Supporting Information

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Diterpenoids from the Seeds of *Euphorbia Lathyris* and their Cytotoxic Acitivity

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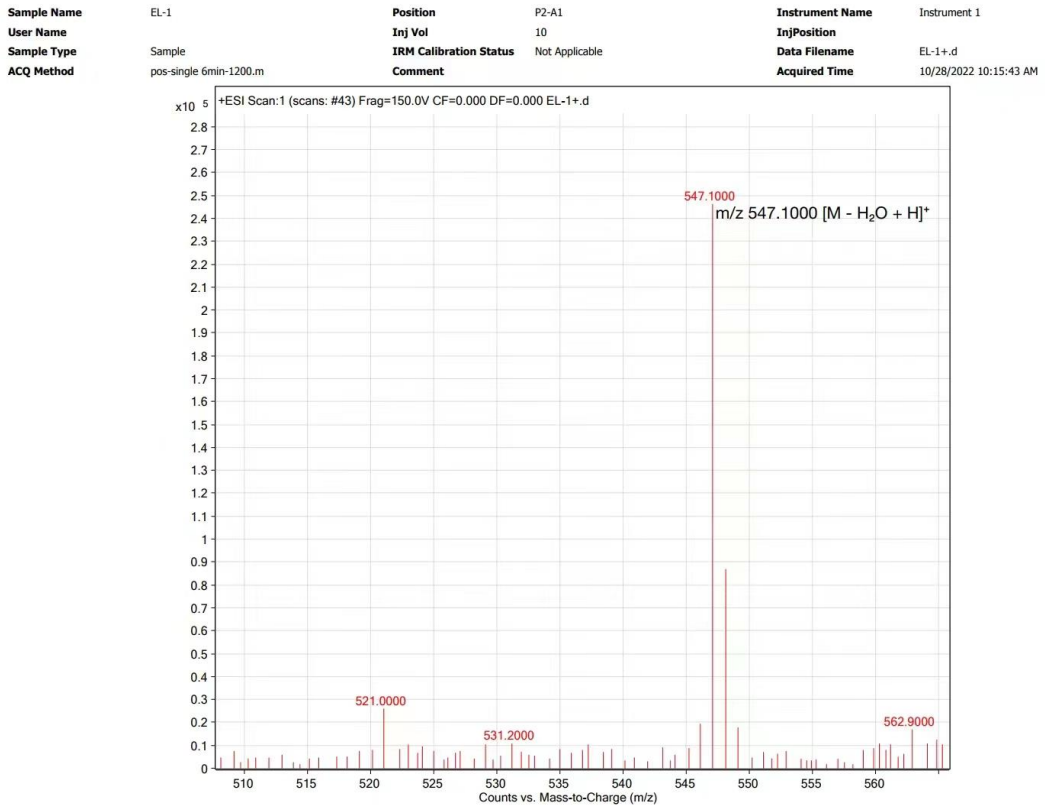


