

Supporting Information

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

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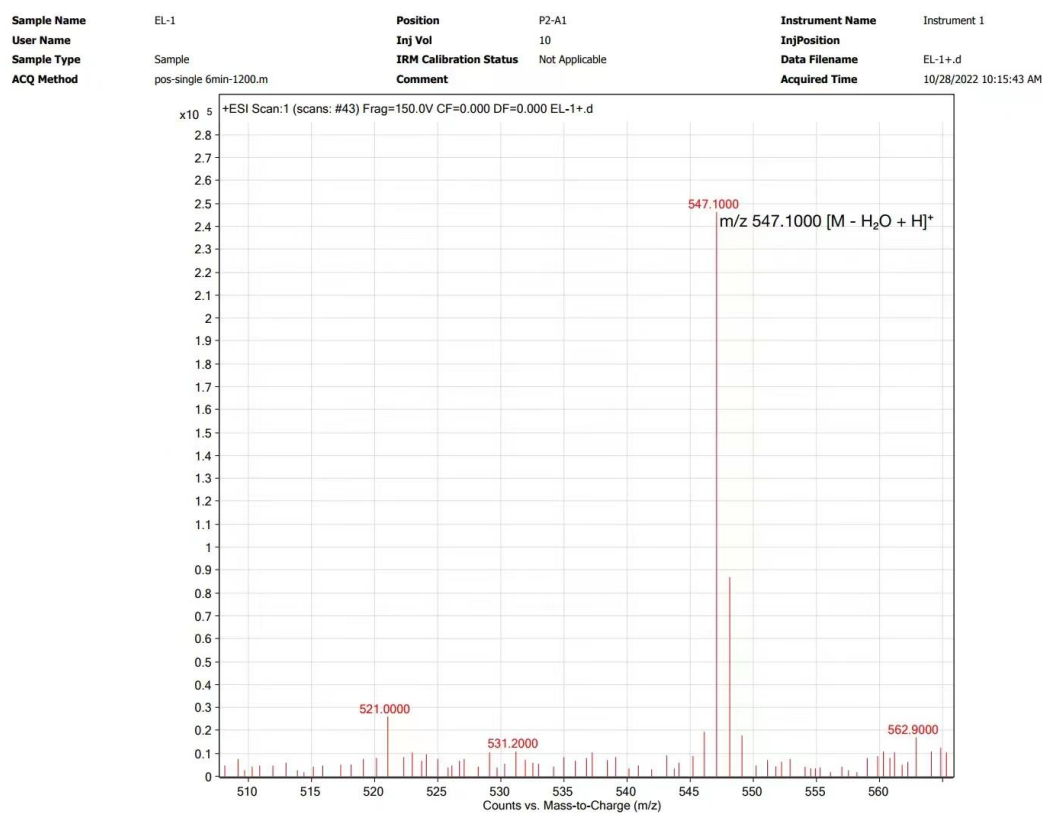


Figure S1: EI-MS spectrum of **1** $[M - H_2O + H]^+$

Sample Name	EL-1	Position	P2-A1	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Not Applicable	Data Filename	EL-1-.d
ACQ Method	NEG -Single 6min-1200.m	Comment		Acquired Time	10/28/2022 10:02:48 AM

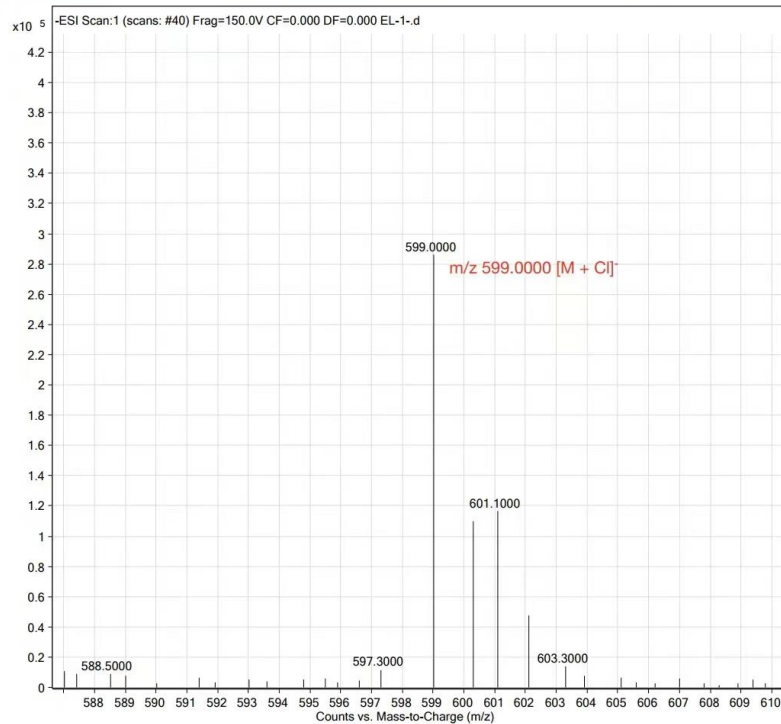


Figure S2: EI-MS spectrum of **1** $[M + Cl]^-$

Compound 1+ #1-13 RT: 0.00-0.06 AV: 13 NL: 3.11E7
T: FTMS + p ESI SIM ms [560.0000-600.0000]

