

## Supporting Information

*Rec. Nat. Prod.* 17:3 (2023) 476-484

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

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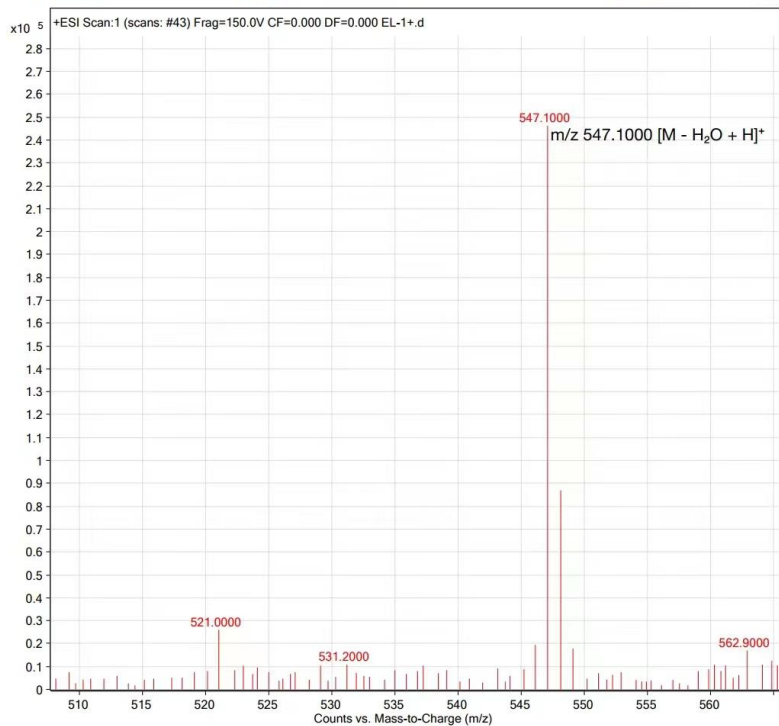
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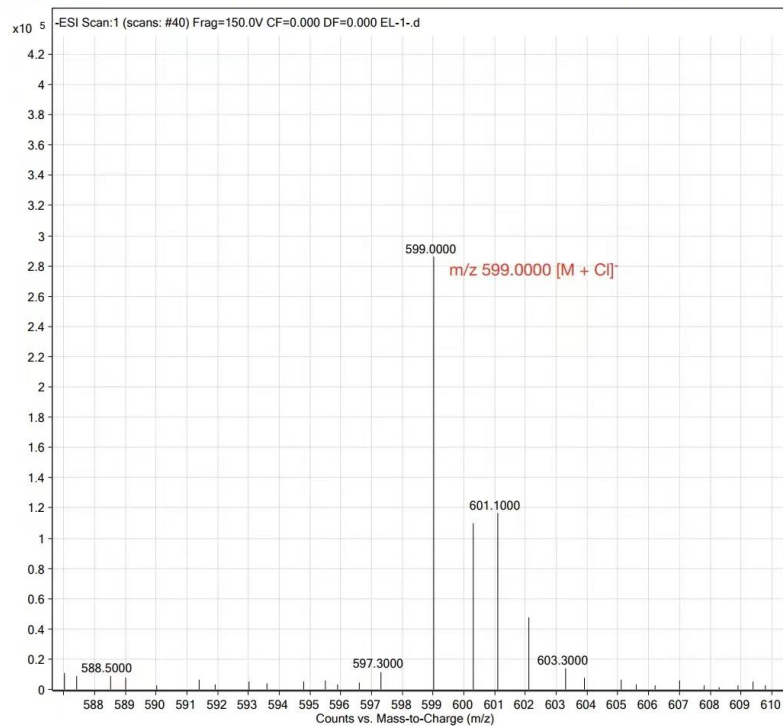
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<b>Sample Name</b>	EL-1	<b>Position</b>	P2-A1	<b>Instrument Name</b>	Instrument 1
<b>User Name</b>		<b>Inj Vol</b>	10	<b>InjPosition</b>	
<b>Sample Type</b>	Sample	<b>IRM Calibration Status</b>	Not Applicable	<b>Data Filename</b>	EL-1+.d
<b>ACQ Method</b>	pos-single 6min-1200.m	<b>Comment</b>		<b>Acquired Time</b>	10/28/2022 10:15:43 AM



