SUPPLEMENTARY MATERIAL

Three new dibenzofurans from Cydonia oblonga Mill.

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Abstract: Phytochemical investigation of *Cydonia oblonga* Mill. collected in Xinjiang province, China, led to the isolation and identification of three new dibenzofurans (1-3) along with one known compound (4). Their structures were elucidated based on HRESIMS, spectroscopic data (IR, UV, 1D, 2D NMR) and X-ray diffraction analysis.

Key words: Cydonia oblonga Mill.; dibenzofurans; Rosaceae

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	1	a	2^{a}			3^b
position	$\delta_{ m H}$	$\delta_{ m C}$	$\delta_{ m H}$	$\delta_{ m C}$	$\delta_{ m H}$	$\delta_{ m C}$
1	7.29 s	98.0		141.2	7.23 s	97.4
2		151.8		137.3		153.8
3		141.6		146.1		143.3
4		140.2		132.6		139.6
4a		143.9		146.3		144.8
5a		146.1		145.5		150.4
6		133.4		133.1		170.5
7		147.8		147.5		159.6
8	7.03 d (8.4)	109.4	7.02 d (8.3)	109.4	5.87 s	107.2
9	7.39 d (8.4)	110.7	7.49 d (8.3)	112.7		183.3
9a		120.8		120.1		123.3
9b		121.2		110.1		118.7
OMe-2	3.92 s	57.7	3.85 s	61.8	3.94 s	56.6
OMe-3	3.85 s	61.7	3.96 s	61.8	3.95 s	61.8
OMe-4	4.16 s	61.5	4.04 s	61.6	4.21 s	61.4
OMe-7	3.92 s	57.1	3.92 s	57.4	3.89 s	57.1
OH-1			8.48 br s			
OH-6	8.25 br s		8.26 br s			
^a Recorded	in acetone- d_6 . ^b	Recorded in	n CDCl ₃ .			

Table S1. ¹H NMR (400 MHz) and ¹³C NMR (100 MHz) data for compounds 1-3 ($\delta_{\rm H}$, $\delta_{\rm C}$ in ppm, *J* in Hz)

Figure S1. Chemical structures of compounds 1-4

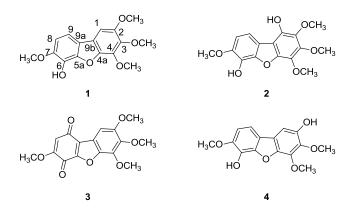


Figure S2. Key COSY, HMBC and NOESY correlations of compound 1

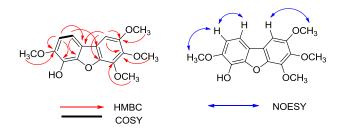


Figure S3. IR spectrum of compound 1

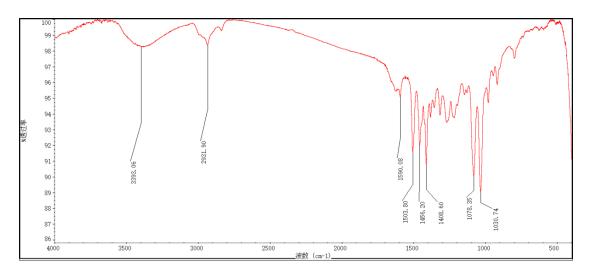
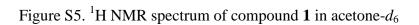


