Supporting Information

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Anti-inflammatory Xanthones from the Fruits of *Hypericum patulum* Thunb.

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Compound **1**:$C_{14}H_8O_4$; ESI-MS *m/z*: 241 $[M+H]^+$.

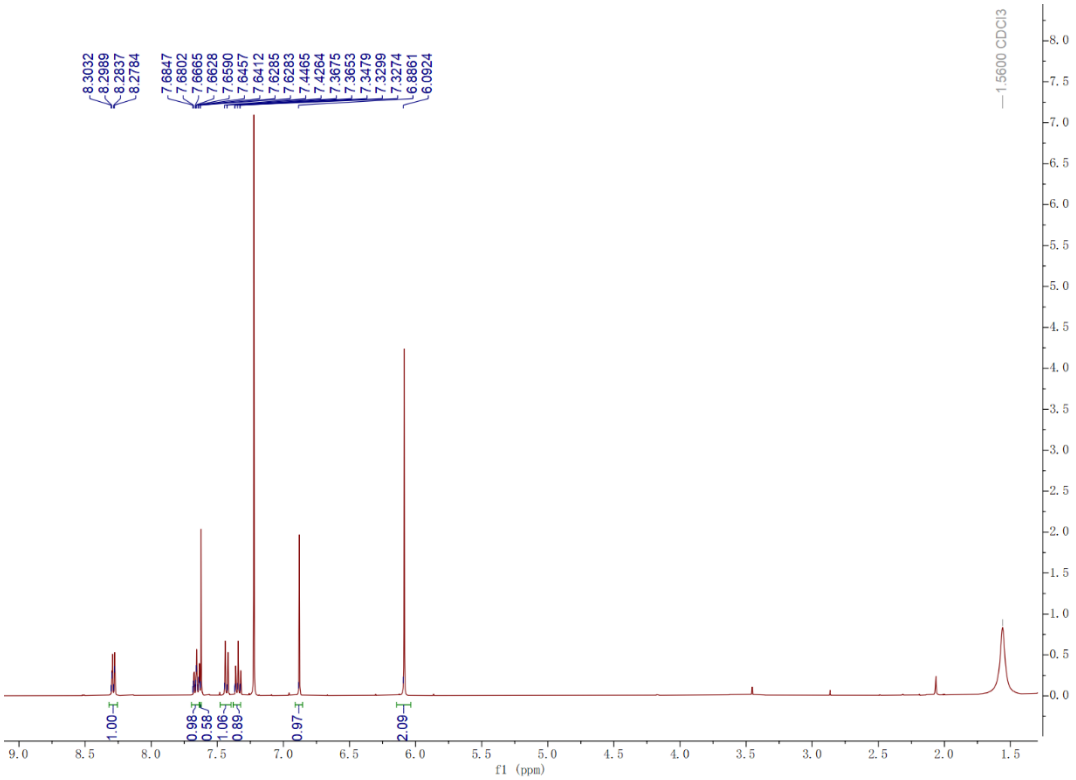


Figure S1: ^{1}H NMR spectrum of compound **1** in $CDCl_3$ (400 MHz).

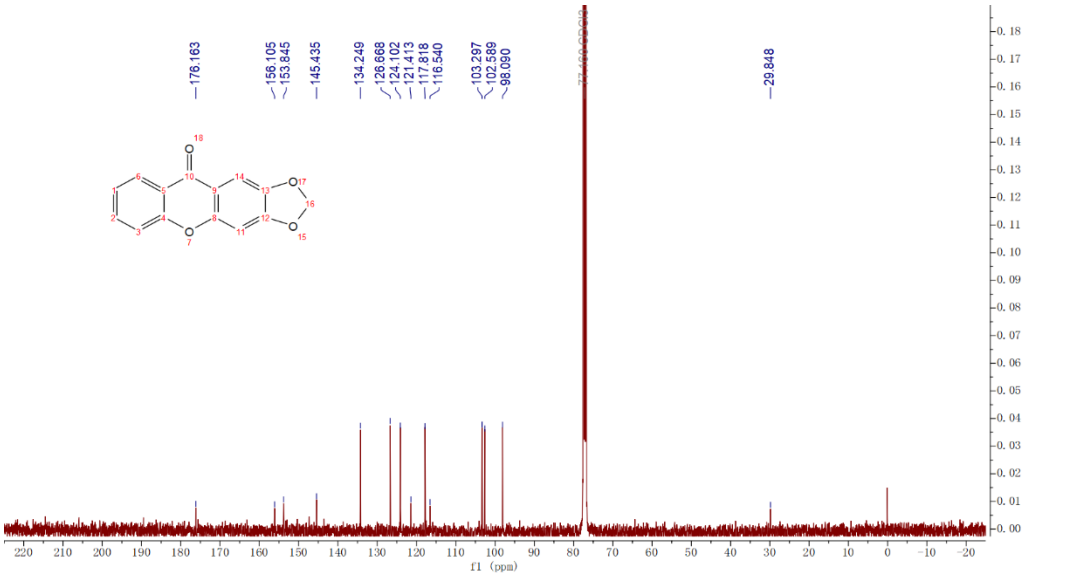


Figure S2: ^{13}C NMR spectrum of compound **1** in $CDCl_3$ (100 MHz).

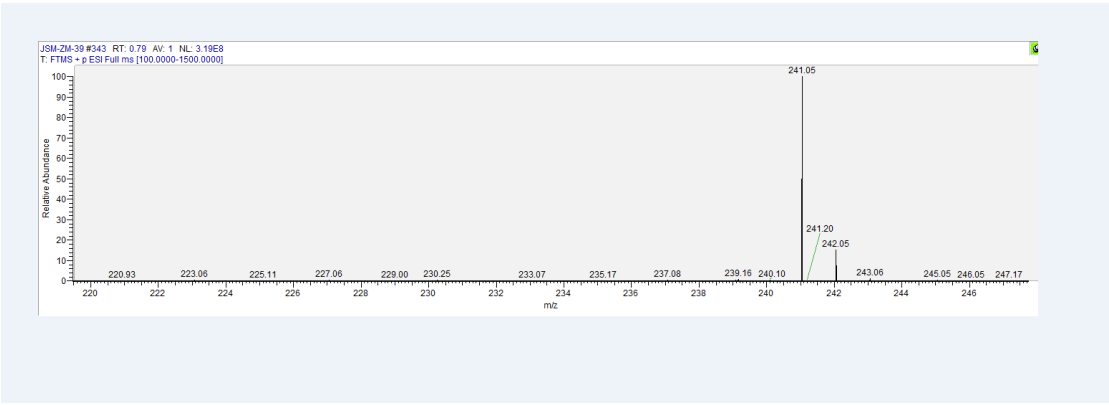


Figure S3: ESI-MS spectrum of compound **1**.

Compound **2**: $C_{13}H_8O_4$; ESI-MS *m/z*: 229 $[M+H]^+$, 227 $[M-H]^-$.

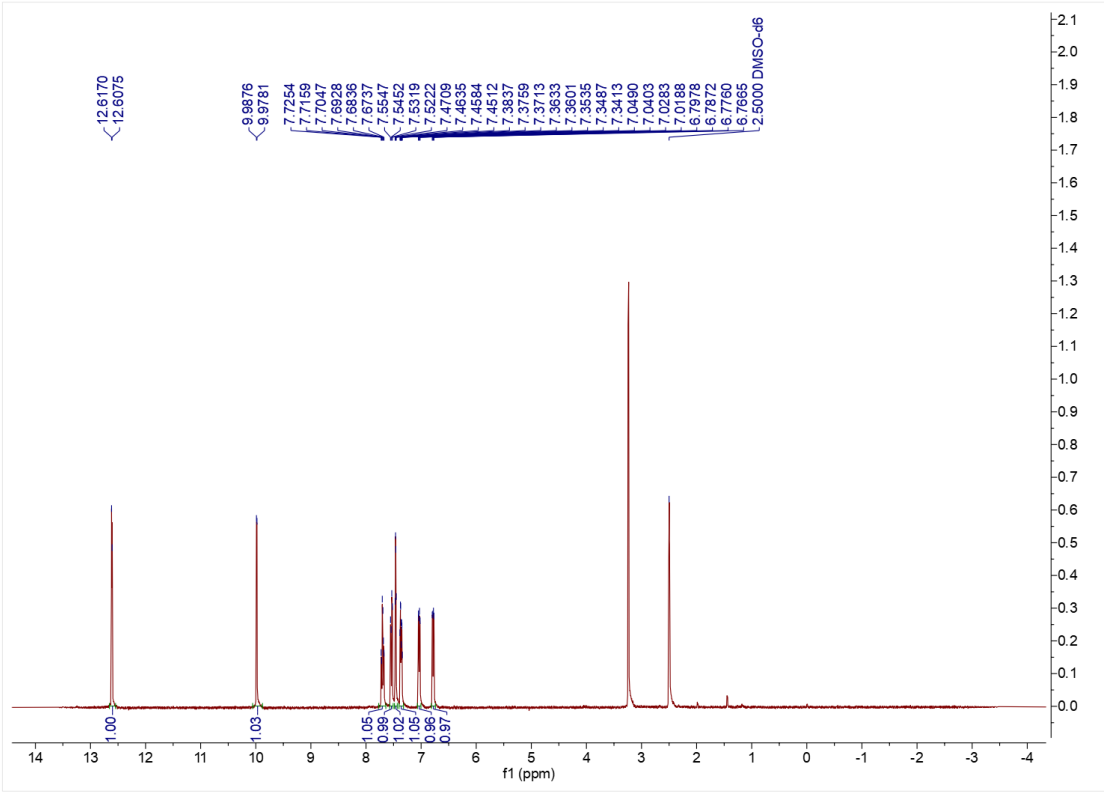


Figure S4: ^{1}H NMR spectrum of compound **2** in DMSO-d_6 (400 MHz).

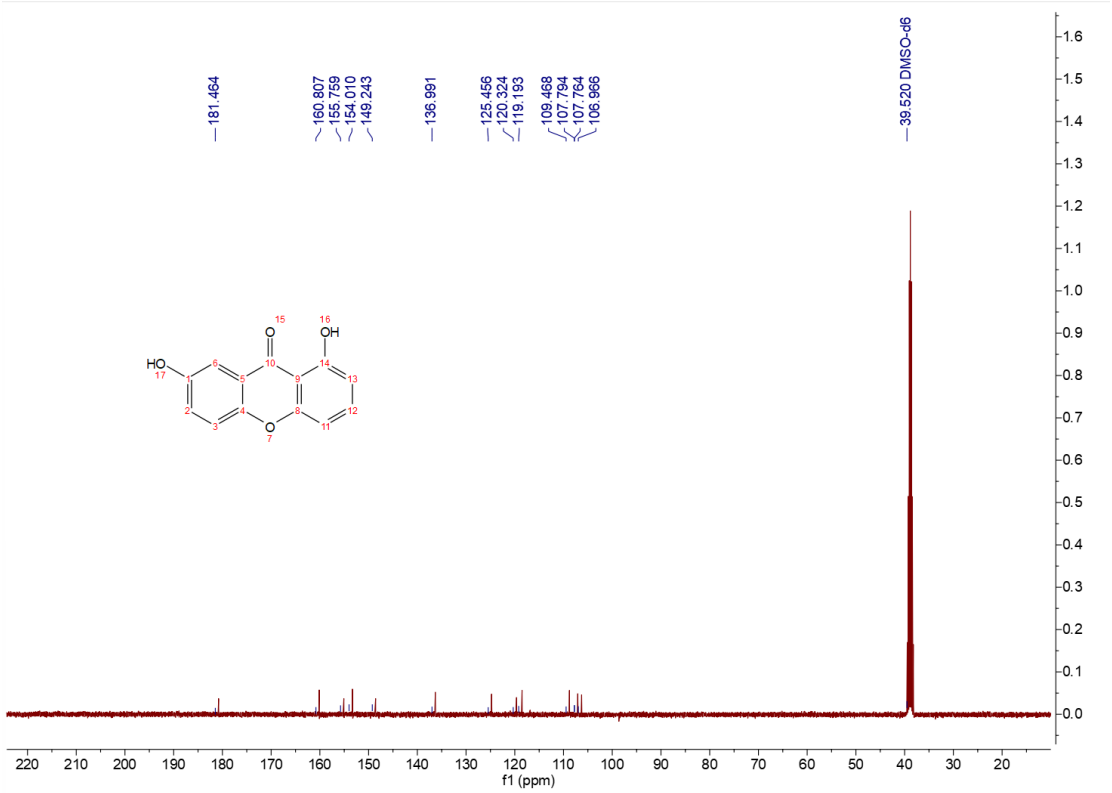
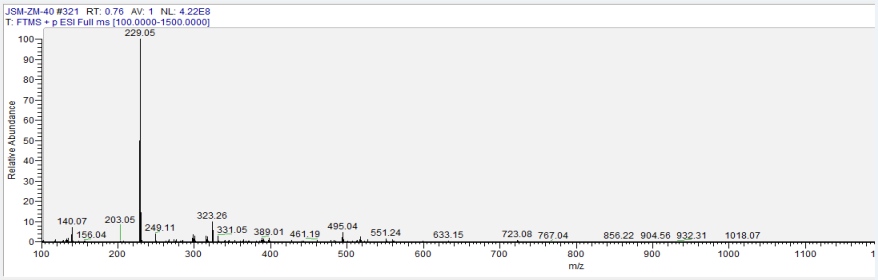


Figure S5: ^{13}C NMR spectrum of compound **2** in DMSO-d_6 (100 MHz).



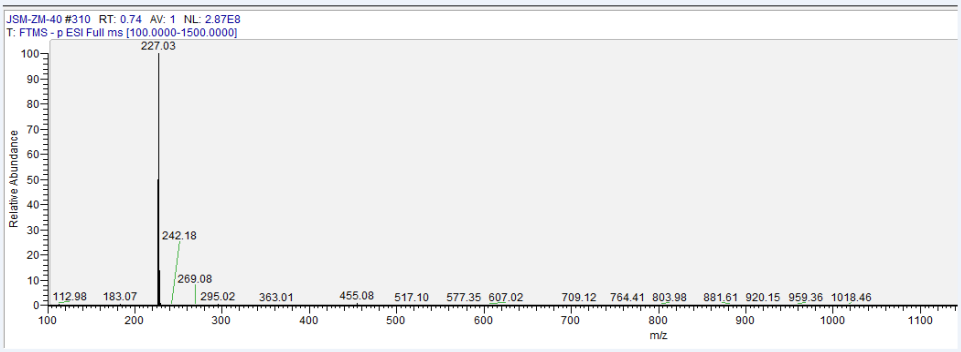


Figure S6: ESI-MS spectrum of compound **2**.

Compound **3**: $C_{14}H_{10}O_4$; ESI-MS *m/z*: 241 $[M-H]^-$, 243 $[M+H]^+$.

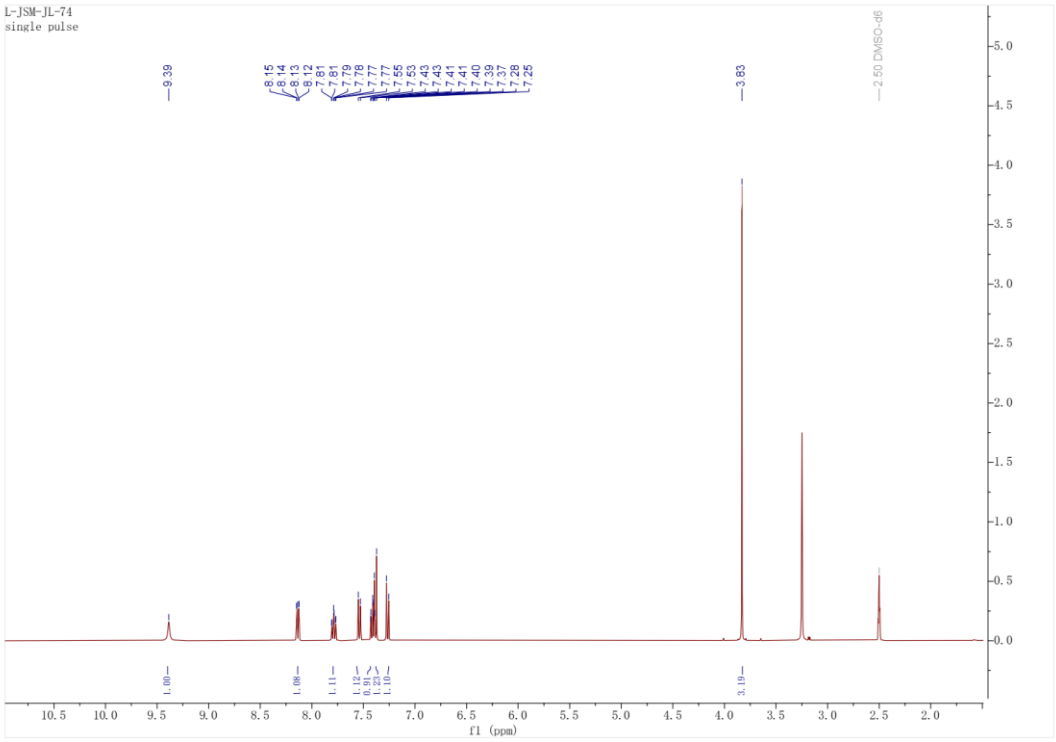


Figure S7: ^{1}H NMR spectrum of compound **3** in DMSO-*d*$_6$ (400 MHz).

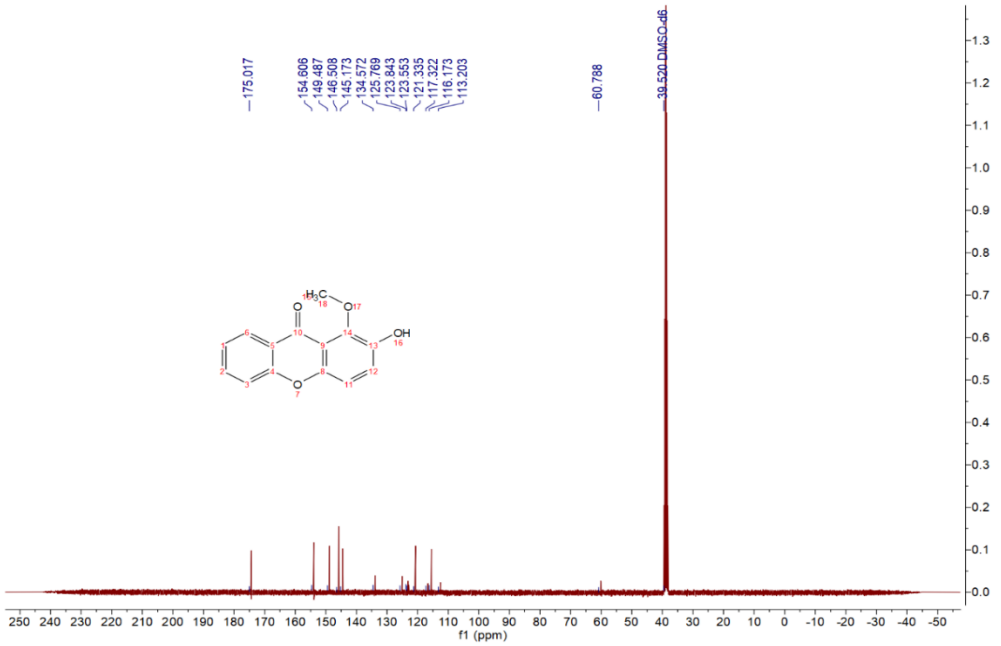


Figure S8: ^{13}C NMR spectrum of compound **3** in DMSO-*d*$_6$ (100 MHz).

Figure S9: ESI-MS spectrum of compound **3**.

Compound **4**: $C_{14}H_{10}O_5$; ESI-MS *m/z*: 257 $[M-H]^-$.

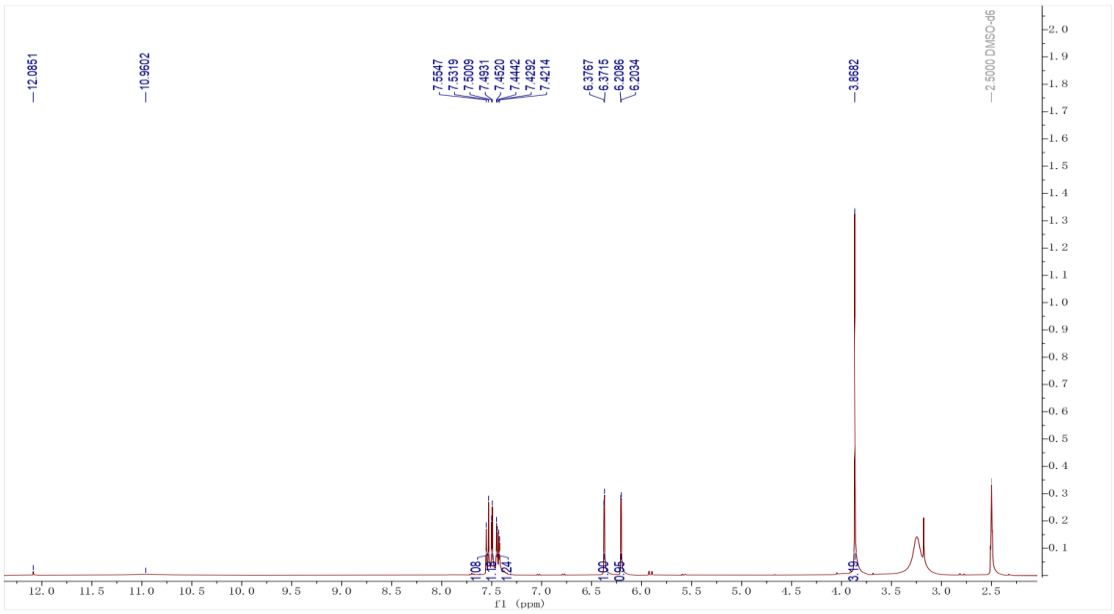


Figure S10: ^{1}H NMR spectrum of compound **4** in DMSO-d_6 (400 MHz).