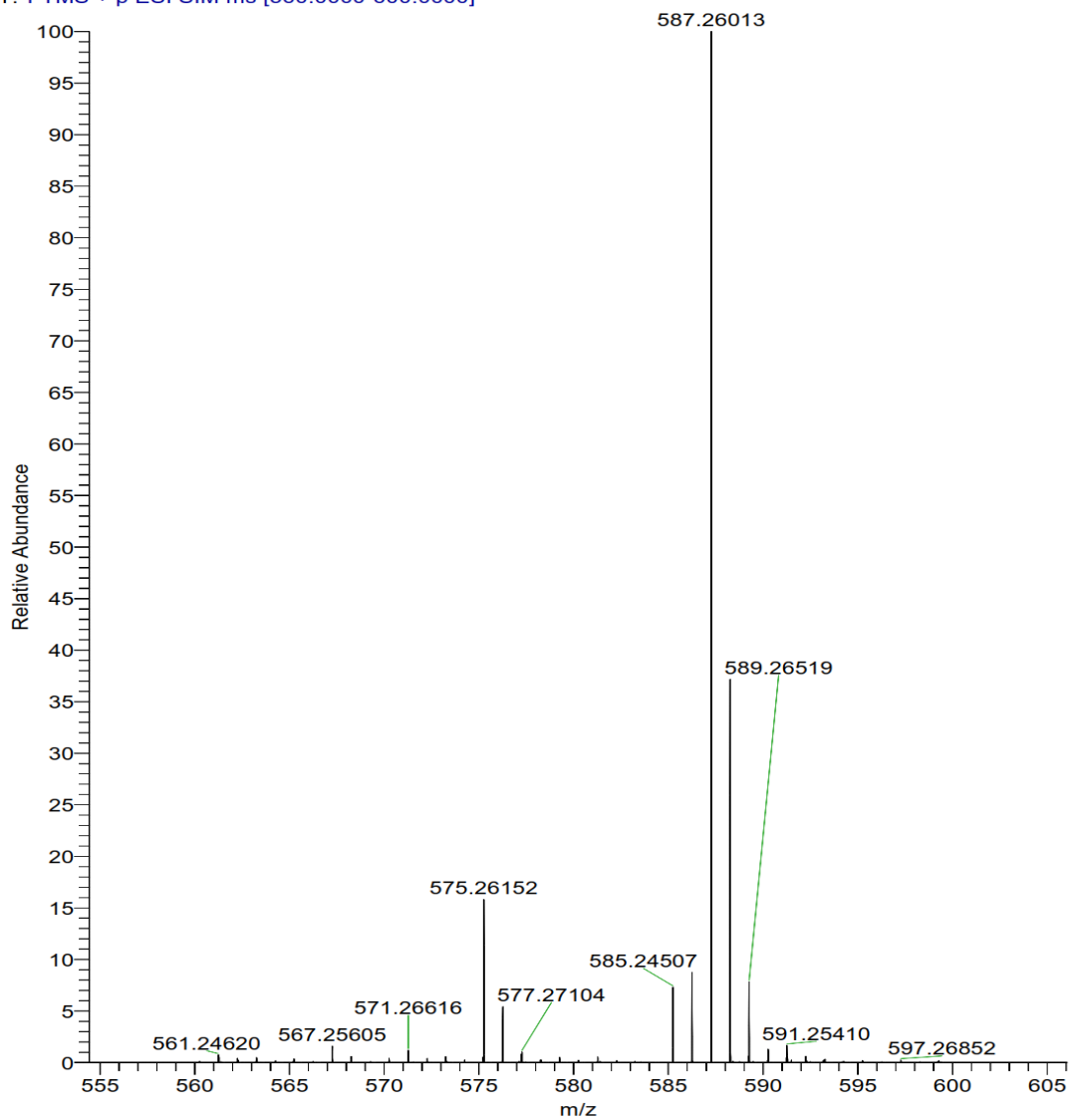
**Figure S1:** EI-MS spectrum of **1**  $[M - H_2O + H]^+$

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



**Figure S2:** EI-MS spectrum of **1** [M + Cl]<sup>-</sup>

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**

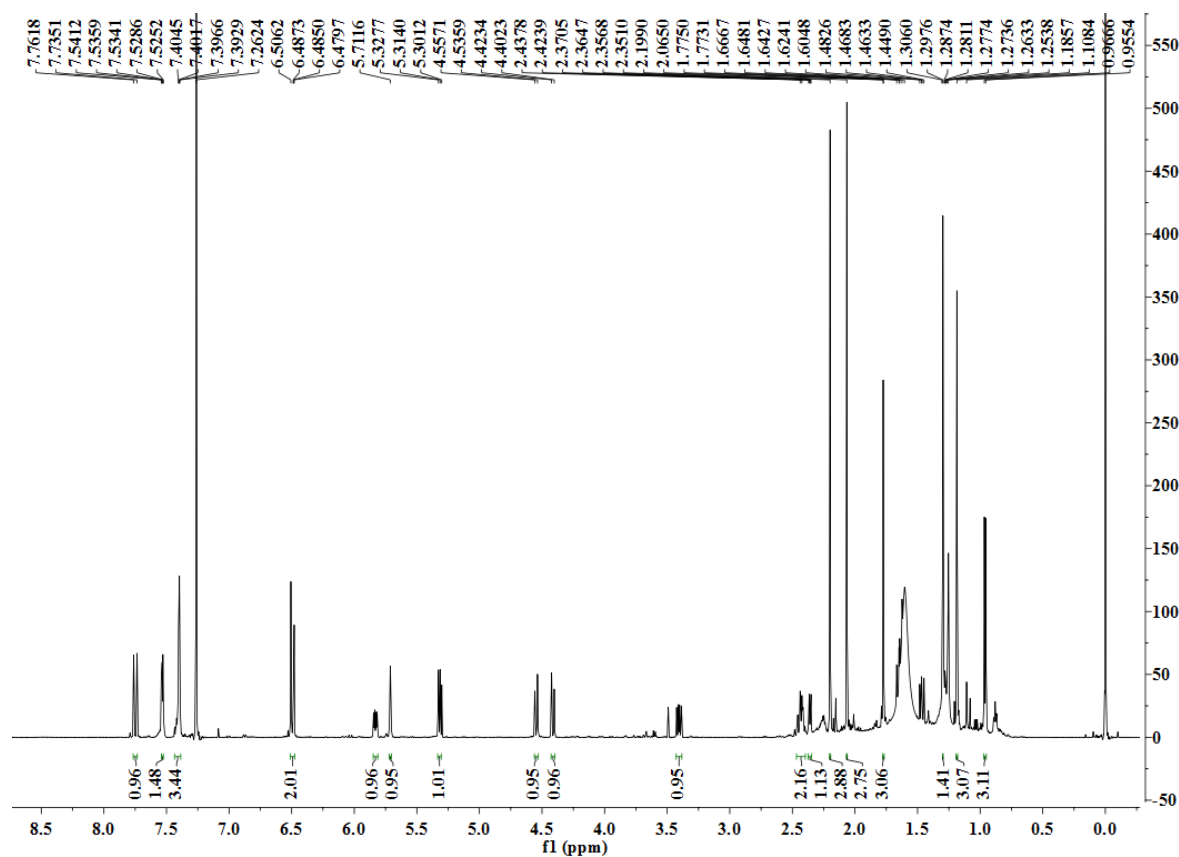


Figure S4: <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>) spectrum of **1**