Figure S4. HRESIMS spectrum of compound 1

Spectrum Sour	ce			Fragmentor V 150	oltage Col	lision Energy 0	Ionization Mod Esi	le
x10 6 +ES	l Sca	an:1 (1.726 ı	nin) Frag=150.	0V C85613.d				
2.5-			* 327	.0878				
2-								
)5.1(/I+H)							
1.5- (1	111)	T .						
1-								
0.5-		311.1014			349.0658			
0			a la la	.				
	305	310 315	5 320 325	<u>33033534</u>	40 345 350	355 360 3	65 370 375	I.
Peak List				Counts vs. Mass	-to-Charge (m/z)			
m/z	z	Abund	Name	For	rmula	Ion	Score (DB)	Hits (DB)
71.1304		319405						
05.1026	1	1367945		C16	5 H17 O6	(M+H)+		
27.0878	1	2539054						
28.0878	1	882112						
89.0549		321253						
76.1233	2	566862						
31.1877		2542311						
		2179514						
	1							
533.184	1	688974						
33.184 53.1611	1	688974 860665	imits					
33.184 53.1611 Formula Calc	1	688974 860665 or Element L	imits					
33.184 53.1611 Formula Calc Element	1 1 ulato	688974 860665 or Element L	imits					
533.184 553.1611 Formula Calc Element	1 1 ulato	688974 860665 or Element L Max	imits					
533.184 553.1611 Formula Calc Element	1 1 ulato	688974 860665 or Element L Max 3 40	imits					<u> </u>
533.184 553.1611 Formula Calc Element C 1 1 0	1 1 ulato	688974 860665 F Element L 3 40 0 80 0 20 0 0	imits					1
533.184 553.1611 Formula Calc Clement C 4 0 0	1 1 ulato	688974 860665 or Element L 3 40 0 80 0 20 0 0 0 0 0 0	imits					1
533.184 553.1611 Formula Calc Element C 1 0 1 0 1 5 5 2	1 1 ulato	688974 860665 or Element L Max 3 40 0 80 0 20 0 0 0 0 0 0 0 0 0 0	imits					
33.184 53.1611 Formula Calc Element 1 1 1	1 ulato	688974 860665 or Element L Max 3 40 0 80 0 20 0 0 0 0 0 0 0 0 0 0 0 0	imits					
532.1837 533.184 553.1611 Formula Calc Clement 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 ulato	688974 860665 or Element L 3 40 0 80 0 20 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	imits	s Diff (ppm)	Ion Species	Score		