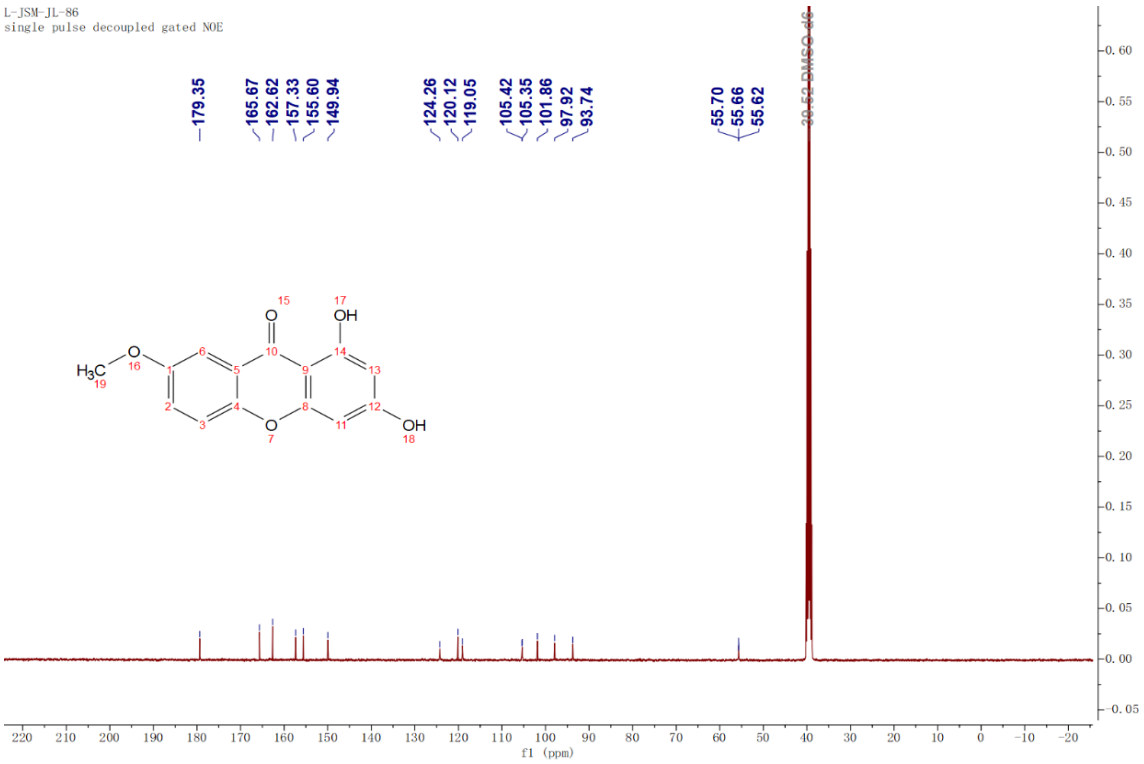


Figure S11: ^{13}C NMR spectrum of compound **4** in DMSO-d_6 (100 MHz).

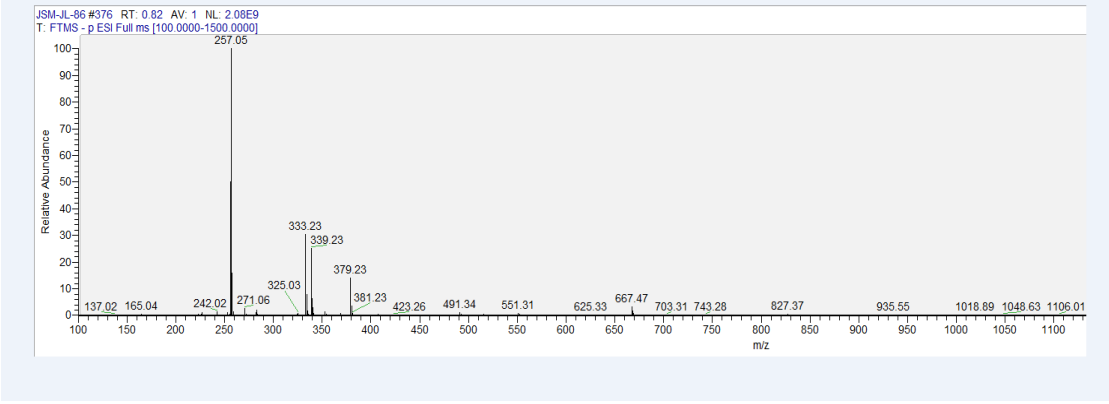


Figure S12: ESI-MS spectrum of compound **4**.

Compound **5**: $C_{14}H_{10}O_5$; ESI-MS *m/z*: 257 $[M-H]^-$, 259 $[M+H]^+$.

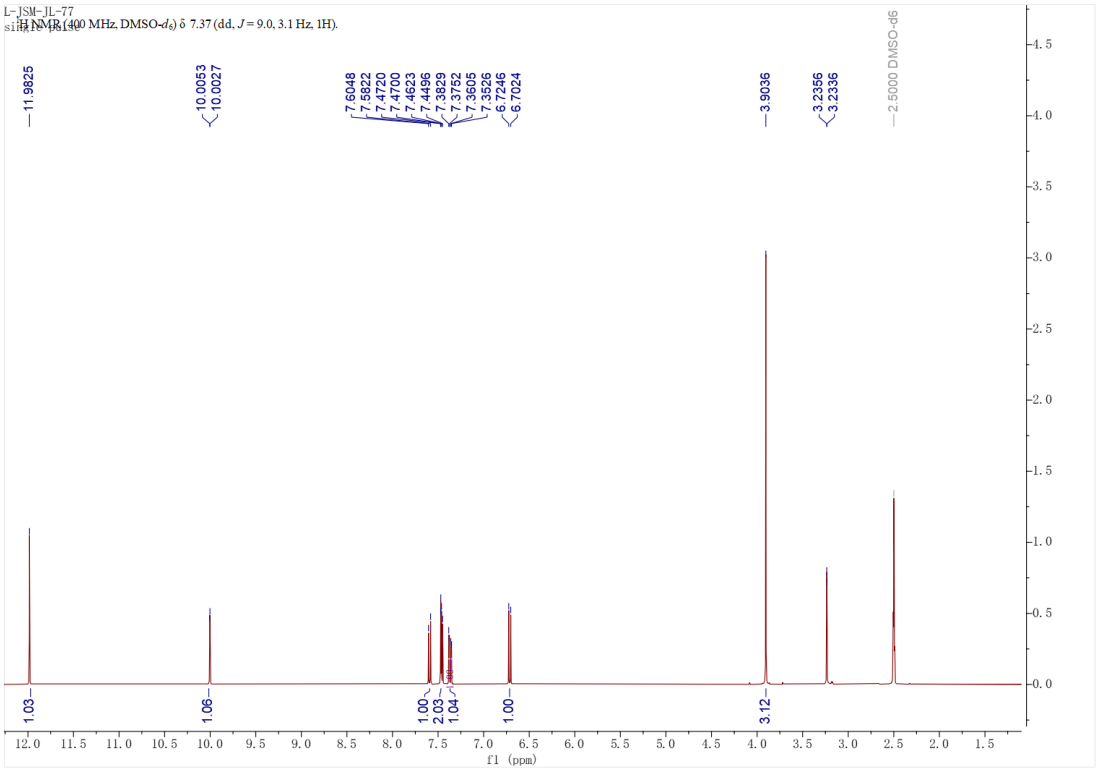


Figure S13: ^{1}H NMR spectrum of compound **5** in DMSO-d_6 (400 MHz).

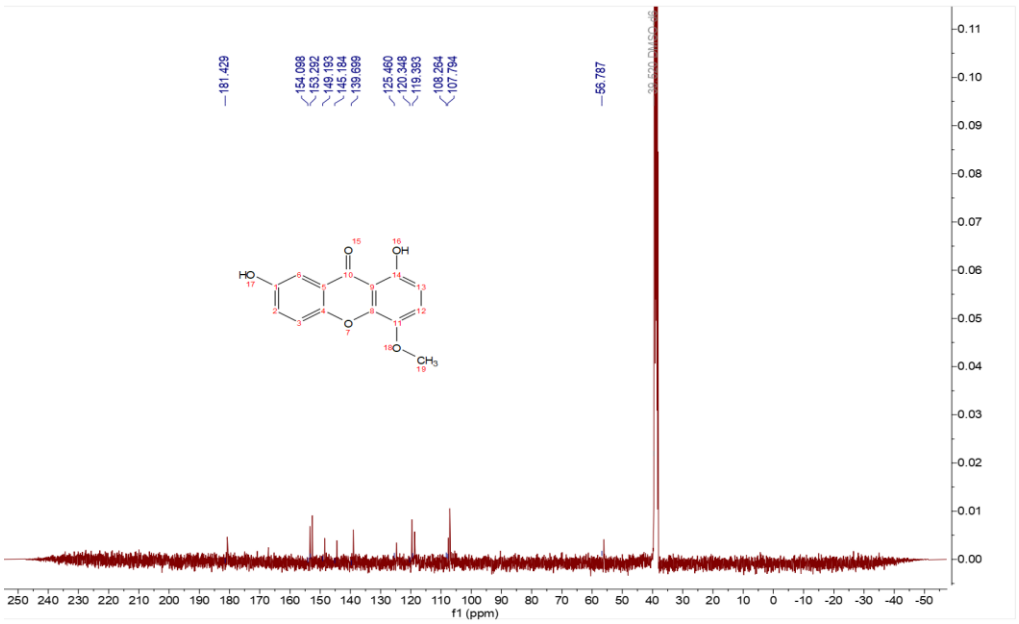


Figure S14: ^{13}C NMR spectrum of compound **5** in DMSO-d_6 (100 MHz).

Figure S15: ESI-MS spectrum of compound **5**.

Compound **6**: $C_{18}H_{14}O_6$; ESI-MS *m/z*: 325 $[M-H]^-$, 327 $[M+H]^+$.

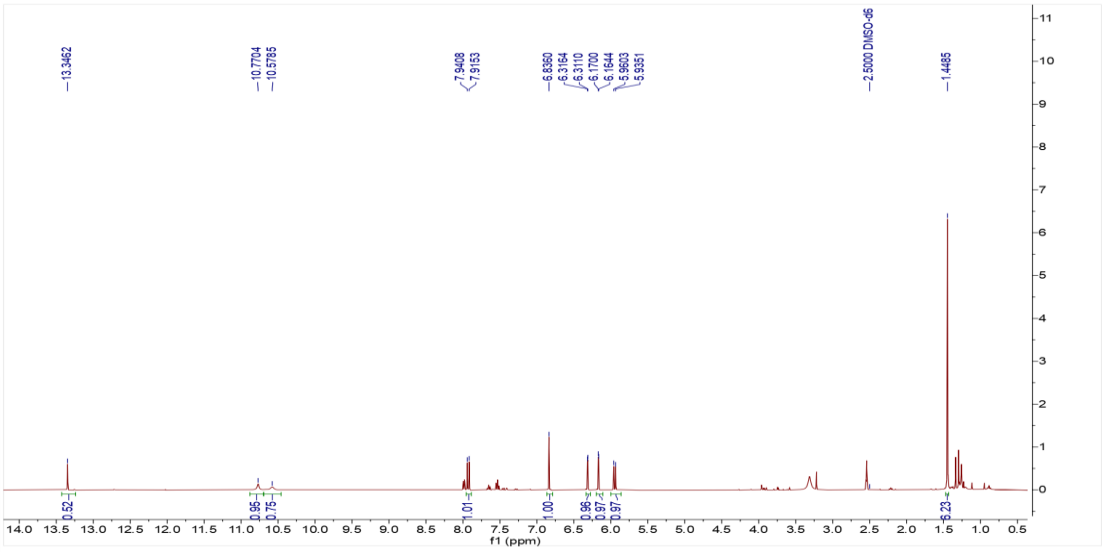


Figure S16: ^{1}H NMR spectrum of compound **6** in DMSO-d_6 (400 MHz).

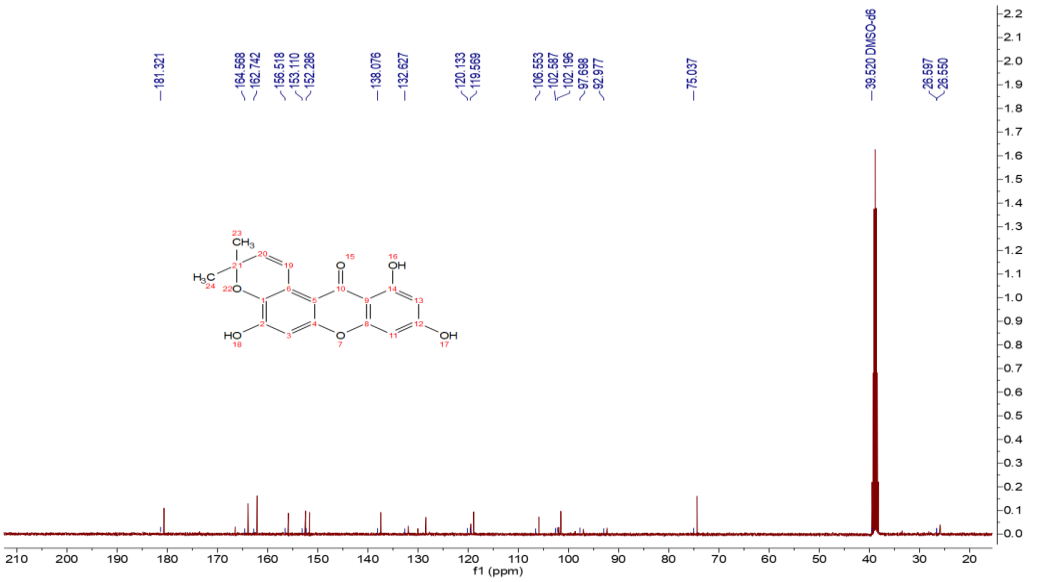
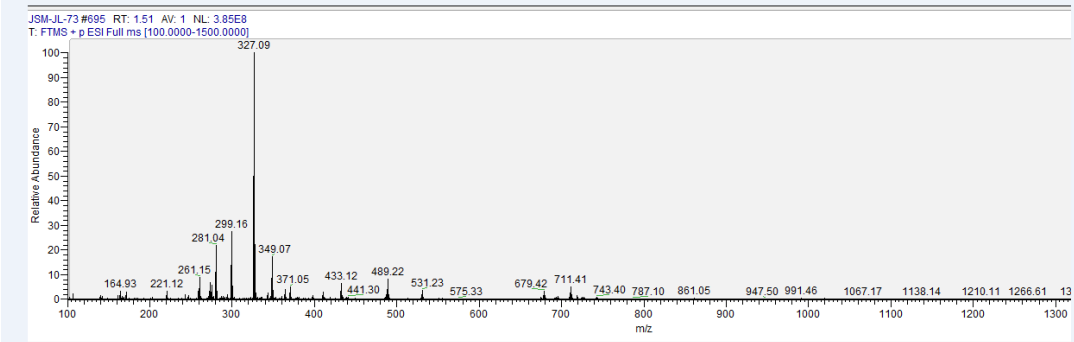


Figure S17: ^{13}C NMR spectrum of compound **6** in DMSO-d_6 (100 MHz).



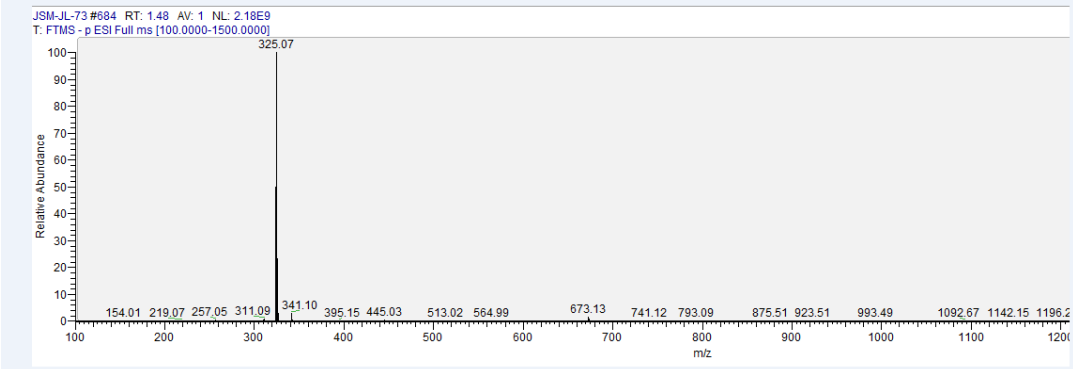


Figure S18: ESI-MS spectrum of compound **6**.

Compound **7**: $C_{14}H_{10}O_5$; ESI-MS *m/z*: 257 $[M-H]^-$.

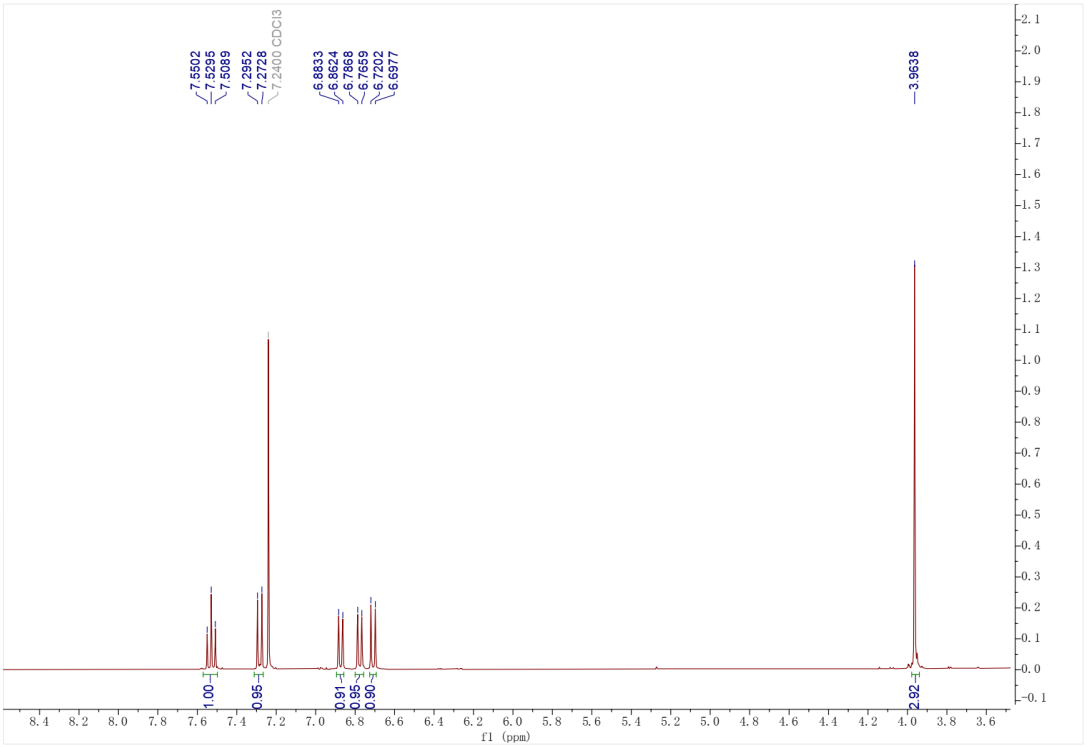


Figure S19: ^{1}H NMR spectrum of compound **7** in $CDCl_3$ (400 MHz).

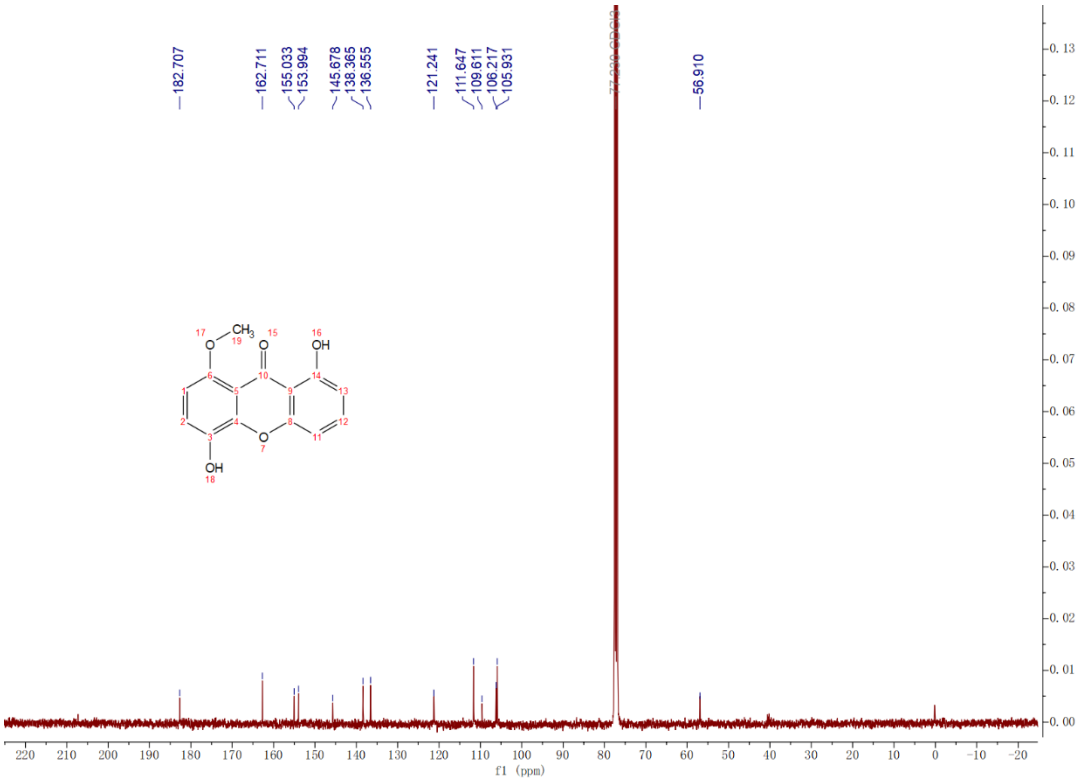


Figure S20: ^{13}C NMR spectrum of compound **7** in $CDCl_3$ (100 MHz).

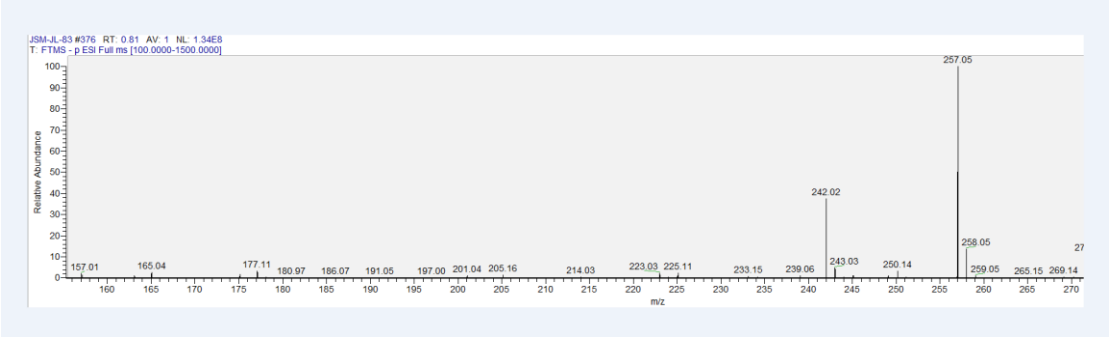


Figure S21: ESI-MS spectrum of compound **7**.