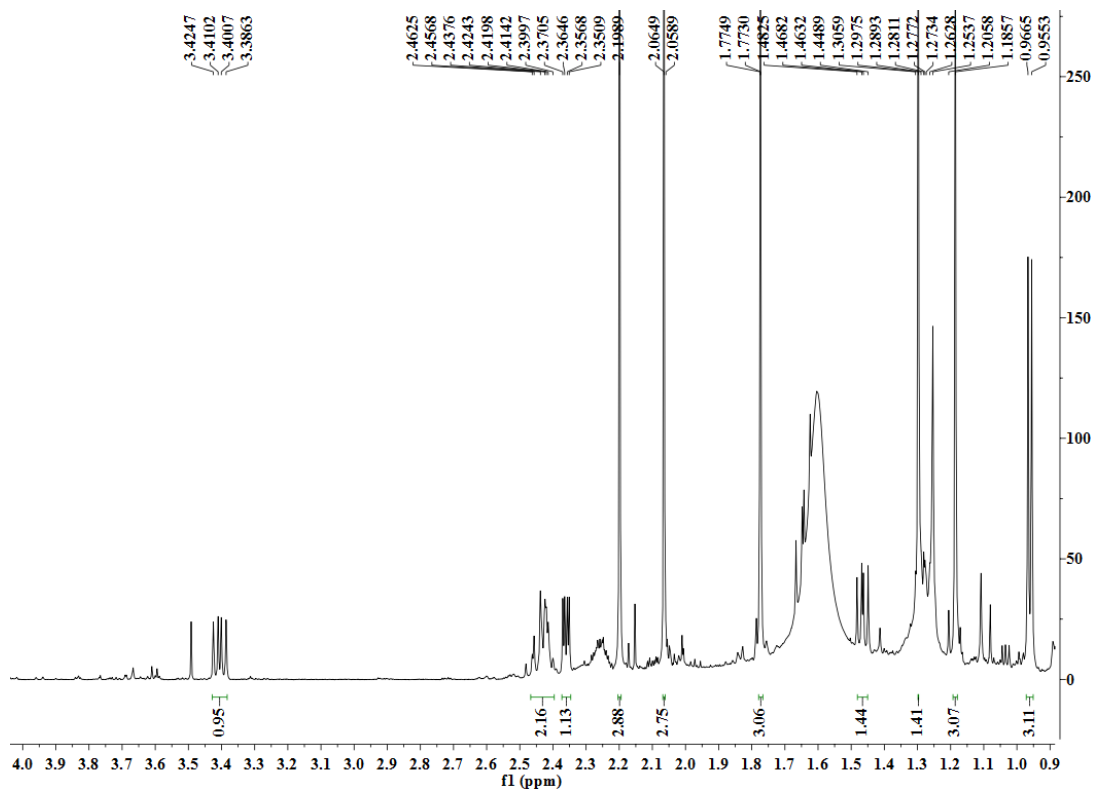
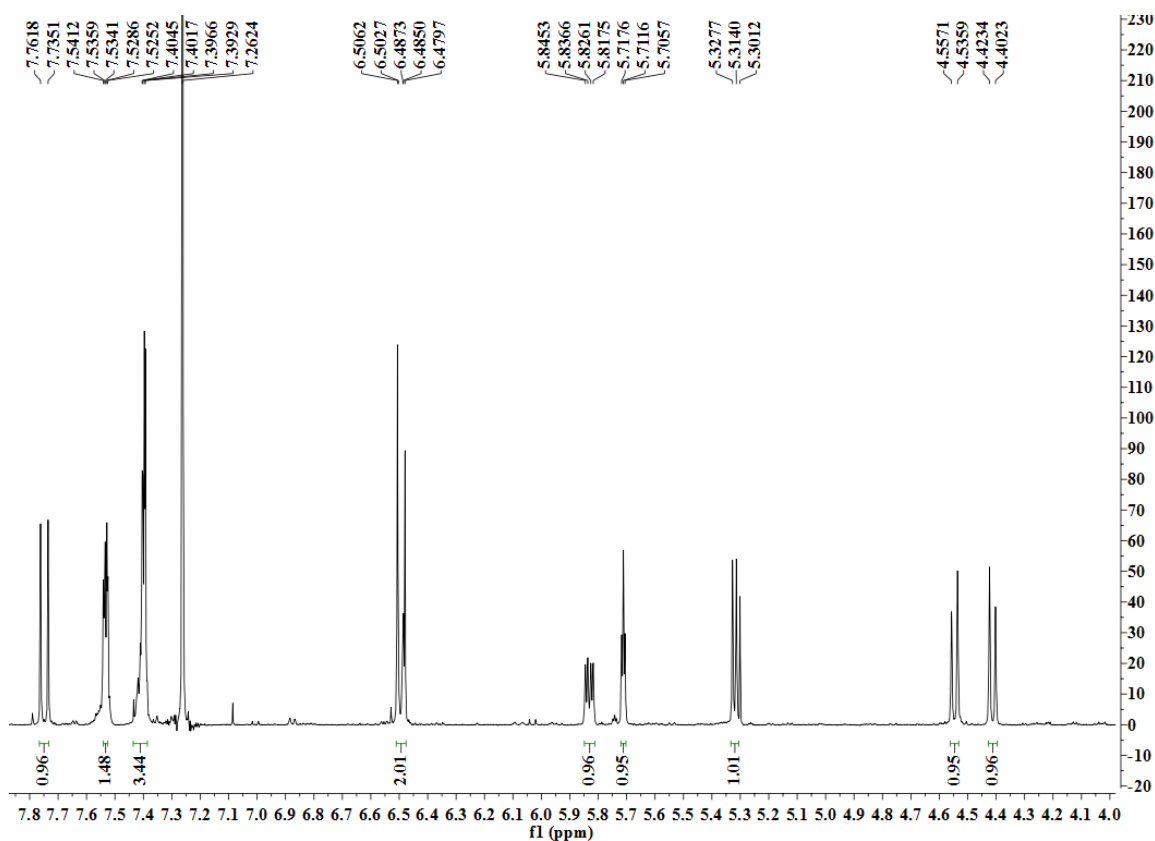
