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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Table S1. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compounds **1-3** (δ_H, δ_C in ppm, *J* in Hz)

	1[a]		**2**[a]		**3**[b]	
position	δ_H	δ_C	δ_H	δ_C	δ_H	δ_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 $CDCl_3$.

Figure S1. Chemical structures of compounds **1-4**

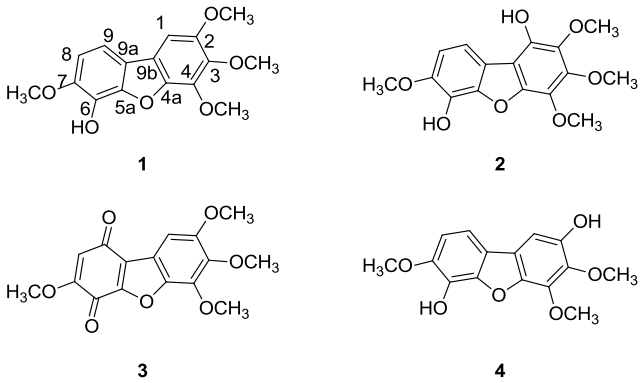


Figure S2. Key COSY, HMBC and NOESY correlations of compound **1**

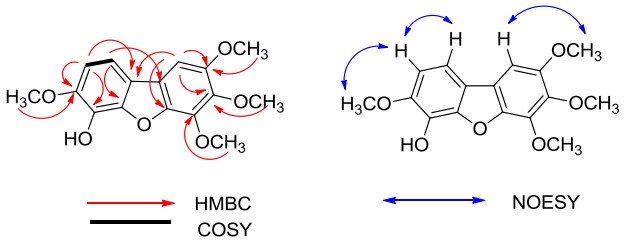


Figure S3. IR spectrum of compound **1**

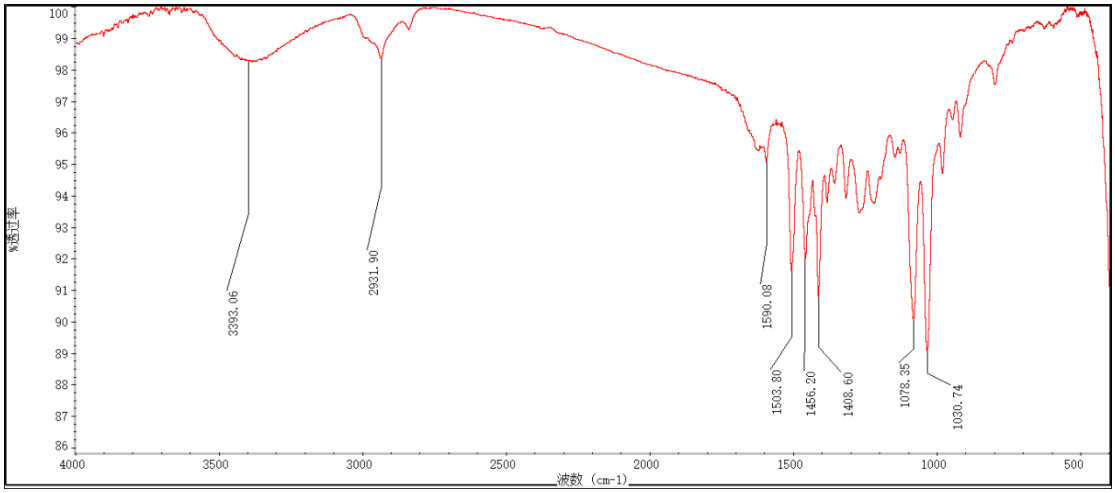
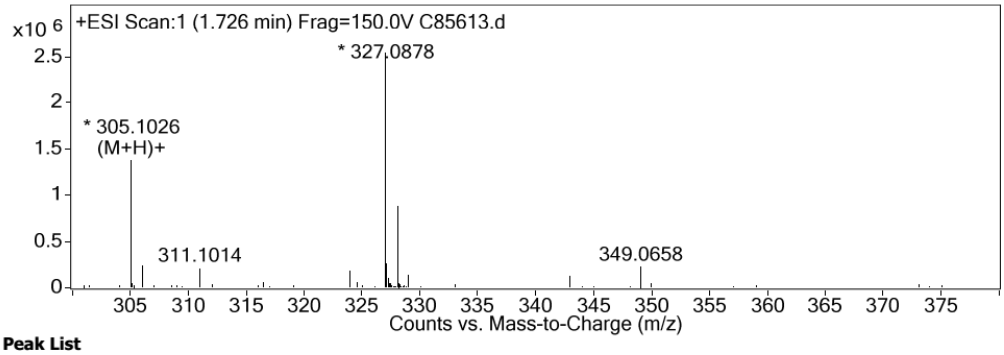


Figure S4. HRESIMS spectrum of compound **1**

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	150	0	Esi



Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
271.1304		319405					
305.1026	1	1367945		C16 H17 O6	(M+H)+		
327.0878	1	2539054					
328.0878	1	882112					
389.0549		321253					
476.1233	2	566862					
631.1877		2542311					
632.1837	1	2179514					
633.184	1	688974					
653.1611	1	860665					

Formula Calculator Element Limits

Element	Min	Max
C	3	40
H	0	80
O	0	20
N	0	0
S	0	0
Cl	0	0
F	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C16 H16 O6	TRUE	304.0954	304.0947	-2.2	C16 H17 O6	97.08