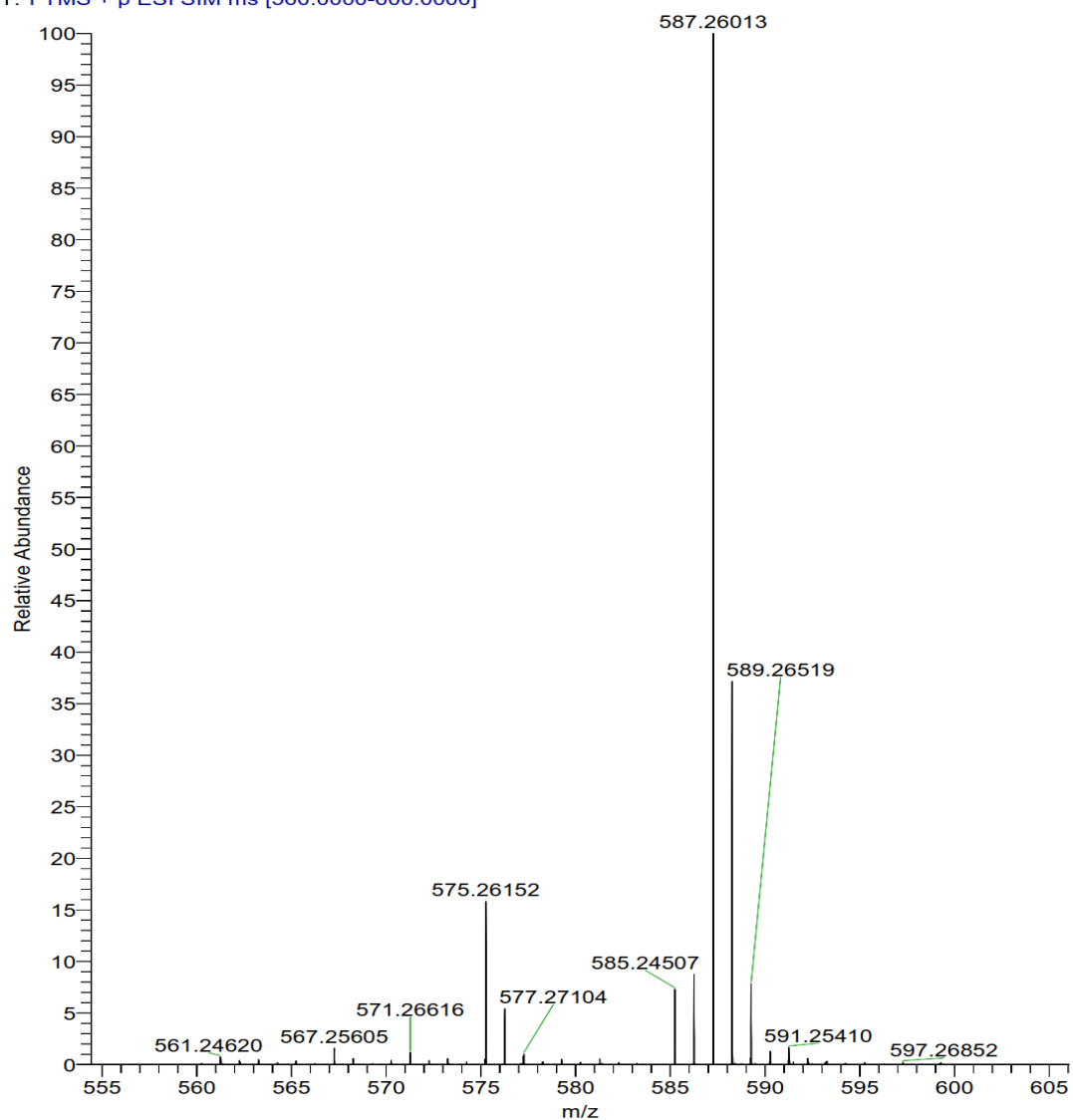


Figure S3: HR-ESI-MS spectrum of **1**



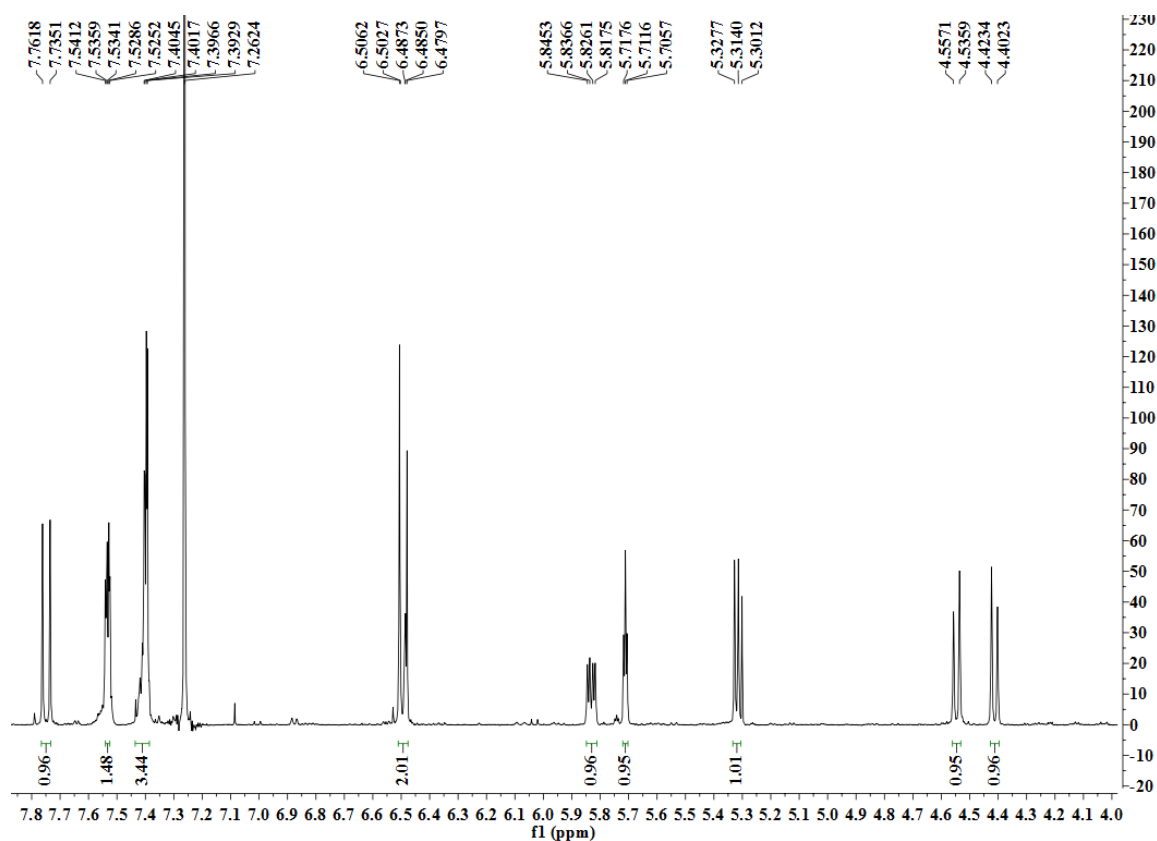


Figure S6: ¹H-NMR (600 MHz, CDCl₃) spectrum of **1** (From δ_H 4.0 ppm to δ_H 7.8 ppm)