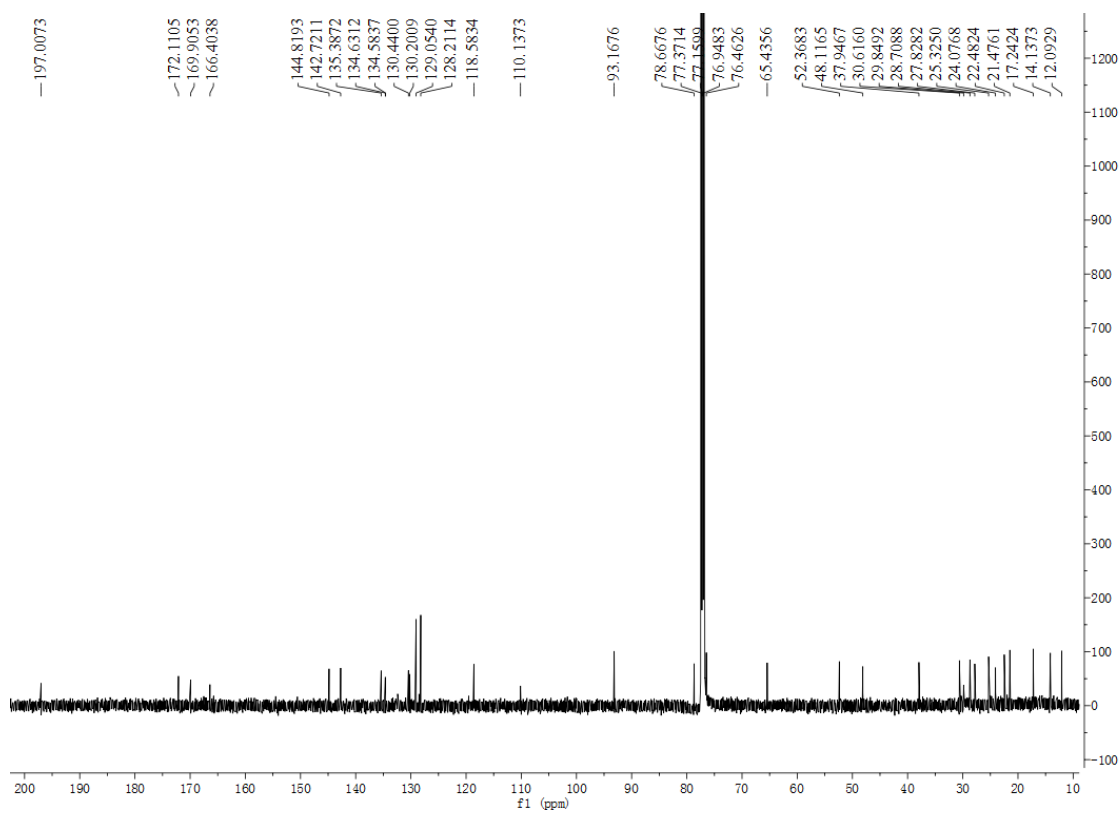