Figure S5. ^{1}H NMR spectrum of compound **1** in acetone-d_6

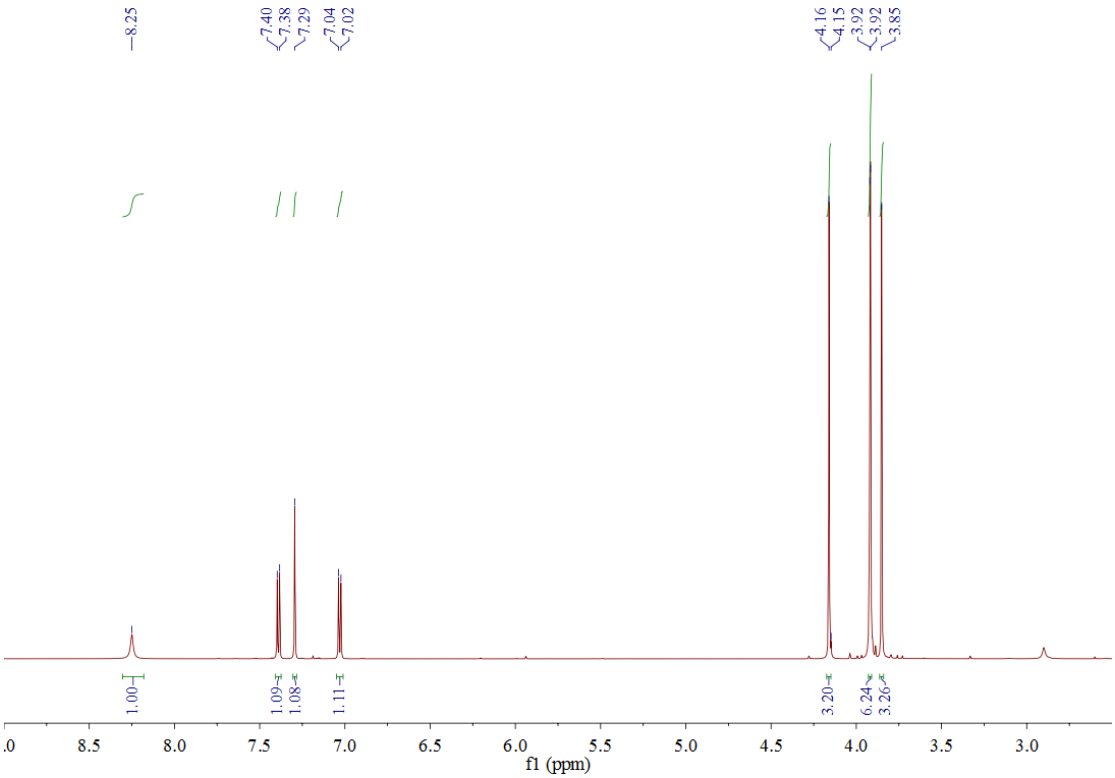


Figure S6. ^{13}C NMR spectrum of compound **1** in acetone-d_6

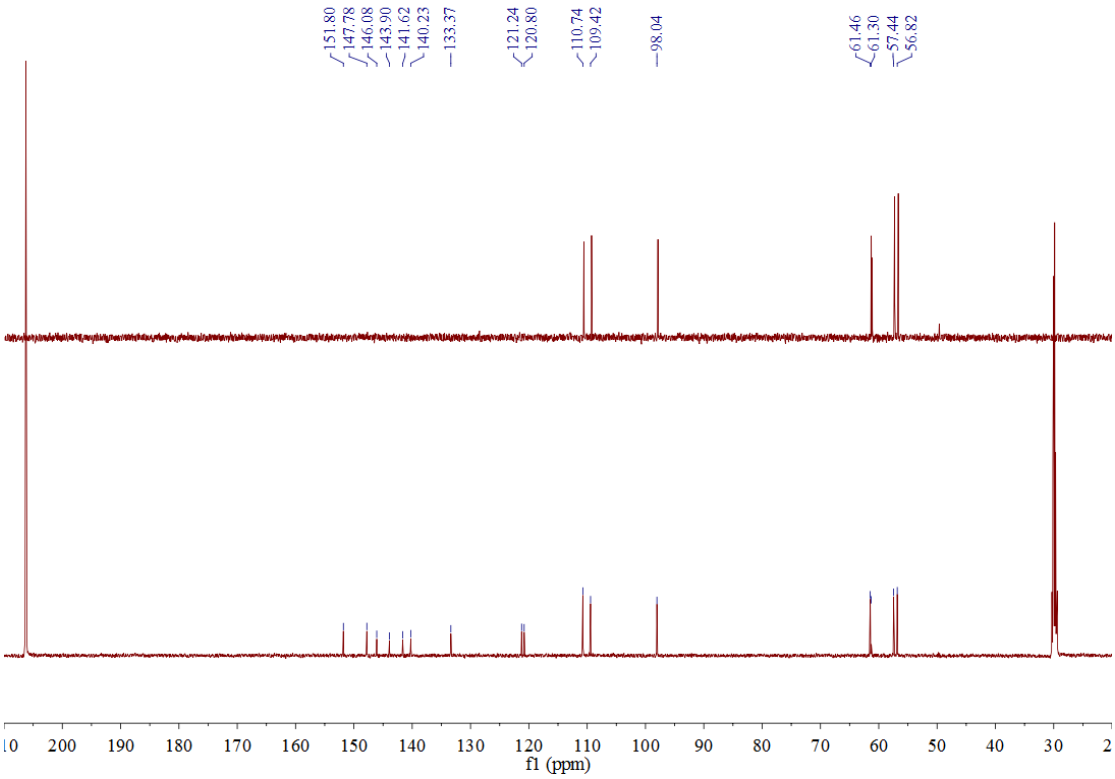


Figure S7. HSQC spectrum of compound **1** in acetone-d_6

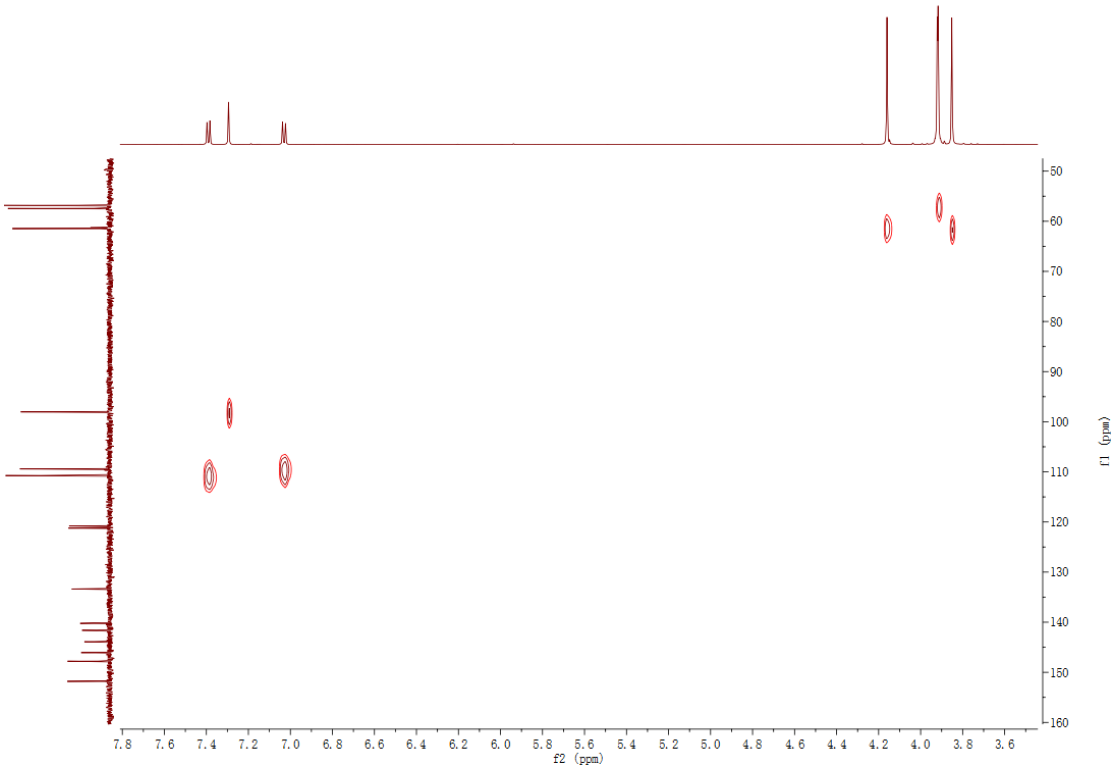


Figure S8. HMBC spectrum of compound **1** in acetone-d_6