Figure S1: EI-MS spectrum of **1** $[M - H_2O + H]^+$

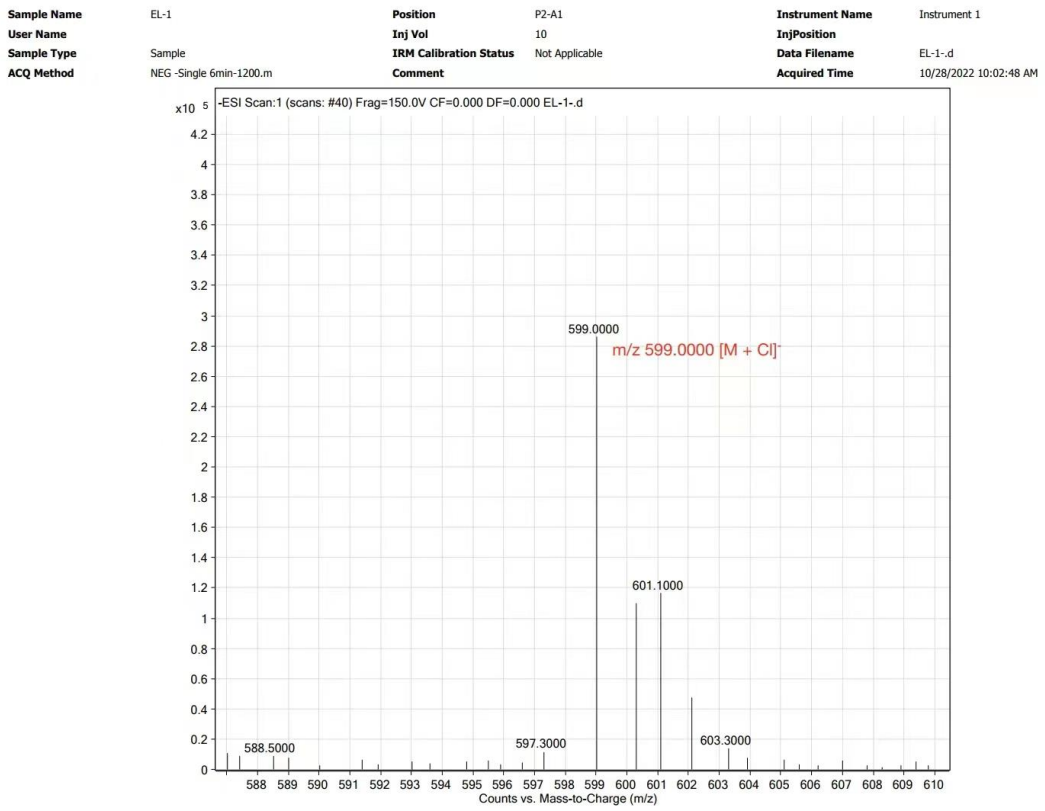


Figure S2: EI-MS spectrum of **1** $[M + Cl]^-$

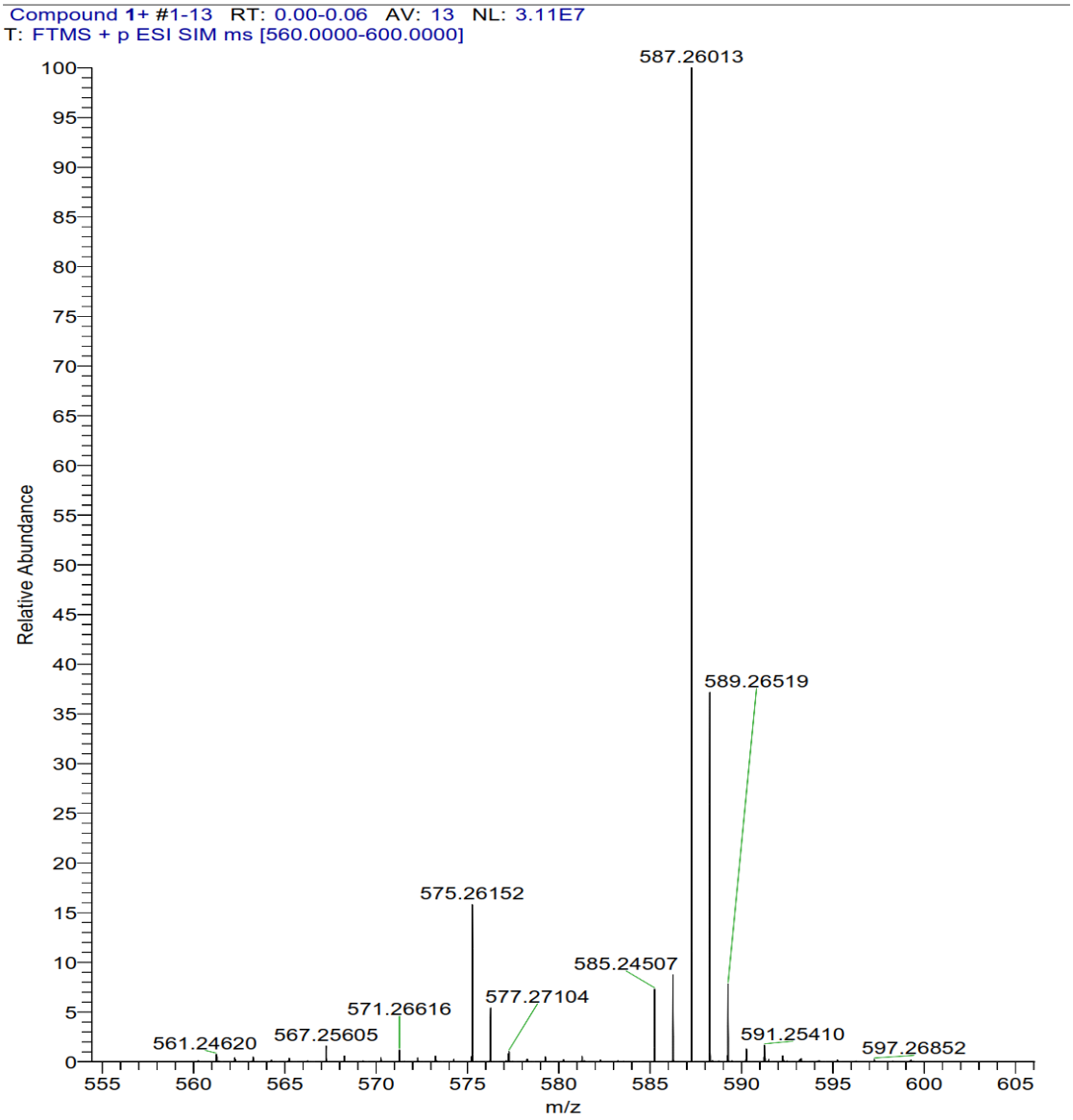


Figure S3: HR-ESI-MS spectrum of **1**

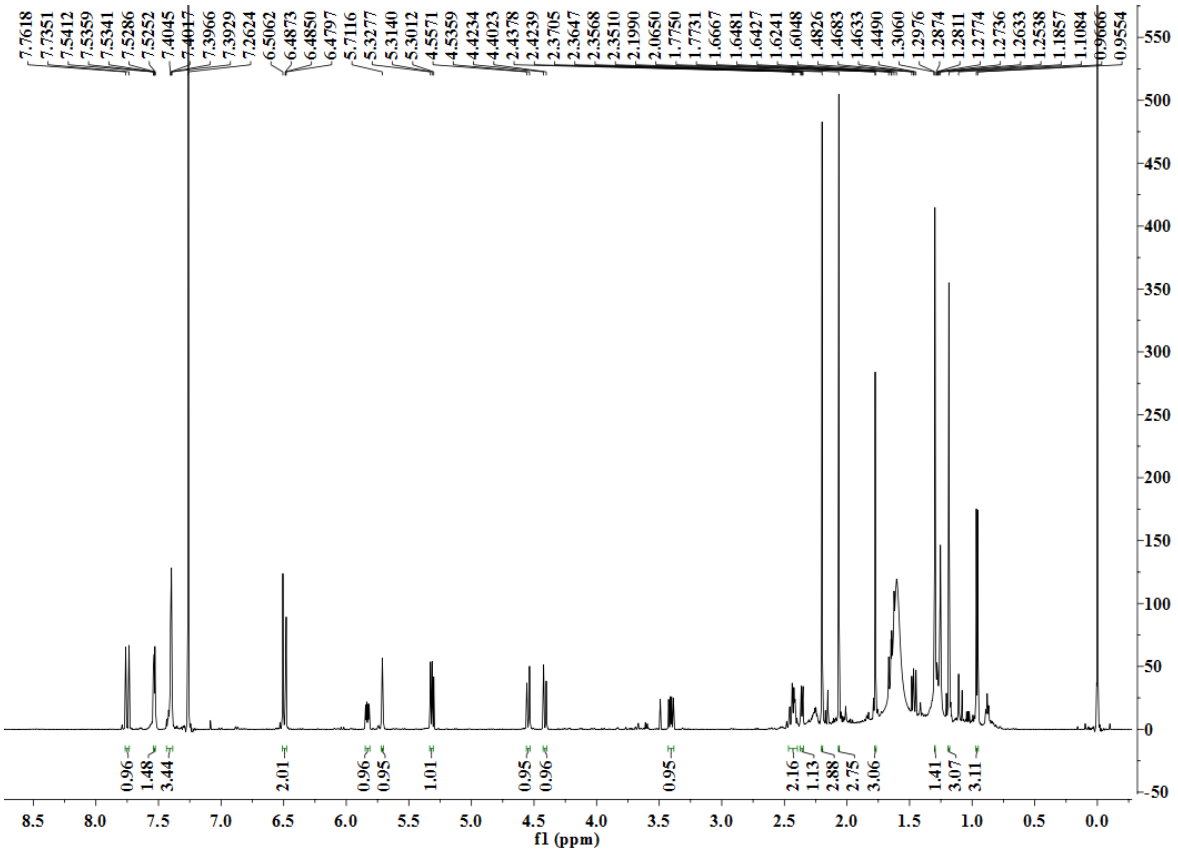


Figure S4: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1**

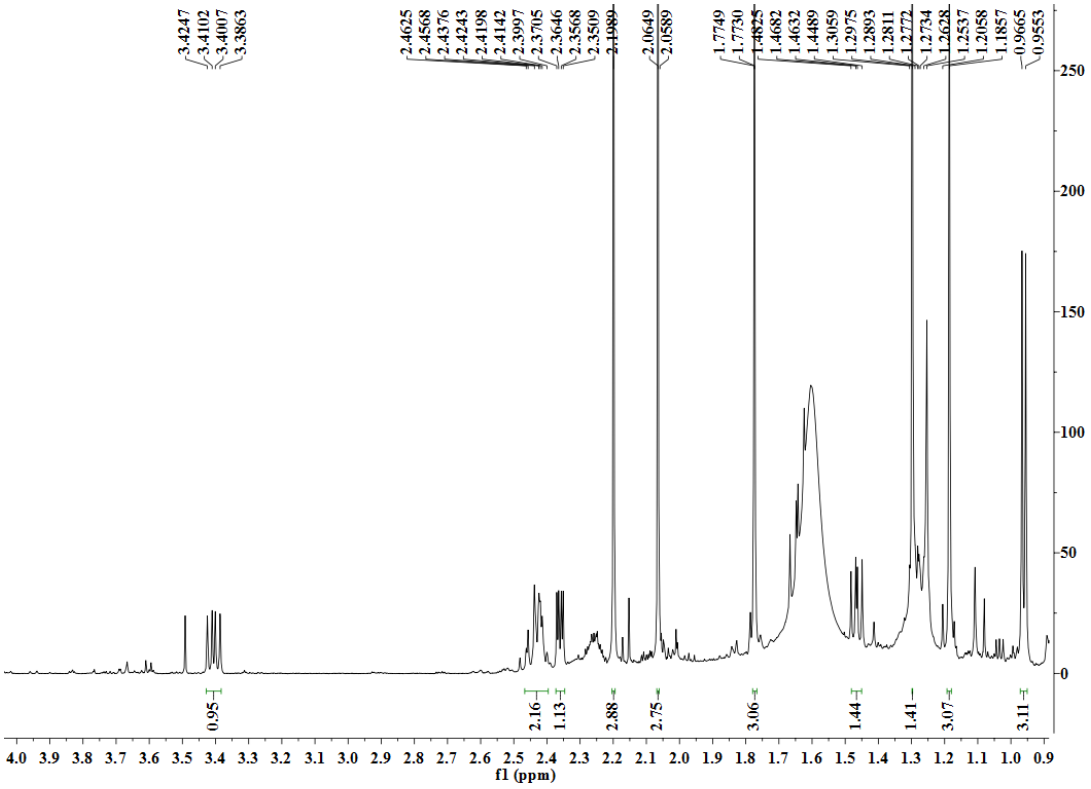


Figure S5: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1** (From δ_H 0.9 ppm to δ_H 4.0 ppm)