Compound **8**: $C_{14}H_{10}O_4$; ESI-MS *m/z*: 243 $[M+H]^+$, 241 $[M-H]^-$.

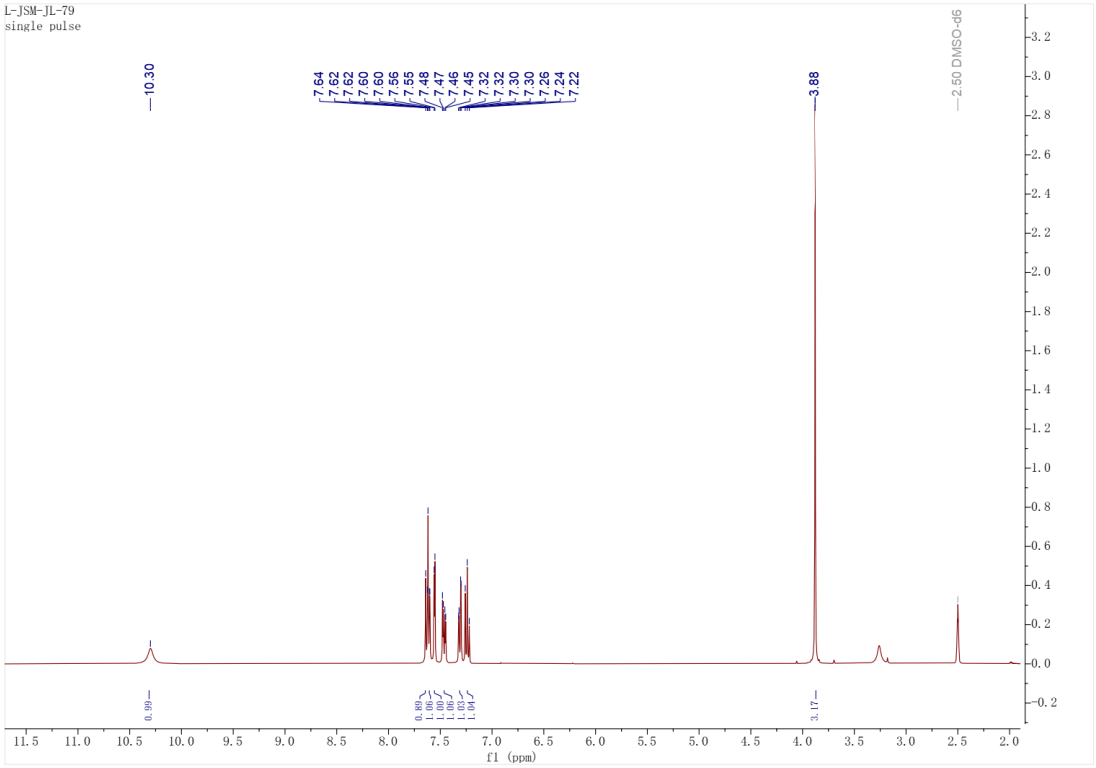


Figure 22: ^{1}H NMR spectrum of compound **8** in DMSO-d_6 (400 MHz).

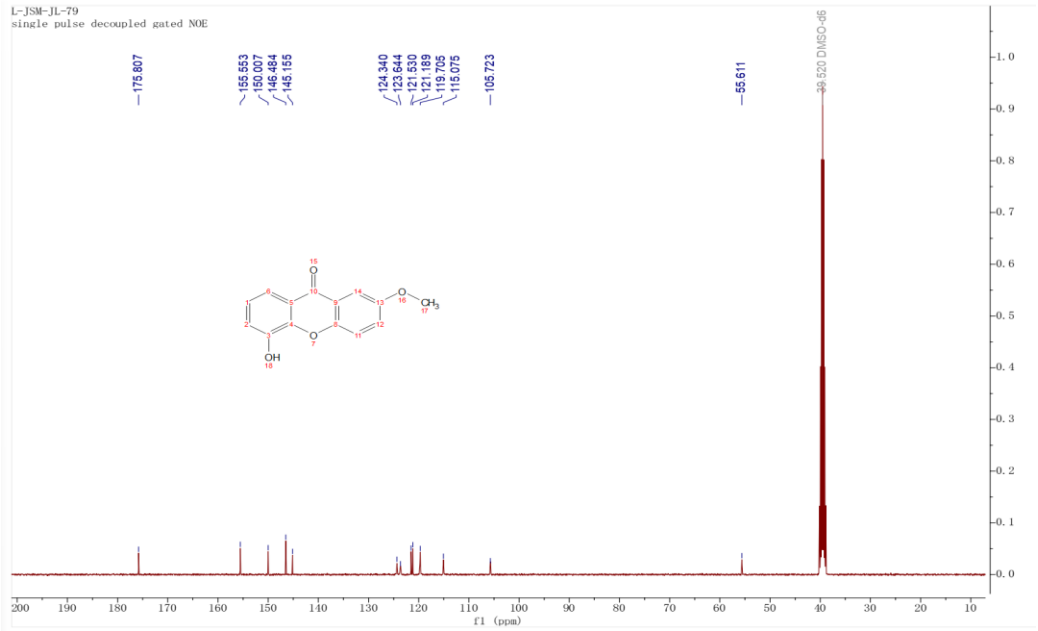


Figure S23: ^{13}C NMR spectrum of compound **8** in DMSO-d_6 (100 MHz).

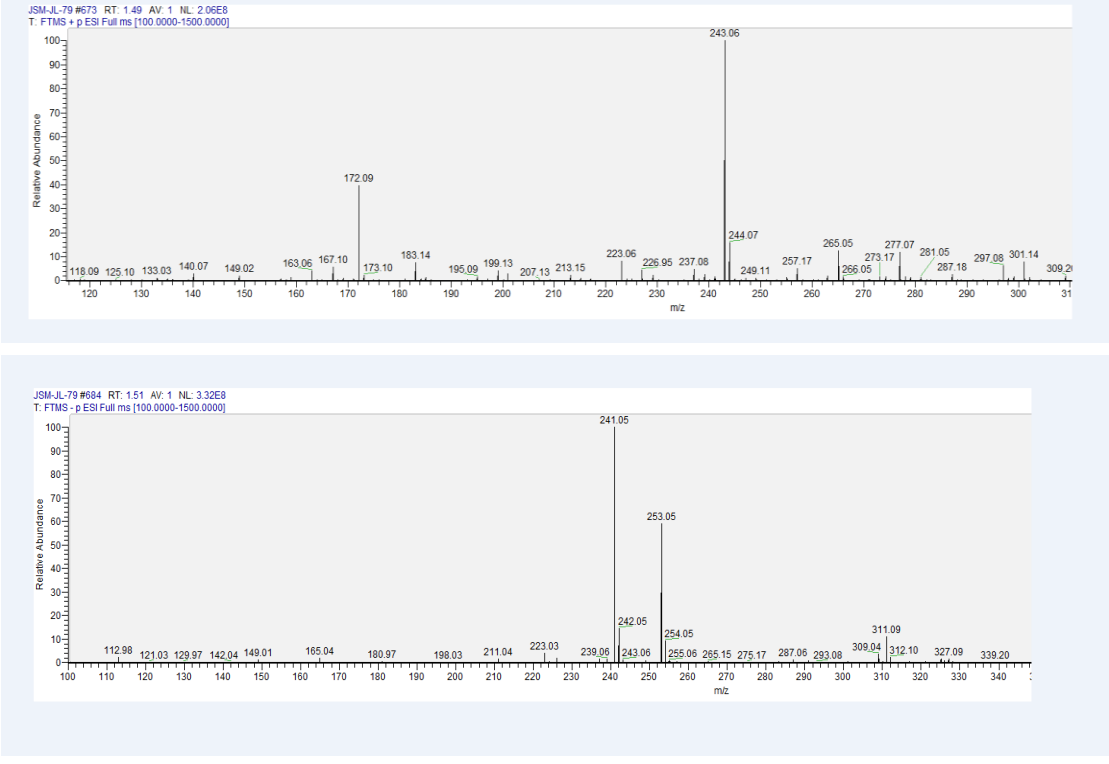


Figure S24: ESI-MS spectrum of compound **8**.

Compound **9**: $C_{14}H_{10}O_4$; ESI-MS *m/z*: 241 $[M-H]^-$.

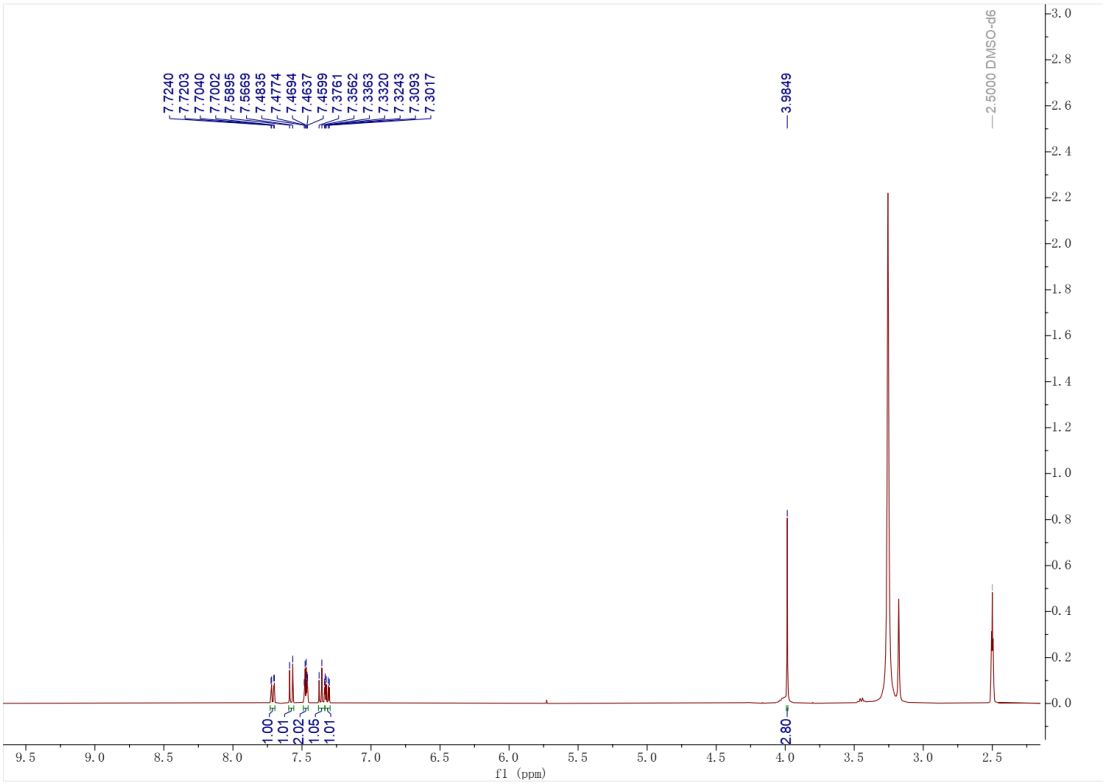


Figure S25: ^{1}H NMR spectrum of compound **9** in DMSO-d_6 (400 MHz).

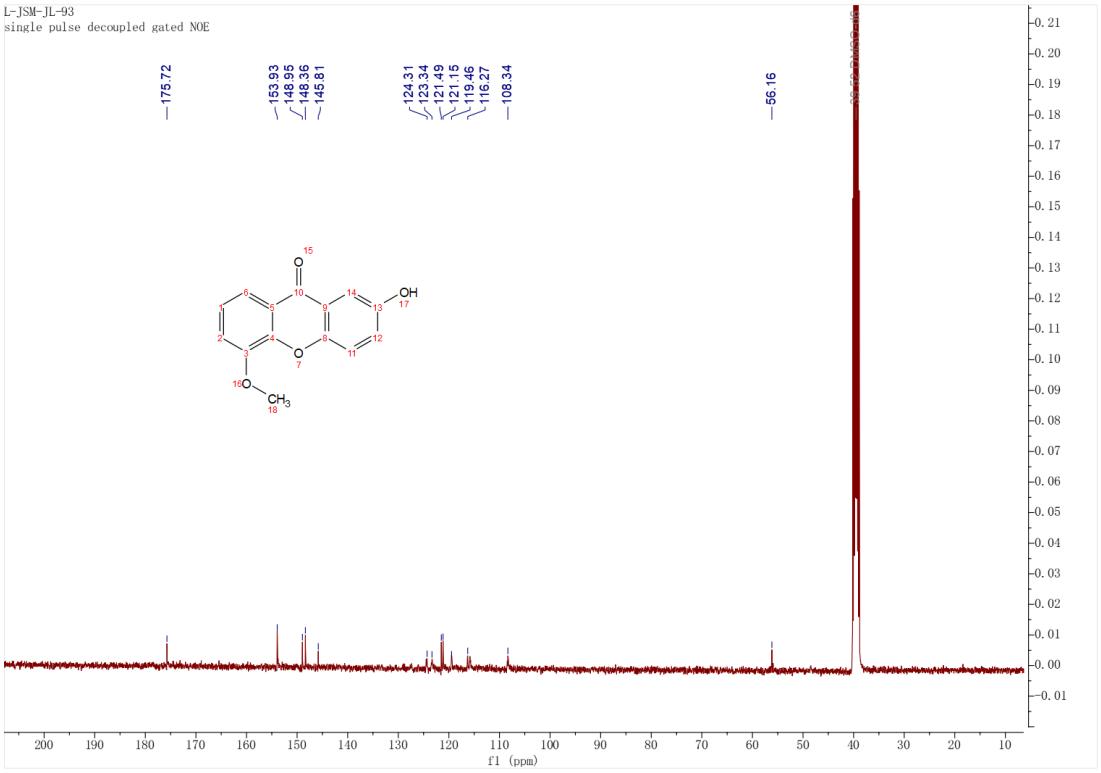


Figure S26: ^{13}C NMR spectrum of compound **9** in DMSO-d_6 (100 MHz).

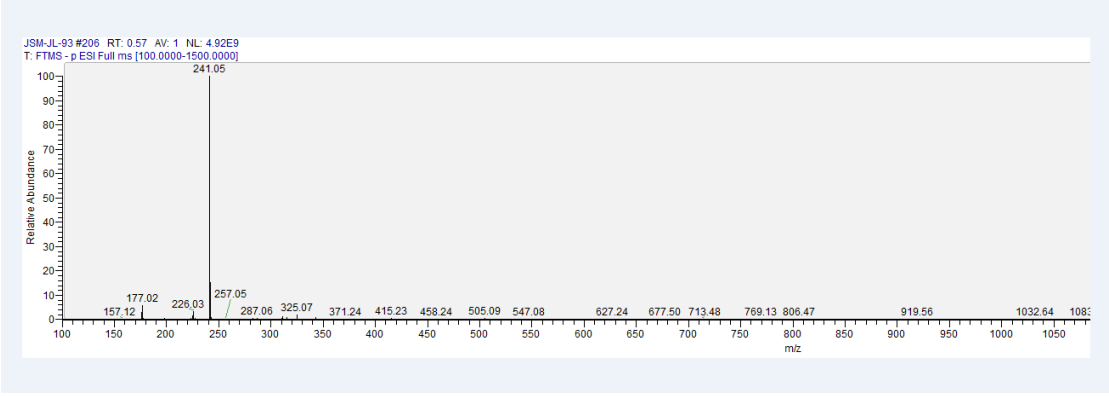


Figure S27: ESI-MS spectrum of compound **9**.

Compound **10**: $C_{13}H_8O_4$; ESI-MS *m/z*: 227 $[M-H]^-$, 229 $[M+H]^+$.

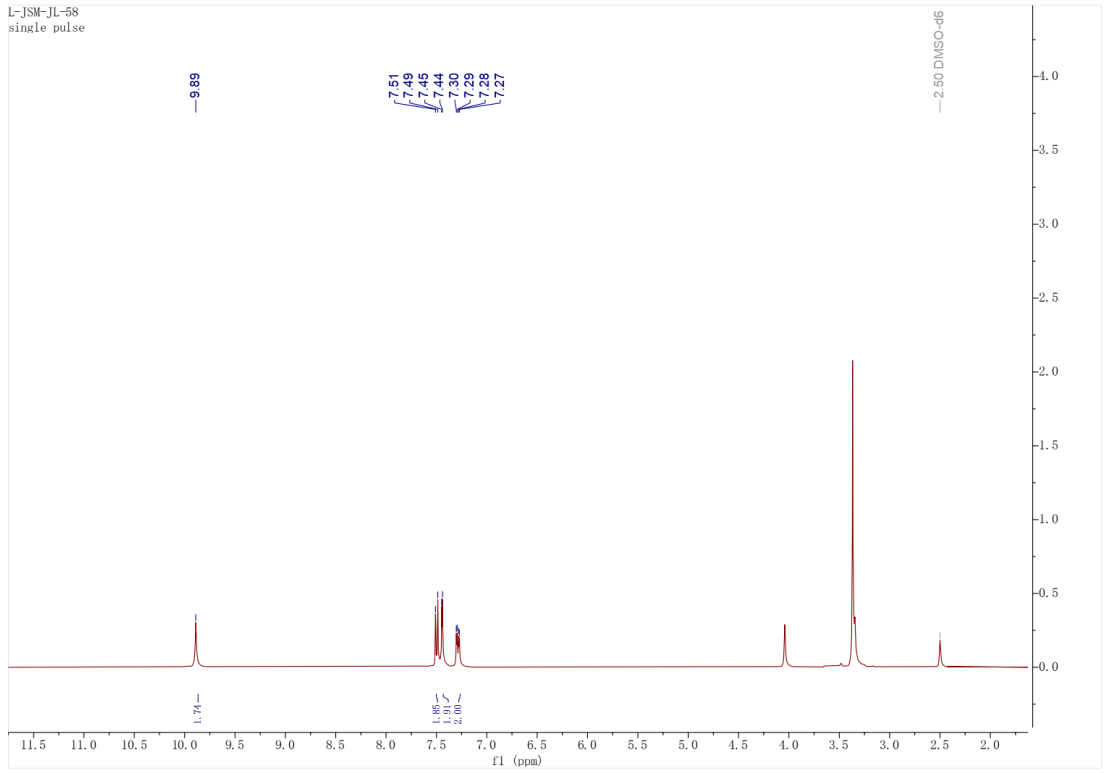


Figure S28: ^{1}H NMR spectrum of compound **10** in DMSO-d_6 (400 MHz).

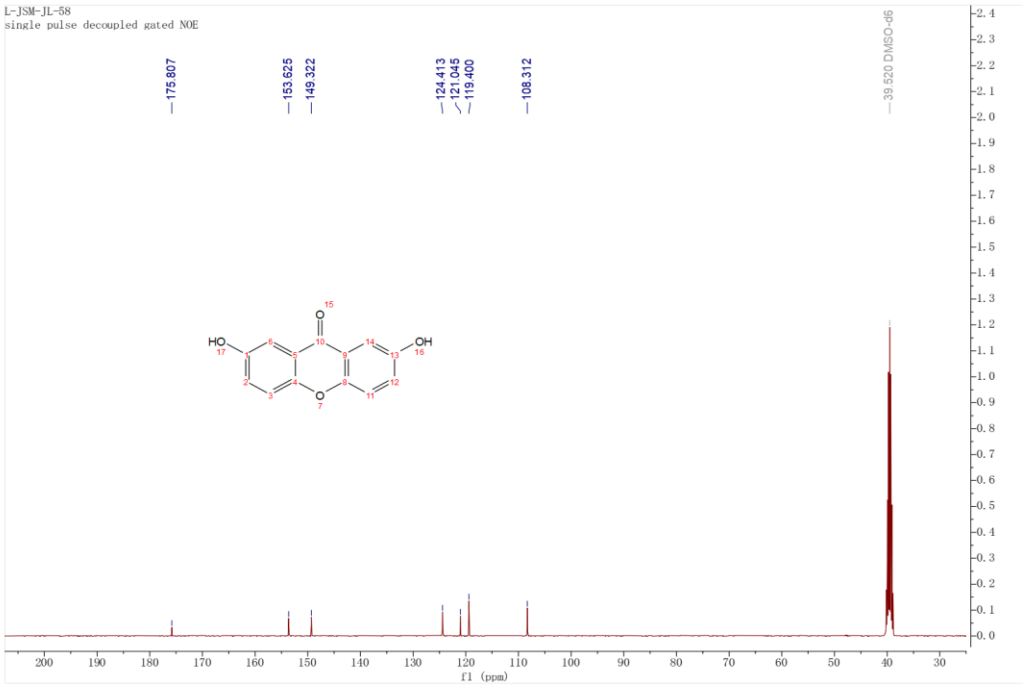
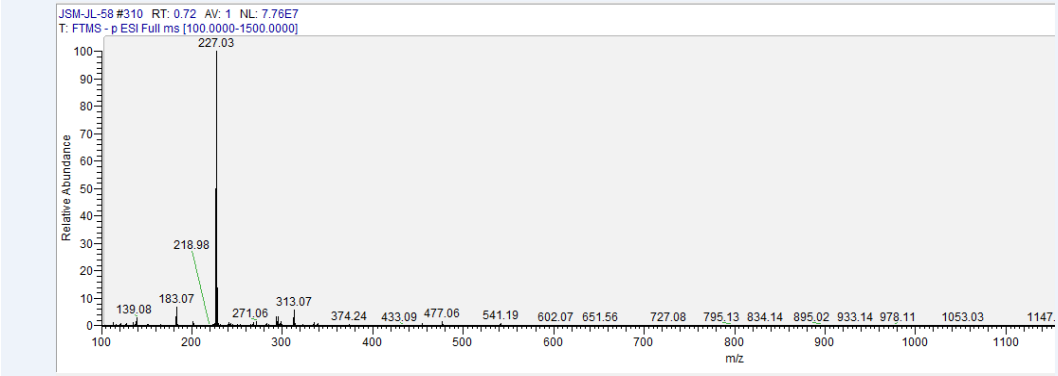


Figure S29: ^{13}C NMR spectrum of compound **10** in DMSO-d_6 (100 MHz).



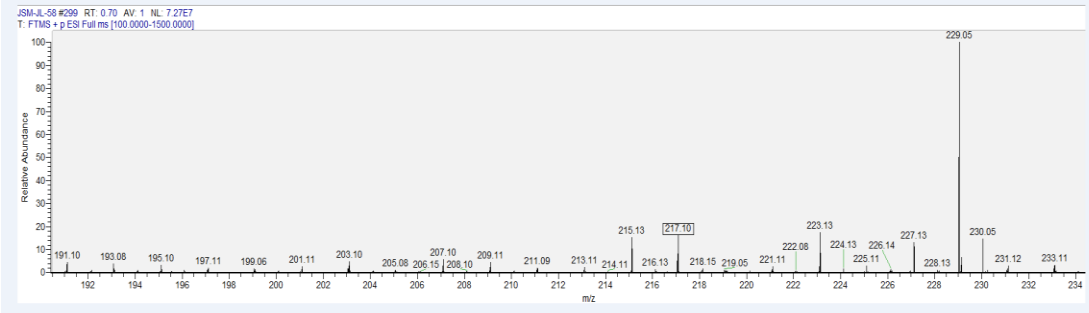


Figure S30: ESI-MS spectrum of compound **10**.