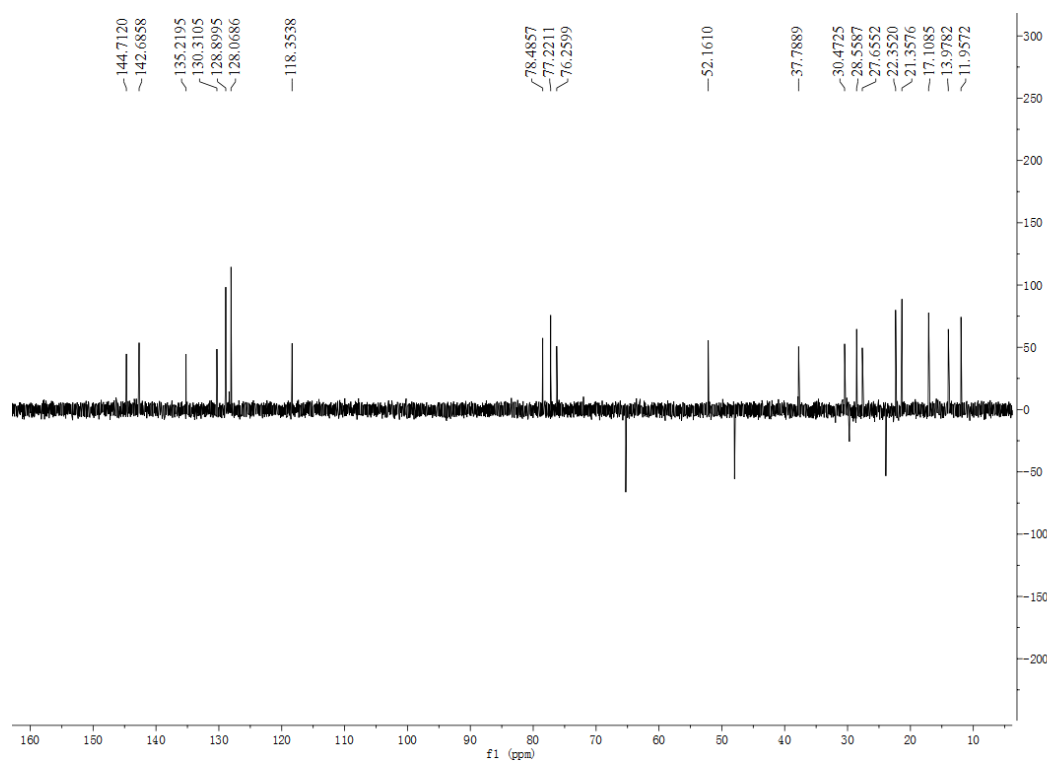
Figure S5: <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>) spectrum of **1** (From  $\delta_H$  0.9 ppm to  $\delta_H$  4.0 ppm)