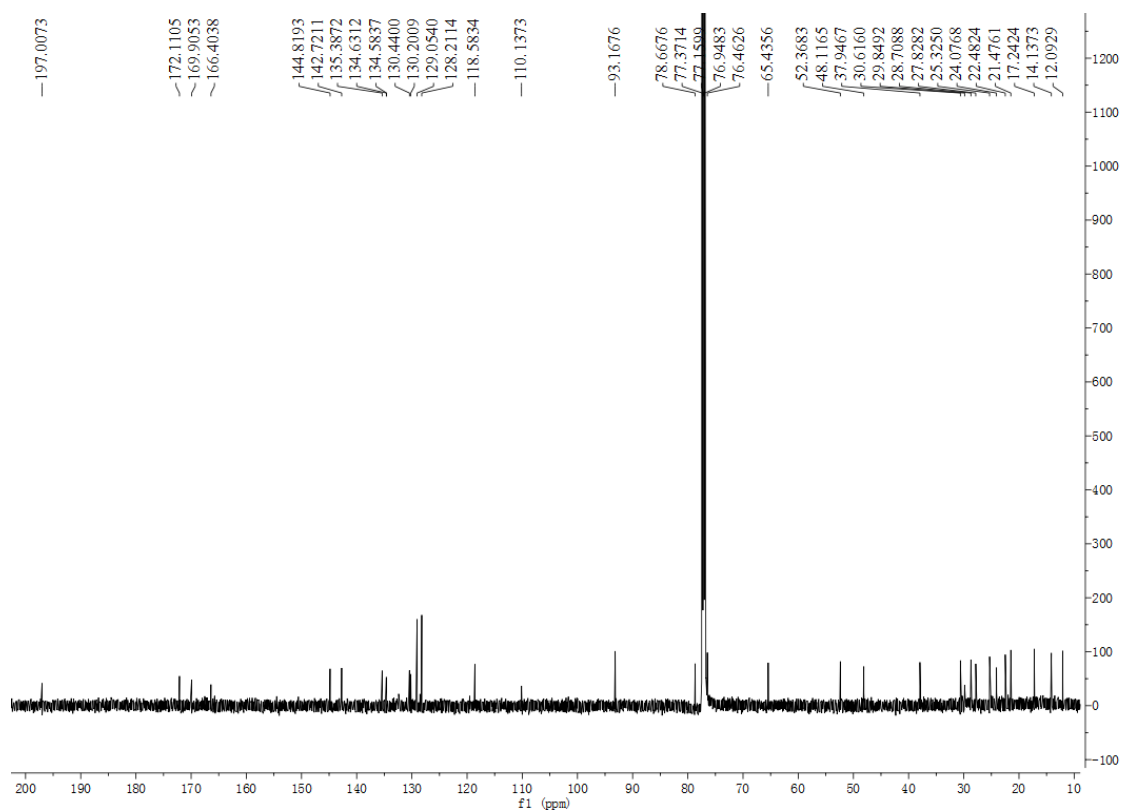


Figure S7: ¹³C-NMR (600 MHz, CDCl₃) spectrum of **1**

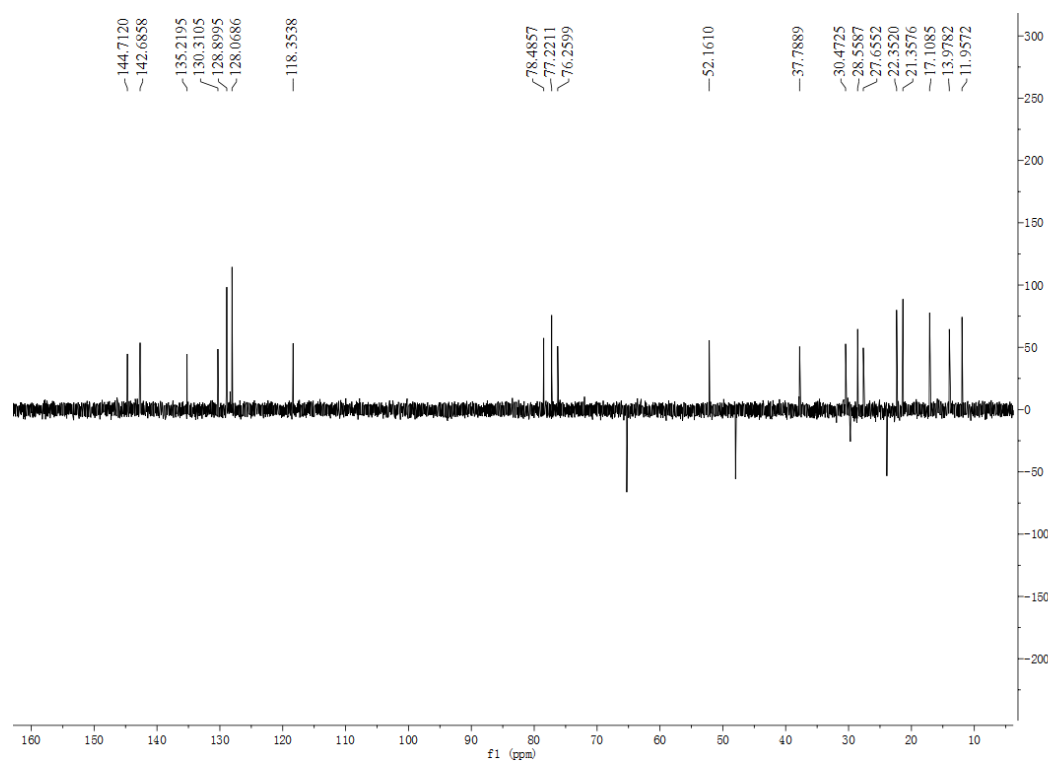


Figure S8: DEPT135 (600 MHz, CDCl_3) spectrum of **1**

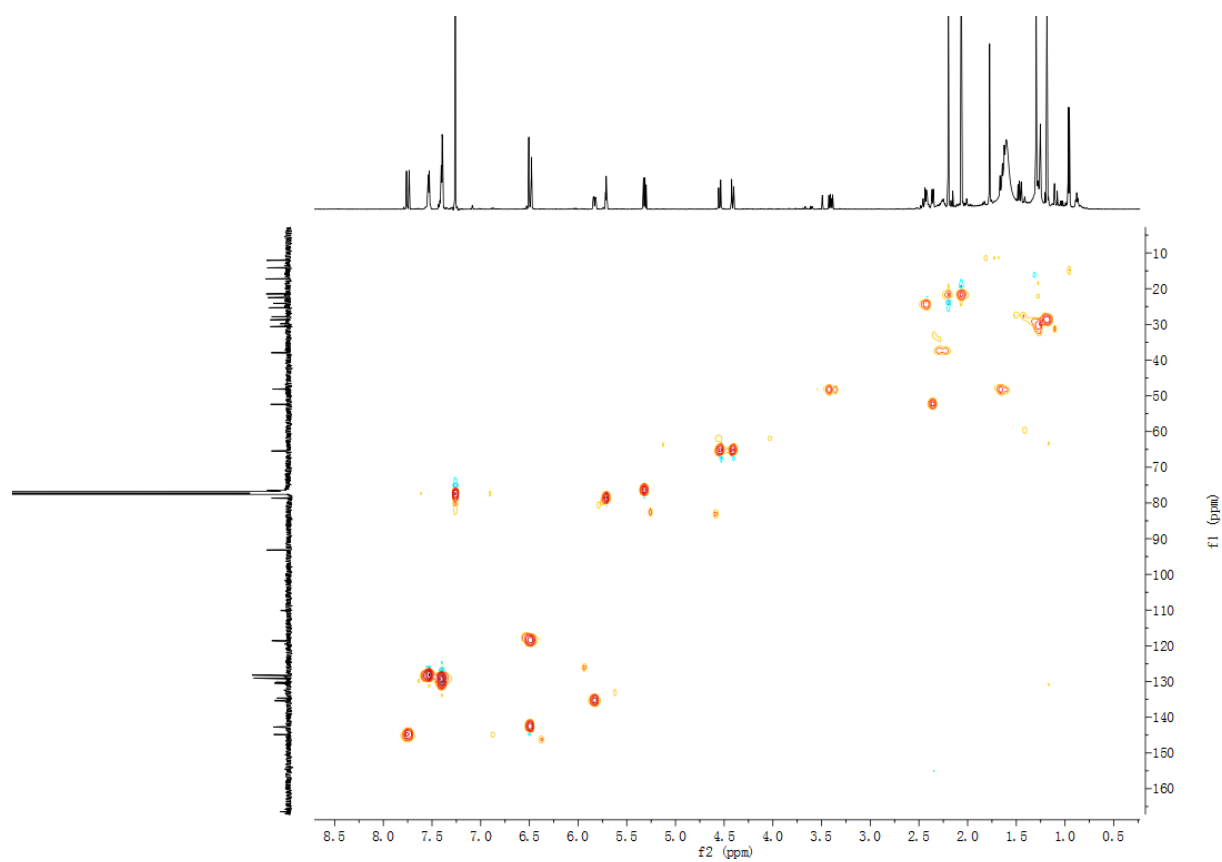