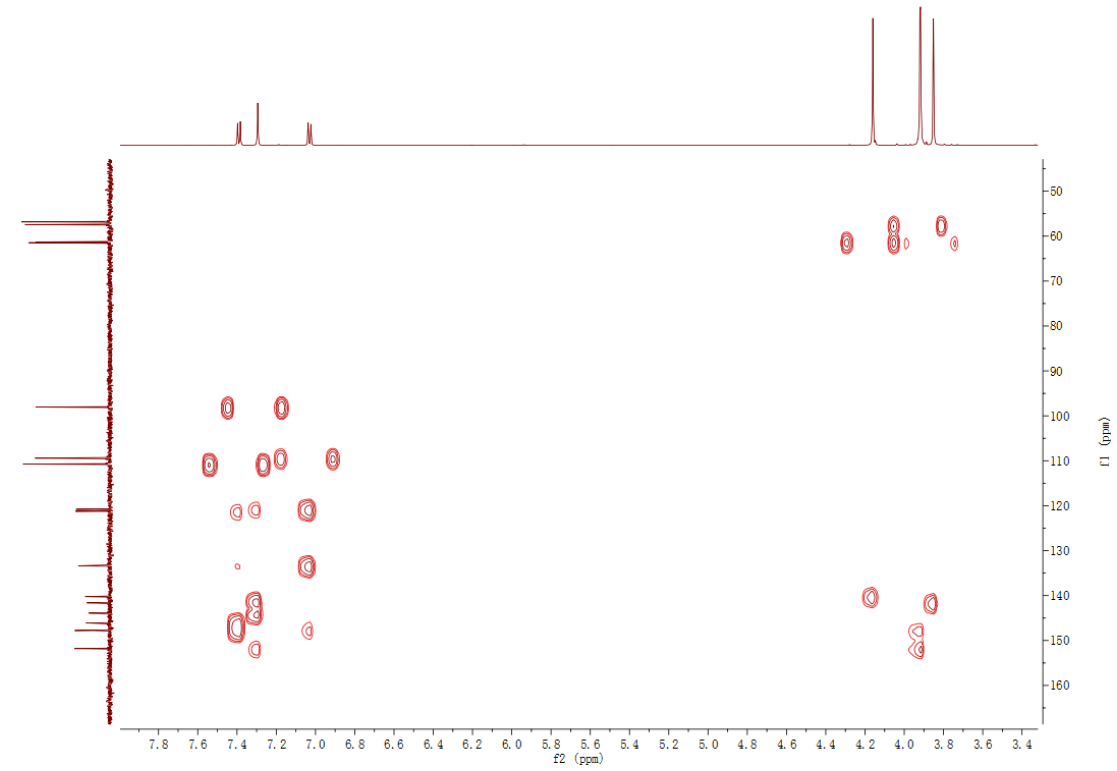


Figure S9. NOESY spectrum of compound **1** in acetone-d_6

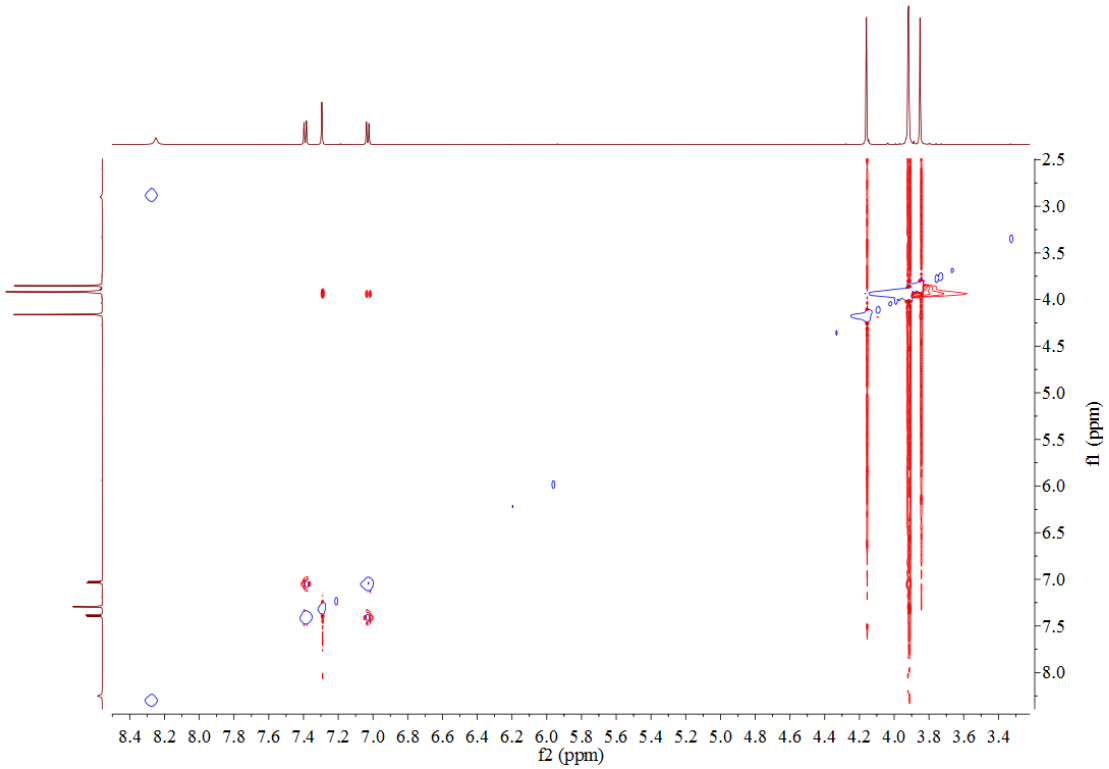


Figure S10. Key COSY, HMBC and NOESY correlations of compound **2**

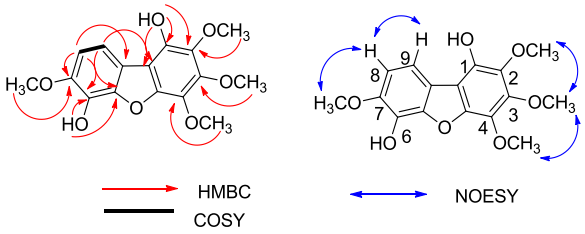


Figure S11. IR spectrum of compound **2**

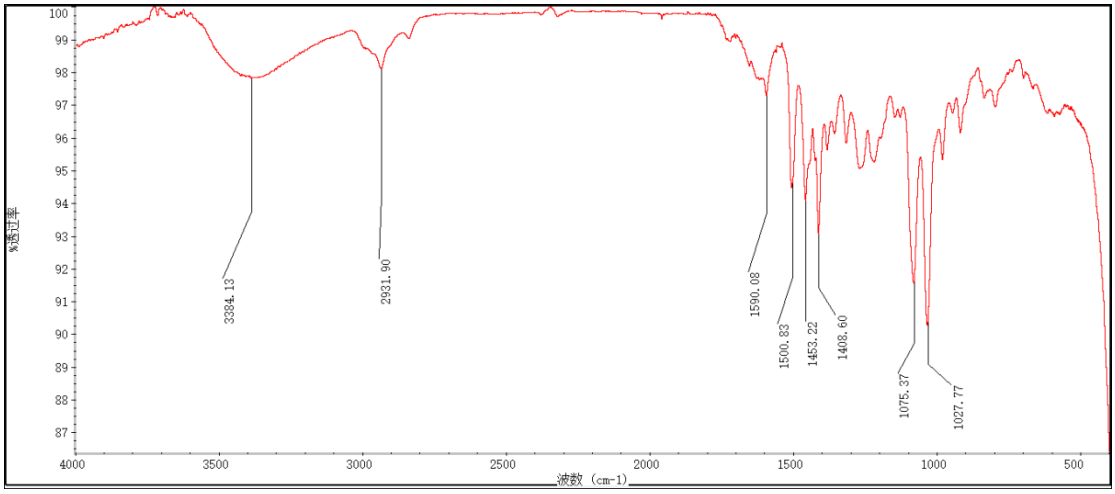
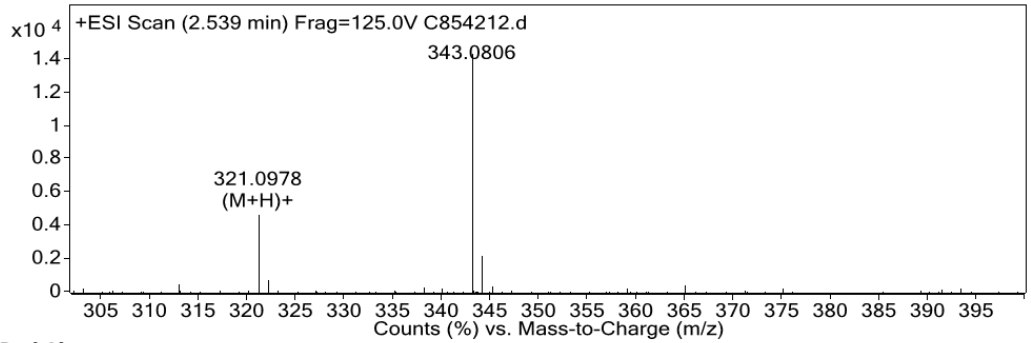