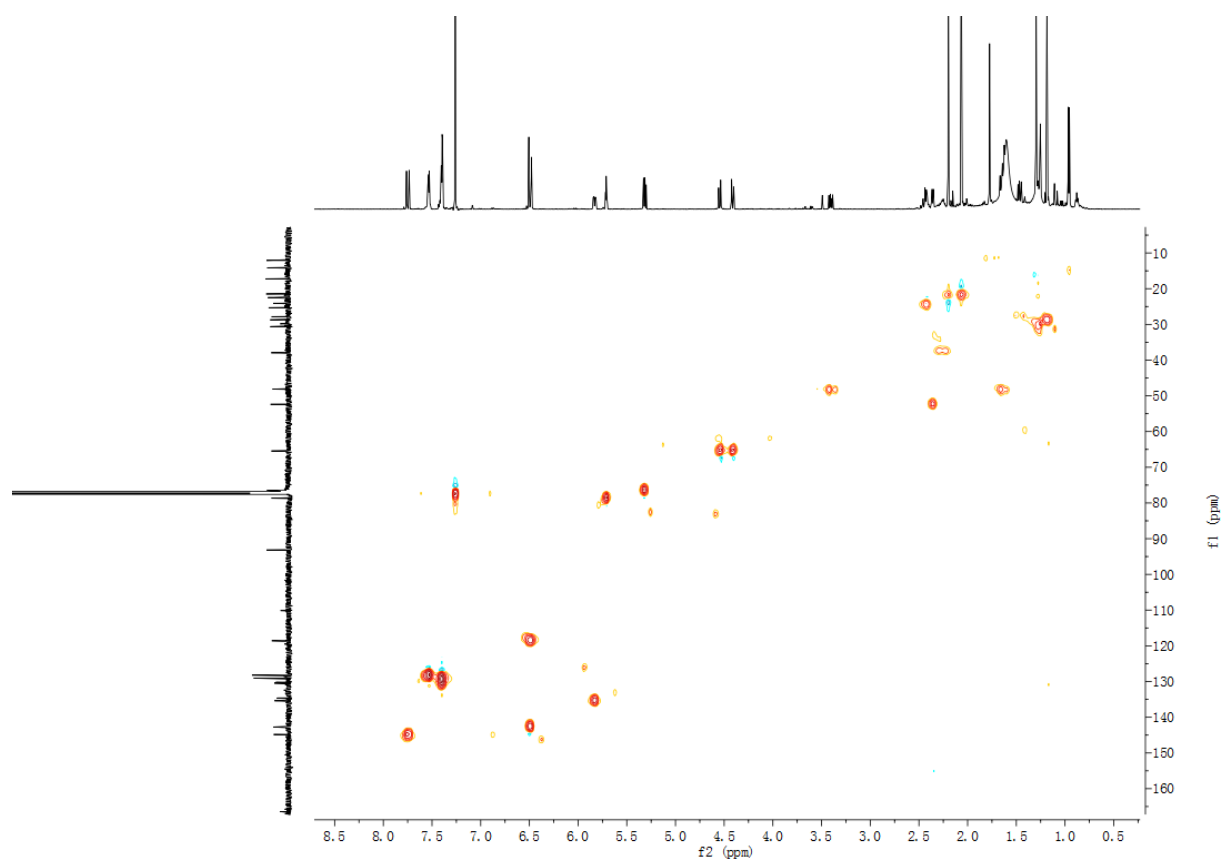
**Figure S6:**  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) spectrum of **1** (From  $\delta_{\text{H}}$  4.0 ppm to  $\delta_{\text{H}}$  7.8 ppm)



**Figure S7:**  $^{13}\text{C-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) spectrum of **1**



**Figure S8:** DEPT135 (600 MHz, CDCl<sub>3</sub>) spectrum of **1**



**Figure S9:** HSQC spectrum of **1**

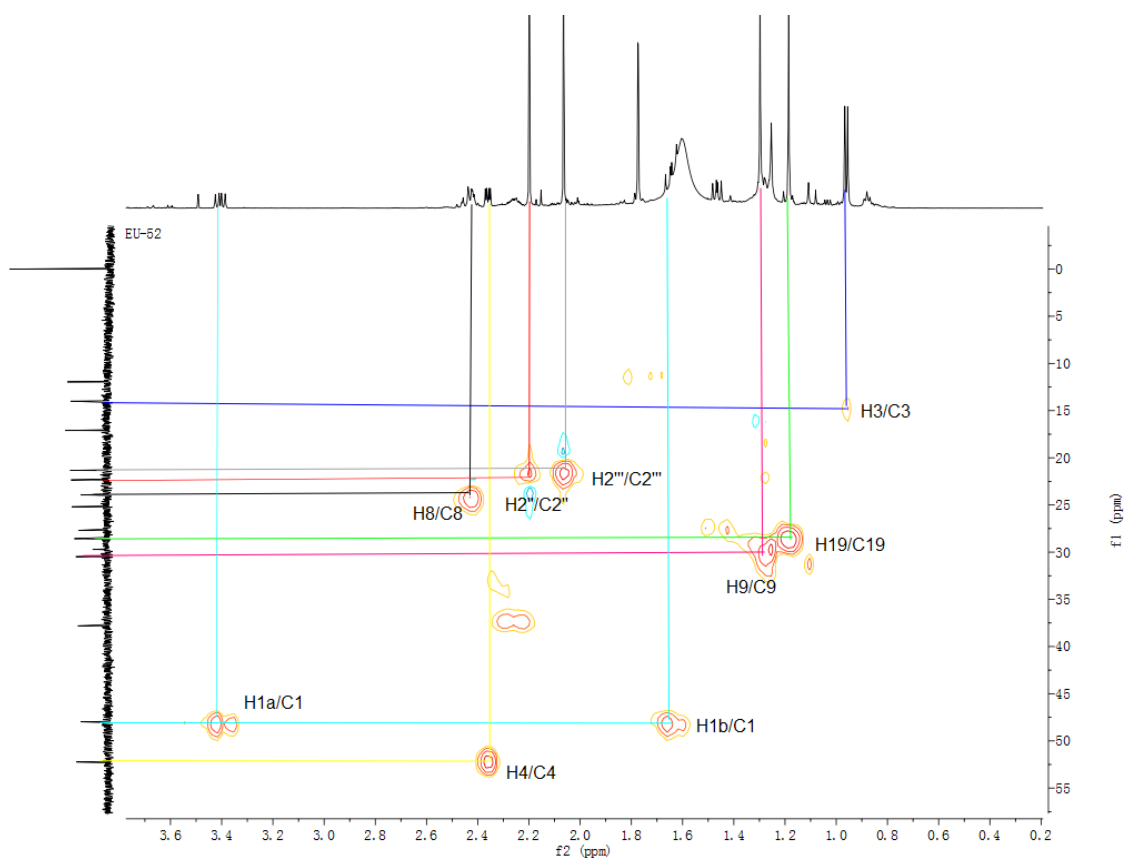


Figure S10: HSQC spectrum of **1** (From  $\delta_H$  0.2 ppm to  $\delta_H$  3.6 ppm)