Figure S9: HSQC spectrum of **1**

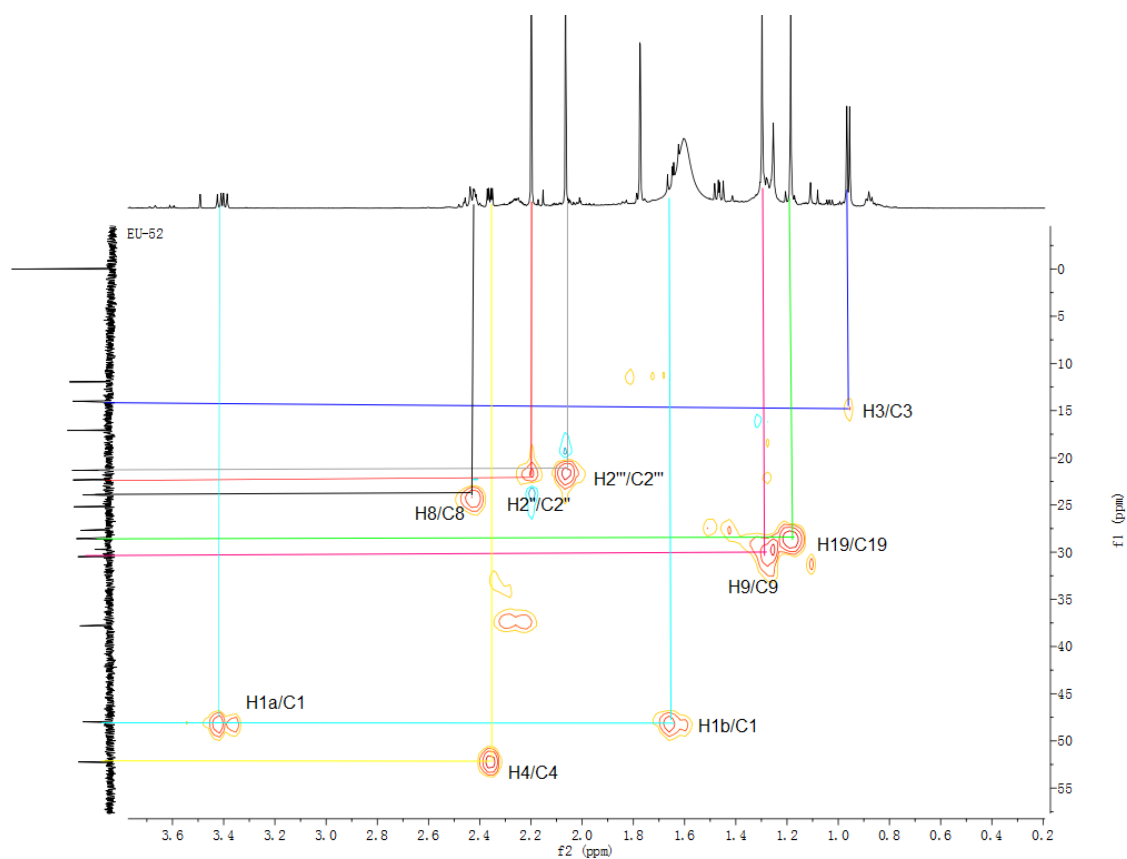


Figure S10: HSQC spectrum of **1** (From δ_{H} 0.2 ppm to δ_{H} 3.6 ppm)

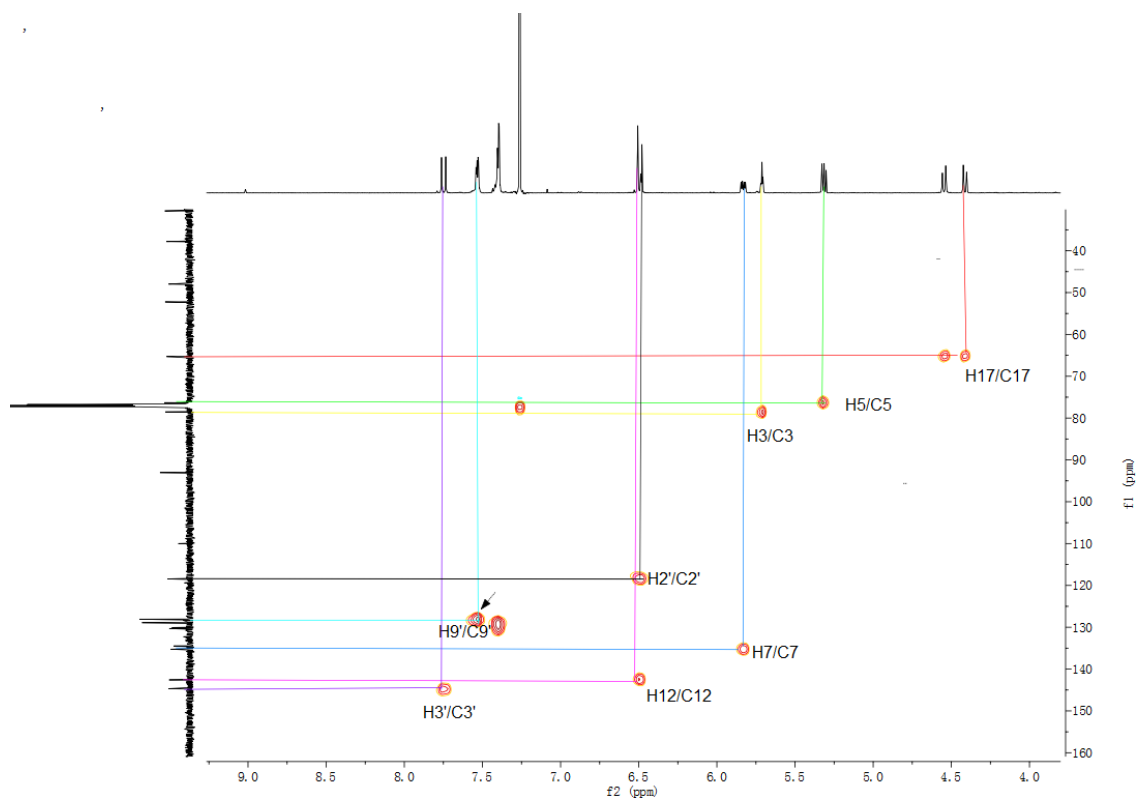


Figure S11: HSQC spectrum of **1** (From δ_{H} 4.0 ppm to δ_{H} 9.0 ppm)