Figure S12. HRESIMS spectrum of compound **2**

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	125	0	Esi



Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
116.9853		26893					
157.0841		63870					
301.1417		34792					
321.0978	1	167569		C16 H17 O7	(M+H)+		
322.0999	1	27353		C16 H17 O7	(M+H)+		
343.0806	1	506686					
344.0829	1	79211					
405.0509		52608					
413.2662		28481					
663.1696		48171					

Formula Calculator Element Limits

Element	Min	Max
C	1	50
H	0	100
O	0	10
N	0	0
S	0	0
Cl	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C16 H16 O7	TRUE	320.0905	320.0896	-2.7	C16 H17 O7	80.73

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

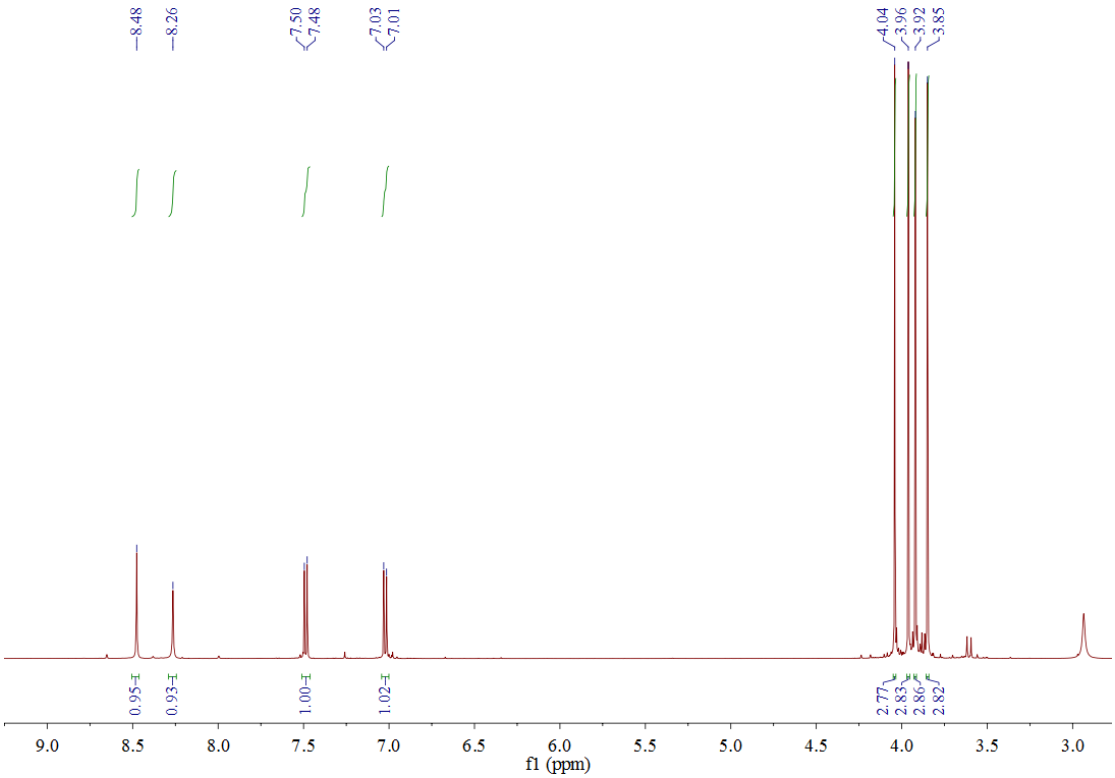


Figure S14. ^{13}C NMR spectrum of compound **2** in acetone-d_6

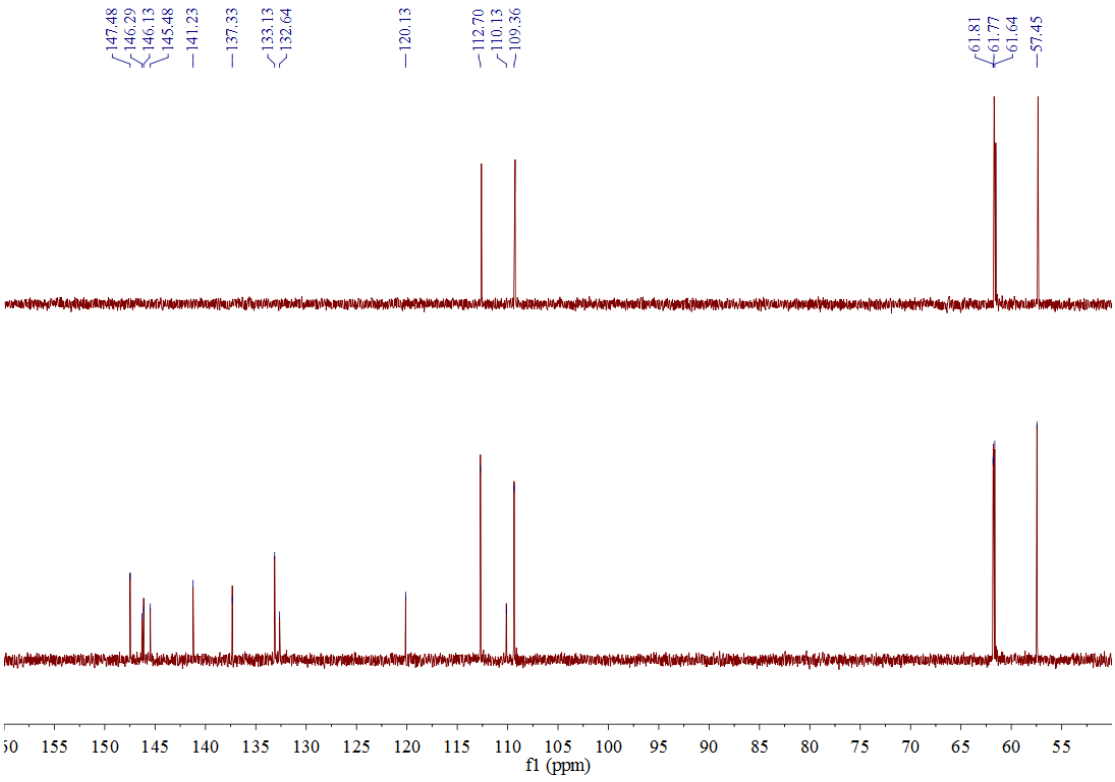


Figure S15. HSQC spectrum of compound **2** in acetone-d_6

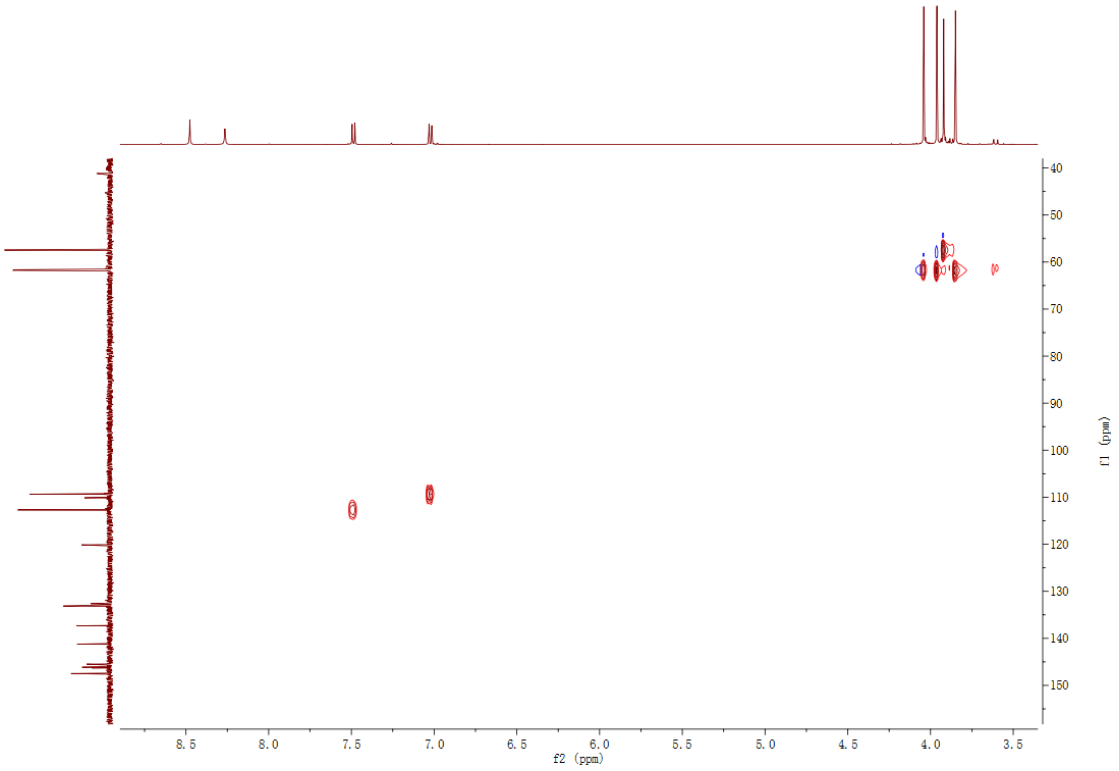


Figure S16. HMBC spectrum of compound **2** in acetone-d_6

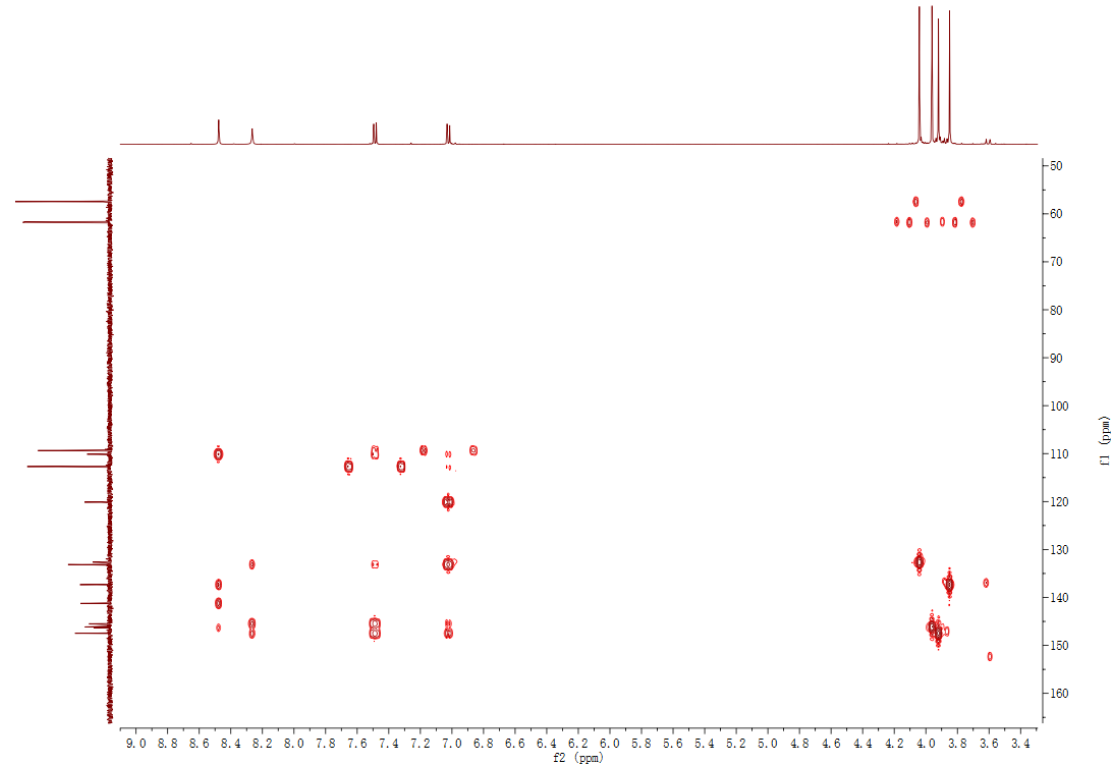


Figure S17. NOESY spectrum of compound **2** in acetone-d_6

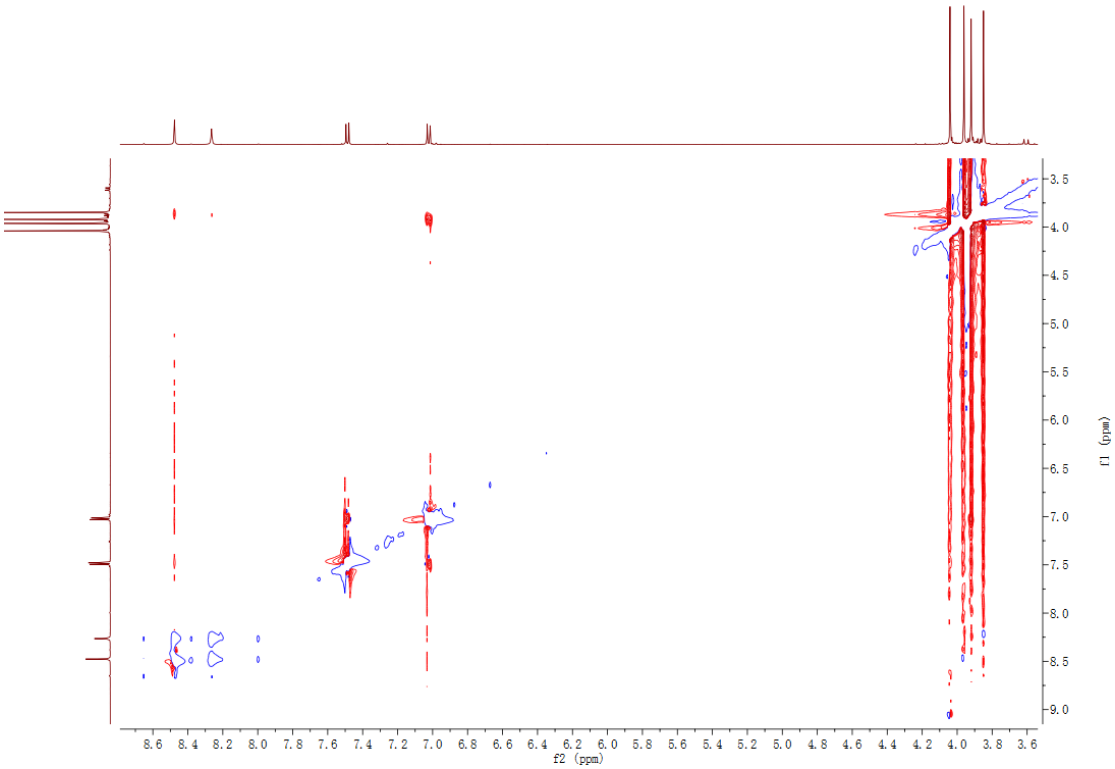


Figure S18. X-ray ORTEP drawing of compound **2**

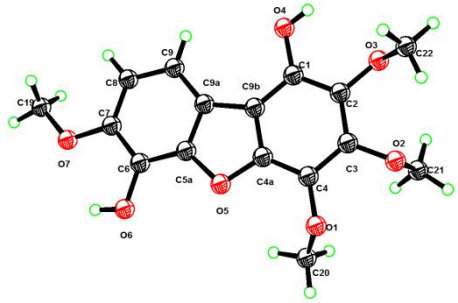


Figure S19. Key COSY, HMBC and NOESY correlations of compound **3**

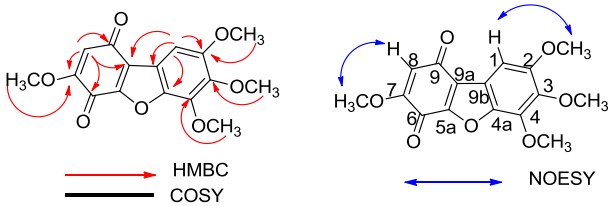