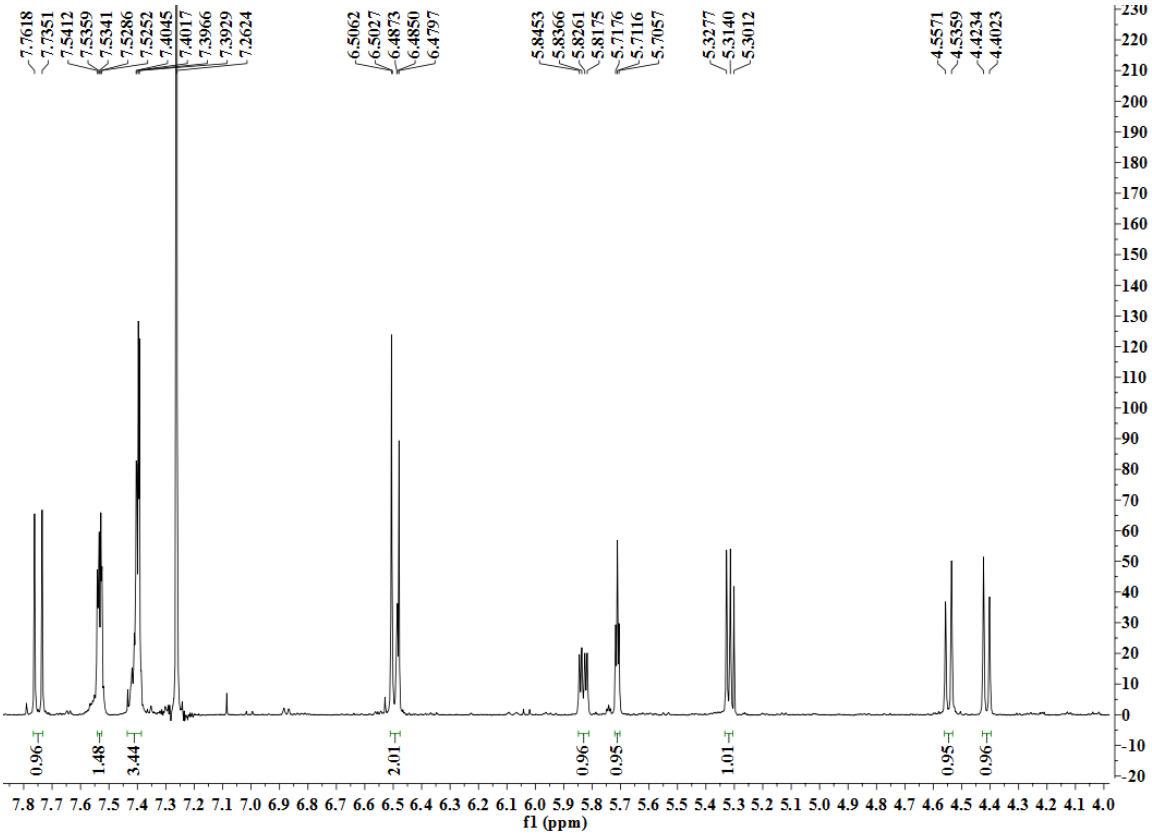


Figure S6: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1** (From δ_H 4.0 ppm to δ_H 7.8 ppm)