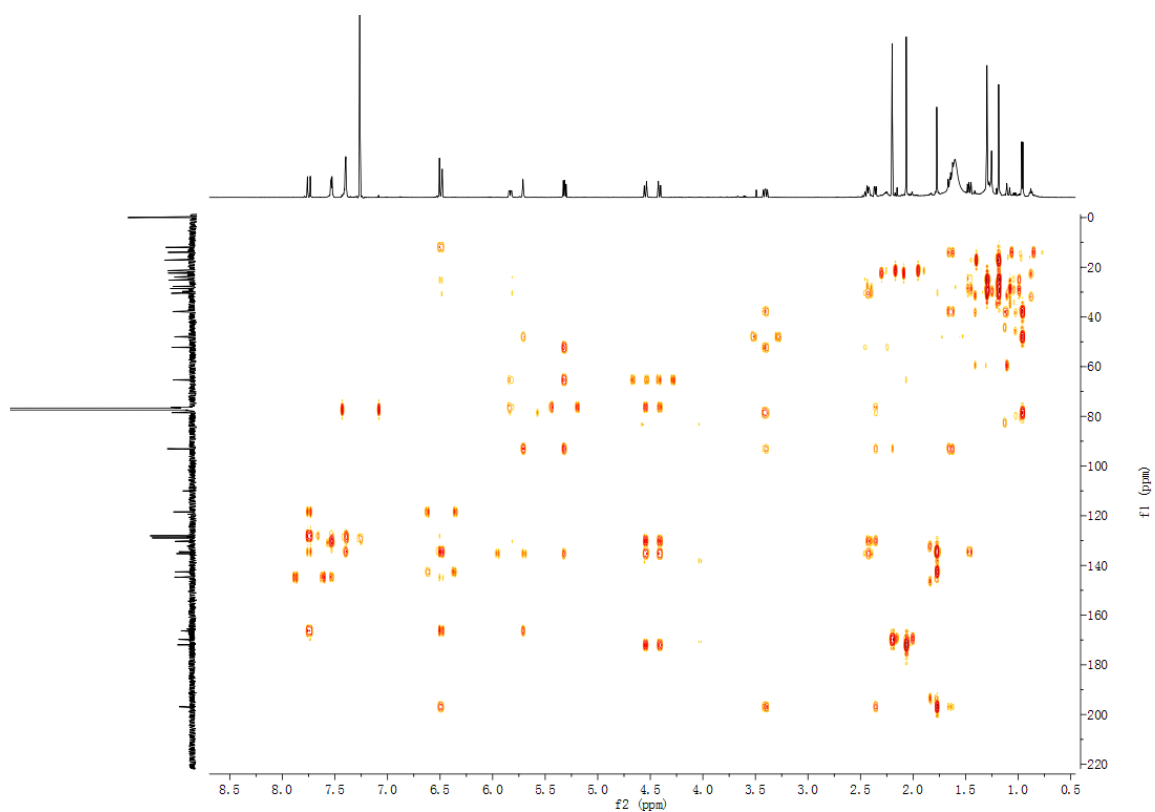


Figure S12: HMBC spectrum of **1**

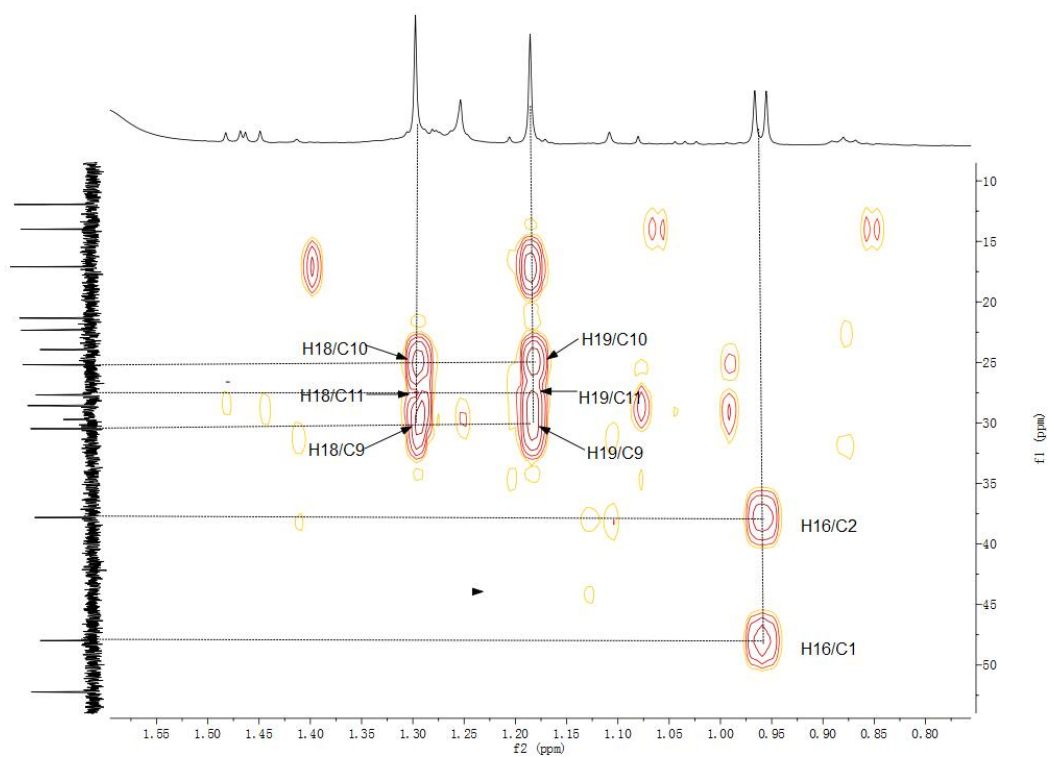


Figure S13: HMBC spectrum of **1** (From δ_C 10 ppm to δ_C 50 ppm)

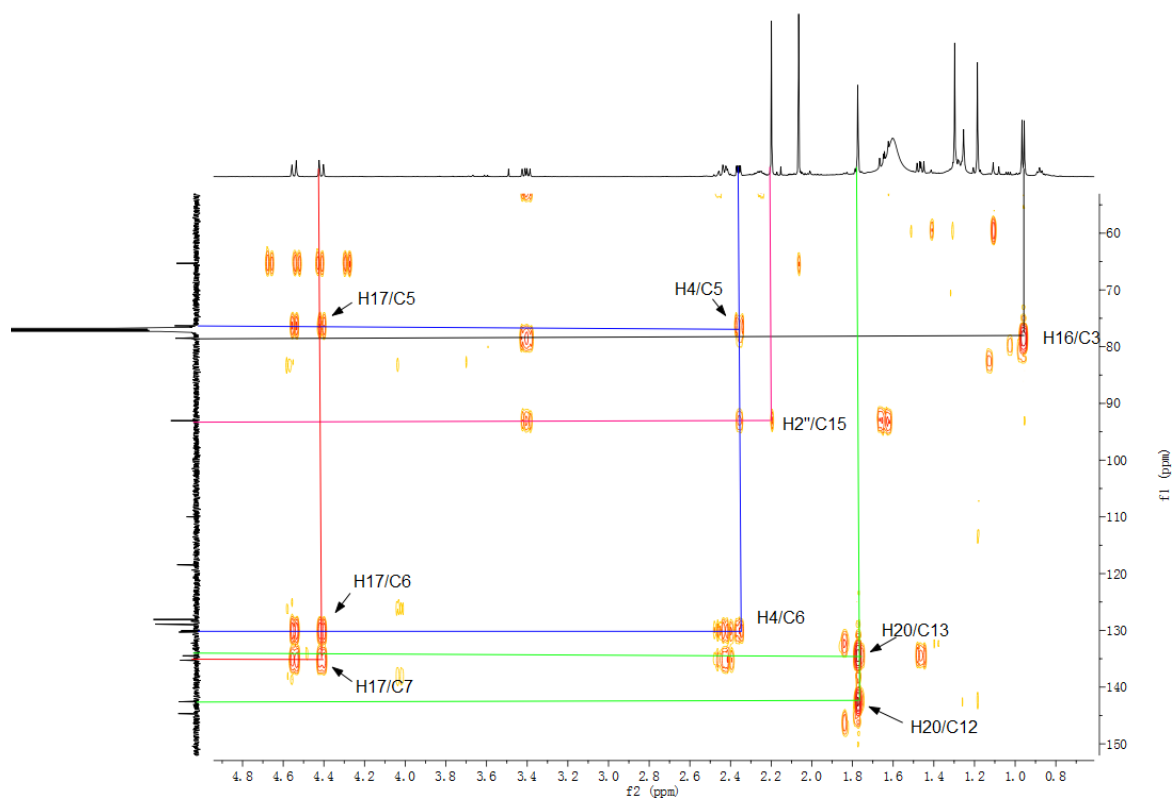


Figure S14: HMBC spectrum of **1** (From δ_c 60 ppm to δ_c 150 ppm)