Figure S20. IR spectrum of compound **3**

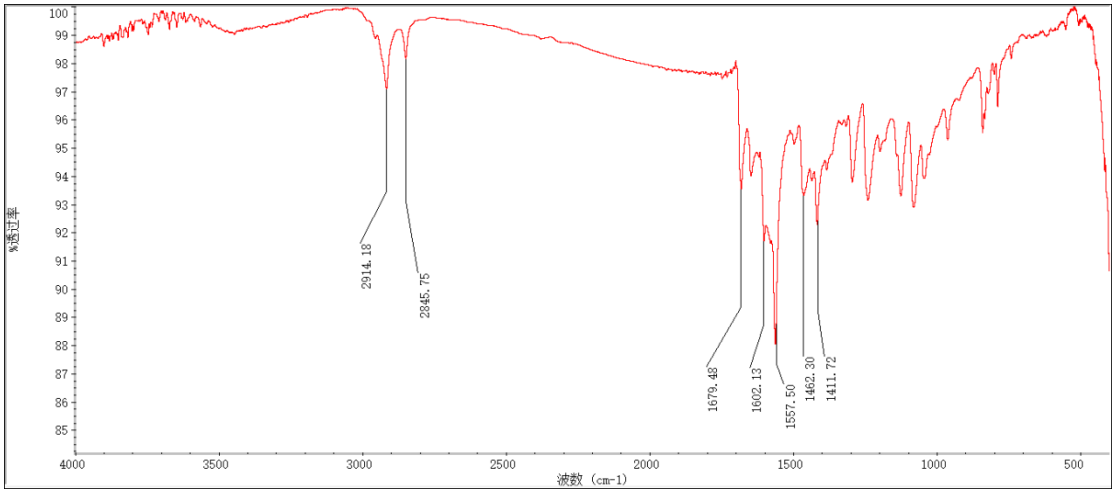
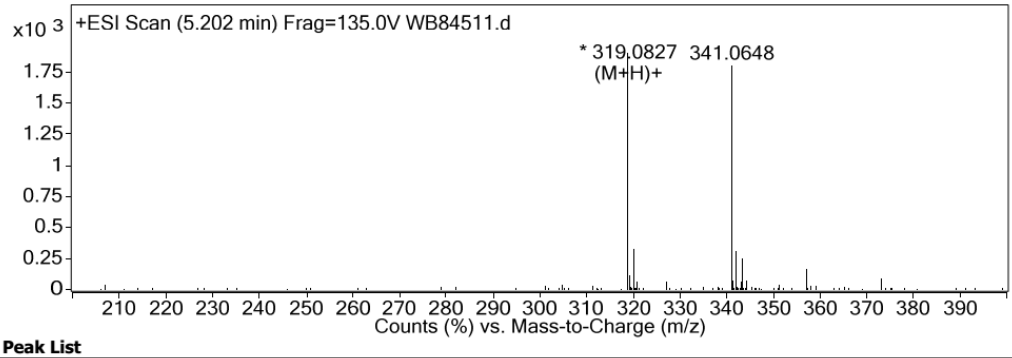


Figure S21. HRESIMS spectrum of compound **3**

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	135	0	Esi



Peak List

m/z	z	Abund	Name	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					
342.067	1	159917					
343.339		127237					
645.1565		98942					
659.1439	1	1855270					
659.4182		110320					
660.1416	1	904572					
661.1427	1	245423					

Formula Calculator Element Limits

Element	Min	Max
C	1	50
H	0	100
O	0	10
N	0	0
S	0	0
Cl	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C16 H14 O7	TRUE	318.0754	318.074	-4.61	C16 H15 O7	90.99