Compound **11**: $C_{19}H_{18}O_{10}$; ESI-MS *m/z*: 405 $[M-H]^-$.

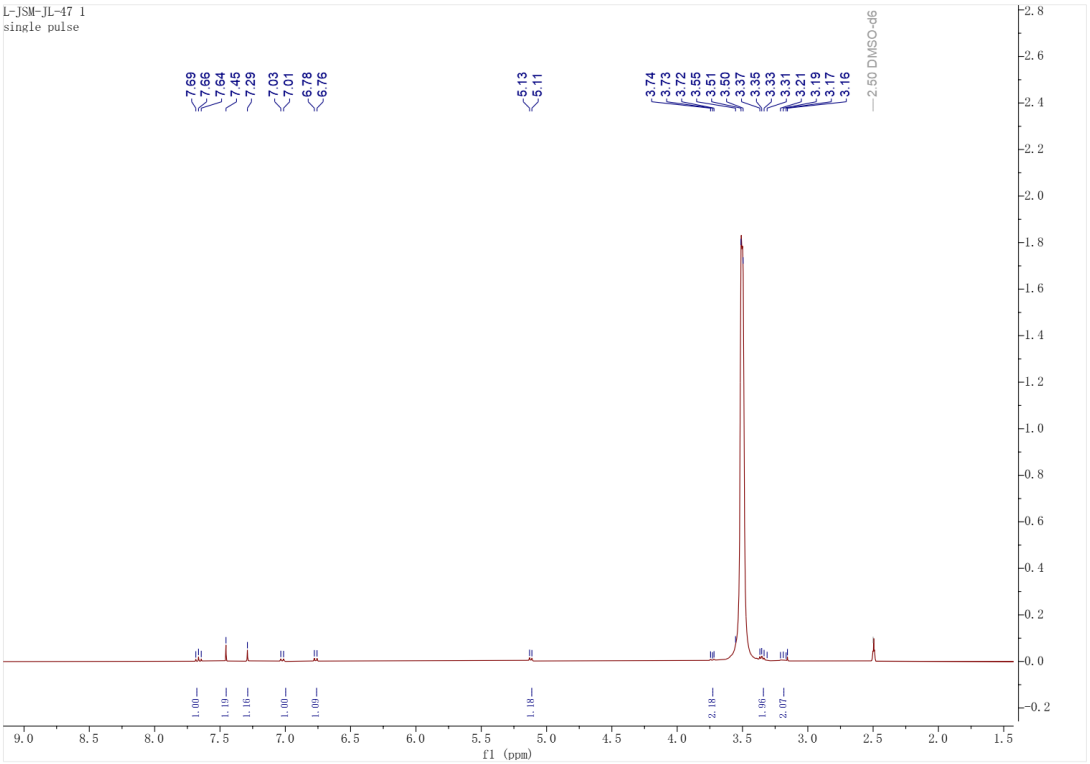


Figure S31: ^{1}H NMR spectrum of compound **11** in DMSO-d_6 (400 MHz).

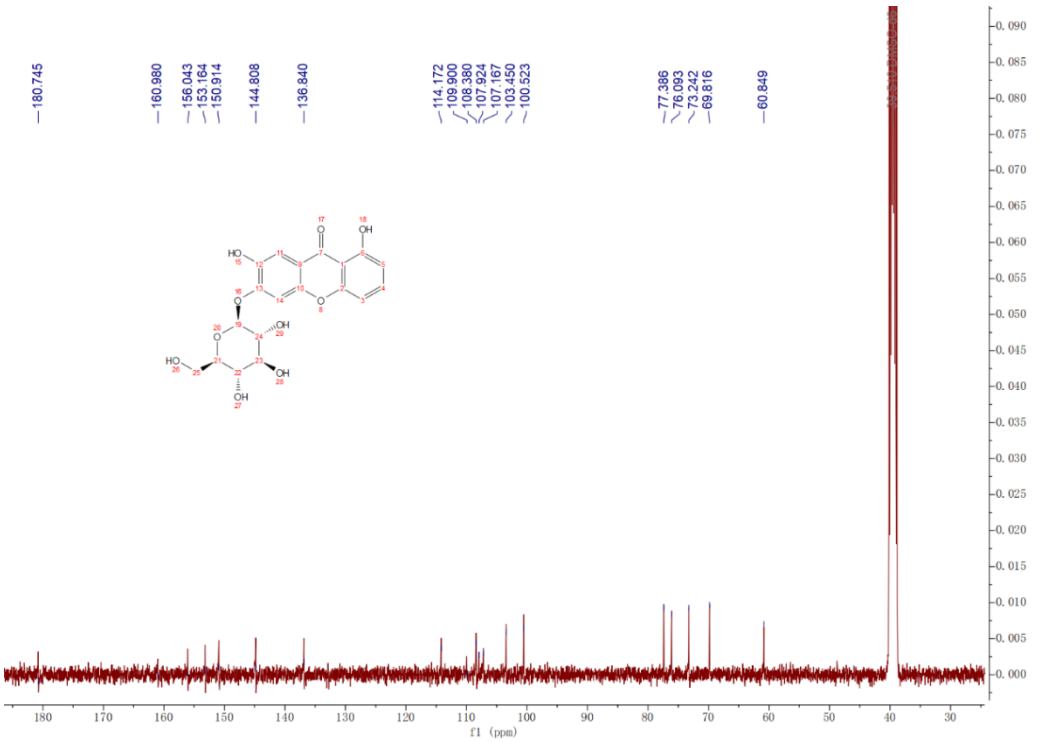


Figure S32: ^{13}C NMR spectrum of compound **11** in DMSO-d_6 (100 MHz).

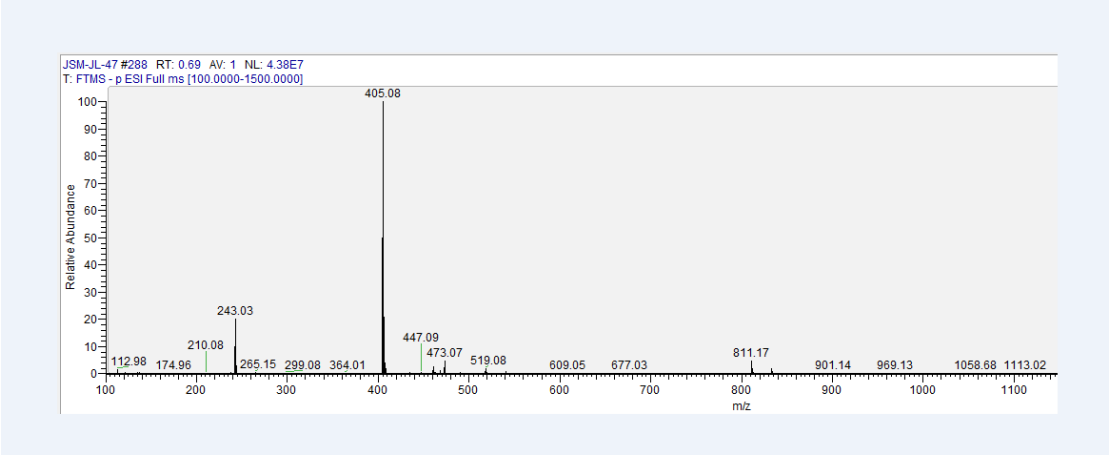


Figure S33: ESI-MS spectrum of compound **11**.

Compound **12**: $C_{13}H_8O_3$; ESI-MS *m/z*: 213 $[M+H]^+$.

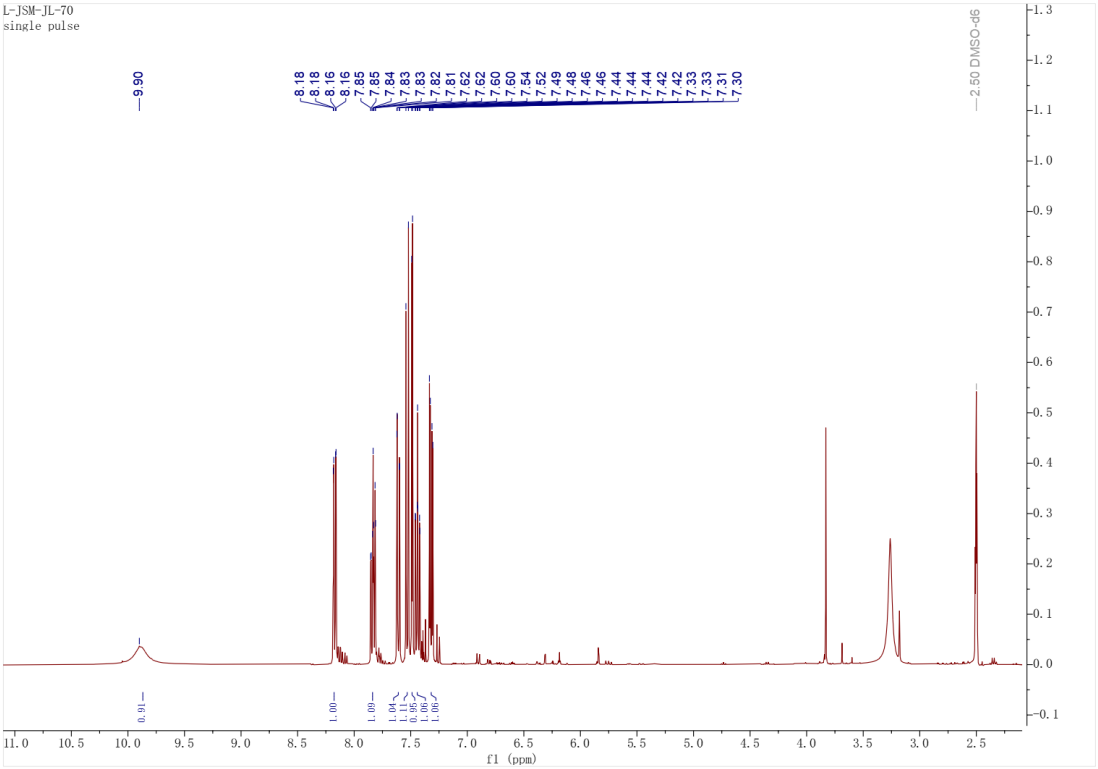


Figure S34: ^{1}H NMR spectrum of compound **12** in DMSO-d_6 (400 MHz).

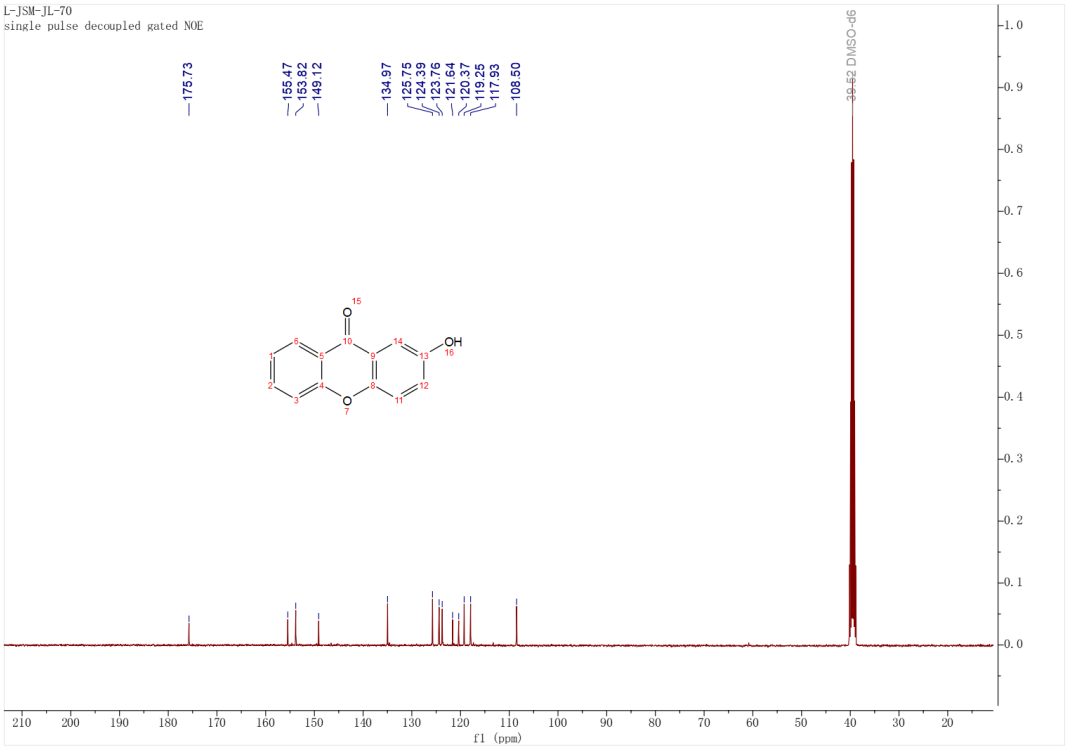


Figure S35: ^{13}C NMR spectrum of compound **12** in DMSO-d_6 (100 MHz).

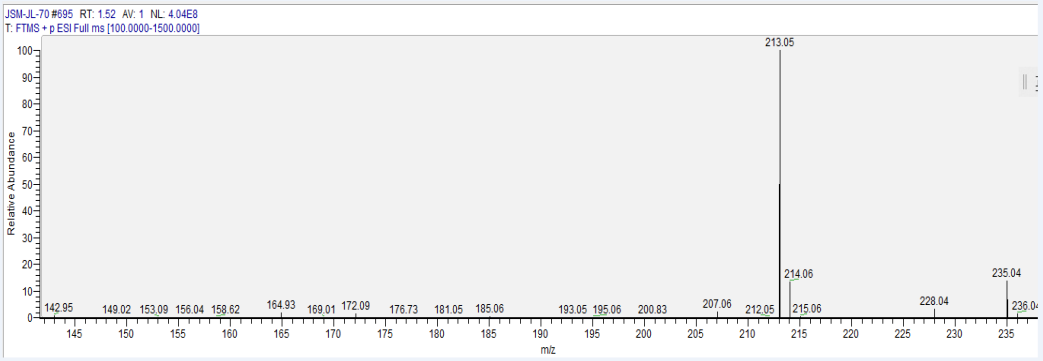


Figure S36: ESI-MS spectrum of compound **12**.

Compound **13**: $C_{18}H_{16}O_6$; ESI-MS *m/z*: 327 $[M-H]^-$.

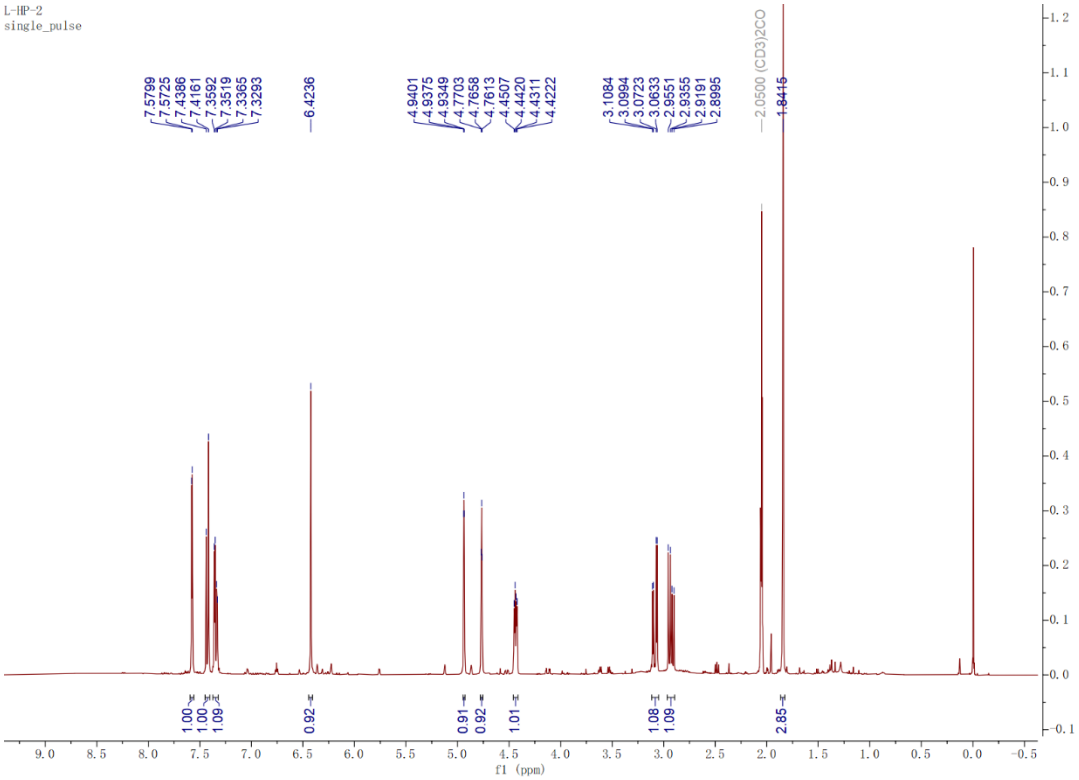


Figure S37: ^{1}H NMR spectrum of compound **13** in Acetone-d_6 (400 MHz).

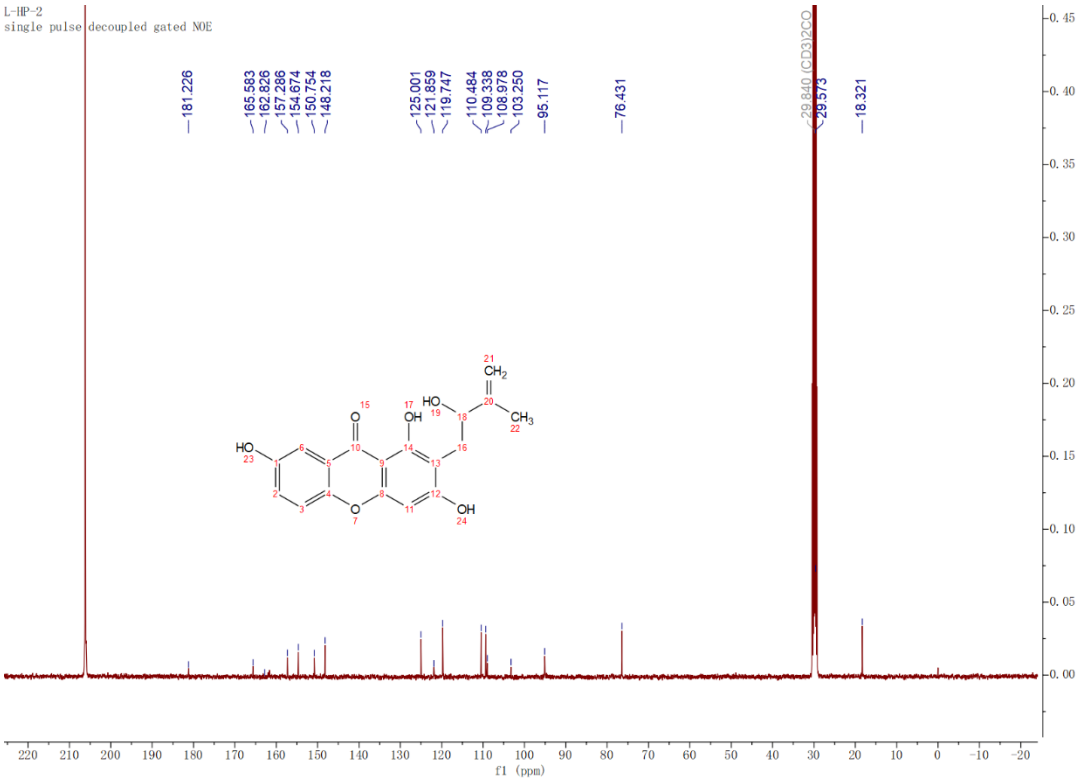


Figure S38: ^{13}C NMR spectrum of compound **13** in Acetone-d_6 (100 MHz).

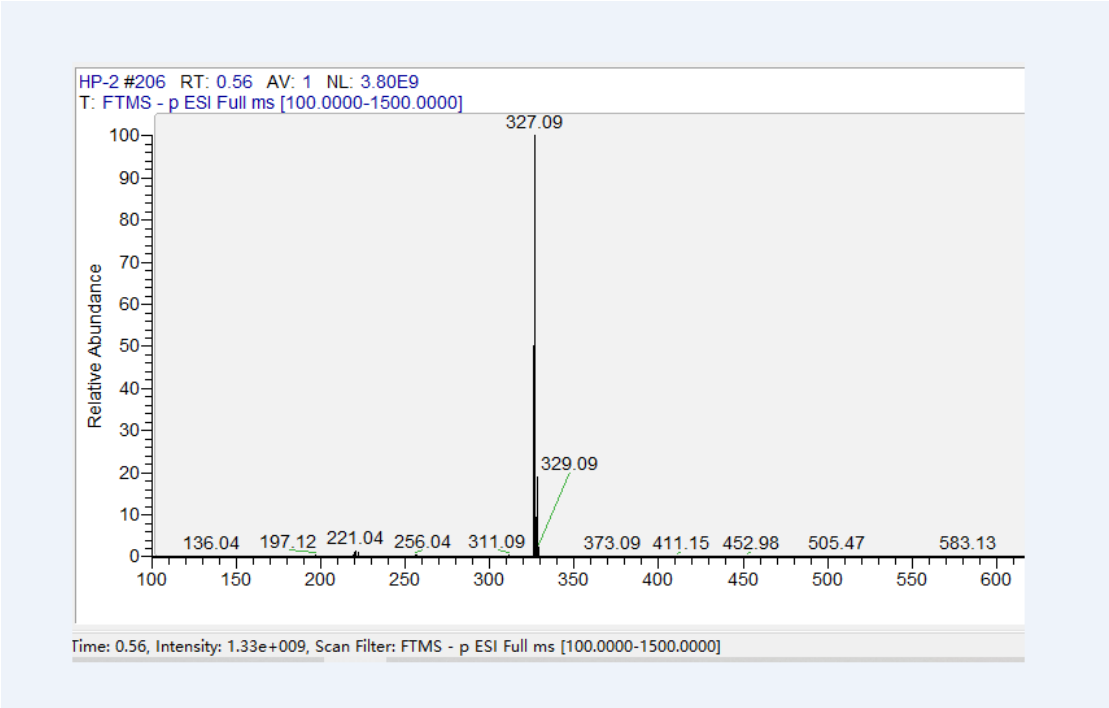


Figure S39: ESI-MS spectrum of compound **13**.

