); δ_C 56.0-56.3 (OCH_3); δ_C 145.9-147.9 (C-5'~C-5'''' and C-6'~C-6'''') , the correlations of which with H-4' ~H-4'''',H-7'~H-7'''' , respectively.

* Assignments were confirmed by DEPT, HMQC and HMBC.

Acknowledgments

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Reference

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