5



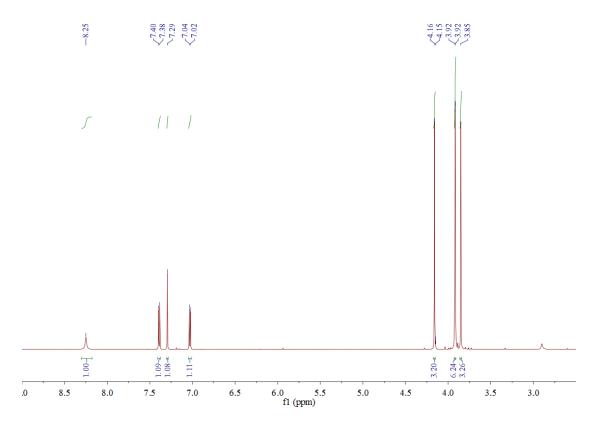


Figure S6. ¹³C NMR spectrum of compound **1** in acetone- d_6

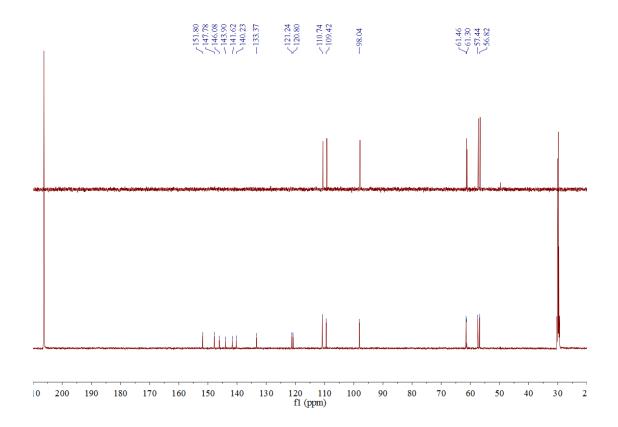


Figure S7. HSQC spectrum of compound $\mathbf{1}$ in acetone- d_6

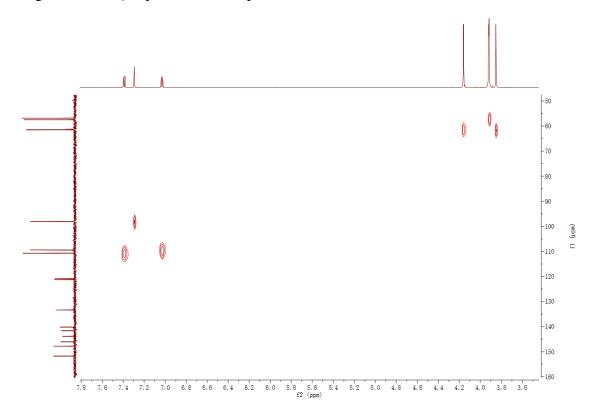


Figure S8. HMBC spectrum of compound $\mathbf{1}$ in acetone- d_6

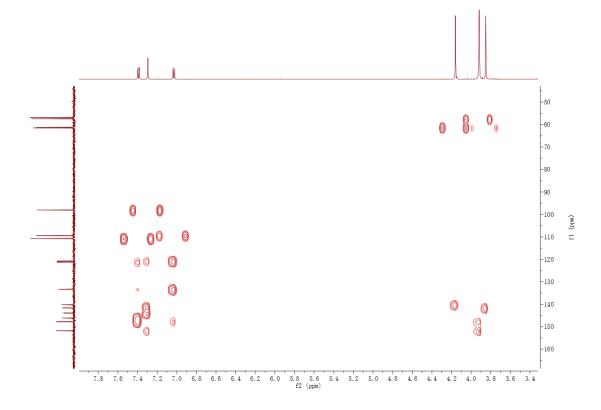


Figure S9. NOESY spectrum of compound 1 in acetone- d_6

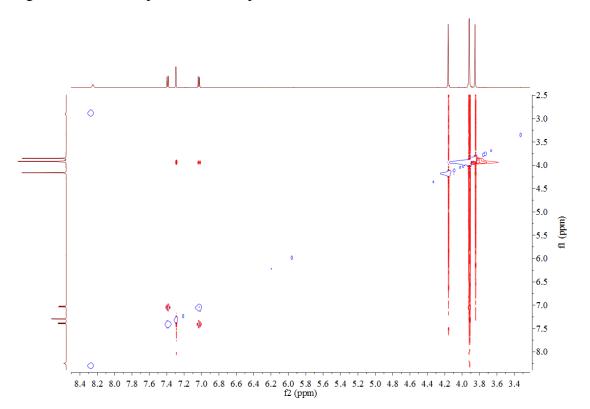
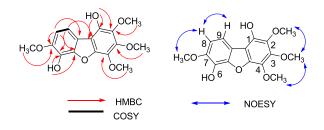
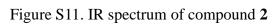