Compound **14**: $C_{18}H_{14}O_6$; ESI-MS *m/z*: 325 $[M–H]^-$.

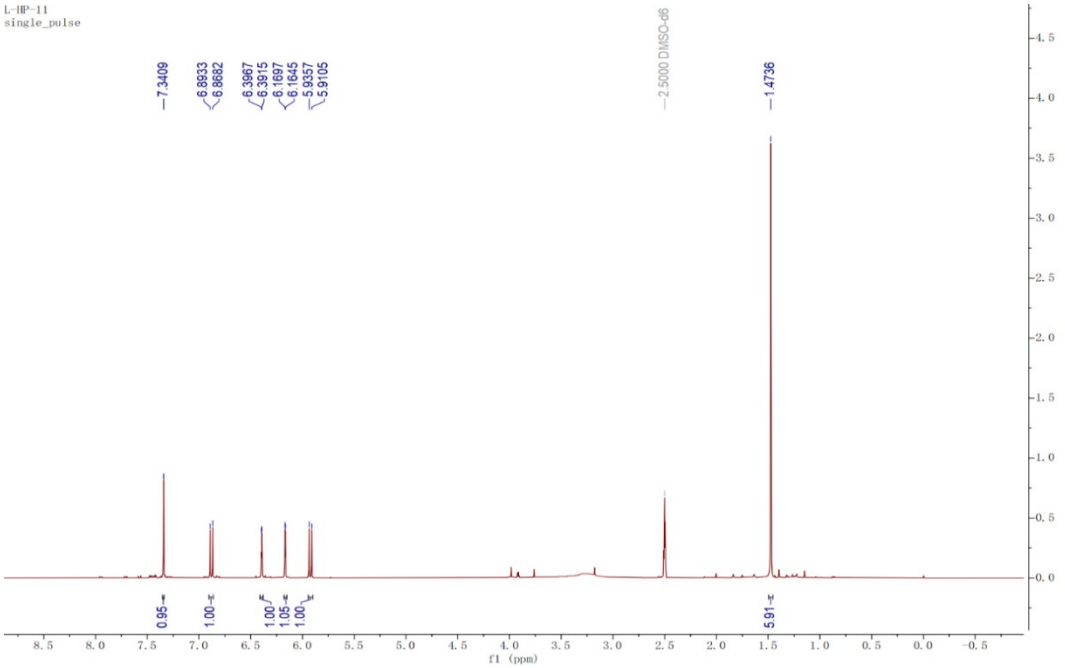


Figure S40: ^{1}H NMR spectrum of compound **14** in DMSO-d_6 (400 MHz).

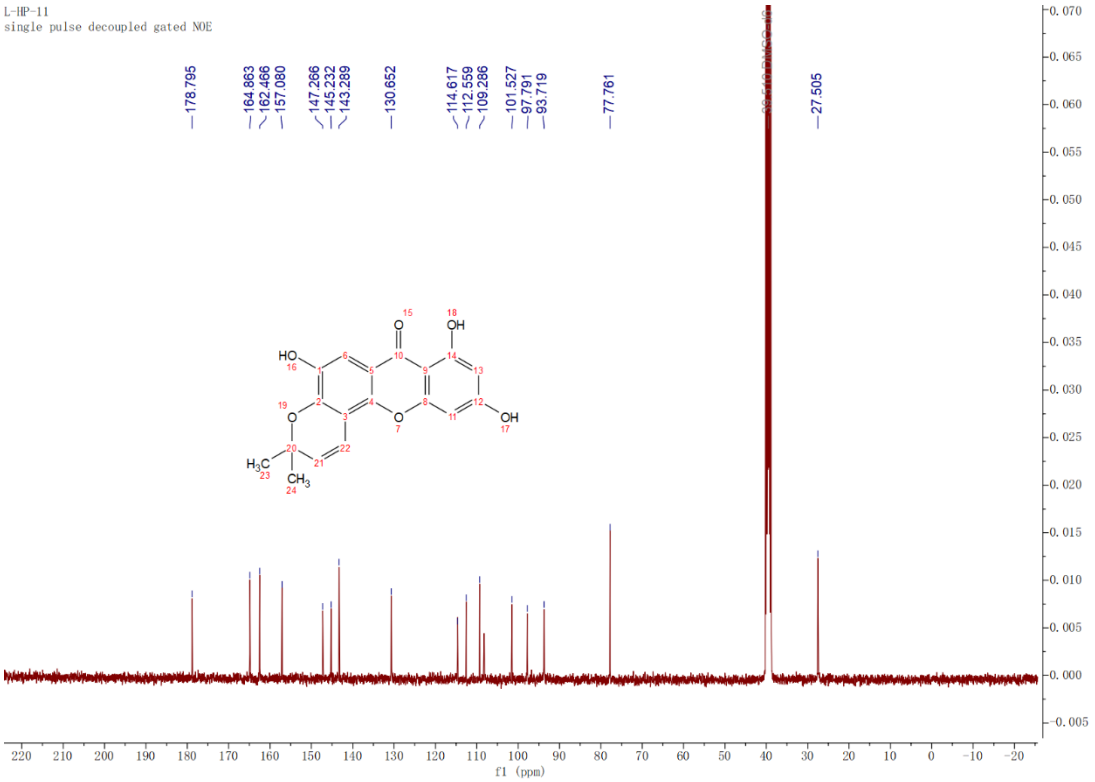


Figure S41: ^{13}C NMR spectrum of compound **14** in DMSO-d_6 (100 MHz).

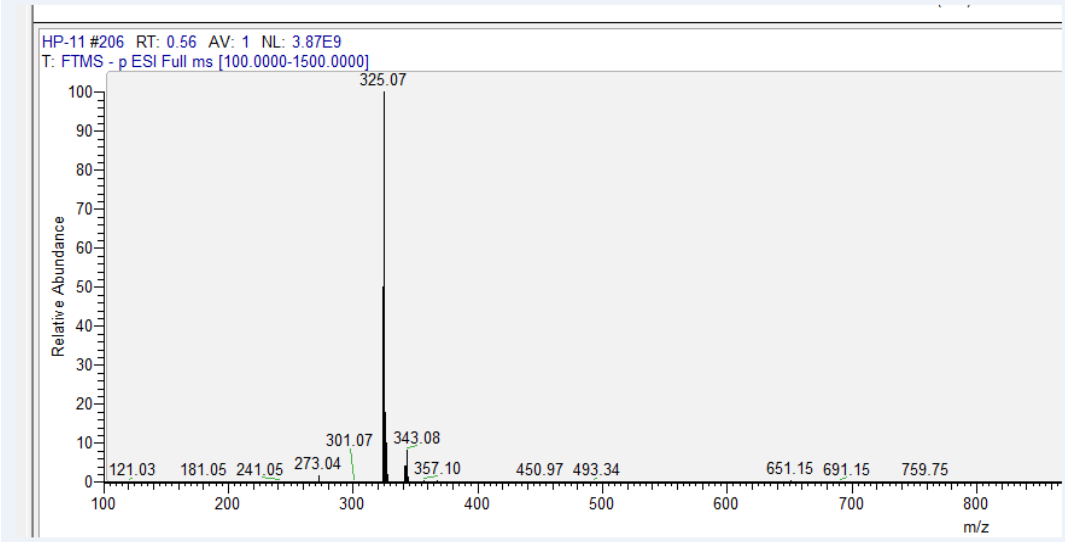


Figure S42: ESI-MS spectrum of compound **14**.

Compound **15**: $C_{18}H_{16}O_5$; ESI-MS *m/z*: 311 $[M–H]^-$.

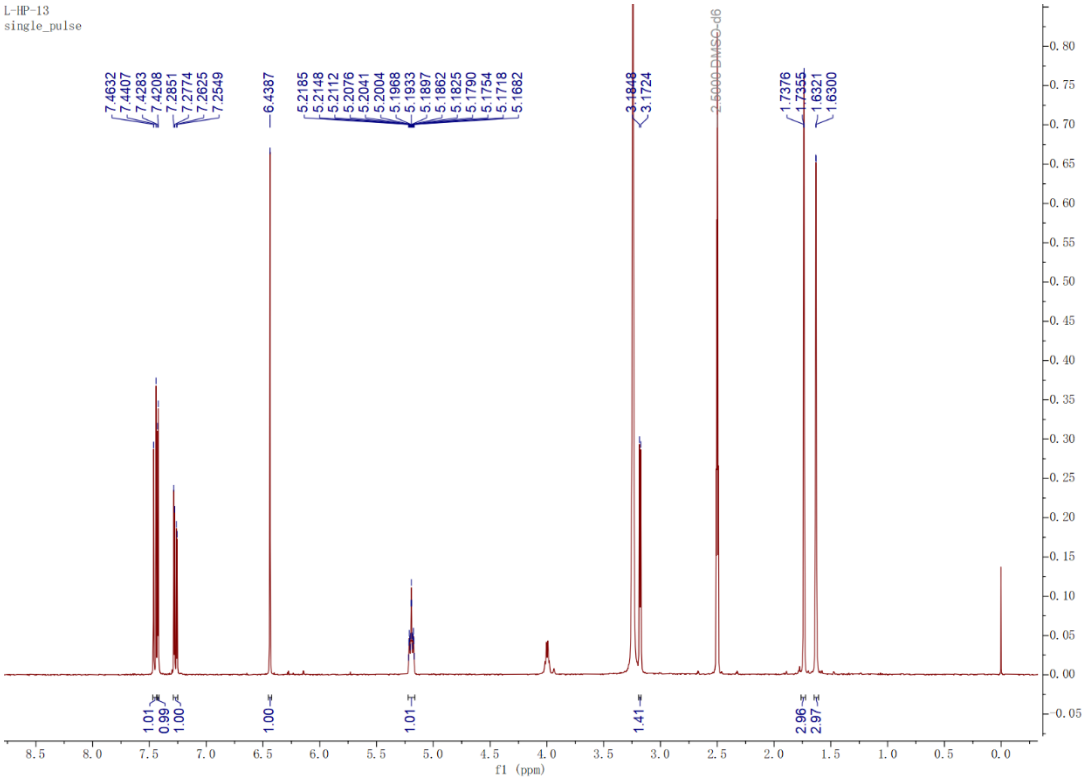


Figure S43: ^{1}H NMR spectrum of compound **15** in DMSO-*d*$_6$ (400 MHz).

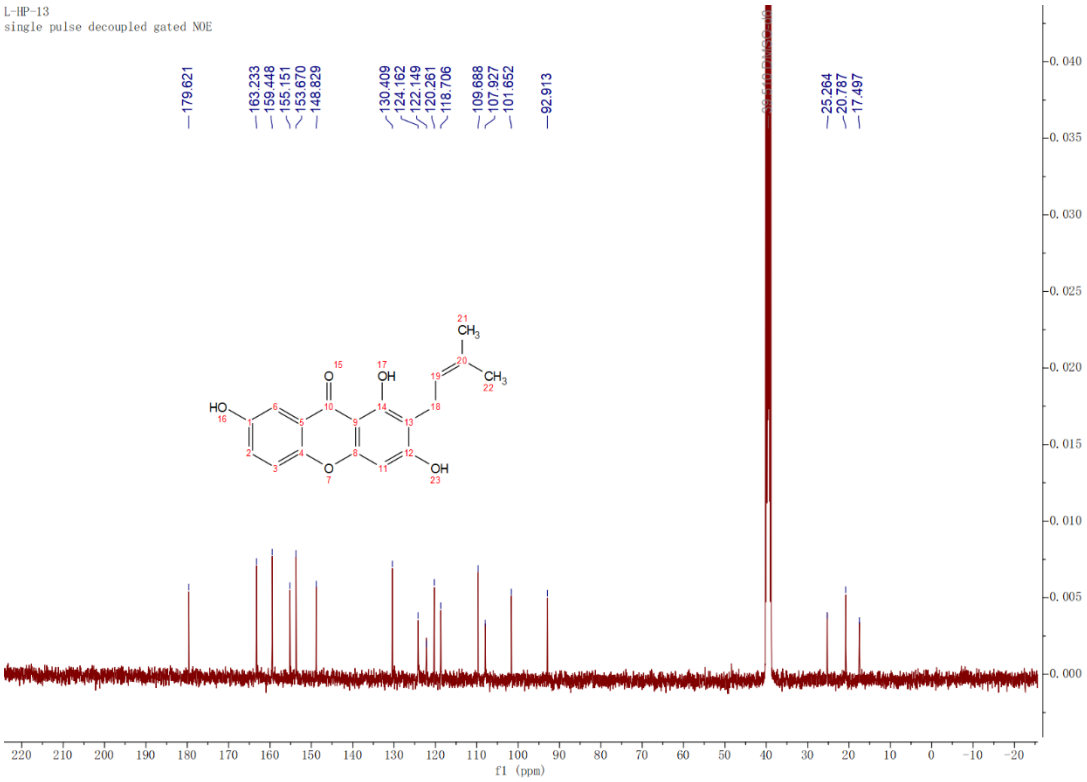


Figure S44: ^{13}C NMR spectrum of compound **15** in DMSO-*d*$_6$ (100 MHz).

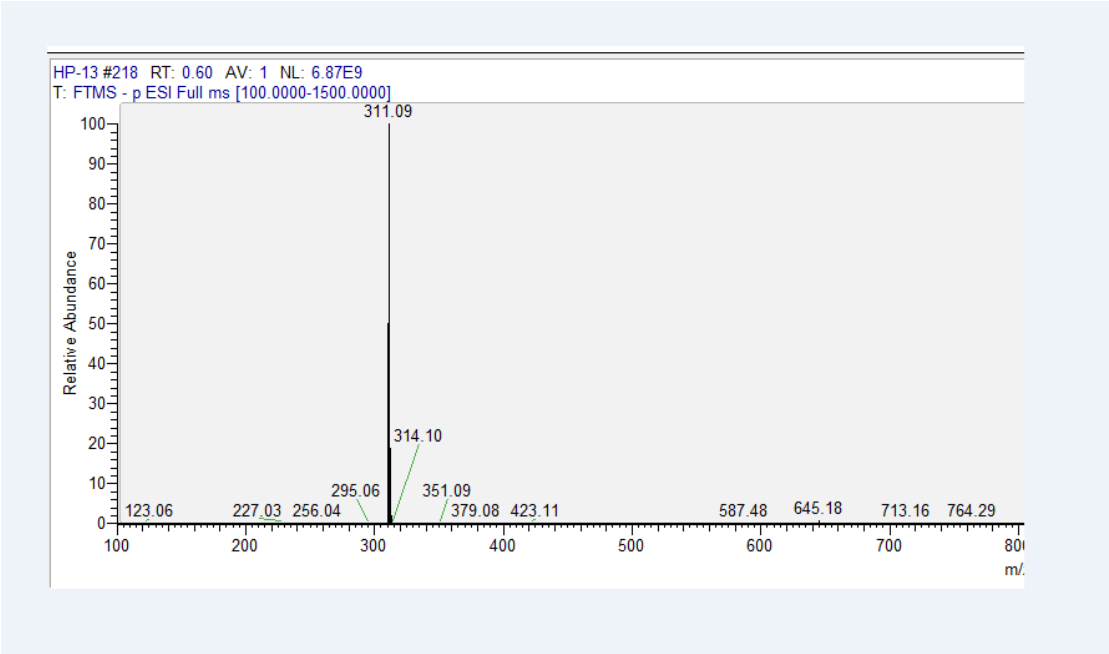


Figure S45: ESI-MS spectrum of compound **15**.

Compound **16**: $C_{14}H_{10}O_6$; ESI-MS *m/z*: 273 $[M–H]^-$.

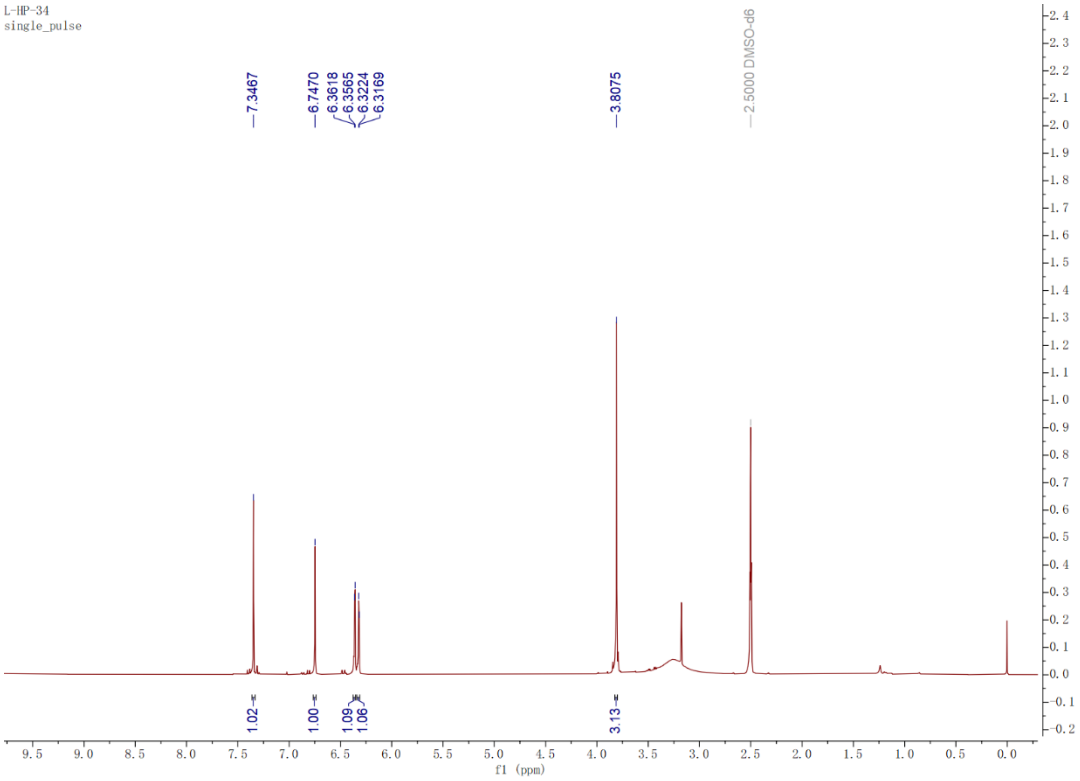


Figure S46: ^{1}H NMR spectrum of compound **16** in DMSO-d_6 (400 MHz).

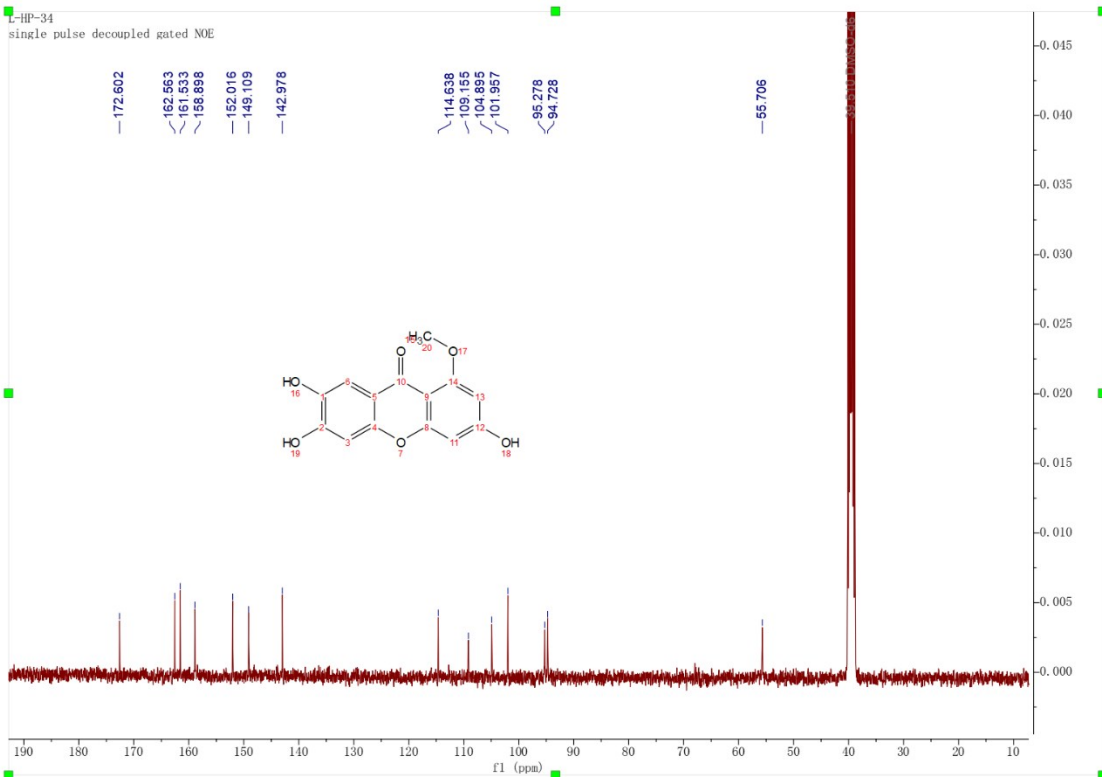


Figure S47: ^{13}C NMR spectrum of compound **16** in DMSO-d_6 (100 MHz).

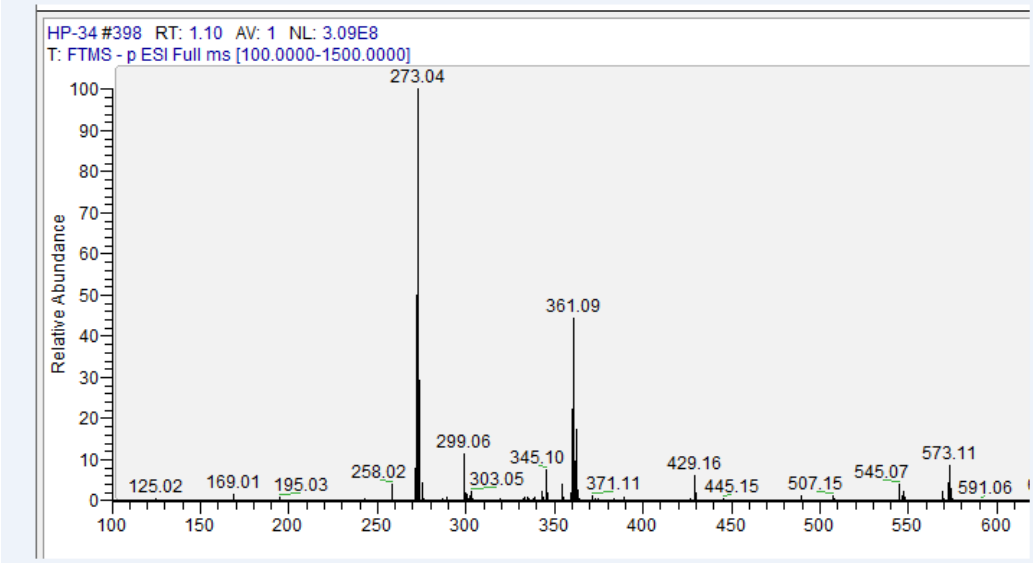


Figure S48: ESI-MS spectrum of compound **16**.