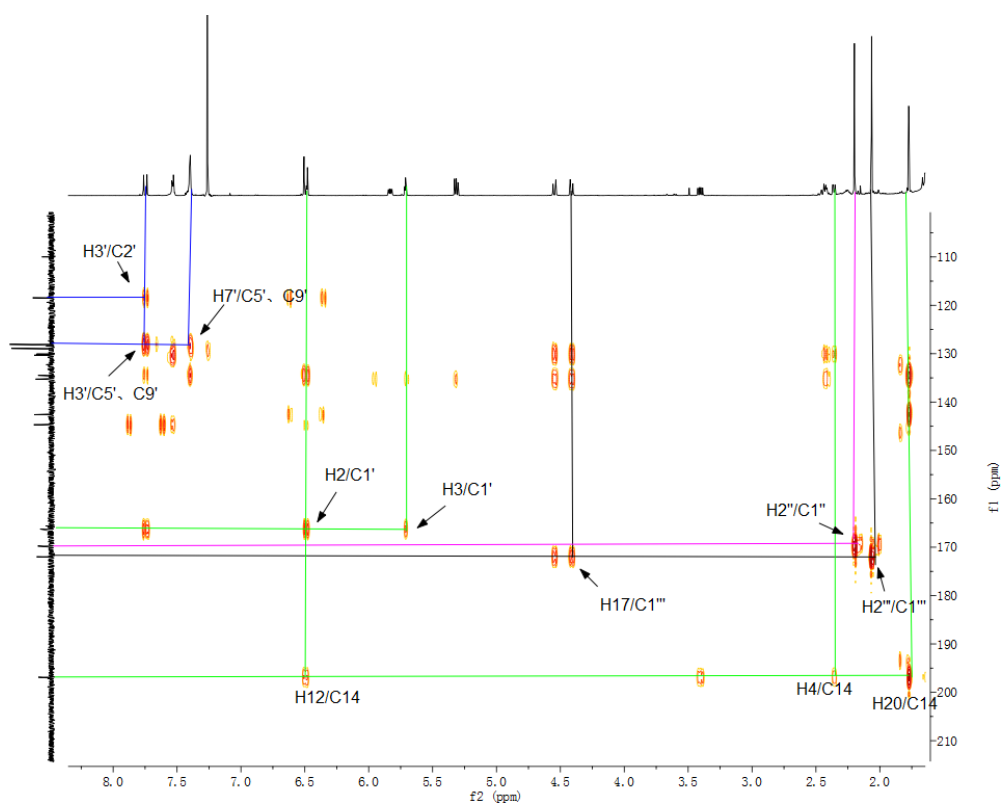


Figure S15: HMBC spectrum of **1** (From δ_c 110 ppm to δ_c 210 ppm)