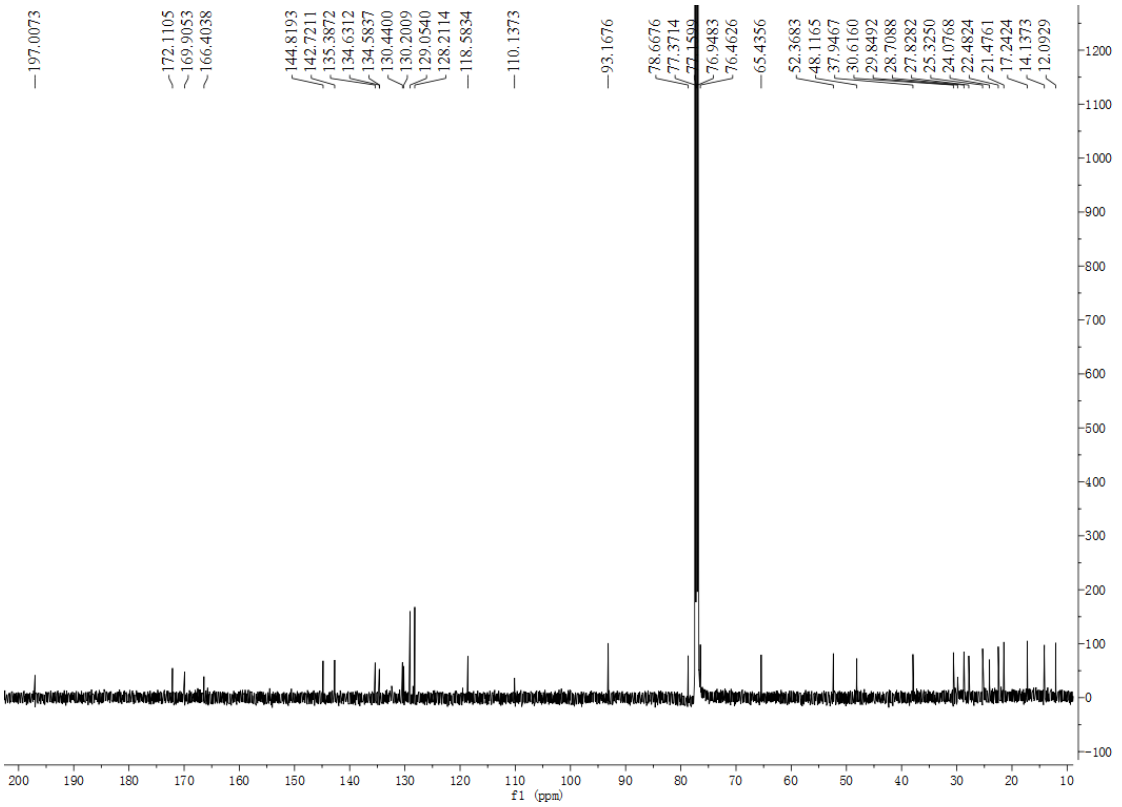


Figure S7: ^{13}C-NMR (600 MHz, $CDCl_3$) spectrum of **1**

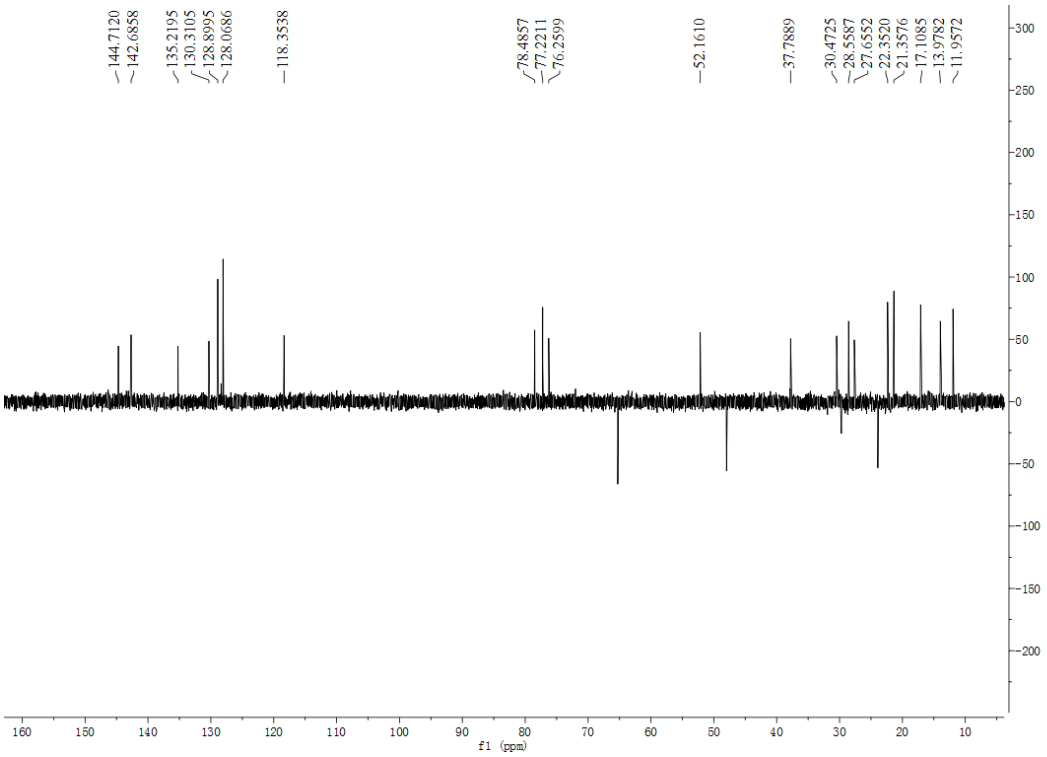
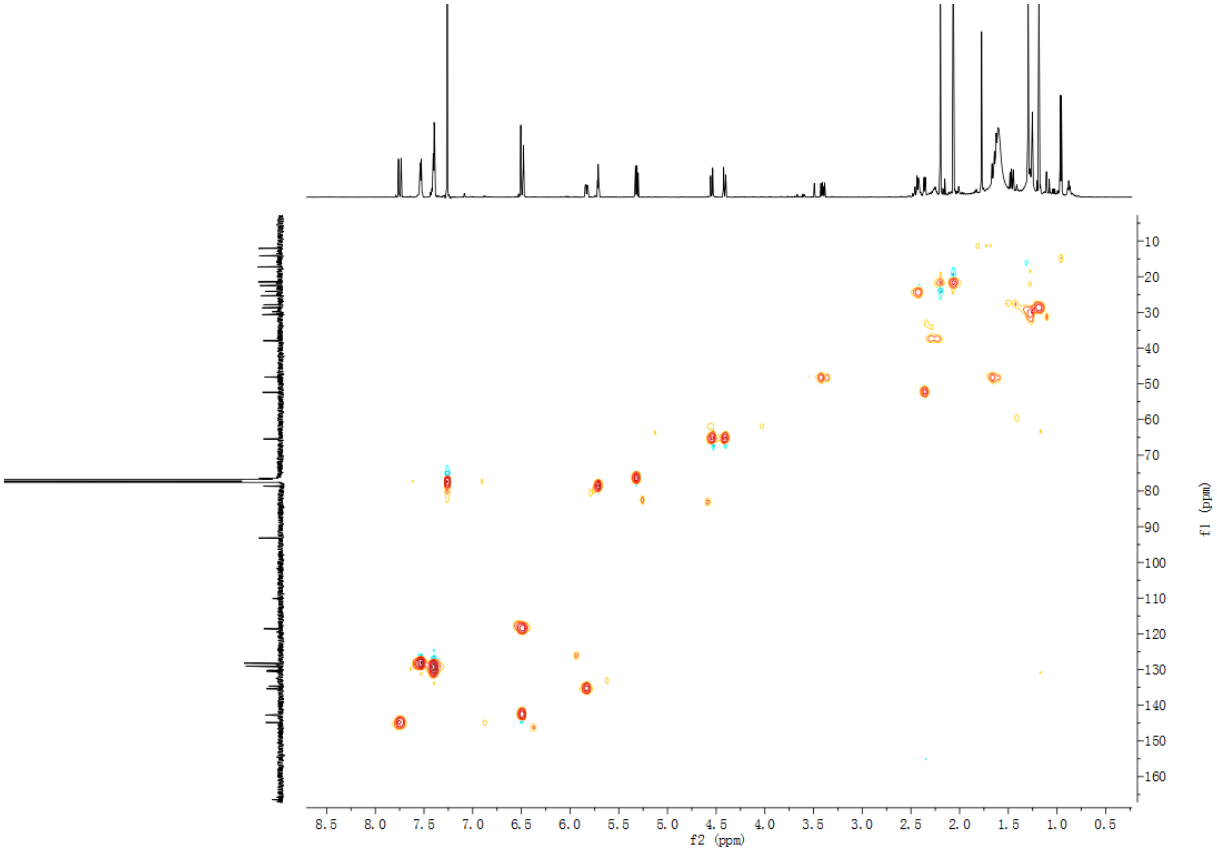
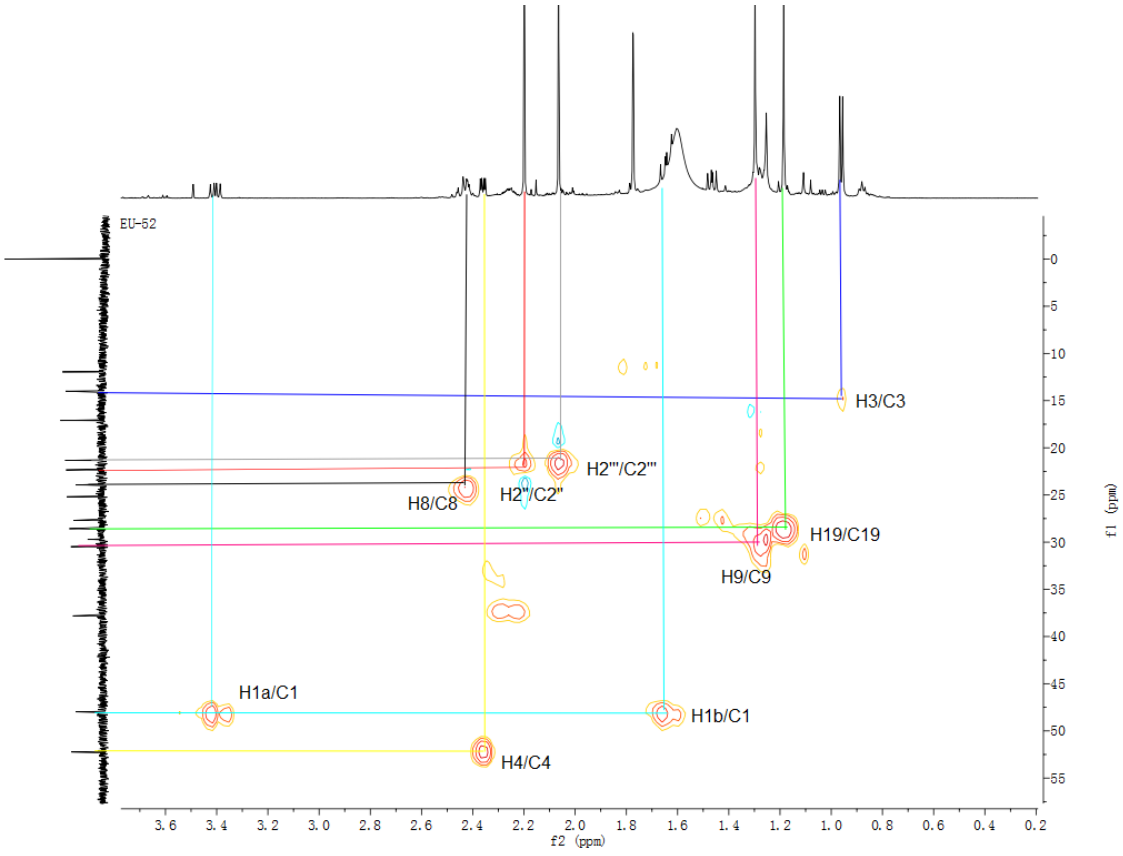


Figure S8: DEPT135 (600 MHz, $CDCl_3$) spectrum of **1**



F**igure S9:** HSQC spectrum of **1**



Fi**gure S10:** HSQC spectrum of **1** (From δ_H 0.2 ppm to δ_H 3.6 ppm)

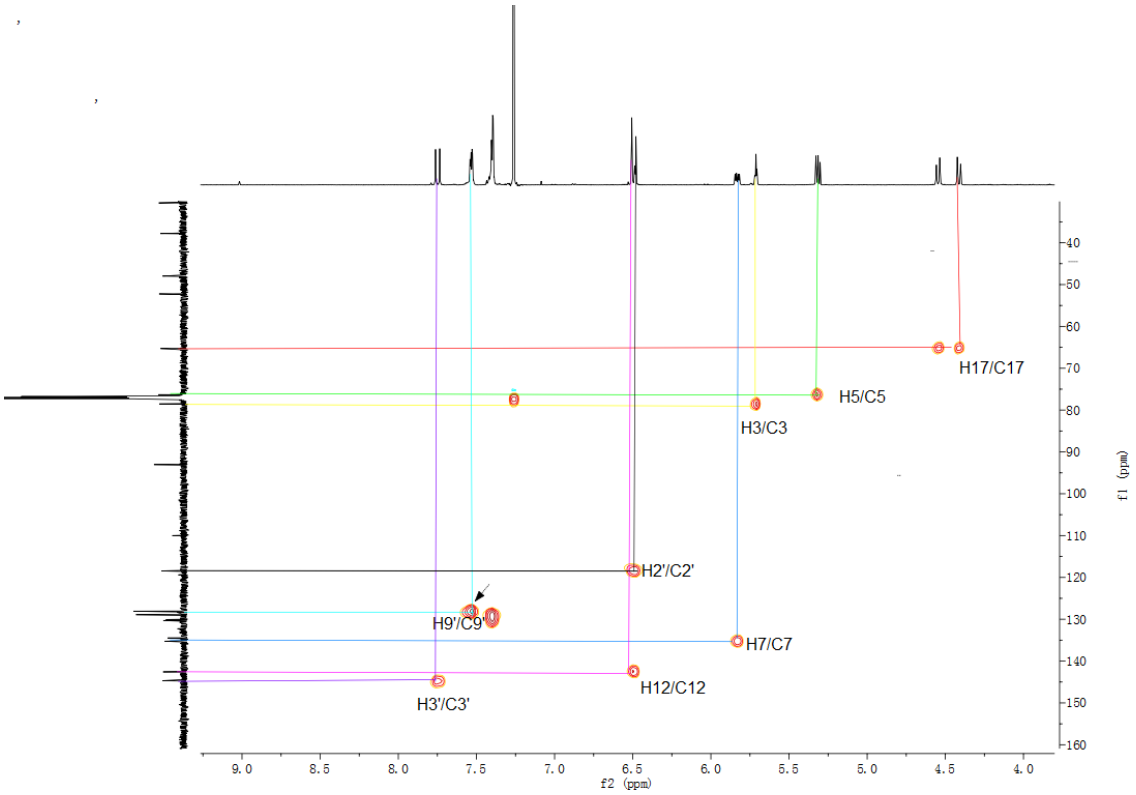


Figure S11: HSQC spectrum of **1** (From δ_H4.0 ppm to δ_H 9.0 ppm)