Figure S10. Key COSY, HMBC and NOESY correlations of compound ${\bf 2}$





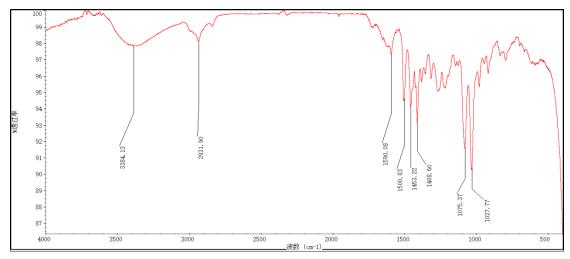


Figure S12. HRESIMS spectrum of compound 2

Spectrum Sou	Source			Fragmentor Voltage 125	Collision Energy		Ionization Mode Esi	
x10 4 +ES	SI Sc	an (2.53	9 min) Fr	ag=125.0V C854212.d				
1.4-				343.0806				
1.2-								
1-								
0.8-								
0.6-			21.0978 M+H)+					
0.4-		(
0.2-								
0.2								
eak List n/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)	
16.9853	<u> </u>	26893						
57.0841		63870						
01.1417		34792						
21.0978	1	167569		C16 H17 O7	(M+H)+			
22.0999	1	27353		C16 H17 O7	(M+H)+			
43.0806	1	506686						
44.0829	1	79211						
		52608						
05.0509								
		28481						
13.2662 63.1696		48171						
13.2662 63.1696 Formula Cale		48171 or Eleme						
13.2662 63.1696 Formula Cale Element	culat Min	48171 or Eleme Max	x					
13.2662 63.1696 formula Cale flement		48171 or Eleme Ma: 1	x 50					
13.2662 63.1696 Formula Cale Element		48171 or Eleme 1 0 1	x					
413.2662 663.1696 Formula Cale Element		48171 or Eleme 1 0 1	x 50 100					
413.2662 663.1696 Formula Cale Element C H D N		48171 or Eleme 1 0 1 0	x 50 100 10					
H13.2662 563.1696 Formula Cald Clement H D N		48171 or Eleme 1 0 1 0 0	x 50 100 10 0				_	
413.2662 563.1696 Formula Cale Element C H H D D N S S Cl Formula Cale	Min	48171 or Eleme 1 0 1 0 0 0 0 0	x 50 100 10 0 0 0					
405.0509 413.2662 663.1696 Formula Cale Element C H O O N S C C Formula Cale Formula Cale	Min	48171 or Eleme 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	x 50 100 10 0 0 0 0 5 5	Tgt Mass Diff (ppm) Ion Spec 320.0896 -2.7 C16 H17				

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Figure S13. ¹H NMR spectrum of compound **2** in acetone- d_6