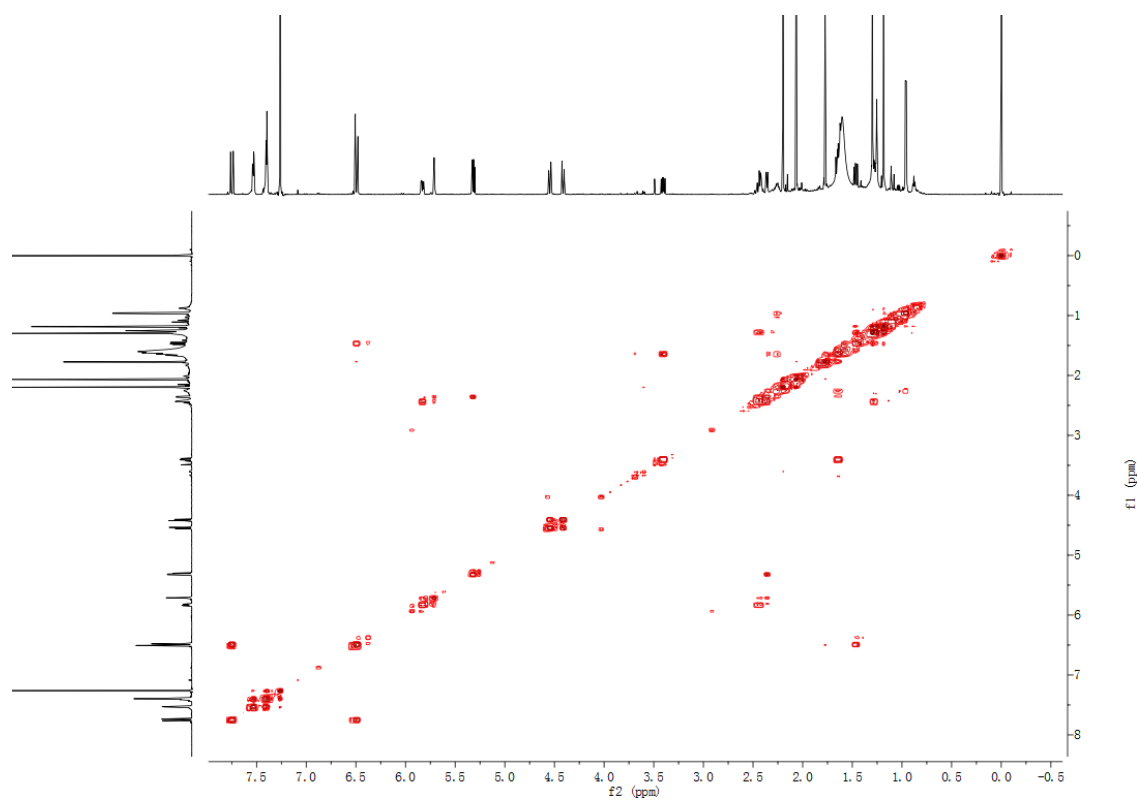


Figure S16: ^1H - ^1H COSY spectrum of **1**

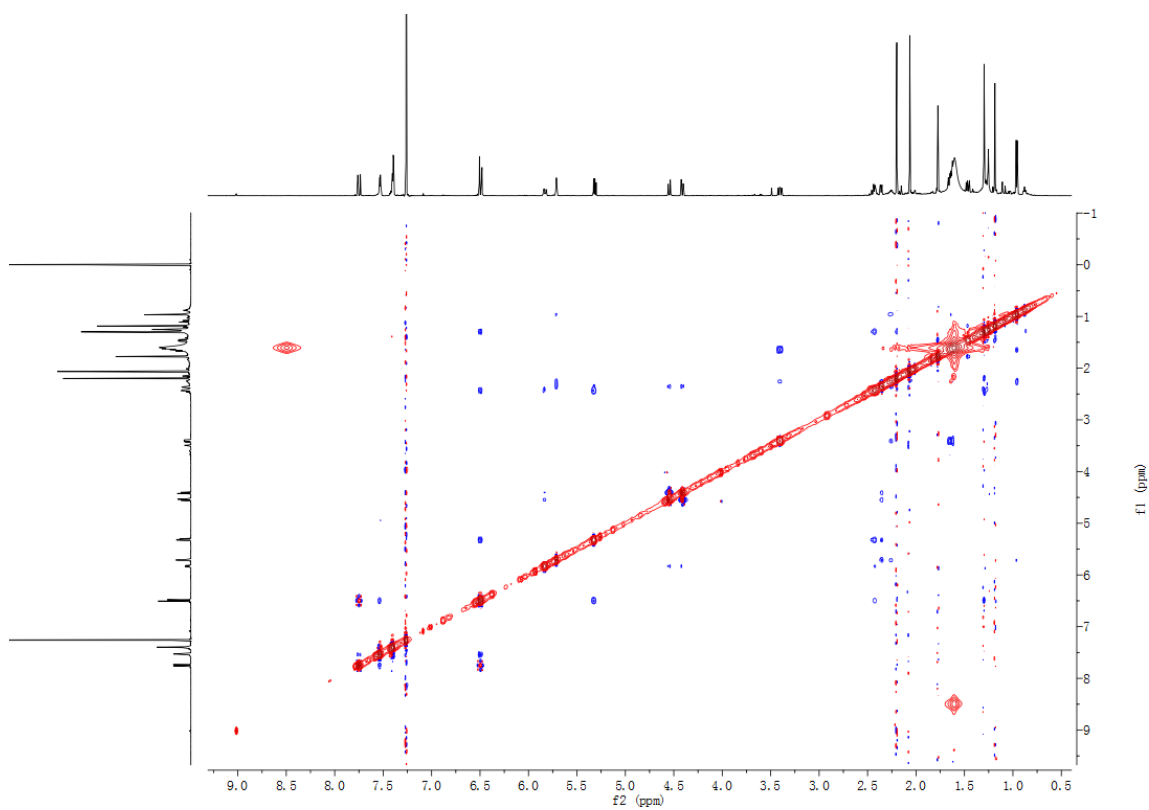


Figure S17: NOESY spectrum of **1**

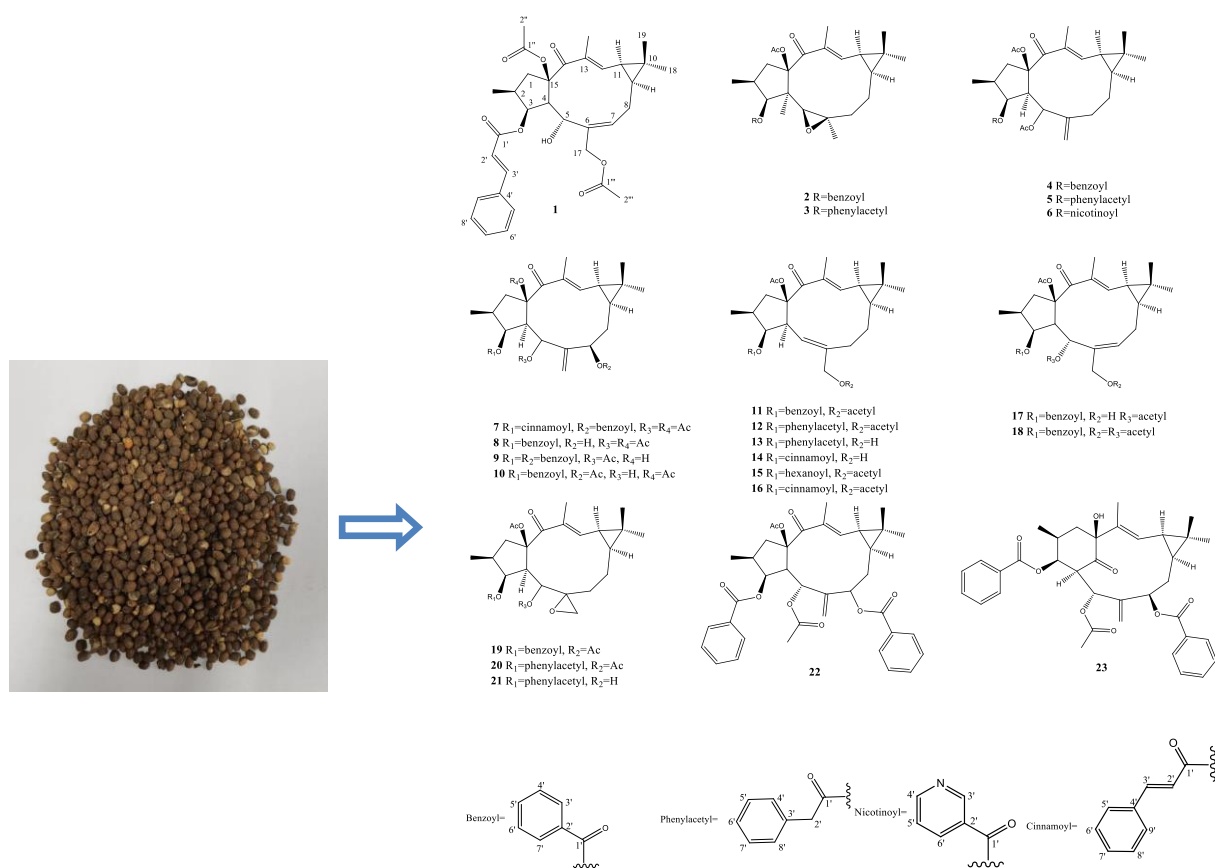


Figure S18: Structures of isolated compounds *Euphorbia lathyris* (1–23)

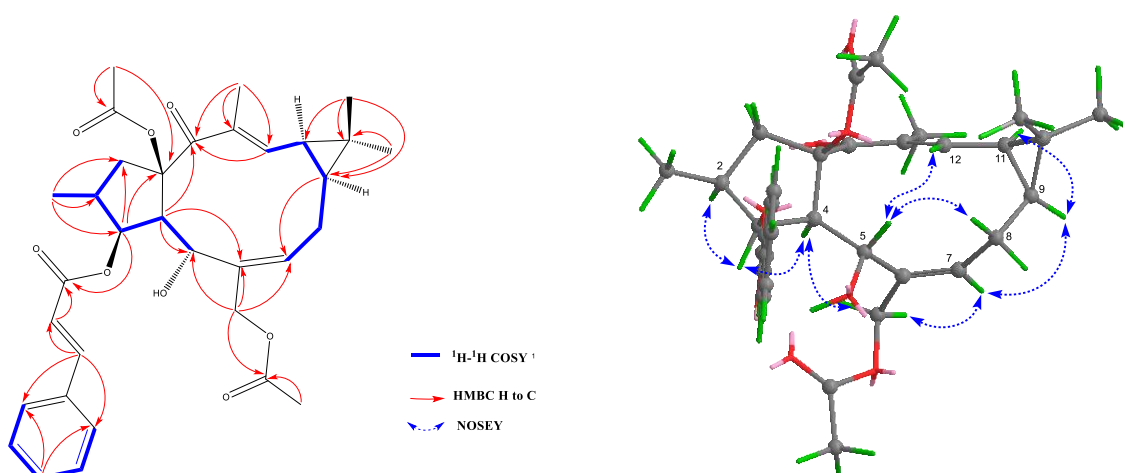


Figure S19: Selected HMBC, $^1\text{H}-^1\text{H}$ COSY and NOESY correlations of compound **1**.

Table S1: ¹H (600 MHz) and ¹³C (150 MHz) NMR data for compound **1** (CDCl₃, δ in ppm, *J* in Hz)

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

^{a, b} Overlapping signals

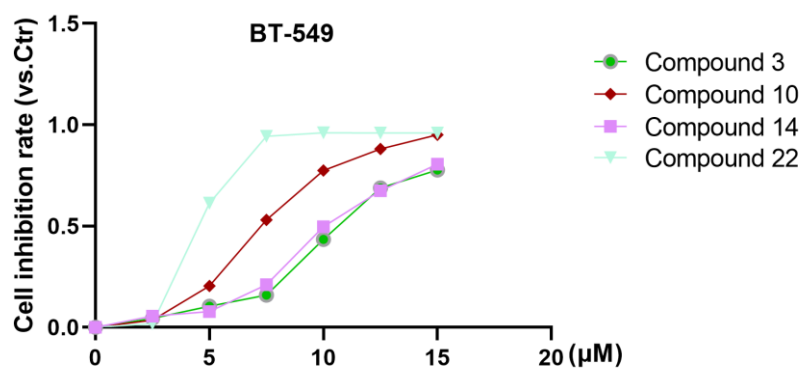


Figure S20: Inhibitory rate of compounds with different concentrations on BT-549 cells.

