SUPPLEMENTARY MATERIAL

A new flavane acid from the fruits of *Illicium verum*

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A new compound, illiciumflavane acid (**1**), along with 13 known compounds (2-14), were isolated from the fruits of *Illicium verum* Hook. F. Their structures were elucidated through various spectroscopic methods, including 1D NMR (^1H NMR, ^{13}C NMR), 2D NMR (HMQC, HMBC and NOESY) and HRMS. The stereochemistry at the chiral centers was determined using CD spectrum, as well as analyses of coupling constants and optical rotation data. Cytotoxicity evaluation of 4 compounds showed that illiciumflavane acid and (*E*)-1,2-bis(4-methoxyphenyl)ethene exhibited potential against A549 activities with IC_{50} values of 4.63 μM and 9.17 μM , respectively.

Fig. S1 The key correlations in HMBC spectrum (H→C) and correlations in NOSEY spectrum (H ↔ H) of **1**

Fig. S2 CD spectrum of **1**

Fig. S3 ¹H-NMR spectrum of **1**

Fig. S4 ^{13}C -NMR spectrum of **1**

Fig. S5 HMBC NMR spectrum of **1**

Fig. S6 HMQC spectrum of **1**

Fig. S7 HR-ESI-MS spectrum of **1**

Fig. S8 NOESY spectrum of **1**

Table S1 ^1H , ^{13}C and HMBC NMR data for compound **1** (CD_3OD).

position	δ_{H}	δ_{C}	HMBC
1			
2	4.68 (1H, <i>d</i> , 7.8)	84.9	C-1', 3, 4, 8a
3	4.63 (1H, <i>td</i> , 7.8, 6.5)	62.4	C-1', 2, 4, 4a
4 α	3.63 (1H, <i>dd</i> , 16.2, 6.5)	36.6	C-4a, 5
4 β	3.70 (1H, <i>dd</i> , 16.2, 6.5)		
4a		114.6	
5	7.15 (1H, <i>s</i>)	119.7	C-4, 4a, 6, 7, 8a, 9
6 α		107.4	
6 β			
7		142.7	
8		139.9	
8a		144.8	
9		169.2	
-OCH ₃	3.76 (3H, <i>s</i>)	54.3	C-8
1'		133.8	
2'	7.04 (1H, <i>d</i> , 8.7)	128.3	
3'	6.84 (1H, <i>d</i> , 8.7)	113.5	
4'		158.6	
5'	6.84 (1H, <i>d</i> , 8.7)	113.5	
6'	7.04 (1H, <i>d</i> , 8.7)	128.3	
1''			
2''			
3''			
4''			
5''			
6''			

Table S2 Cytotoxicity activities of compounds **1**, **5**, **6**, **7**

Compound	Cytotoxicity (IC ₅₀ , μM)			
	P-388	NUGC	HT-29	A549
1	78.36 ± 1.24	39.47 ± 2.13	14.72 ± 1.42	4.63 ± 0.13
5	22.36 ± 1.32	38.48 ± 1.94	35.39 ± 2.57	9.17 ± 0.42
6	>100	76.83 ± 3.56	72.17 ± 3.75	69.78 ± 2.13
7	>100	77.25 ± 2.78	73.55 ± 2.95	70.35 ± 2.01
Cisplatin	21.56 ± 1.06	22.47 ± 1.32	18.71 ± 0.45	15.94 ± 0.76

^a All values are means of three independent experiments.^b Cisplatin, an antitumor agent used as positive control.