Compound **17**: $C_{19}H_{18}O_8$; ESI-MS *m/z*: 373 $[M–H]^-$.

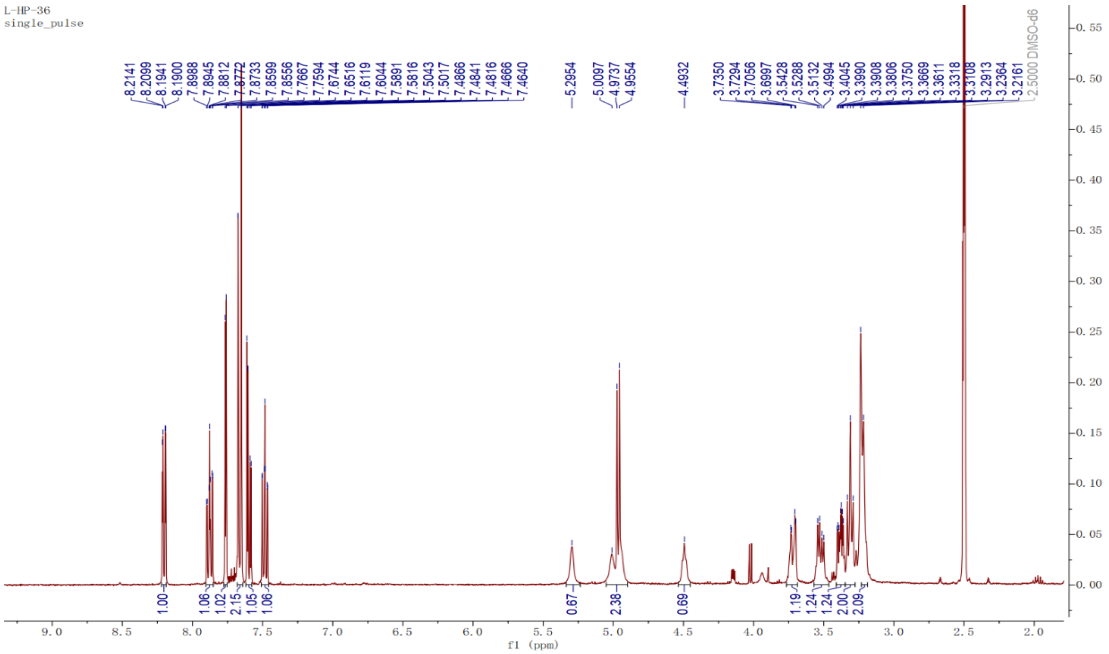


Figure S49: ^{1}H NMR spectrum of compound **17** in DMSO-*d*$_6$ (400 MHz).

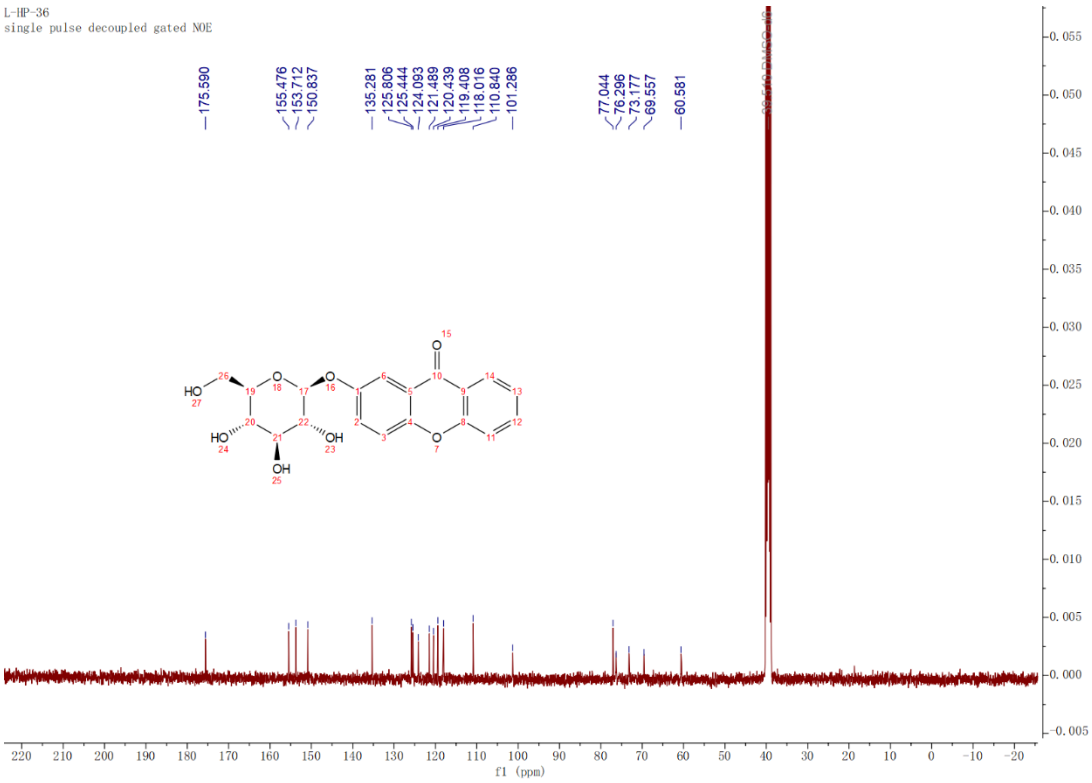


Figure S50: ^{13}C NMR spectrum of compound **17** in DMSO-*d*$_6$ (100 MHz).

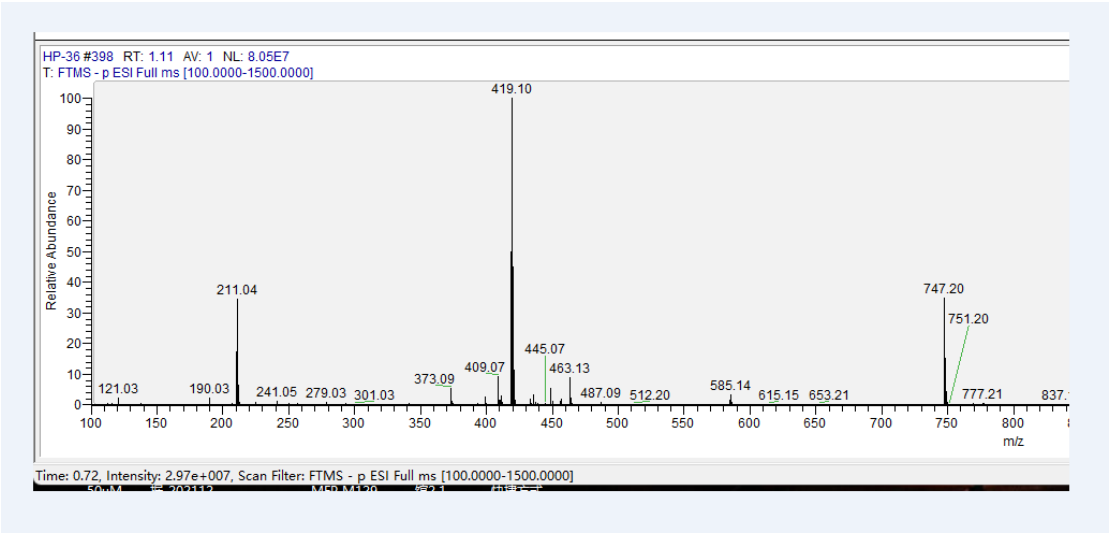


Figure S51: ESI-MS spectrum of compound **17**.

Compound **18**: $C_{20}H_{20}O_{10}$; ESI-MS *m/z*: 419 $[M–H]^-$.

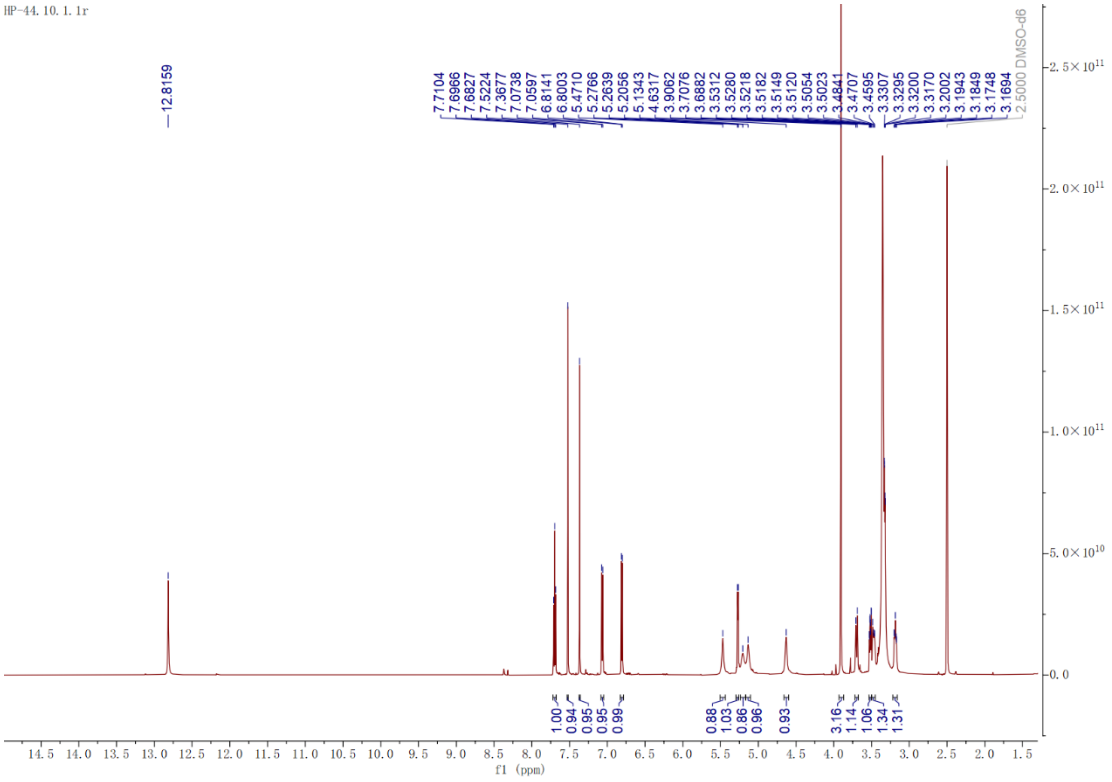


Figure S52: ^{1}H NMR spectrum of compound **18** in DMSO-d_6 (600 MHz).

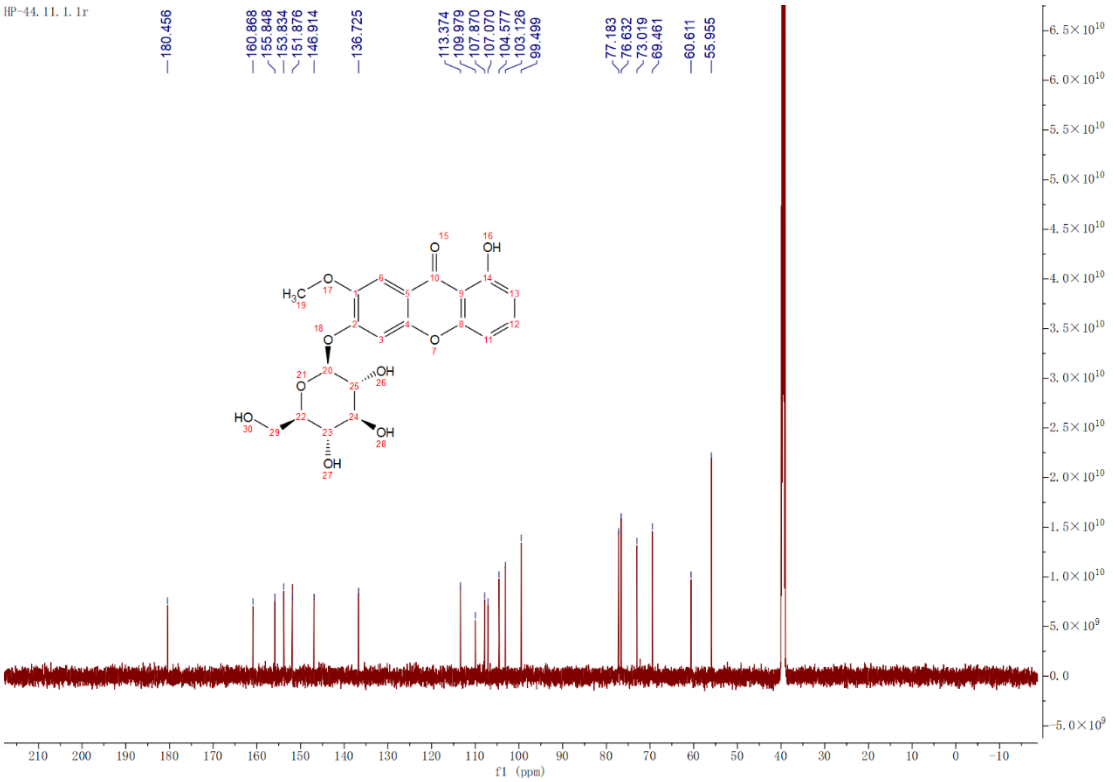


Figure S53: ^{13}C NMR spectrum of compound **18** in DMSO-d_6 (150 MHz).

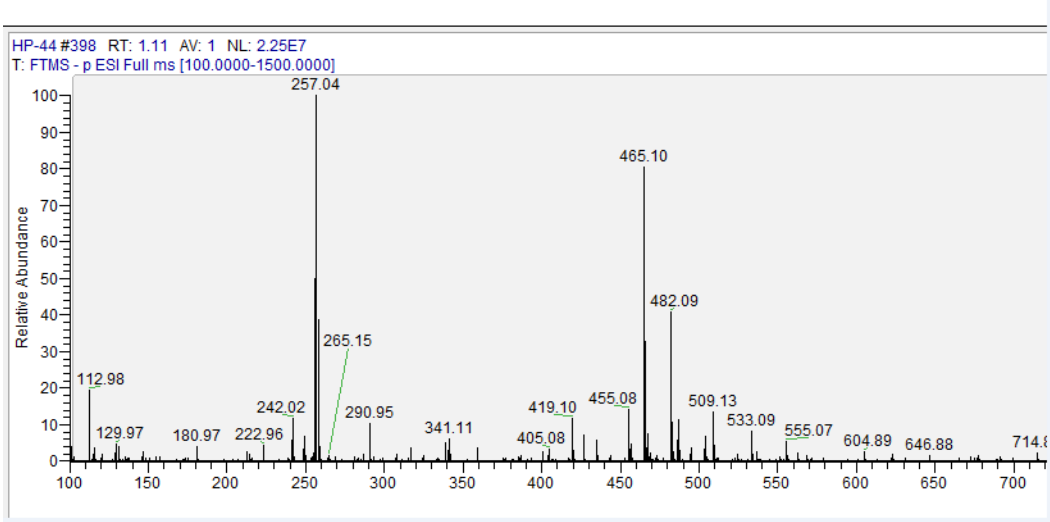


Figure S54: ESI-MS spectrum of compound **18**.

Compound **19**: $C_{19}H_{18}O_9$; ESI-MS *m/z*: 389 $[M–H]^-$.

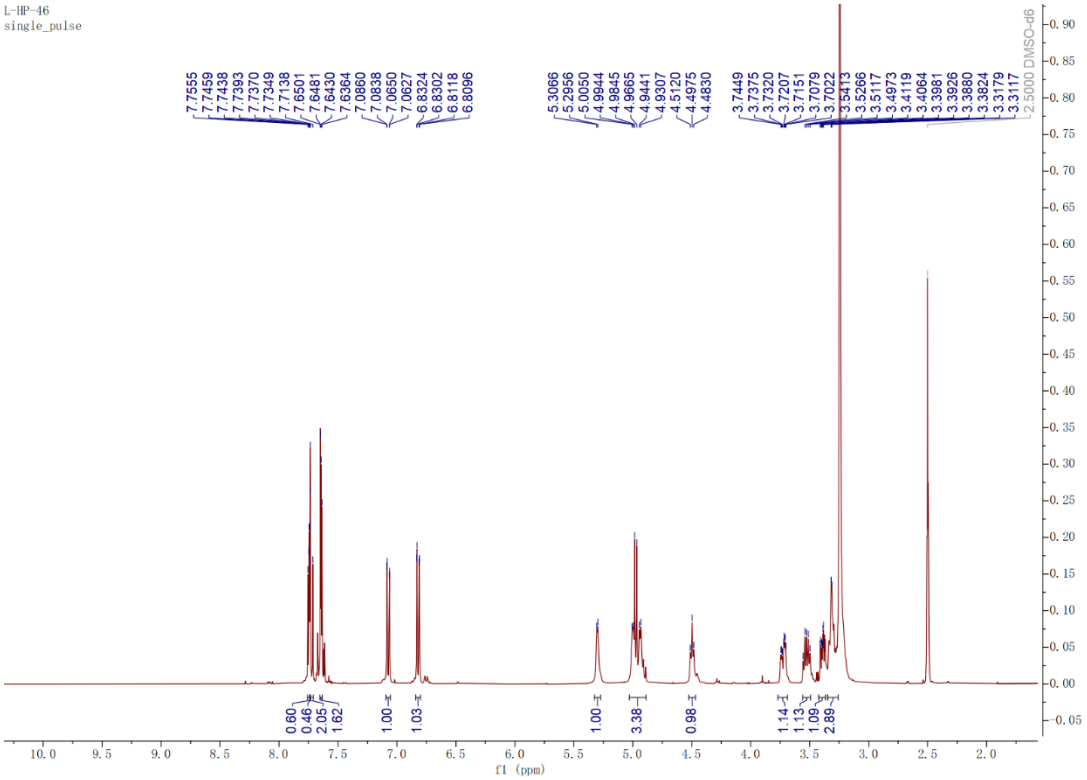


Figure S55: ^{1}H NMR spectrum of compound **19** in DMSO-d_6 (400 MHz).

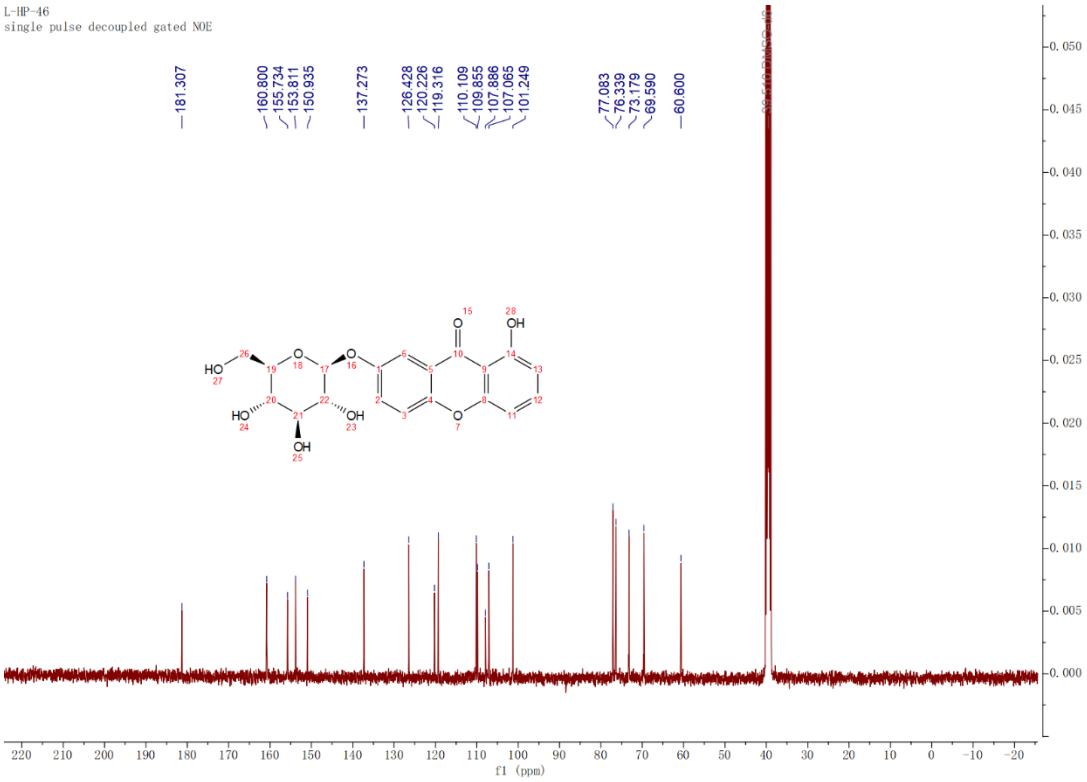


Figure S56: ^{13}C NMR spectrum of compound **19** in DMSO-d_6 (100 MHz).

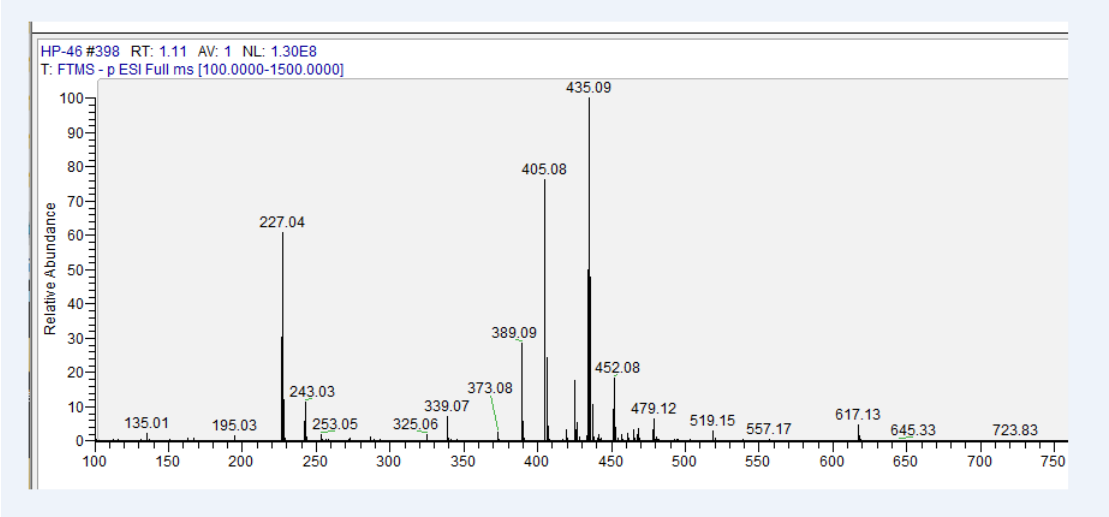


Figure S57: ESI-MS spectrum of compound **19**.