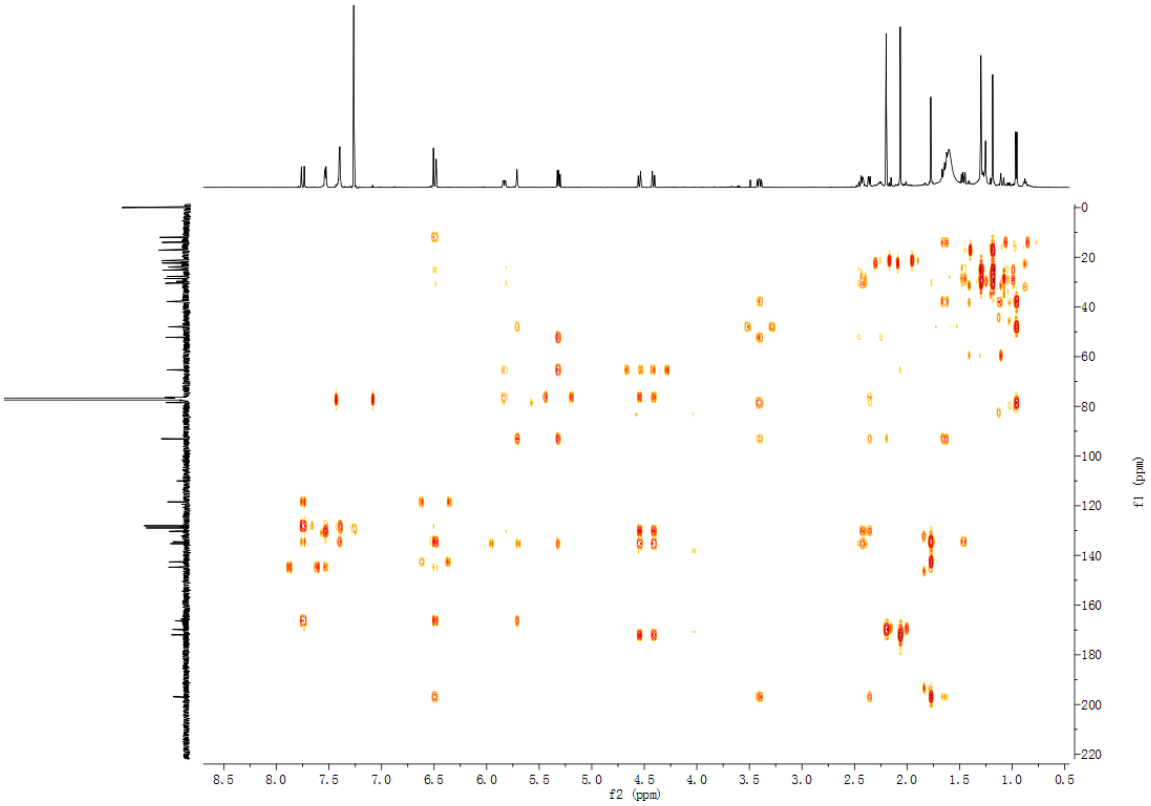


Figure S12: HMBC spectrum of **1**

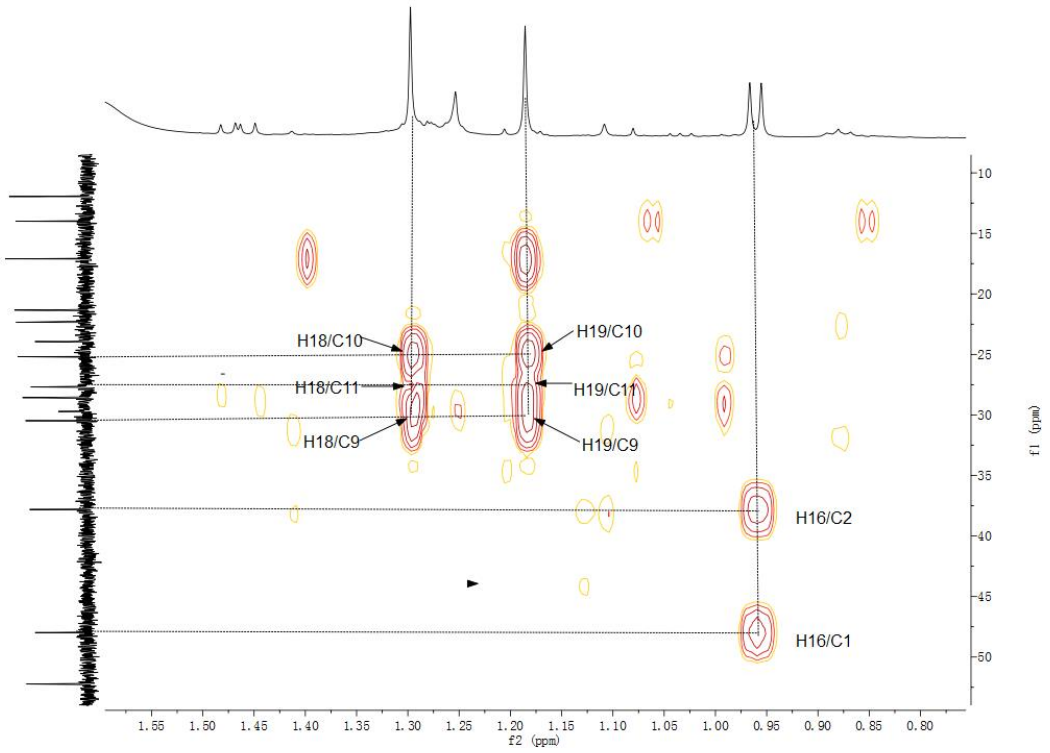


Figure S13: HMBC spectrum of **1** (From δ_C 10 ppm to δ_C 50 ppm)

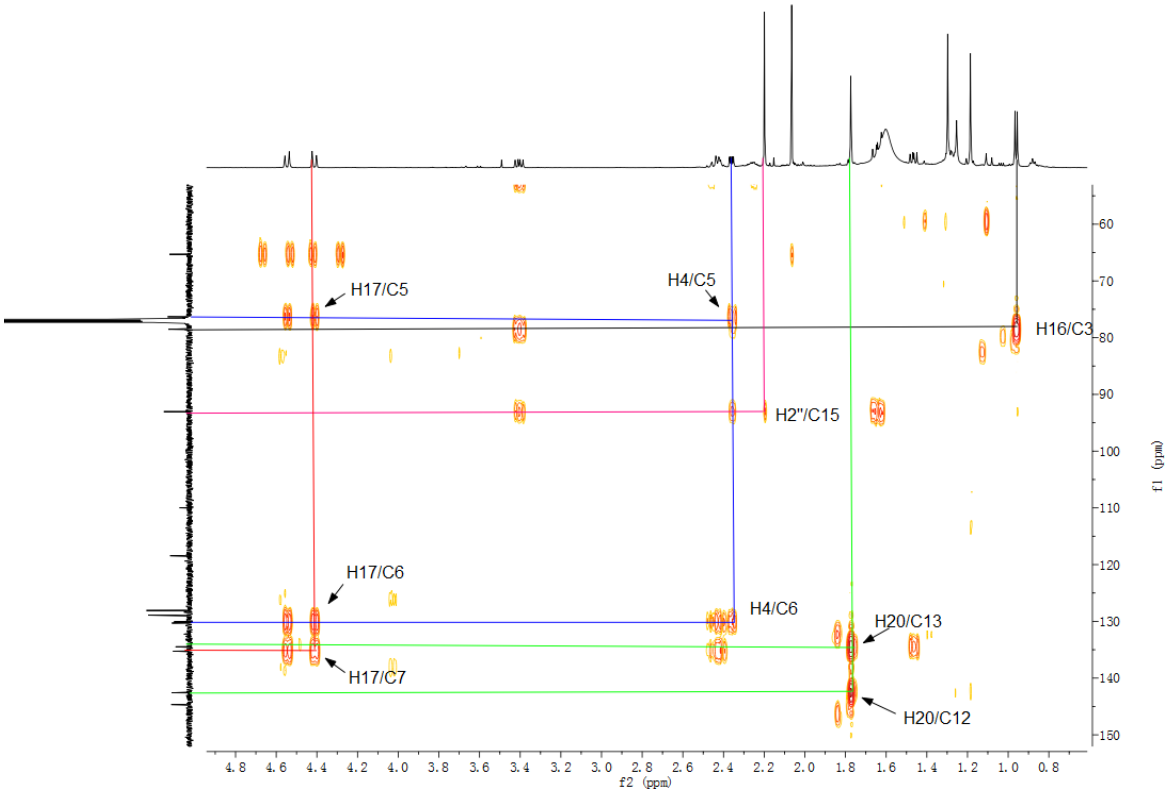


Figure S14: HMBC spectrum of **1**(From δ_C 60 ppm to δ_C 150 ppm)