Figure S22. ^{1}H NMR spectrum of compound **3** in $CDCl_3$

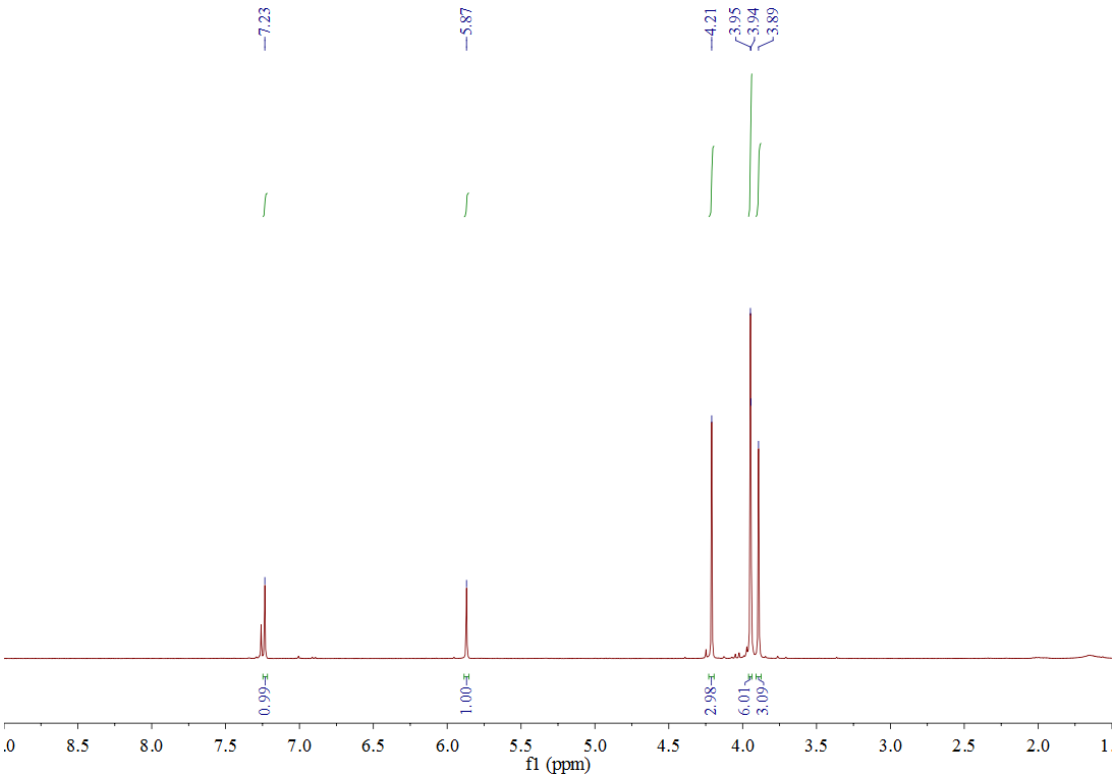


Figure S23. ^{13}C NMR spectrum of compound **3** in $CDCl_3$

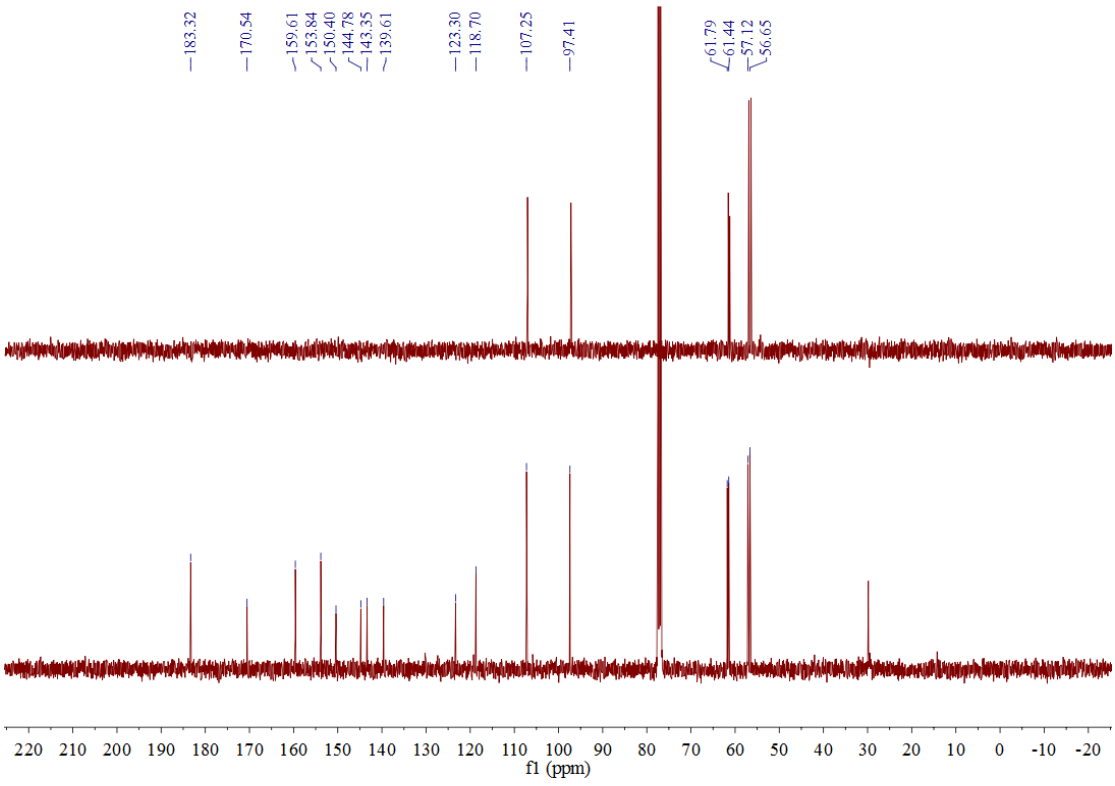


Figure S24. HSQC spectrum of compound **3** in $CDCl_3$

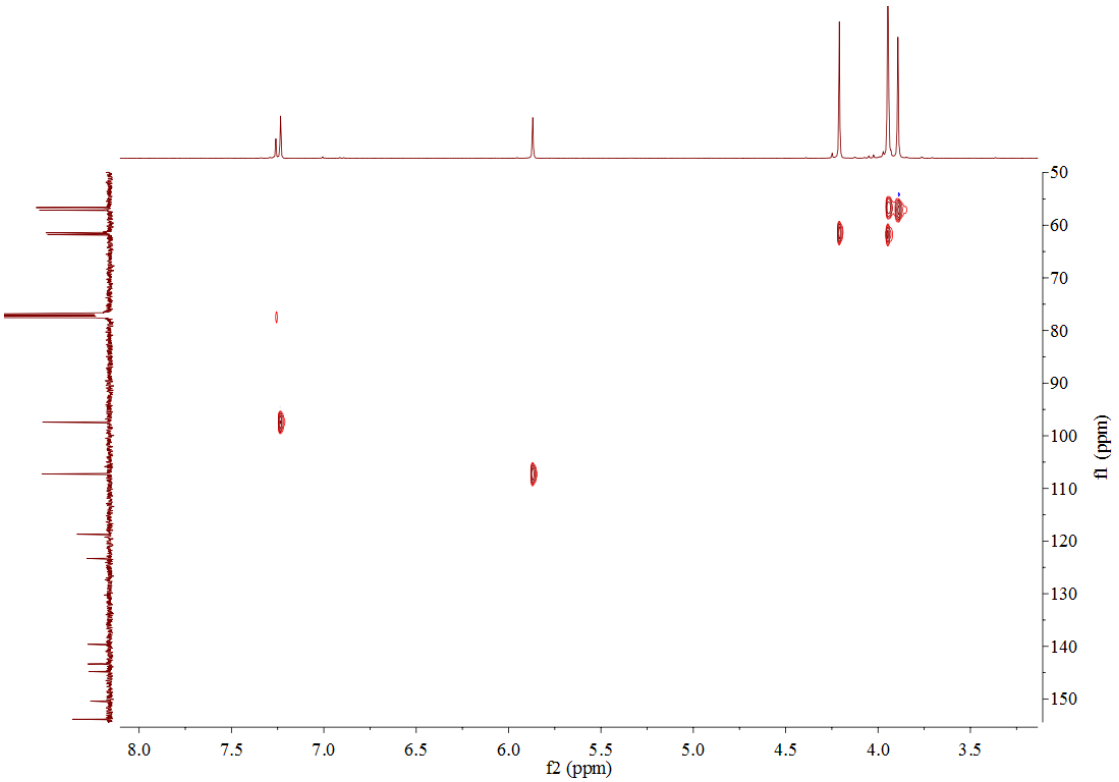


Figure S25. HMBC spectrum of compound **3** in $CDCl_3$