Compound **20**: $C_{14}H_{10}O_6$; ESI-MS *m/z*: 273 $[M–H]^-$.

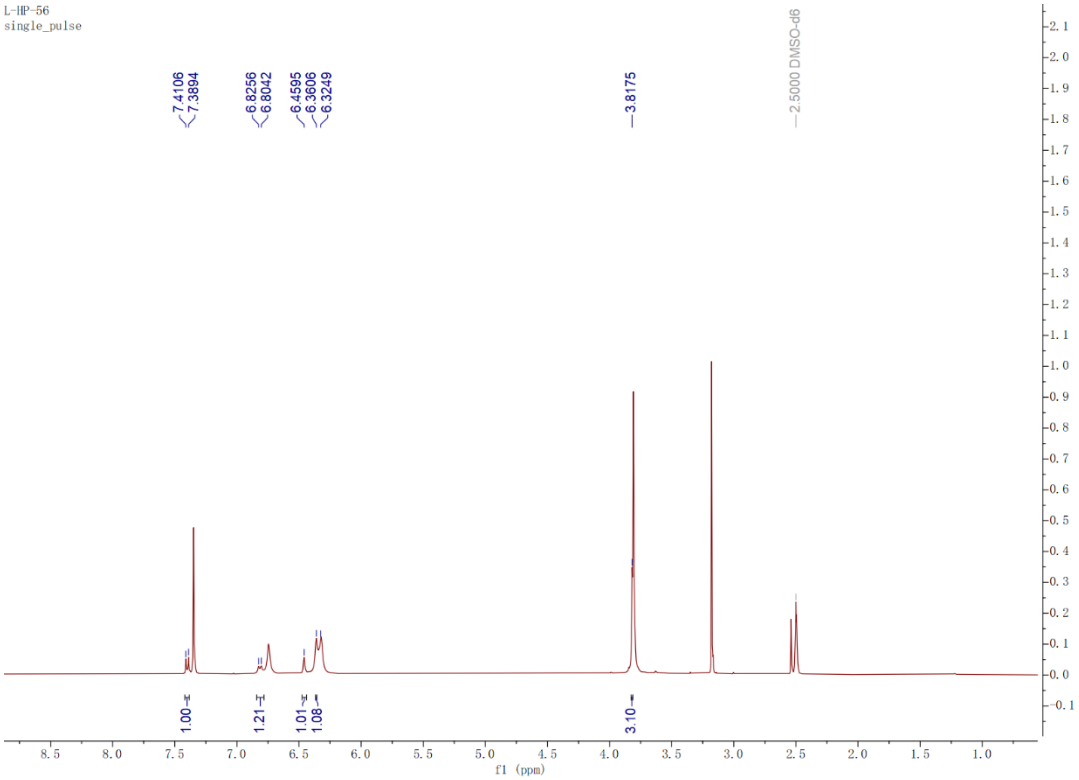


Figure S58: ^{1}H NMR spectrum of compound **20** in DMSO-d_6 (400 MHz).

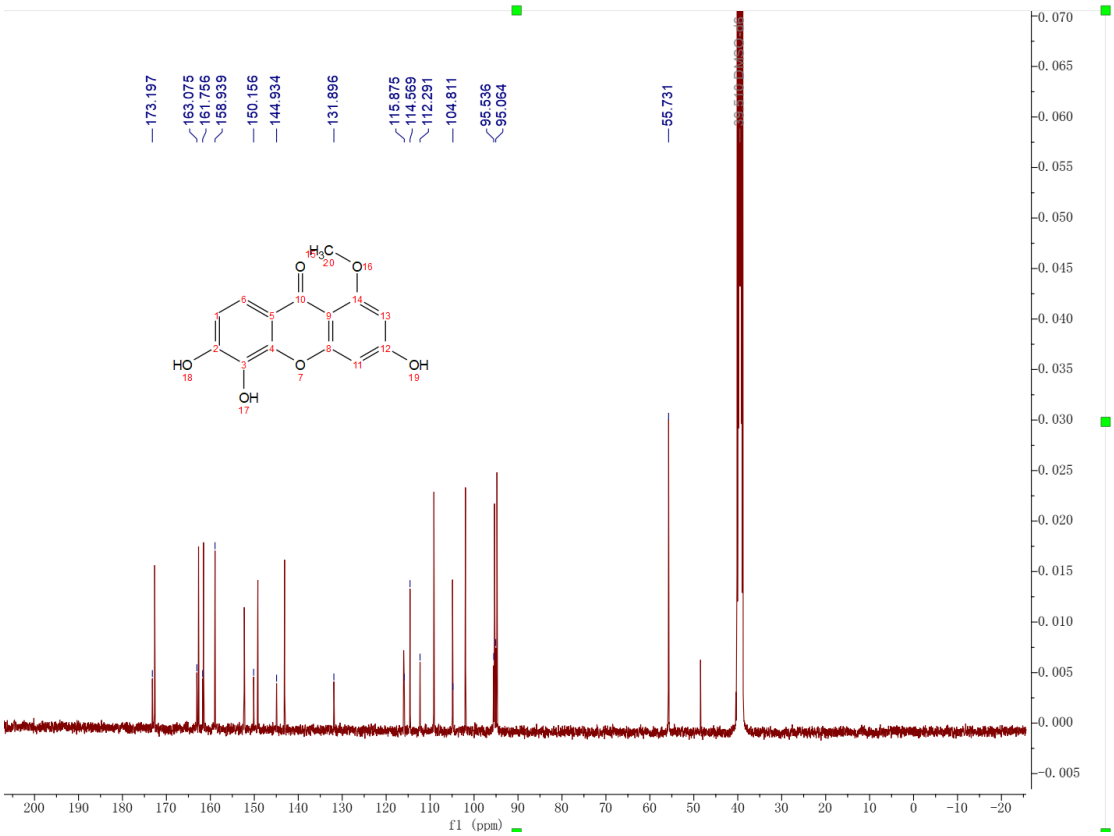


Figure S59: ^{13}C NMR spectrum of compound **20** in DMSO-d_6 (100 MHz).

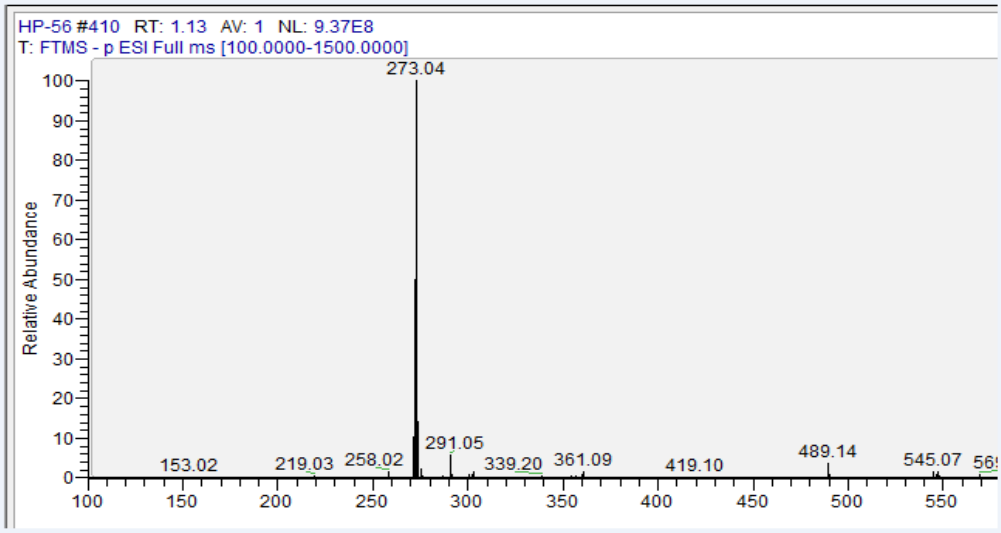


Figure S60: ESI-MS spectrum of compound **20**.

Compound **21**: $C_{15}H_{12}O_5$; ESI-MS *m/z*: 271 $[M-H]^-$

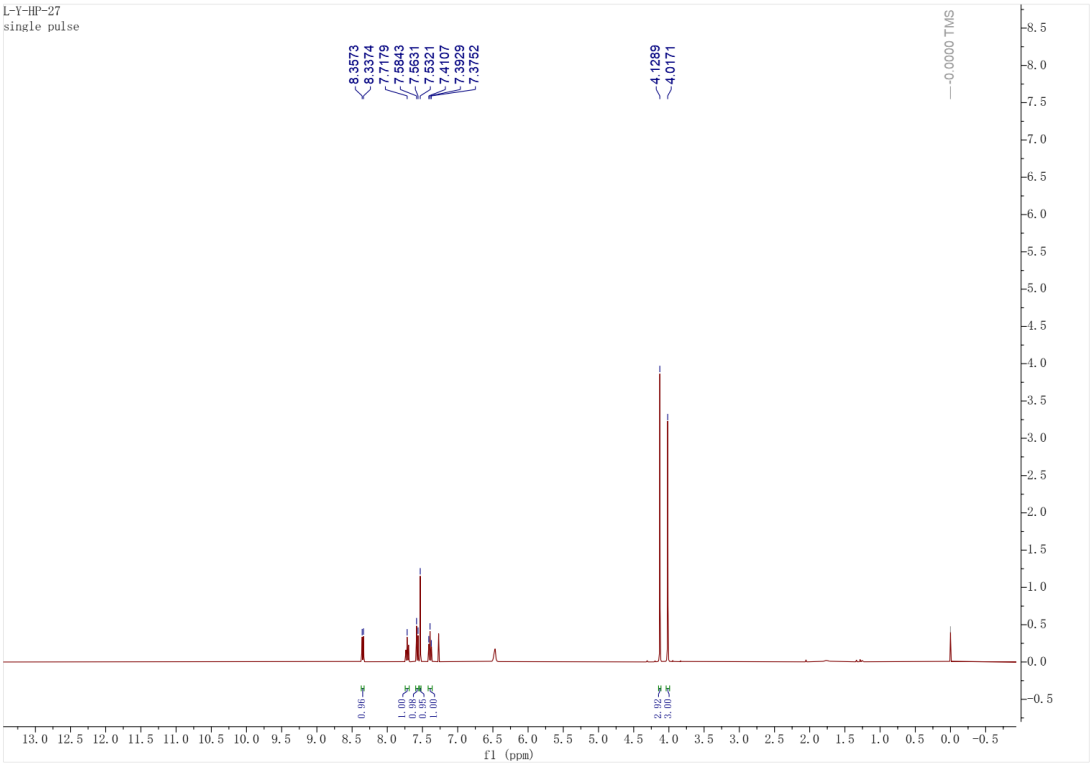


Figure S61: ^{1}H NMR spectrum of compound **21** in $CDCl_3$ (400 MHz).

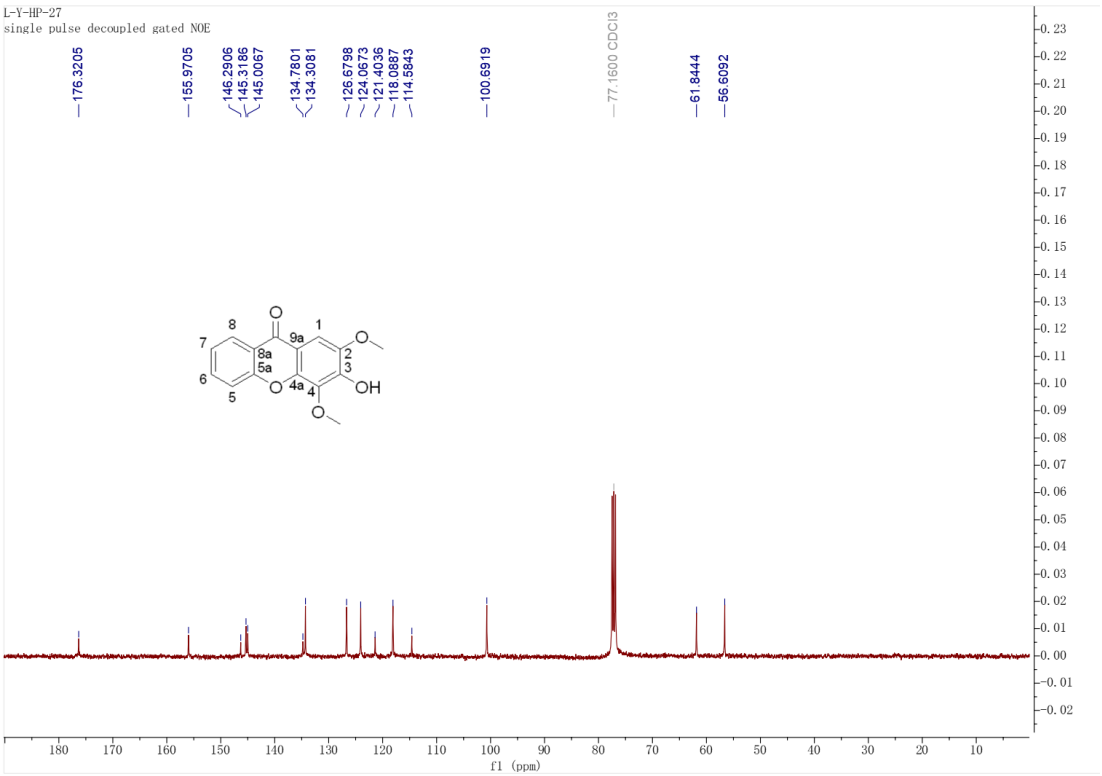


Figure S62: ^{13}C NMR spectrum of compound **21** in $CDCl_3$ (100 MHz).

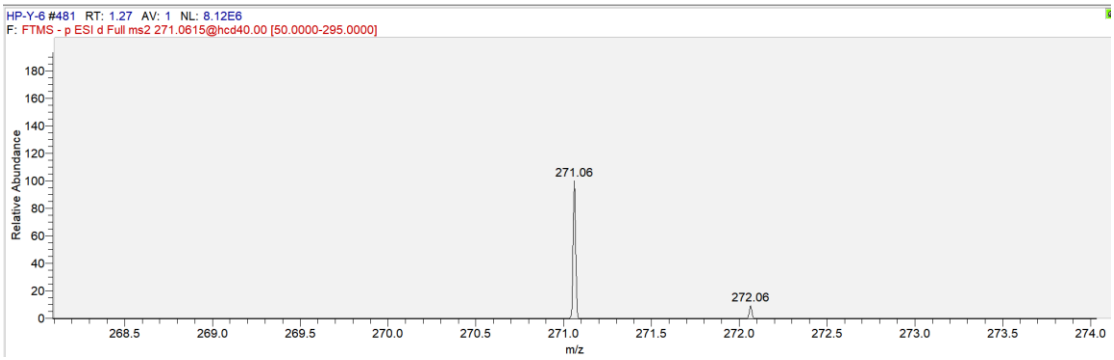


Figure S63: ESI-MS spectrum of compound **21**.

Compound **22**: $C_{14}H_{10}O_5$; ESI-MS *m/z*: 281 $[M+Na]^+$, 257 $[M-H]^-$.

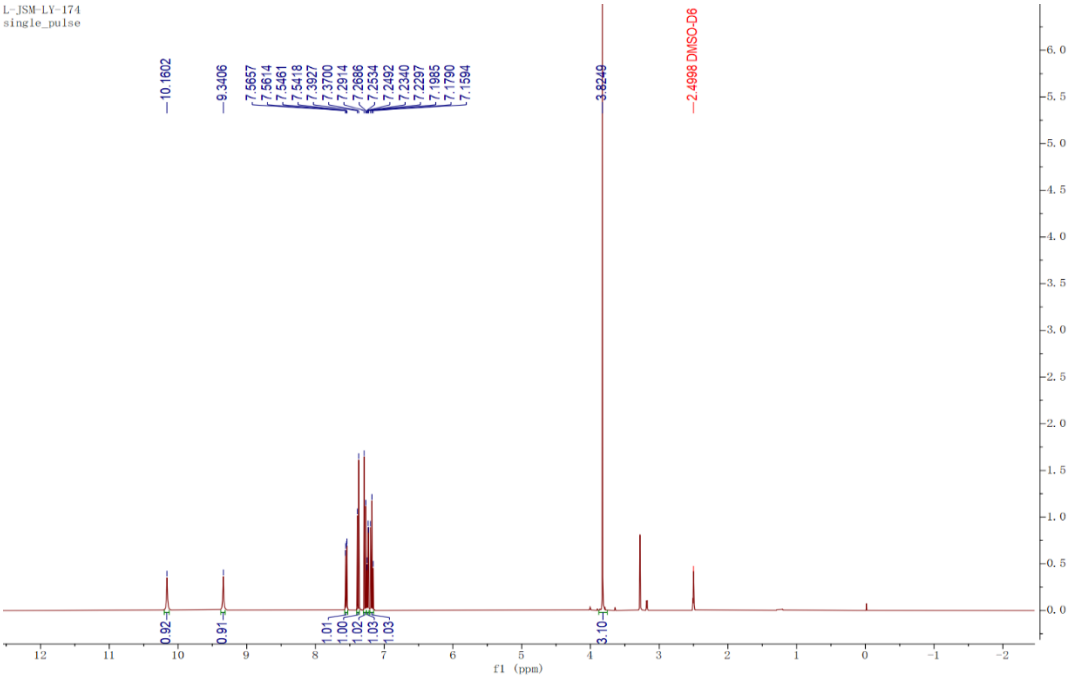


Figure S64: ^{1}H NMR spectrum of compound **22** in DMSO-d_6 (400 MHz).

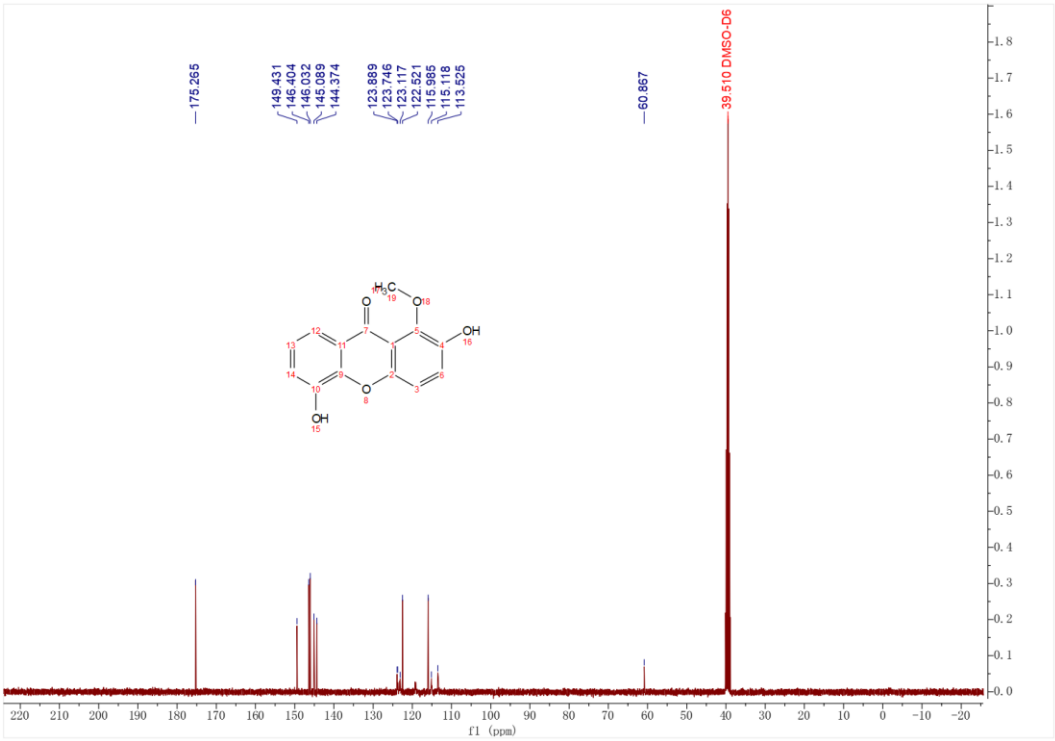


Figure S65: ^{13}C NMR spectrum of compound **22** in DMSO-d_6 (100 MHz).

Figure S66: ESI-MS spectrum of compound **22**.

Compound **23**: $C_{14}H_{10}O_6$; ESI-MS *m/z*: 273 $[M-H]^-$, 297 $[M+Na]^+$.

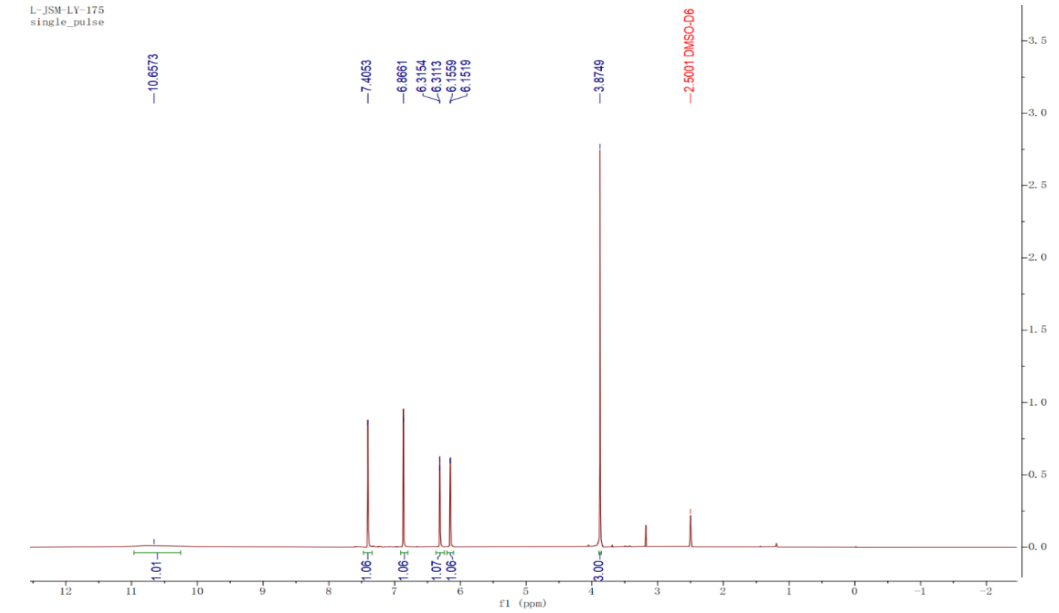


Figure S67: ^{1}H NMR spectrum of compound **23** in DMSO-d_6 (400 MHz).