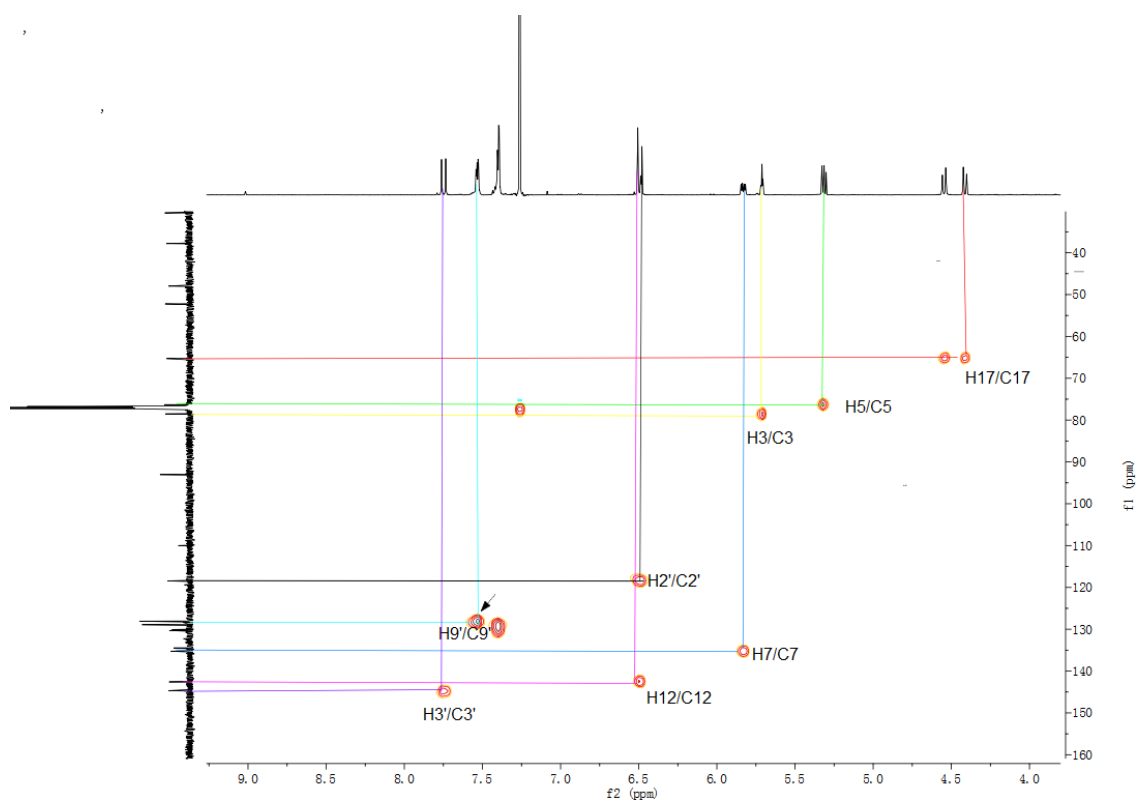
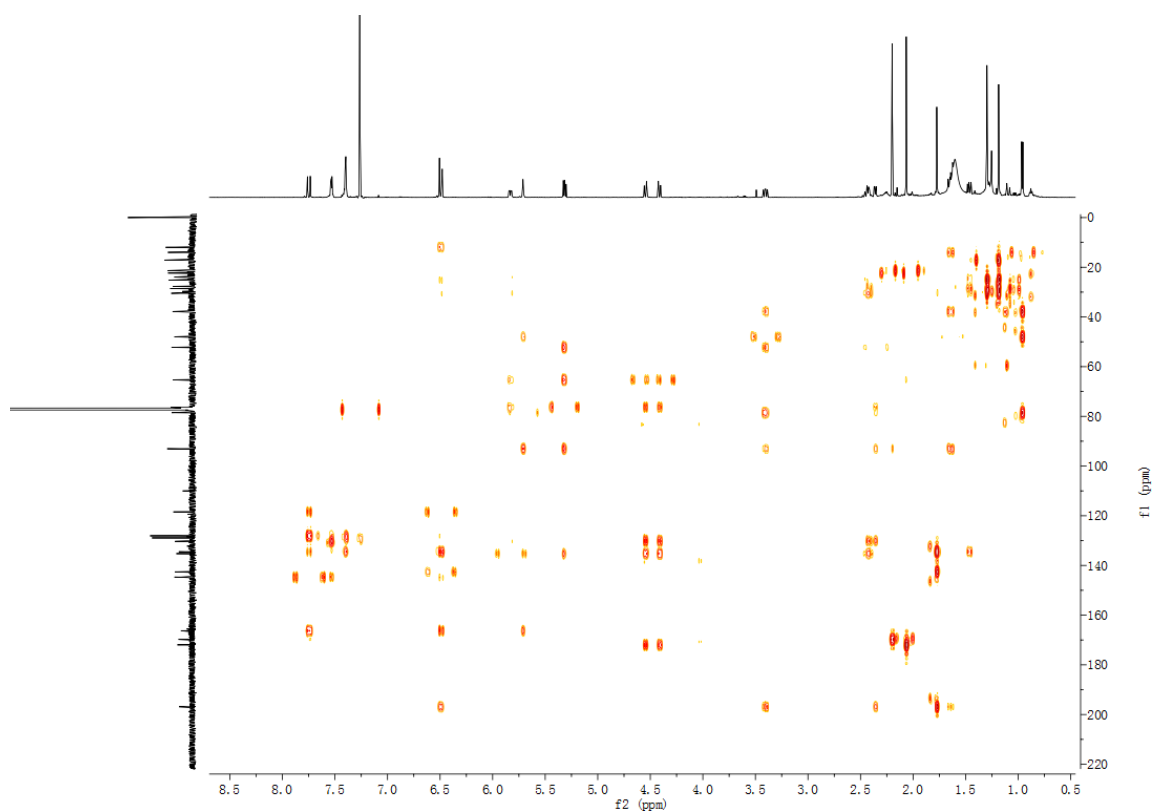
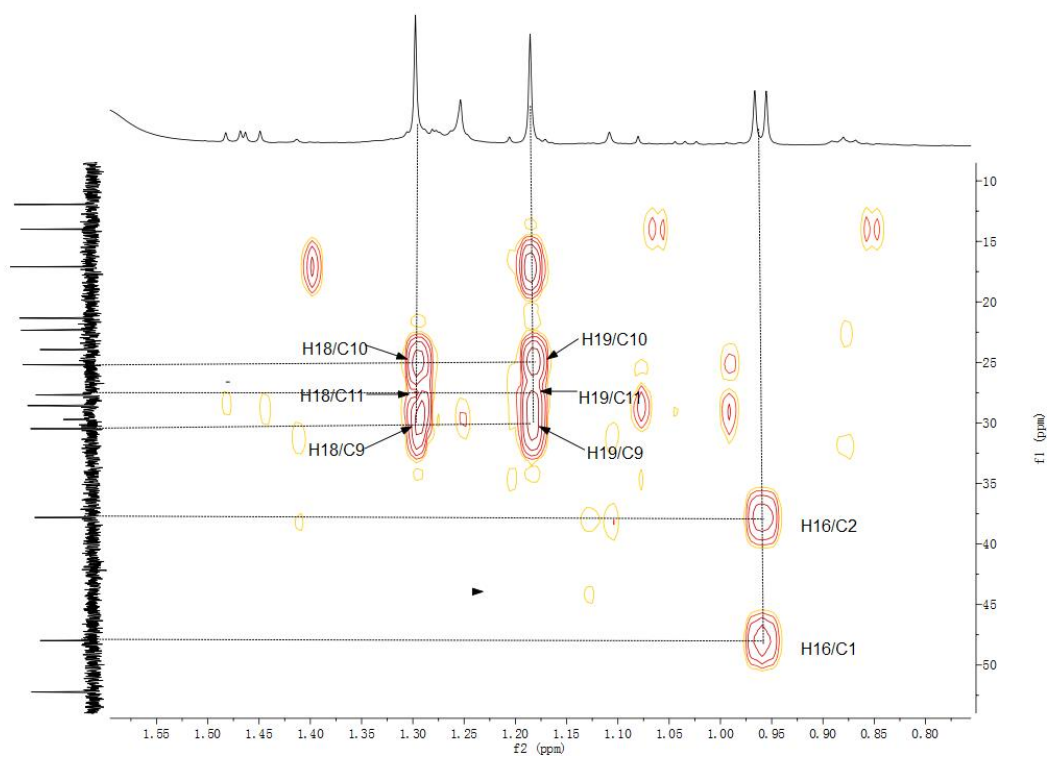