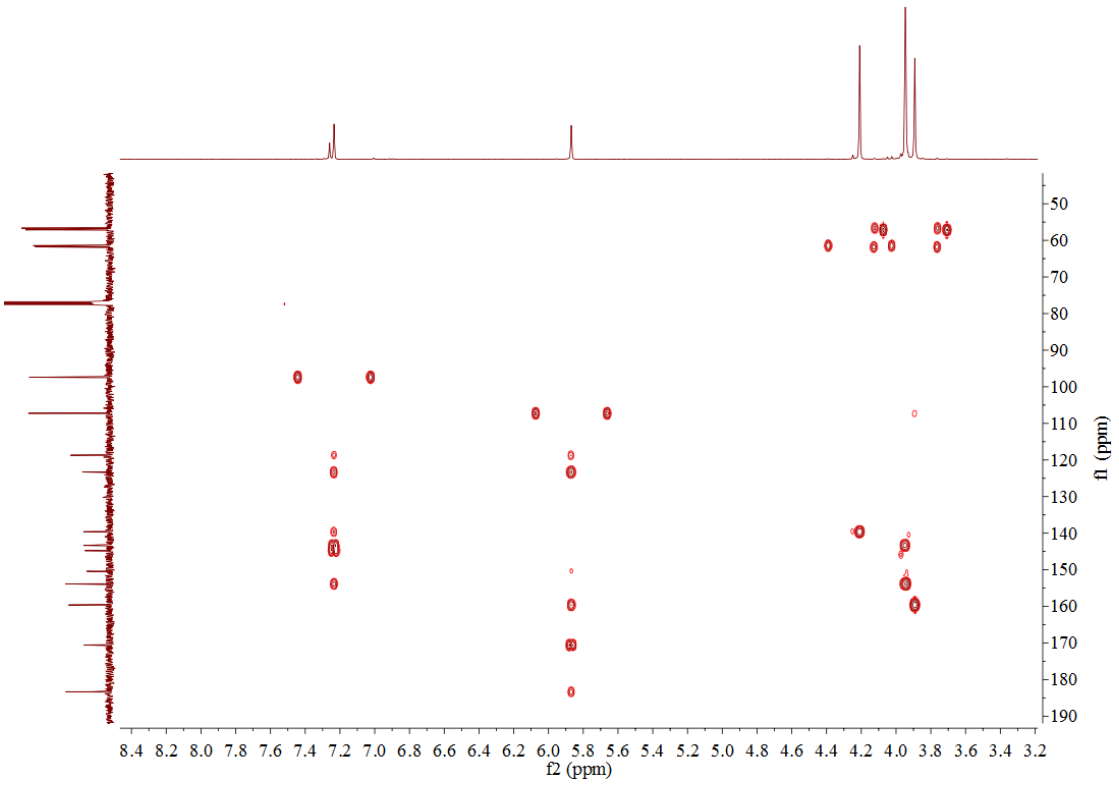


Figure S26. NOESY spectrum of compound **3** in $CDCl_3$

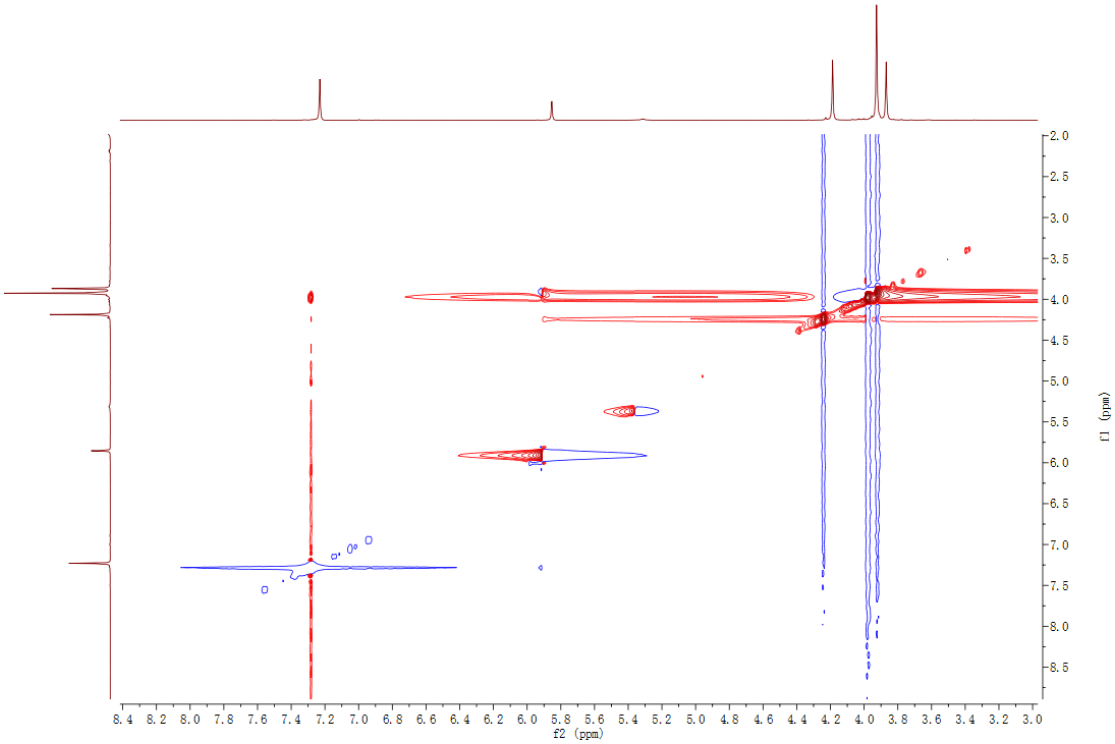


Figure S27. UV spectrum of compound **1**

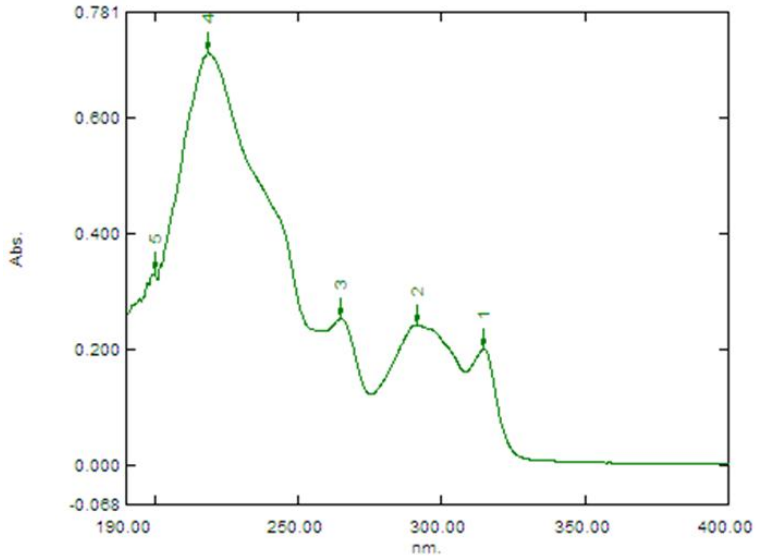


Figure S28. UV spectrum of compound **2**

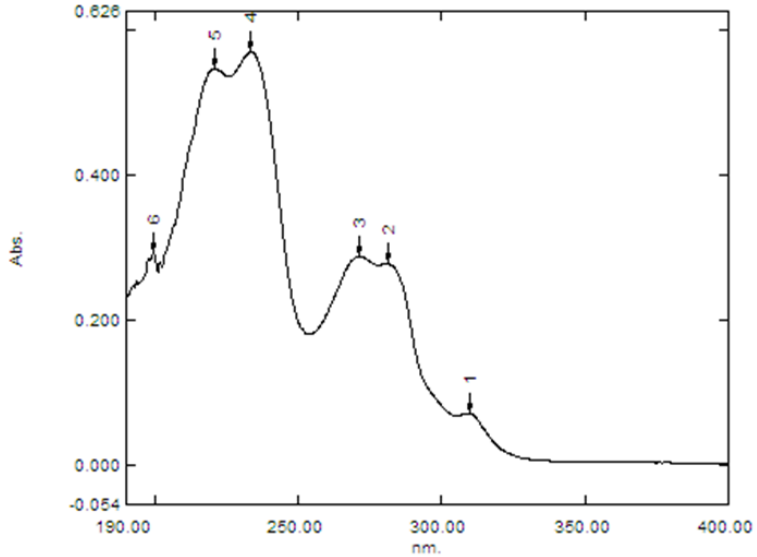


Figure S29. UV spectrum of compound **3**