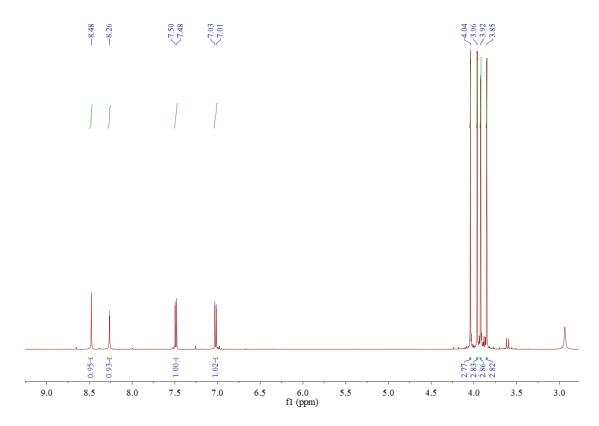


Figure S14. ¹³C NMR spectrum of compound **2** in acetone- d_6

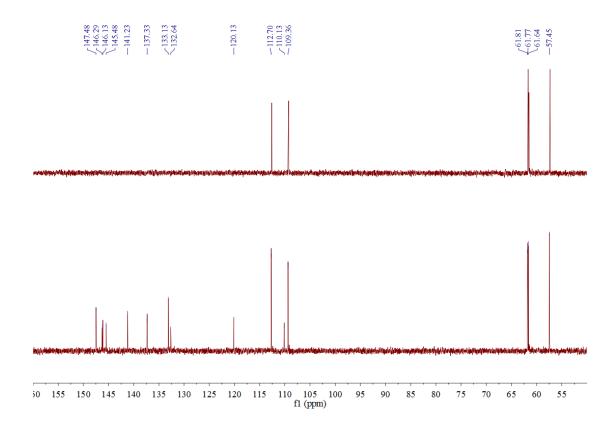


Figure S15. HSQC spectrum of compound $\mathbf{2}$ in acetone- d_6

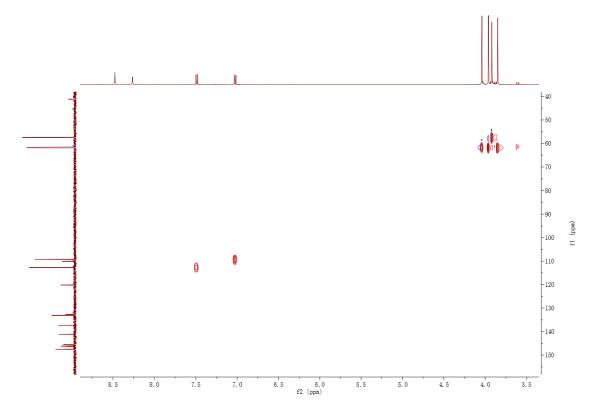


Figure S16. HMBC spectrum of compound $\mathbf{2}$ in acetone- d_6

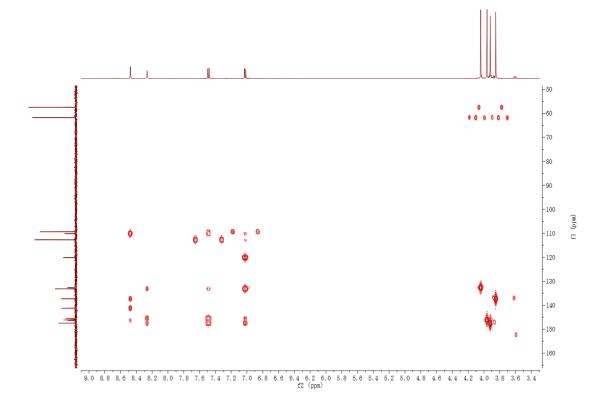


Figure S17. NOESY spectrum of compound 2 in acetone- d_6

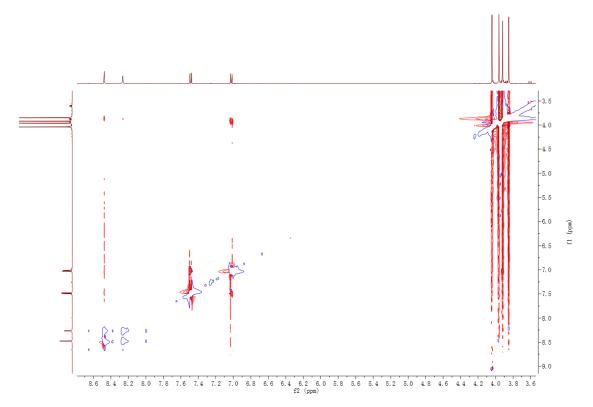


Figure S18. X-ray ORTEP drawing of compound 2

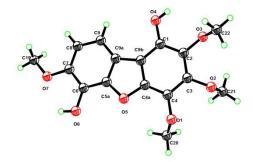
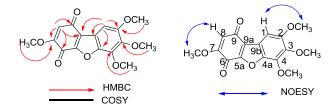
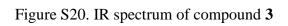