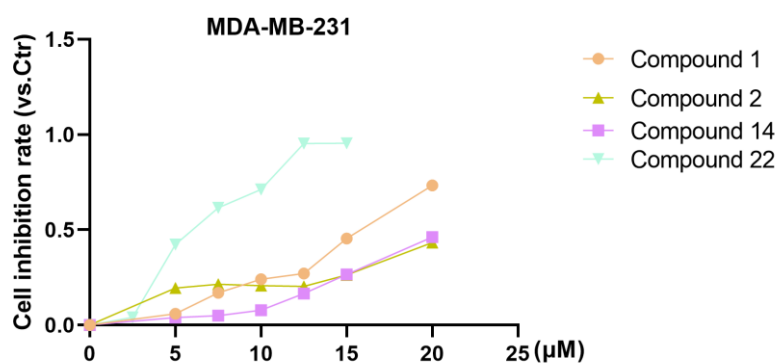


Figure S21: Inhibitory rate of compounds with different concentrations on MDA-MB-231 cells

Table S2 : Cytotoxic activity (IC₅₀ 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

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- Journal
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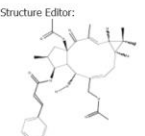
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Similarity Range	Substances
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90-94	7
85-89	60
80-84	664
75-79	1511
70-74	4028
65-69	14398
0-64 (least similar)	55889

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Substance Role

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Preparation 4

Reactant or Reagent 3

Process 2

Properties 2

Uses 2

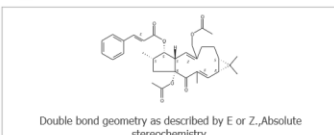
Analytical Study 1

Occurrence 1

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Score: 97

1. 93550-94-8



Double bond geometry as described by E or Z, Absolute stereochemistry.

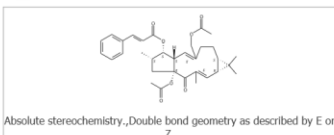
$C_{33}H_{40}O_7$
2-Propenoic acid, 3-phenyl-, (1aR,2E,4aR,6S,7S,7aS,8E,11aS)-4a-(acetyloxy)-9-[(acetyloxy)methyl]-1a,4,4a,5,6,7,7a,10,11,11a-decahydro-1,1,3,6-tetramethyl-4-oxo-1H-cyclopenta[a]cyclopropa[f]cycloundecen-7-yl ester, (2E)-

Key Physical Properties

Experimental Properties

Score: 97

2. 2415153-32-9



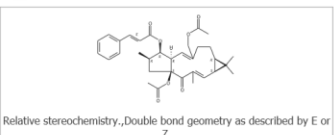
Absolute stereochemistry, Double bond geometry as described by E or Z.

$C_{33}H_{40}O_7$
INDEX NAME NOT YET ASSIGNED

Key Physical Properties

Score: 97

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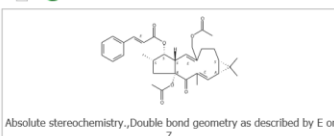
Relative stereochemistry, Double bond geometry as described by E or Z.

$C_{33}H_{40}O_7$
2-Propenoic acid, 3-phenyl-, (1aR,2E,4aR,6S,7S,7aS,8E,11aS)-4a-(acetyloxy)-9-[(acetyloxy)methyl]-1a,4,4a,5,6,7,7a,10,11,11a-decahydro-1,1,3,6-tetramethyl-4-oxo-1H-cyclopenta[a]cyclopropa[f]cycloundecen-7-yl ester, (2E)-ref

Key Physical Properties

Score: 97

4. 2687264-12-4

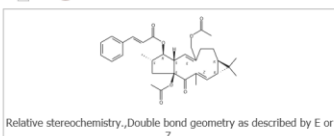


Absolute stereochemistry, Double bond geometry as described by E or Z.

$C_{33}H_{40}O_7$
2-Propenoic acid, 3-phenyl-, (1aR,2E,4aR,6S,7S,7aS,8E,11aS)-4a-(acetyloxy)-9-[(acetyloxy)methyl]-1a,4,4a,5,6,7,7a,10,11,11a-decahydro-1,1,3,6-tetramethyl-4-oxo-1H-cyclopenta[a]cyclopropa[f]cycloundecen-7-yl ester, (2E)-

Score: 97

5. 2699621-48-0

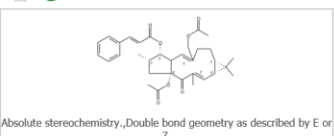


Relative stereochemistry, Double bond geometry as described by E or Z.

$C_{33}H_{40}O_7$
2-Propenoic acid, 3-phenyl-, (1aR,2E,4aR,6S,7S,7aS,8E,11aS)-4a-(acetyloxy)-9-[(acetyloxy)methyl]-1a,4,4a,5,6,7,7a,10,11,11a-decahydro-1,1,3,6-tetramethyl-4-oxo-1H-cyclopenta[a]cyclopropa[f]cycloundecen-7-yl ester, ref

Score: 97

6. 2727249-93-4



Absolute stereochemistry, Double bond geometry as described by E or Z.

$C_{33}H_{40}O_7$
INDEX NAME NOT YET ASSIGNED

Key Physical Properties

Figure S22: The Scifinder similarity report for new compound 1

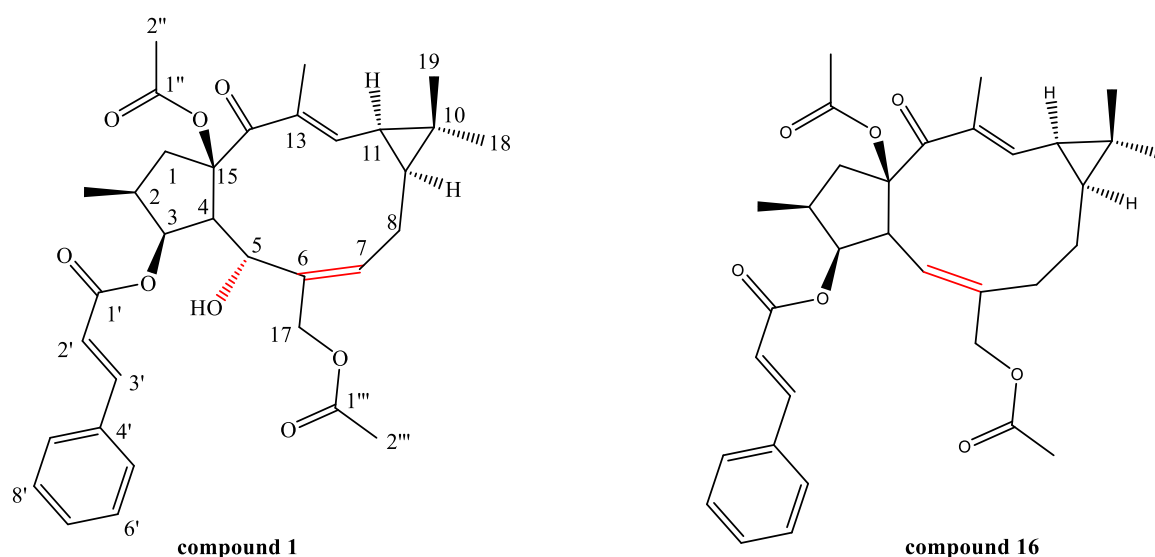


Figure S23: The structure is most similar to compound **1**

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

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

^{a, b} Overlapping signals

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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