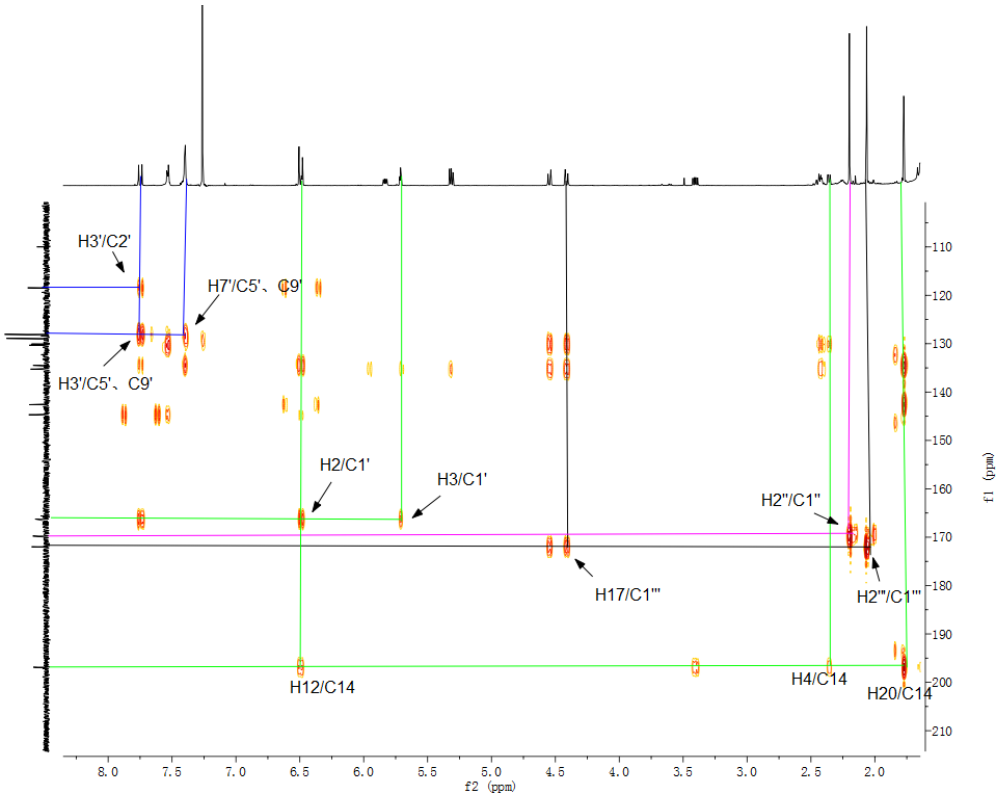


Figure S15: HMBC spectrum of **1** (From δ_C 110 ppm to δ_C 210 ppm)