Figure S19. Key COSY, HMBC and NOESY correlations of compound ${\bf 3}$





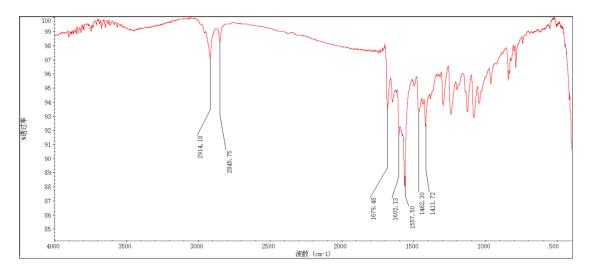


Figure S21. HRESIMS spectrum of compound 3

Spectrum Sou	rce				Fragmentor Voltage 135	Collision Energy 0	Ionization Mode Esi	
x10 3 +ES	SI Sca	an (5.20	02 min) Fra	ag=135.0V W				
1.75-					* 319. (M+	0827 341.0648		
1.5-					(141)	·)·		
1.25-								
1-								
0.75-								
0.5-								
0.25-							1	
02	10	220 23	30 240 25		280 290 300 310 3		60 370 380 390	<u> </u>
Peak List				Count	s (%) vs. Mass-to-Char	ge (m/z)		
m/z	z	Abund	Nar	ne	Formula	Ion	Score (DB)	Hits (DB)
319.0827	1	990922			C16 H15 O7	(M+H)+		
320.0847	1	172971			C16 H15 O7	(M+H)+		
341.0648	1	939085	i					
342.067	1	159917	,					
	1	159917 127237						
343.339 545.1565	1	127237 98942	,					
343.339 645.1565 659.1439	1	127237 98942 185527	/0					
343.339 645.1565 659.1439 659.4182	1	127237 98942 185527 110320	, 70)					
343.339 645.1565 659.1439 659.4182 660.1416	1	127237 98942 185527 110320 904572	/0) 2					
343.339 545.1565 559.1439 559.4182 560.1416 561.1427	1	127237 98942 185527 110320 904572 245423	70 0 2 3					
343.339 545.1565 559.1439 559.4182 560.1416 561.1427 Formula Cale	1	127237 98942 185527 110320 904572 245423 or Elem	70 0 2 3					
343.339 645.1565 659.1439 659.4182 660.1416 661.1427 Formula Calo Element	1 1 1 culate	127237 98942 185527 110320 904572 245423 or Elem	70 0 2 ent Limits					
343.339 645.1565 659.1439 659.4182 660.1416 661.1427 Formula Calo Element C	1 1 1 culate	127237 98942 185527 110320 904572 245423 or Elem	70 0 2 ent Limits ax					
342.067 343.339 645.1565 659.1439 659.4182 660.1416 661.1427 Formula Calo Element C H O	1 1 1 culate	127237 98942 185527 110320 904572 245423 or Elem M 1	70 0 2 3 ent Limits ax 50					
343.339 645.1565 659.1439 659.4182 660.1416 661.1427 Formula Cald Element C H	1 1 1 culate	127237 98942 185527 110320 904572 245423 or Elem M 1 0	70 2 3 6 6 6 70 70 70 70 70 70 70 70 70 70					
343.339 645.1565 659.1439 659.4182 660.1416 661.1427 Formula Cald Element C H O	1 1 1 culate	127237 98942 185527 110320 904572 245423 57 Elem M 1 0 0	70 2 2 2 2 2 2 3 2 3 4 5 100 10					
343.339 645.1565 659.1439 669.4182 660.1416 660.1416 661.1427 Formula Cald Element C C H C N S C	1 1 1 culate Min	127237 98942 185527 110320 904572 245423 DF Elem M 1 0 0 0 0 0 0	70 70 9 9 9 9 9 9 9 9 9 9 9 9 9					
343.339 645.1565 659.1439 659.4182 660.1416 661.1427 Formula Calo Element C H O N S	1 1 1 culate Min	127237 98942 185527 110320 904572 245423 or Elem M 1 0 0 0 0 0 0 0 0	70 70 9 9 9 9 9 9 9 9 9 9 9 9 9	Tqt Mass	Diff (ppm) Ion Spec	es Score		

User Spectra

Figure S22. ¹H NMR spectrum of compound **3** in CDCl₃

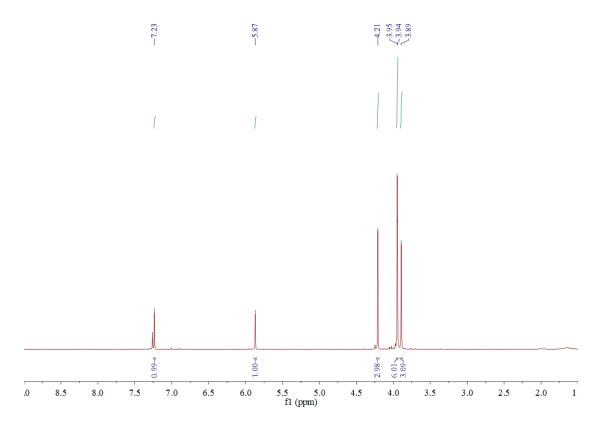
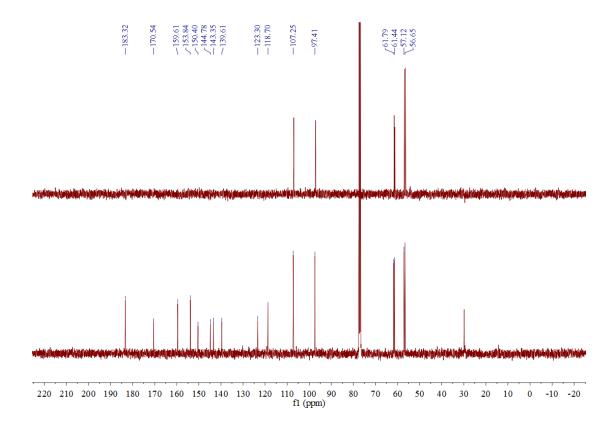
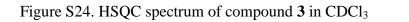


