SUPPLEMENTARY MATERIAL

Lignans and phenylpropanoids from the liquid juice of

Phyllostachys edulis

De-Tao Wang¹, Ying-Ying Xue¹, Ying-Fang Zhang¹, Hang Xun¹, Qi-Rong Guo², Feng Tang¹, Jia Sun¹*, Fei-Fei Qi³*

¹ State Forestry Administration Key Open Laboratory, International Centre for Bamboo and Rattan, Beijing 100102, China;

² Co-Innovation Center for Sustainable Forestry in Southern China, College of Forestry, Nanjing Forestry University, Nanjing 210037, China;

³ Shandong Provincial Key Laboratory of Synthetic Biology, CAS Key Laboratory of Biofuels, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao, Shandong 266101, China.

Seven lignans and eight phenylpropanoids, including one new lignan, 7S, 8R, 8'R-5, 5'-dimethoxyariciresinol-4-*O*- β -*D*-glucopyranoside (1), were isolated from the liquid juice of *Phyllostachys edulis*. Their structures were established by extensive spectroscopic analyses. The absolute configuration of the new compound was determined by comparing its experimental electronic circular dichroism (ECD) spectra with calculated ECD spectra. All compounds were evaluated for their anti-inflammatory activity and xanthine oxidase inhibitor activity, and the results showed that compound **9** exhibited a moderate activity in these two bioassays. In addition, all the compounds can be detected in health panda faeces by LC-MS.

Keywords: lignan; phenylpropanoid; Phyllostachys edulis; activity; panda faeces

*Corresponding author. E-mail: <u>sunjia@icbr.ac.cn</u>, qiff@qibebt.ac.cn

Figure S1. ¹H NMR spectrum of compound **1**

Figure S2. ¹C NMR spectrum of compound **1**

Figure S3. DEPT-135 spectrum of compound 1

Figure S4. HSBC spectrum of compound **1**

Figure S5. HMQC spectrum of compound 1

Figure S6. HRESIMS spectrum of compound 1

Figure S7. UV spectrum of compound 1

Figure S8. Experimental and calculated ECD spectrum of compound 1 in MeOH

Figure S9. Compounds 1-15 detected in panda faeces

Table S1 ¹H and ¹³C NMR spectral data for compound **1** in DMSO-d6



Figure S1. ¹H NMR spectrum of compound **1**



Figure S2. ¹C NMR spectrum of compound **1**



Figure S3. DEPT-135 spectrum of compound 1



Figure S4. HSBC spectrum of compound $\mathbf{1}$







Figure S6. HRESIMS spectrum of compound 1



Figure S7. UV spectrum of compound 1



Figure S8. Experimental and calculated ECD spectrum of compound 1 in MeOH



Figure S9. Compounds 1-15 detected in panda faeces

	Compound 1				
	$\delta_{H}, J(Hz)$	δ_C		δ_{H} , $J\left(Hz ight)$	δ_C
1		131.4	1″	4.87 (1H, <i>d</i> , 7.0)	103.2
2,6	6.44 (2H, <i>s</i>)	106.3	2″	3.11 (<i>m</i> , 1H)	74.7
3,5		148.4	3″	3.18 (<i>m</i> , 1H)	77.0
4		133.8	4″	3.03 (<i>m</i> , 1H)	70.4
7	2.83 (1H, <i>dd</i> , 4.5, 13.5) 2.41 (1H, <i>dd</i> , 11.5, 13.5)	33.2	5″	3.09 (<i>m</i> , 1H)	77.7
8	2.60 (1H, <i>m</i>)	42.5	6''	3.58 (<i>m</i> , 1H)	61.4
9	3.90 (1H, <i>dd</i> , 7.0, 8.0) 3.60 (1H, <i>dd</i> , 7.5, 8.0)	72.5		3.40 (<i>m</i> , 1H)	
3,5-OCH ₃	3.72 (6H, <i>s</i>)	56.4			
1′		140.1			
2',6'	6.59 (<i>s</i> , 2H)	104.3			
3',5'		153.0			
4'		134.0			
7′	4.72 (1H, <i>d</i> , 6.0)	82.3			
8'	2.23 (1H, <i>m</i>)	52.9			
9'	3.75 (1H, <i>m</i>) 3.51 (1H, <i>m</i>)	59.2			
3',5'-OCH ₃	3.74 (6H, s)	56.9			

Table S1 ¹H and ¹³C NMR spectral data for compound **1** in DMSO-d6.^a

^a The ¹H and ¹³C NMR spectral data were measured at 500 MHz and 125 MH_z.