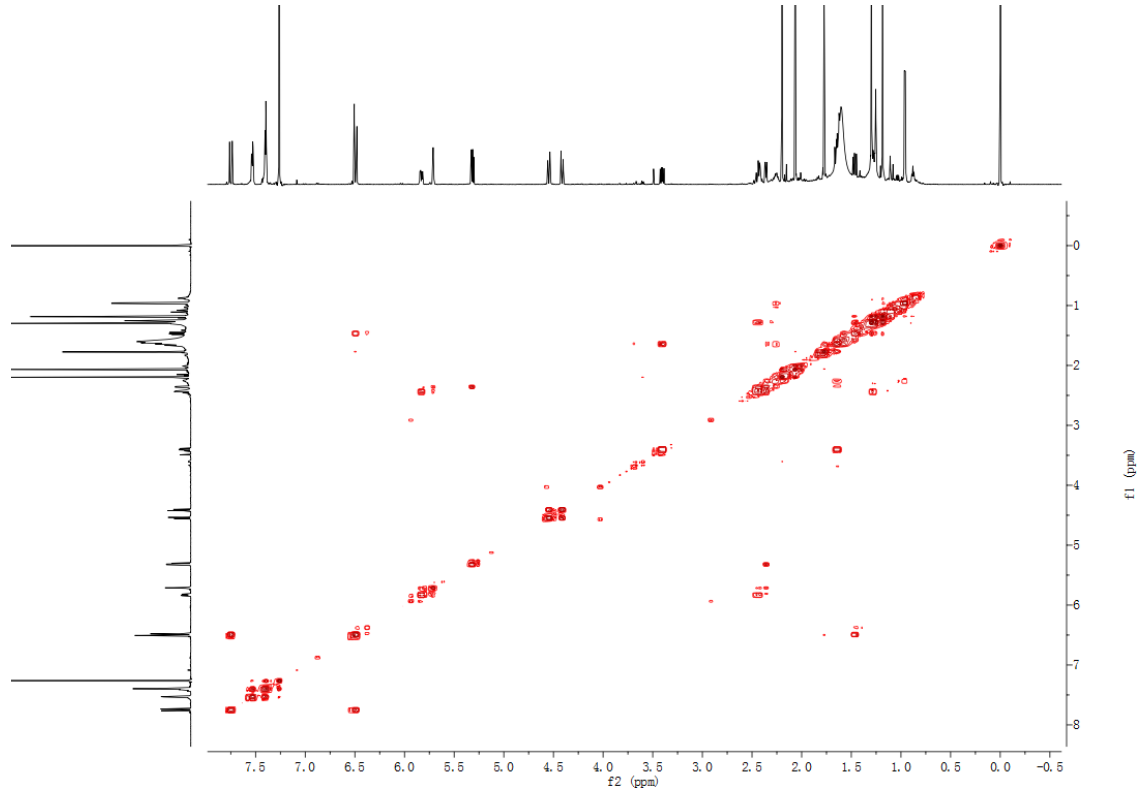


Figure S16: ^{1}H-^{1}H COSY spectrum of **1**

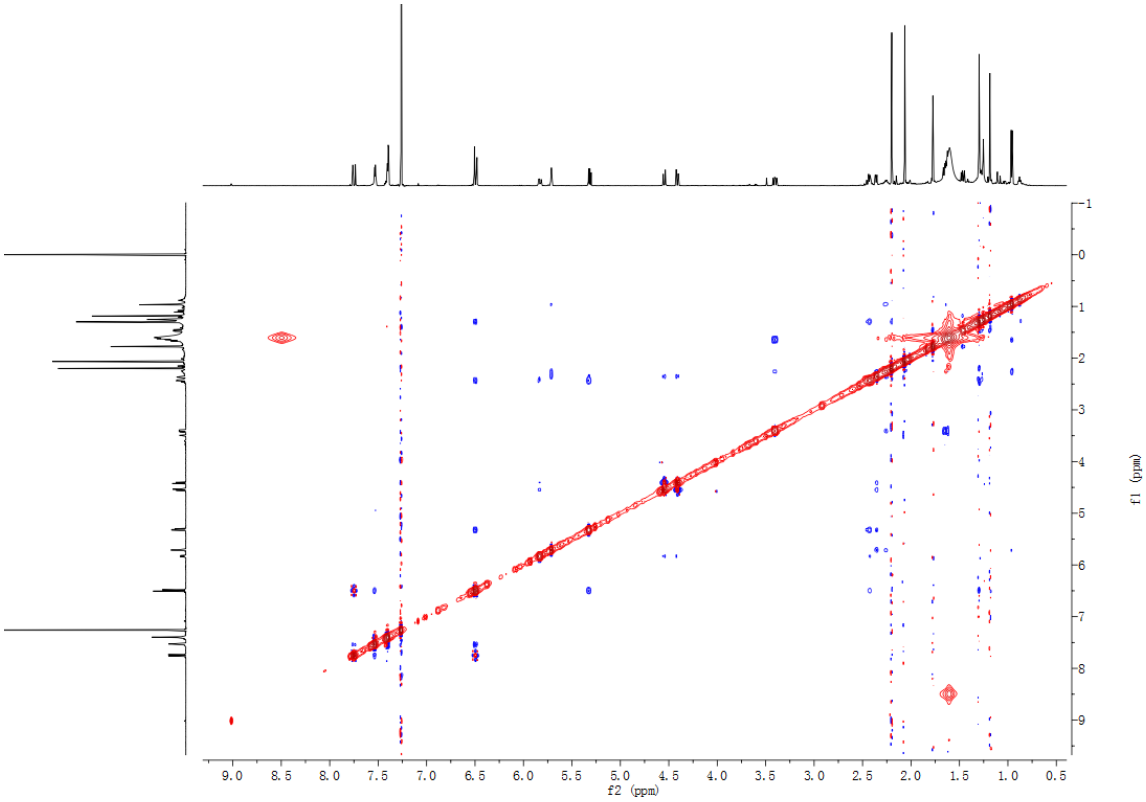


Figure S17: NOESY spectrum of **1**

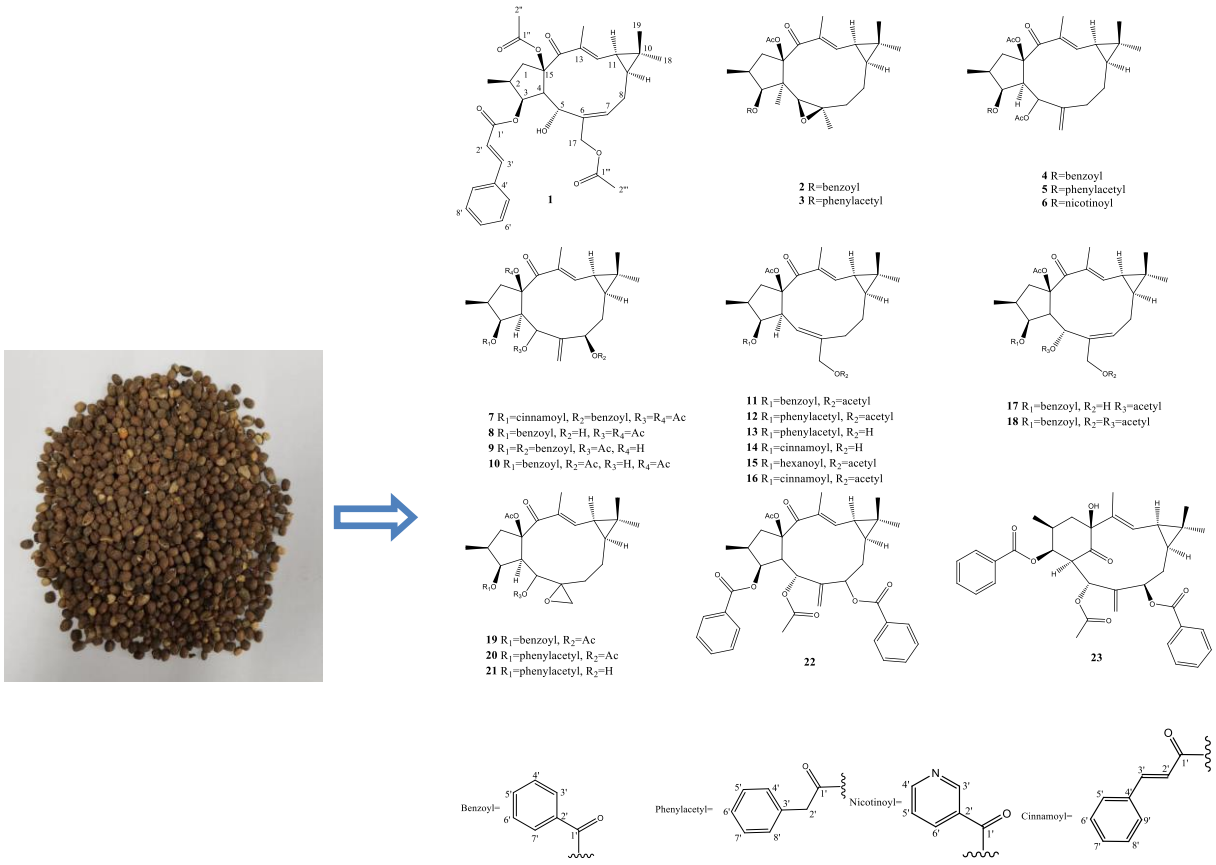


Figure S18: Structures of isolated compounds *Euphorbia lathyris* (**1–23**)

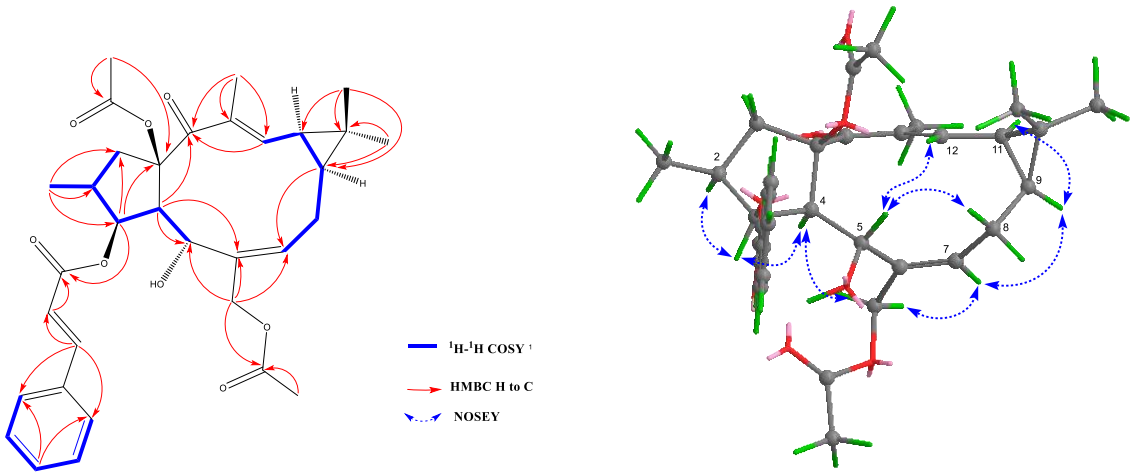


Figure S19: Selected HMBC, ^{1}H–^{1}H COSY and NOESY correlations of compound **1**.

Table S1: ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data for compound **1** ($CDCl_3$, δ in ppm, *J* in Hz)

position	*δ*H	*δ*C
1	3.41 (1H, *dd*, *J* = 14.4, 8.7)	48.1
	1.65 (1H, *m*)	
2	2.26 (1H, *m*, H-2)	37.9
3	5.71 (1H, *t*, *J* = 3.6)	78.7
4	2.36 (1H, *dd*, *J* = 8.2, 3.5)	52.3
5	5.32 (1H, *d*, *J* = 8.2)	76.4
6		130.2
7	5.83 (1H, *dd*, *J* = 11.5, 5.2)	135.4
8	2.41 - 2.46 (2H, *m*)	24.1
9	1.29 (1H, *m*, H-9)[b]	30.6
10		25.3
11	1.47 (1H, *dd*, *J* = 11.6, 8.6)	27.8
12	6.49 (1H, *m*)[a]	142.7
13		134.6
14		197.0
15		93.2
16	0.96 (3H, *d*, *J* = 6.7)	14.1
17	4.55 (1H, *d*, *J* = 12.7)	65.4
	4.41 (1H, *d*, *J* = 12.7)	
18	1.30 (3H, *s*, H-18)[b]	17.2
19	1.19 (3H, *s*, H-19)	28.7
20	1.77 (3H, *s*)	12.1
1'		166.4
2'	6.49 (1H, *d*[a])	118.6
3'	7.74 (1H, *d*)	144.8
4'		134.5
5'		128.1
6'	7.40 (1H, *m*)	129.1
7'	7.40 (1H, *m*)	130.3
8'	7.40 (1H, *m*)	129.1
9'	7.53 (1H, *m*)	128.1
1"		169.7
2"	2.20 (3H, *s*)	22.4
1"'		172.1
2"'	2.06 (3H, *s*)	21.5

[a, b] Overlapping signals

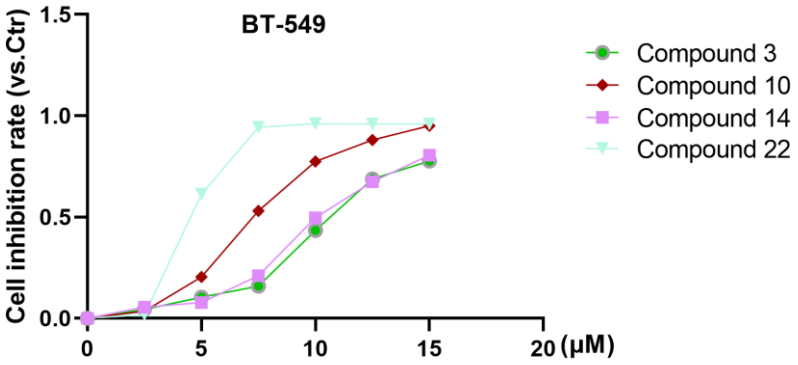


Figure S20: Inhibitory rate of compounds with different concentrations on BT-549 cells.

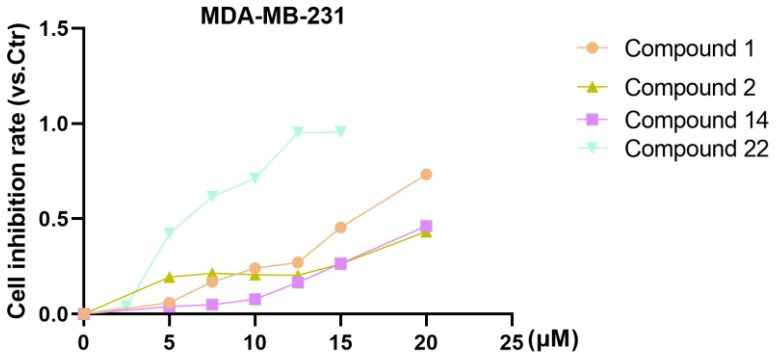


Figure S21: Inhibitory rate of compounds with different concentrations on MDA-MB-231 cells

Table S2 : Cytotoxic activity (IC_{50} in μM)

Compound	IC_{50}（μM）	
	MDA-MB-231	BT-549
1	21.3	>30
2	15.3	>30
3	>30	10.1
10	>30	7.4
14	16.3	9.9
22	5.7	4.7

