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Biphenyl Ferulate from *Glehnia littoralis*

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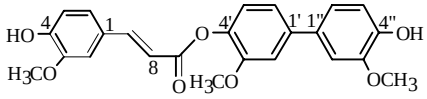
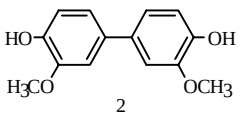
Abstract: From the underground parts of *Glehnia littoralis* Fr. Schmidt ex Miquel (Umbelliferae), a new compound named glehnilate was obtained. Its structure was determined by analysis of its spectral data.

Keywords: *Glehnia littoralis*, biphenyl ferulate, glehnilate.

Glehnia littoralis FR. SCHMIDT ex MIQUEL (Umbelliferae) is a perennial herb growing on the sandy beaches of China. The dried roots and rhizomes of this plant are used in traditional Chinese medicine as tonic, antiphlogistic, and mucolytic for the treatment of respiratory and gastrointestinal disorders. We report here the isolation and structure elucidation of a new biphenyl ferulate, glehnilate (**1**) from EtOAc-soluble fraction of *Glehnia littoralis* extract.



1



2

A concentrated ethanolic extract of the underground part of *G. littoralis* was suspended in water and defatted with petroleum ether, then extracted with EtOAc and *n*-BuOH successfully. The EtOAc-soluble fraction was separated by repeated silica gel column chromatography to afford **1**.

Glehnilate (**1)** was obtained as pale yellow amorphous solid, $[\alpha]_D$ –2.6 (c 0.37,

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MeOH). The EI-MS spectrum showed $[M+H]^+$ at *m/z* 423, consistent with the molecular formula $C_{24}H_{22}O_7$. The ^{1}H-NMR spectrum of **1** displayed the signals of three 1,3,4-trisubstituted benzene rings, a *trans*-olefine, and three methoxyl groups. Its ^{13}C-NMR spectrum showed the signals of twenty-four carbons, including a carboxyl carbon and an olefine. Detailed analysis of the HMQC and HMBC spectra of **1** suggested the presence of a biphenyl moiety which was formed by two symmetrically fused guaiacol units, and a *trans*-feruloyl group. Alkaline hydrolysis of **1** furnished **2** and ferulic acid. The TLC behavior and ^{1}H-NMR data of **2** were almost identical with those reported data[1]. The location of the *trans*-feruloyl group was determined to be at C-4′ of the biphenyl moiety, based on the shielding effect of *O*-acetylation on C-4′ and deshielding effect on C-1′ [2]. From these data, glehnilate was determined to have the structure formula **1**.

Table 1 ^{1}H- and ^{13}C-NMR Data for Compound **1** (in CD_3OD)

Position	Correlation in HMQC		^{13}C-^{1}H long range correlation in HMBC
	δ_H [α)]	δ_C	
1		130.6	H-5, H-8
2	7.30 d (2.0)	112.7	H-6, H-7
3		150.5	H-5, 3-OCH_3
4		149.3	H-2, H-6
5	6.77 d (8.3)	114.9	
6	7.05 dd (8.3, 2.0)	123.2	H-2, H-7
7	7.60 d (15.8)	146.0	H-2, H-6
8	6.37 d (15.8)	117.9	
9		170.7	H-7
1′		128.6	H-5′
2′	7.57 d (2.0)	114.4	H-6′
3′		150.0	H-5′, 3′-OCH_3
4′		148.6	H-2′, H-6′
5′	6.72 d (8.3)	116.2	
6′	7.07dd (8.3, 2.0)	125.5	H-2′
1″		125.8	H-5″
2″	7.34 d (2.0)	113.7	H-6″
3″		148.9	H-5″, 3″-OCH_3
4″		149.6	H-2″, H-6″
5″	6.72 d (8.3)	116.2	
6″	7.03 dd (8.3, 2.0)	126.4	H-2″
3-OMe	3.95 s	56.8	
3′-OMe	3.75 s	56.3	
3″-OMe	3.56 s	56.0	

α) *J* values (in Hz) in parentheses

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