SUPPLEMENTARY MATERIAL

A new anthraquinone from seed of *Cassia obtusifolia*

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Abstract: Seeds of *Cassia obtusifolia* L. are known as homology of medicine and food material, which is a commonly consumed beverage in China. One new compound,

8-hydroxy-1,7-dimethoxy-3-methylanthracene-9,10-dione-2-*O*- β -D-glucoside (**1**), together with 11 known compounds, including seven anthraquinones (**2-8**) were isolated from the seeds. The 2D NMR data of compound **2** are reported for the first time. The structures of the compounds were established on the basis of 1D and 2D NMR, IR, HRESI-MS spectra. All the compounds' cytotoxic activities to five cells (L02, HCT-116, A549, HepG2 and SGC7901) are evaluated by CCK8 methods. Compound **1**, **3**, and **7** show moderate cytotoxicity to HCT 116 cells as comparing to oxaliplatin.

Keywords: *Cassia obtusifolia*, Anthraquinone, Antineoplastic activity

List of Supplementary materials

Table S1 ^1H NMR (500 MHz, DMSO), ^{13}C NMR (125 MHz, DMSO) and HMBC spectroscopic data for 1-2 with J values (in Hz) in parentheses.

Fig. S1 Key Key HMBC correlation of compound 1 and 2.

Fig. S2 ^1H NMR spectrum of compound 1

Fig. S3 ^{13}C NMR spectrum of compound 1

Fig. S4 HSQC spectrum of compound 1

Fig. S5 HMBC spectrum of compound 1

Table S1 ¹H NMR (500 MHz, DMSO), ¹³C NMR (125MHz, DMSO) and HMBC spectroscopic data for **1-2** with *J* values (in Hz) in parentheses.

No.	1			2		
	δ_{H}	δ_{C}	HMBC	δ_{H}	δ_{C}	HMBC
1	-	153.3		-	153.2	
2	-	154.3			154.6	
3	-	141.5	-	-	140.7	-
4	7.86 s	125.0	C-4a, 2,10,11	7.82(1H,s)	125.1	C-4a, 2, 10,11
5	7.68d(8.4)	119.8	C- 7, 8a, 10	7.18(1H,s)	107.9	C-6, 7, 10, 8a, 10a
6	7.40d(8.4)	116.3	C- 8, 10a	-	156.7	-
7	-	153.7	-	-	139.8	-
8	-	151.8	-	-	156.9	-
9	-	188.3	-	-	186.7	-
10	-	180.2	-	-	180.8	-
4a		124.7			124.6	
8a	-	116.5	-	-	111.1	-
9a		130.1			129.5	
10a	-	124.0	-	-	128.2	-
8-OH	13.11(1H,Br s)		C-7, 8a	13.25(1H,Br s)		C-7, 8,8a
3-CH ₃	2.43(3H,s)	17.6	C-2,3,4	2.41(3H,s)	17.5	C-2,3,4
1-OCH ₃	3.89(3H,s)	61.4	C-1	3.87(3H,s)	61.4	C-1
7-OCH ₃	3.93(3H,s)-	56.2	C-7	3.85(3H,s)-	60.0	C-7
1'	5.01 d (1H, 7.4)	103.7	C-2, 3'	5.01 d (1H, 7.5)	103.8	C-2
2'	3.30(1H,m)	74.0	C-4'	3.28(1H,m)	74.0	C-4'
3'	3.09t(1H,9.0)	77.3		3.09t(1H,9.0)	77.3	
4'	3.16t(1H,9.0)	69.8		3.15t(1H,9.0)	69.8	
5'	3.25t (1H,9.0)	76.4	C-4'	3.25t (1H,9.0)	76.4	C-4'
6'	3.61 d (1H,12.2)	60.9	C-5'	3.61d (1H,11.5)	60.9	C-5'
	3.42dd(1H,9.0,12.2)			3.42dd(1H,9.0,11.5)

Fig. S1 Key Key HMBC correlation of compound 1 and 2.

Fig. S2 ^1H NMR spectrum of compound 1

Fig. S3 ¹³C NMR spectrum of compound 1

Fig. S4 HSQC spectrum of compound 1

Fig. S5 HMBC spectrum of compound 1