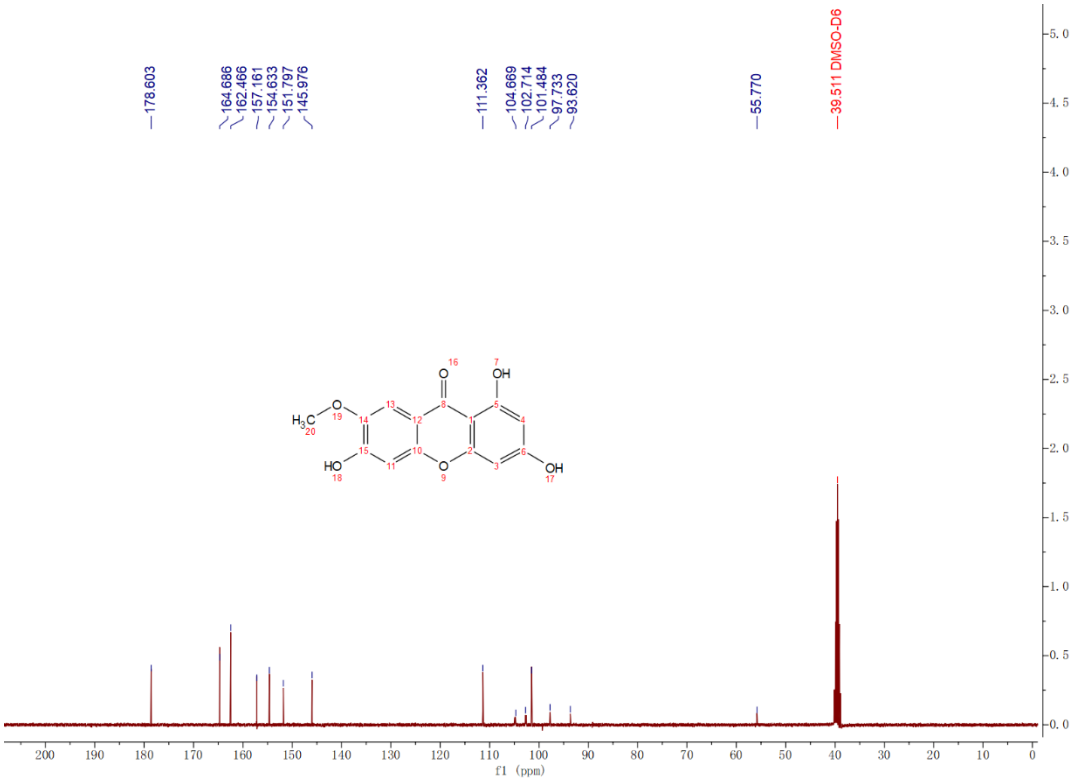


Figure S68: ^{13}C NMR spectrum of compound **23** in DMSO-d_6 (100 MHz).

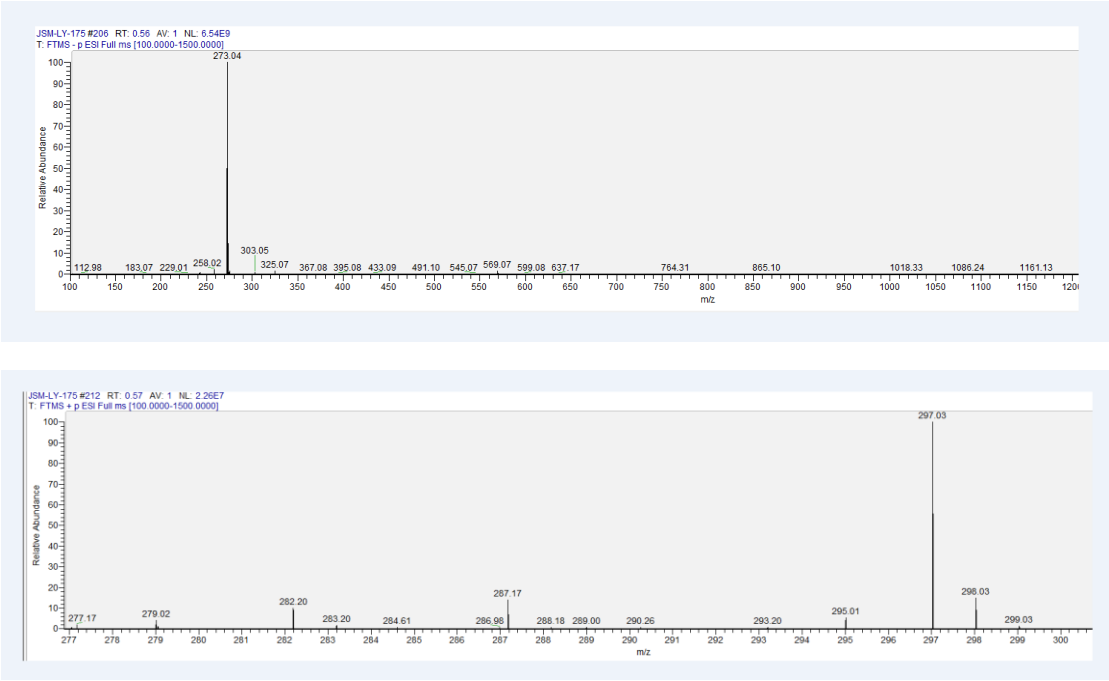


Figure S69: ESI-MS spectrum of compound **23**.

Compound **24**: $C_{18}H_{14}O_6$; ESI-MS *m/z*: 325 $[M-H]^-$, 327 $[M+H]^+$.

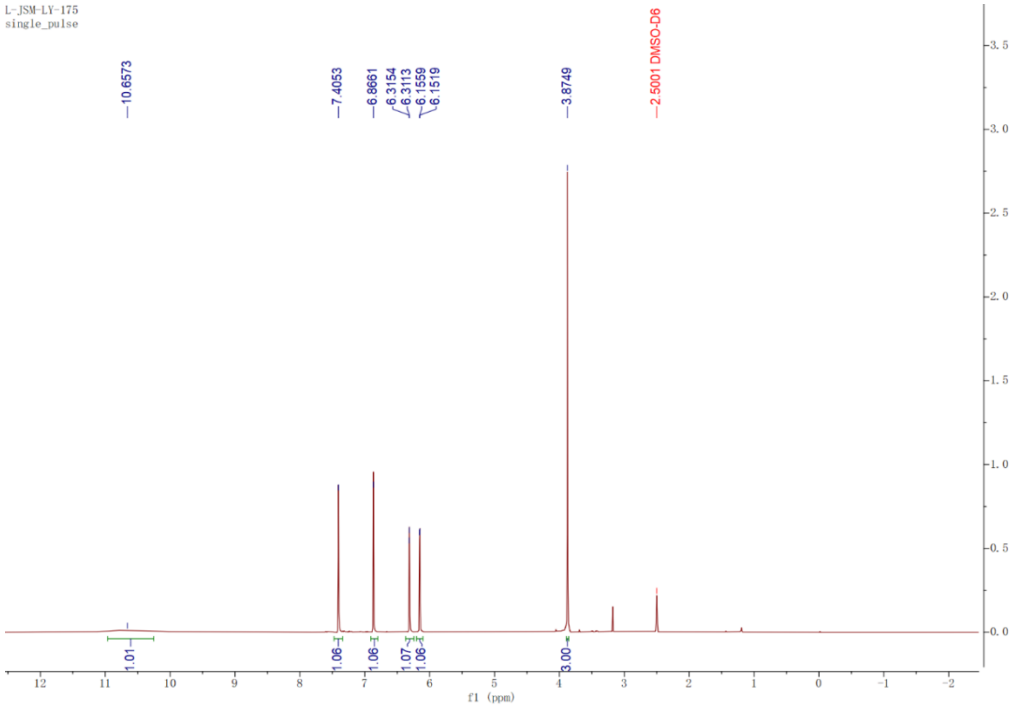


Figure S70: ^{1}H NMR spectrum of compound **24** in DMSO-d_6 (400 MHz).

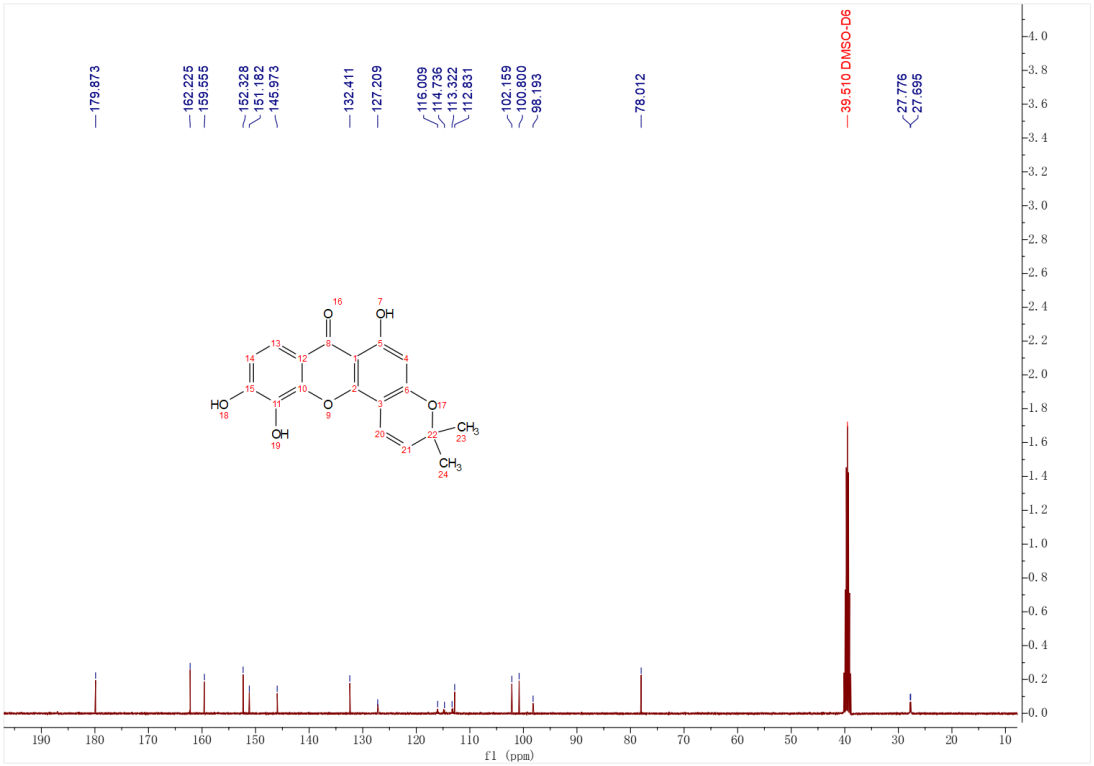
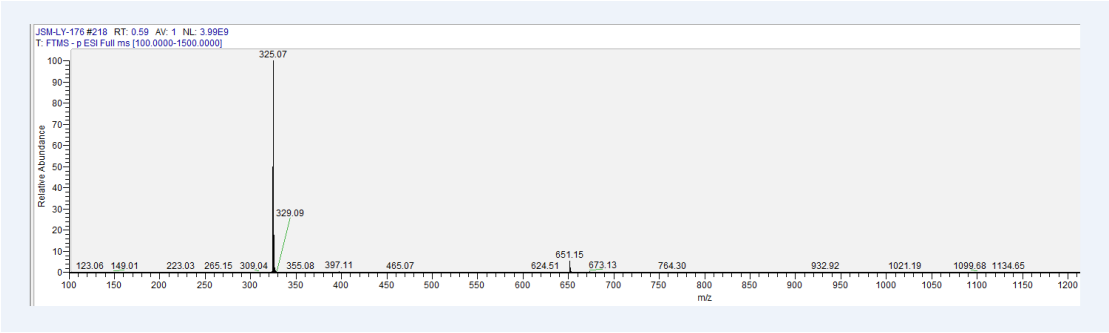


Figure S71: ^{13}C NMR spectrum of compound **24** in DMSO-d_6 (100 MHz).



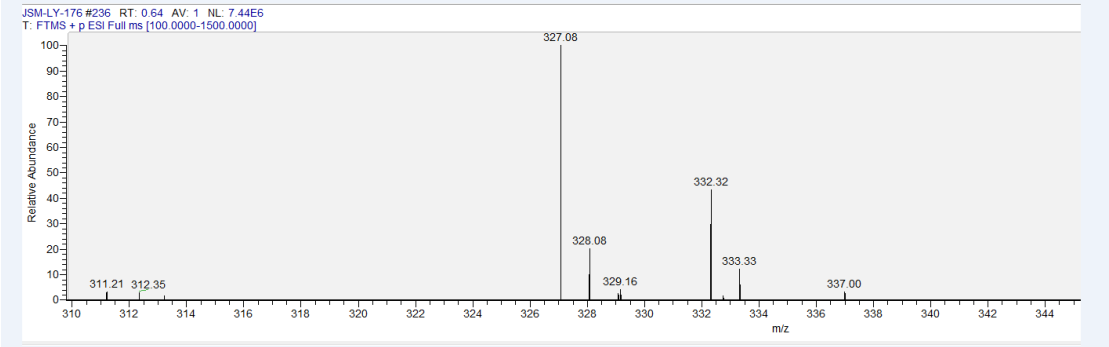


Figure S72: ESI-MS spectrum of compound **24**.

Table 1: ^{1}H (400 MHz) and ^{13}C (100 MHz) data for compounds **1**,**3**,**4** and **7** (δ in ppm).

	1 ($CDCl_3$)		**3** (DMSO-d_6)		**4** (DMSO-d_6)		**7** ($CDCl_3$)	
H/C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C
1	7.64,1H,s	103.3		145.2		162.6		162.7
2		145.5		146.5	6.21,1H,d (2.1,Hz)	97.9	6.77,1H,d (8.4 Hz)	111.6
3		153.9	7.38,1H,d (9.1 Hz)	123.6		165.7	7.53,1H,t (8.4 Hz)	136.6
4	6.90,1H,s	98.1	7.27,1H,d (9.2 Hz)	113.2	6.37,1H,d (2.1,Hz)	93.7	6.87,1H,d (8.4 Hz)	106.2
5	7.45,1H,d (8.0 Hz)	117.9	7.54,1H,d (8.5 Hz)	117.4	7.44,1H,dd (9.1,3.1 Hz)	119.1		138.4
6	7.67,1H,m	134.3	7.79,1H,td (7.9,1.7 Hz)	134.6	7.54,1H,d (9.1 Hz)	124.3	7.28,1H,d (8.8 Hz)	121.2
7	7.36,1H,td (8.0,0.9 Hz)	124.1	7.41,1H,m	123.9		155.6	6.71,1H,d (8.8 Hz)	105.9
8	8.30,1H,dd (8.0,1.9 Hz)	126.7	8.14,1H,dd (7.9,1.7 Hz)	125.8	7.50,1H,d (3.1 Hz)	105.4		154.0
9		176.2		175.0		179.4		182.7
10	6.10,2H,s	102.6						
4a		153.9		149.5		149.9		155.0
5a		156.1		154.6		157.3		145.7
8a		121.4		121.4		120.1		111.6
9a		116.6		116.2		101.9		109.6
1-OH					12.09,1H,s			
2-OH			9.39,1H,s					
7-OH					10.96,1H,s			
1-OCH_3			3.83,3H,s	60.8				
7-OCH_3					3.87,1H,s	55.6		
8-OCH_3							3.96,3H,s	56.9

Table 2: ^{1}H (400 MHz) and ^{13}C (100 MHz) data for compounds **9**,**10**,**13** and **14** (δ in ppm).

	9 (DMSO-d_6)		**10** (DMSO-d_6)		**13** (Acetone)		**14** (DMSO-d_6)	
H/C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C
1	7.47,2H,m	108.3	7.44,2H,d (3.0 Hz)	108.3		162.8		162.4
2		153.9		153.6		108.9	6.16,1H,d (2.0 Hz)	97.8
3	7.32,1H,dd (9.0,3.1 Hz)	123.5	7.29,2H,dd (9.0,3.0 Hz)	124.4		166.6		164.8
4	7.58,1H,d (9.0 Hz)	119.5	7.50,2H,d (9.0 Hz)	119.4	6.42,1H,s	95.1	6.39,1H,d (2.0 Hz)	93.7
5		148.4	7.50,2H,d (9.0 Hz)	119.4	7.42,1H,d (9.0 Hz)	119.7		109.3
6	7.47,2H,m	116.3	7.29,2H,dd (9.0,3.0 Hz	124.4	7.34,1H,dd (9.1,2.9 Hz)	125.0		145.2
7	7.36,1H,t (8.0 Hz)	124.5		153.6		154.6		143.3
8	7.71,1H,dd (8.0,1.5 Hz)	119.5	7.44,2H,d (3.0 Hz)	108.3	7.58,1H,d (3.0 Hz)	109.3	7.34,1H,s	
9		175.7		175.8		181.2		178.8
11							6.87,1H,d (10.0 Hz)	114.6
12							5.92,1H,d (10.1 Hz)	130.7
13								77.7
14							1.47,3H,s	27.5
15							1.47,3H,s	
1'a					3.07,1H,dd (14.4,7.8 Hz)	29.6		
1'b					2.93,1H,dd (14.4,7.8 Hz)			
2'					4.44,1H,dd (7.8,3.5 Hz)	76.4		
3'						148.2		
4'a					4.93,1H,t (1.0 Hz)	110.5		
4'b					4.76,1H,t (1.0 Hz)			
5'					1.84,3H,s	18.3		
4a		149.0		149.3		157.3		157.0
5a		145.8		149.3		150.7		147.2
8a		121.2		121.0		121.8		112.5
9a		121.5		121.0		103.3		101.5
2-OH			9.89,1H,s					
7-OH			9.89,1H,s					
5-OCH_3	3.98,3H,s	56.2						

Table 3: ^{1}H (400 MHz) and ^{13}C (100 MHz) data for compounds **15**,**16**,**20** and **21** (δ in ppm).

	15 (DMSO-d_6)		**16** (DMSO-d_6)		**20** (DMSO-d_6)		**21** ($CDCl_3$)	
H/C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C
1		159.4		158.9		158.9	7.53,1H,s	100.7
2		109.7	6.31,1H,d (2.1 Hz)	95.3	6.34,1H,brs	95.5		145.3
3		163.2		162.6		163.1		146.3
4	6.44,1H,s	92.9	6.35,1H,d (2.1 Hz)	94.7	6.46,1H,brs	95.1		134.8
5	7.45,1H,d (9.0 Hz)	118.7	6.74,1H,s	102.0		131.9	7.58,1H,d (8.4 Hz)	118.1
6	7.26,1H,dd (9.0,3.1 Hz)	122.1		149.1		150.2	7.71,1H,t (7.8 Hz)	134.3
7		153.7		149.2	6.81,1H,d (8.6 Hz)	114.2	7.39,1H,t (7.2 Hz)	124.1
8	7.42,1H,d (3.0 Hz)	107.9	7.34,1H,s	109.2	7.40,1H,d (8.5 Hz)	115.9	8.35,1H,d (7.8 Hz)	126.7
9		179.6		172.6		173.2		176.2
4a		155.2		161.5		161.8		145.0
5a		148.8		152.0		145.5		156.0
8a		120.3		114.6		112.3		121.4
9a		101.7		104.9		104.8		114.6
1'	3.17,1H,d (5.0 Hz)	20.8						
2'	5.20,1H,m	124.2						
3'		130.4						
4'	1.63,3H,s	25.2						
5'	1.73,3H,s	17.5						
1-OCH_3			3.81,3H,s	55.7	3.82,3H,s	55.7		
2-OCH_3							4.02,3H,s	56.6
4-OCH_3							4.13,3H,s	61.8

Table 4: ^{1}H (400 MHz) and ^{13}C (100 MHz) data for compounds **11**,**17** and **19** (δ in ppm). ^{1}H (600 MHz) and ^{13}C (150 MHz) data for compound**18** (δ in ppm).

	11 (DMSO-d_6)		**17** (DMSO-d_6)		**18** (DMSO-d_6)		**19** (DMSO-d_6)	
H/C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C
1		161.0	7.75,1H,d (2.9 Hz)	110.8		160.9		160.8
2	6.77,1H,d (8.3 Hz)	109.9		153.7	6.81,1H,d (8.3 Hz)	110.0	6.82,1H,dd (8.4,1.0 Hz)	110.1
3	7.67,1H,t (8.3 Hz)	136.8	7.59,1H,dd (9.1,3.0 Hz)	125.4	7.69,1H,t (8.3 Hz)	136.7	7.73,1H,dd (8.4,8.4 Hz)	137.3
4	7.03,1H,d (8.3 Hz)	107.2	7.66,1H,d (9.1 Hz)	119.4	7.06,1H,d (8.5 Hz)	107.9	7.07,1H,dd (8.4,1.0 Hz)	107.1
5	7.30,1H,s	103.4	7.65,1H,d (9.1 Hz)	118.0	7.37,1H,s	103.1	7.64, 2H,,dd (5.4,2.6 Hz)	119.3
6		153.2	7.87,1H,ddd (7.0,7.1,1.7 Hz)	135.3		153.8	7.64, 2H,,dd (5.4,2.6 Hz)	126.4
7		144.8	7.48,1H,ddd (7.1,7.1,1.0 Hz)	124.1		151.9		153.8
8	7.46,1H,s	108.4	8.20,1H,dd (8.0,1.6 Hz)	125.8	7.52,1H,s	104.6	7.75,1H,brs	109.9
9		180.7		175.6		180.4		181.3
4a		156.0		150.8		155.8		155.7
5a		150.9		155.5		146.9		150.9
8a		114.2		120.4		113.4		120.2
9a		107.9		121.5		107.1		107.9
1'	5.13,1H,d (7.1 Hz)	100.5	4.96,1H,d (7.3 Hz)	101.3	5.25,1H,d (7.6 Hz)	99.5	4.98,1H,d (7.2 Hz)	101.2
2'	3.16-3.75 6H,m	73.2	3.40-3.21 4H,m	73.2	3.7-3.31 6H,m	73.0	3.72-3.25 6H,m	73.2
3'		76.1		76.3		76.6		76.3
4'		69.8		69.6		69.5		69.6
5'		77.4		77.0		77.2		77.1
6'		60.8	3.71,1H,dd (11.7,2.2 Hz)	60.6		60.6		60.6
1-OH					12.81,1H,s		12.52,1H,s	
2'-OH			5.29,1H,brs		5,47-4,63 4H,m		5.29-4.49 4H,m	
3'-OH			5.00,1H,brs					
4'-OH								
6'-OH			4.49,1H,brs					
7-OCH$_3$					3.90,3H,s	56.0		