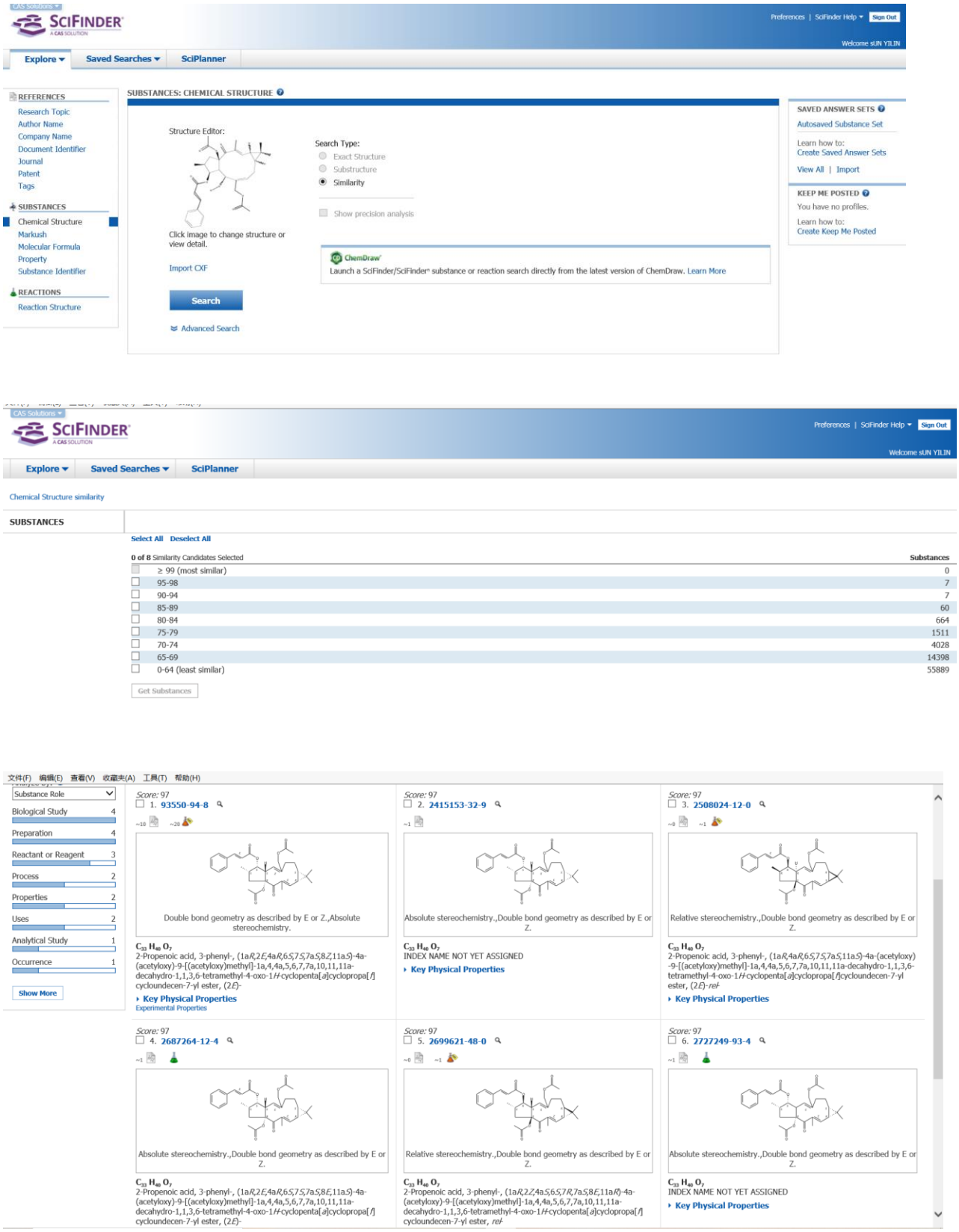
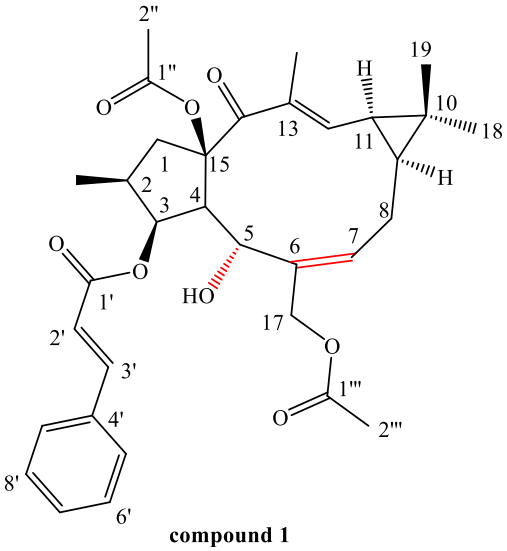


Figure S22: The Scifinder similarity report for new compound **1**



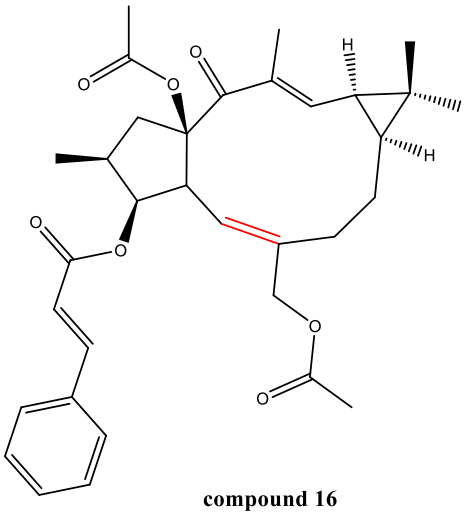


Figure S23: The structure is most similar to compound **1**

Table S3: The ^{1}H NMR data for compound **1** and the similar compound

position	1	16
1	3.41 (1H, *dd*, *J* = 14.4, 8.7)	3.60 (1H, *dd*, *J* = 14.0, 8.1)
	1.65 (1H, *m*)	1.55 (1H, *m*)
2	2.26 (1H, *m*, H-2)	
3	5.71 (1H, *t*, *J* = 3.6)	5.43 (1H, *t*, *J* = 3.5)
4	2.36 (1H, *dd*, *J* = 8.2, 3.5)	2.80 (1H, *dd*, *J* = 11.0, 3.5)
5	5.32 (1H, *d*, *J* = 8.2)	5.67 (1H, *d*, *J* =11.0)
6		
7	5.83 (1H, *dd*, *J* = 11.5, 5.2)	2.20, 2.38 (2H, *m*)
8	2.41 - 2.46 (2H, *m*)	1.52, 2.24 (2H, *m*)
9	1.29 (1H, *m*, H-9)[b]	1.10 (1H, *m*, H-9)
10		
11	1.47 (1H, *dd*, *J* = 11.6, 8.6)	1.43 (1H, *dd*, *J* = 11.5, 8.0)
12	6.49 (1H, *m*)[a]	6.58 (1H, *d*, *J* =11.5)
13		
14		
15		
16	0.96 (3H, *d*, *J* = 6.7)	1.01 (3H, *d*, *J* = 6.7)
17	4.55 (1H, *d*, *J* = 12.7)	4.14 (1H, *d*, *J* = 12.2)
	4.41 (1H, *d*, *J* = 12.7)	4.38 (1H, *d*, *J* = 12.2)
18	1.30 (3H, *s*, H-18)[b]	1.17 (3H, *s*, H-18)
19	1.19 (3H, *s*, H-19)	1.05 (3H, *s*, H-19)
20	1.77 (3H, *s*)	1.85 (3H, *s*)
2'	6.49 (1H, *d*[a])	6.49 (1H, *d*[a])
3'	7.74 (1H, *d*)	7.73 (1H, *d*)
6'	7.40 (1H, *m*)	7.41 (1H, *m*)
7'	7.40 (1H, *m*)	7.41 (1H, *m*)
8'	7.40 (1H, *m*)	7.41 (1H, *m*)
9'	7.53 (1H, *m*)	7.55 (1H, m)
2"	2.20 (3H, *s*)	2.02 (3H, *s*)
2'"	2.06 (3H, *s*)	2.06 (3H, *s*)

[a, b] Overlapping signals

Table S4: The ^{13}C NMR data for compound **1** and the similar compound

position	1	16
1	48.1	44.8
2	37.9	38.7
3	78.7	80.9
4	52.3	50.6
5	76.4	140.4
6	130.2	145.0
7	135.4	34.1
8	24.1	29.1
9	30.6	32.3
10	25.3	24.8
11	27.8	28.5
12	142.7	147.0
13	134.6	134.3
14	197.0	194.4
15	93.2	94.6
16	14.1	13.8
17	65.4	64.0
18	17.2	29.3
19	28.7	16.1
20	12.1	12.3
1'	166.4	166.2
2'	118.6	118.2
3'	144.8	124.9
4'	134.5	132.4
5'	128.1	128.0
6'	129.1	128.9
7'	130.3	130.4
8'	129.1	128.9
9'	128.1	128.0
1"	169.7	169.4
2"	22.4	20.9
1'"	172.1	170.7
2'"	21.5	21.5