Figure S23. ¹³C NMR spectrum of compound **3** in CDCl₃





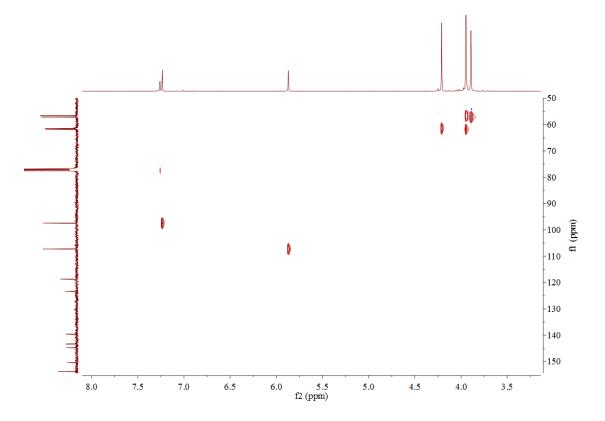


Figure S25. HMBC spectrum of compound 3 in CDCl₃

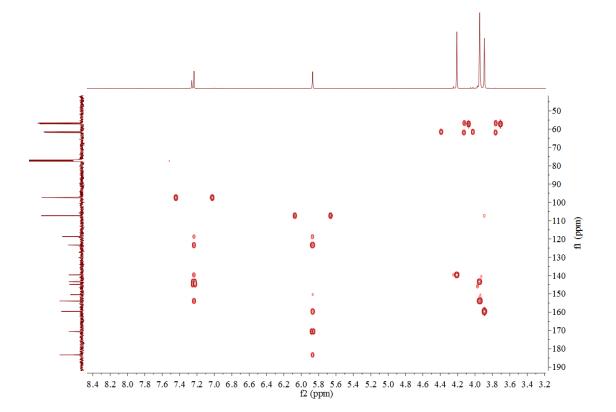


Figure S26. NOESY spectrum of compound 3 in CDCl₃

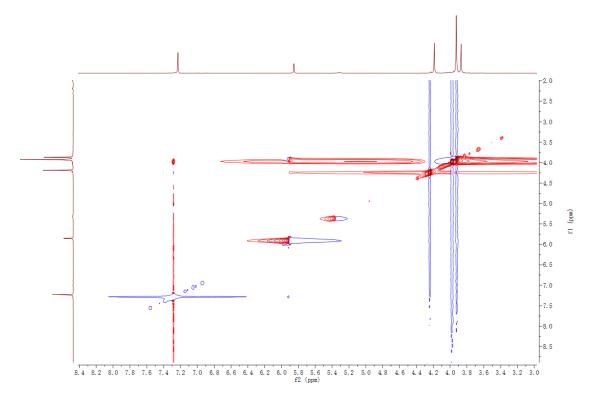


Figure S27. UV spectrum of compound 1

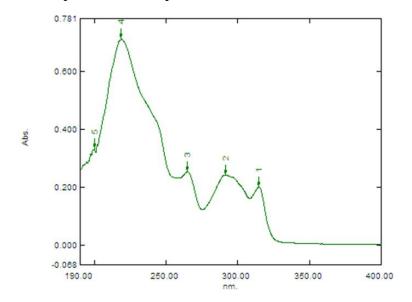


Figure S28. UV spectrum of compound 2

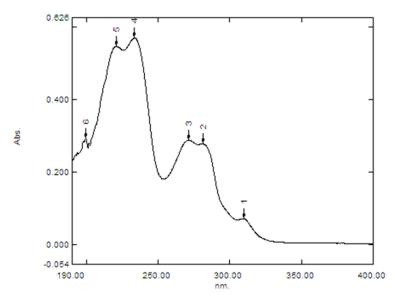


Figure S29. UV spectrum of compound 3