Figure S11: HSQC spectrum of **1** (From  $\delta_H$  4.0 ppm to  $\delta_H$  9.0 ppm)

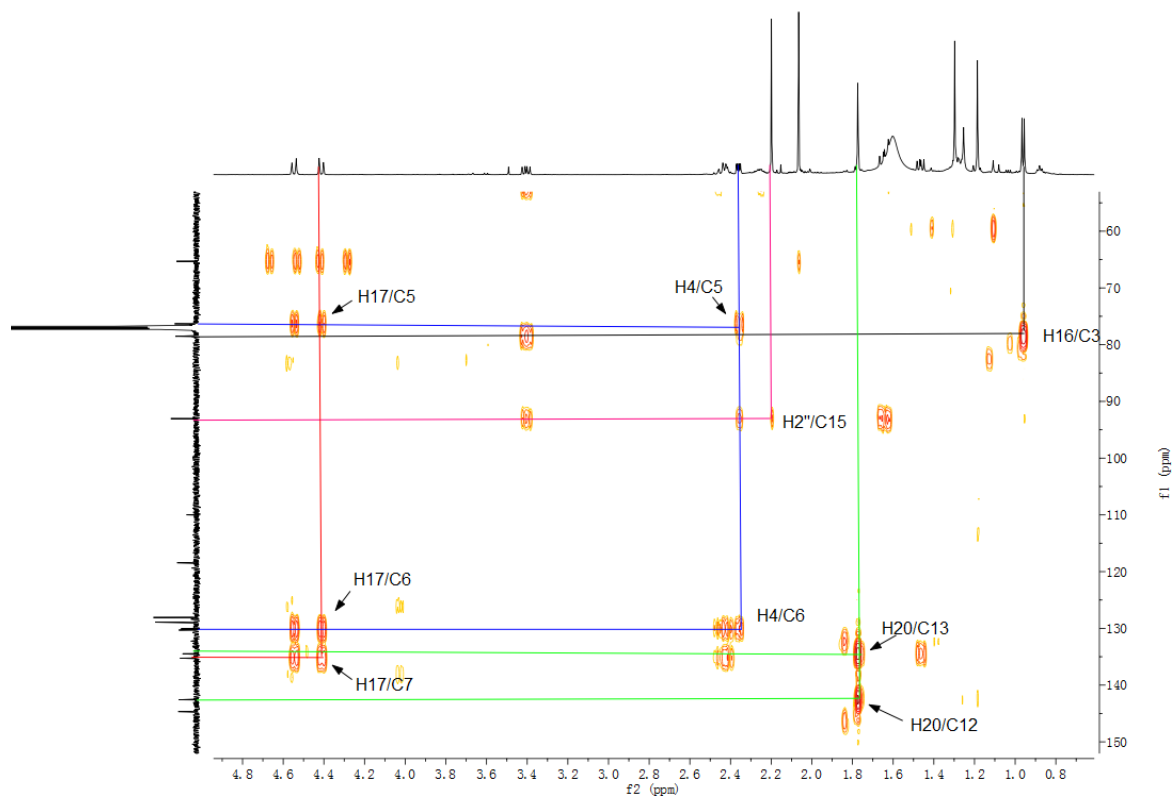




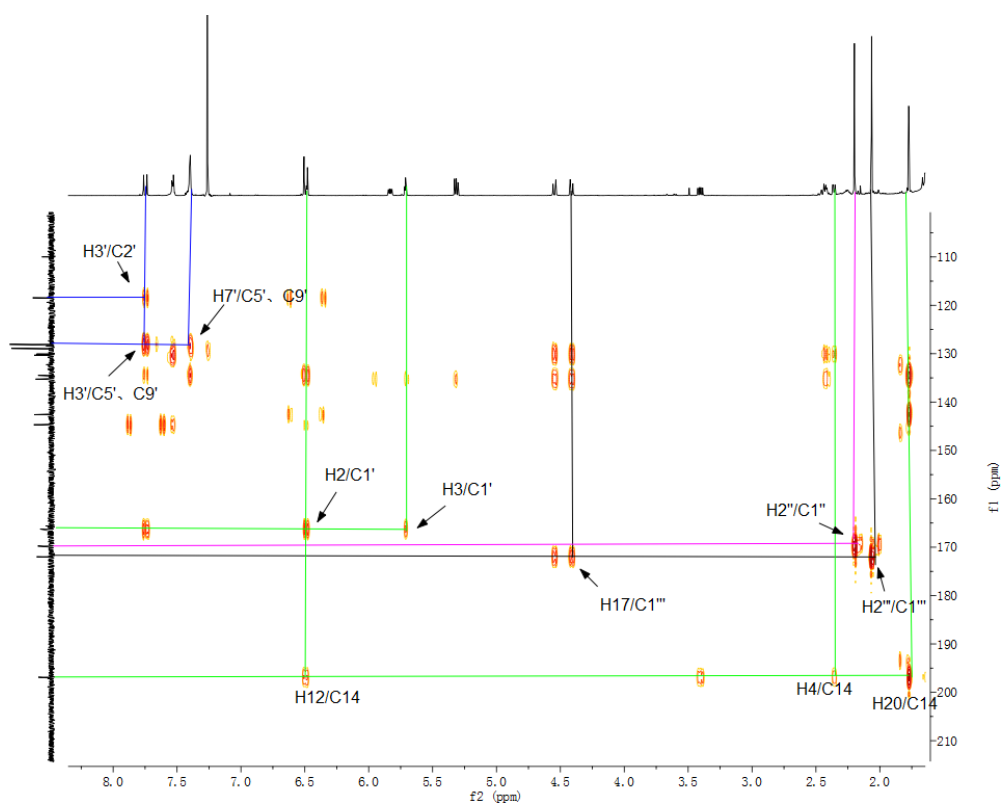
**Figure S12:** HMBC spectrum of **1**



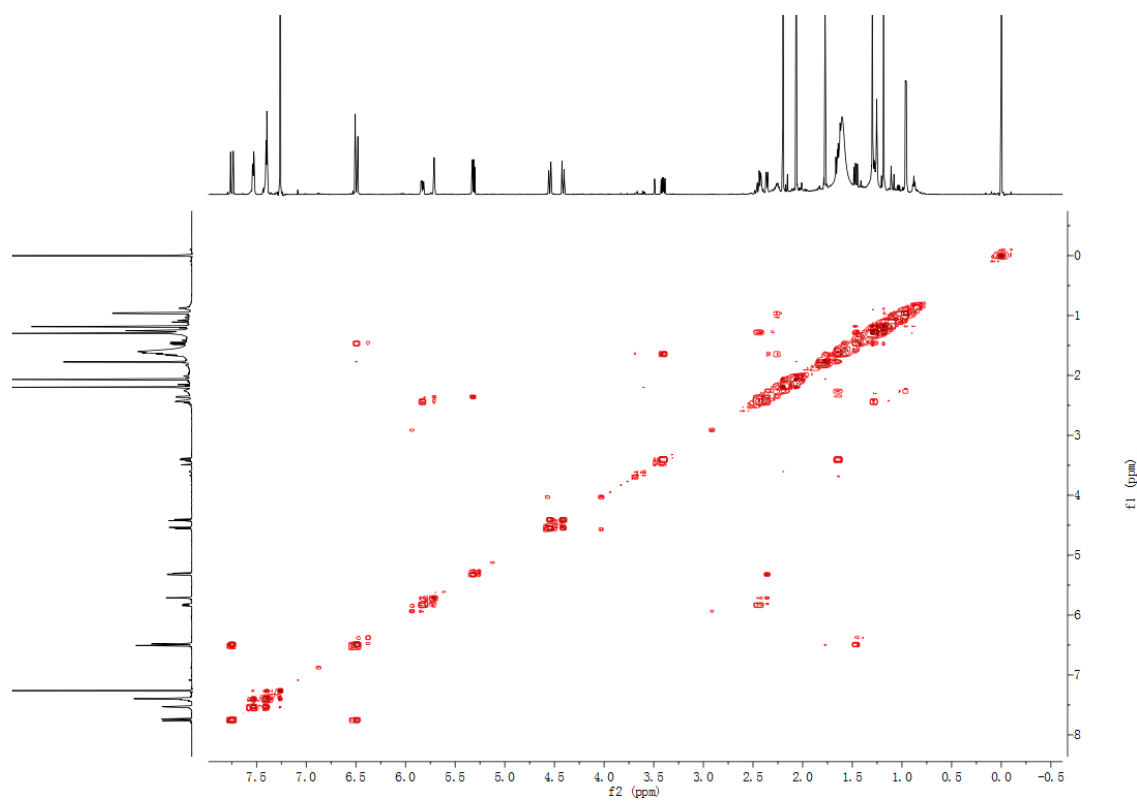
**Figure S13:** HMBC spectrum of **1** (From  $\delta_c$  10 ppm to  $\delta_c$  50 ppm )



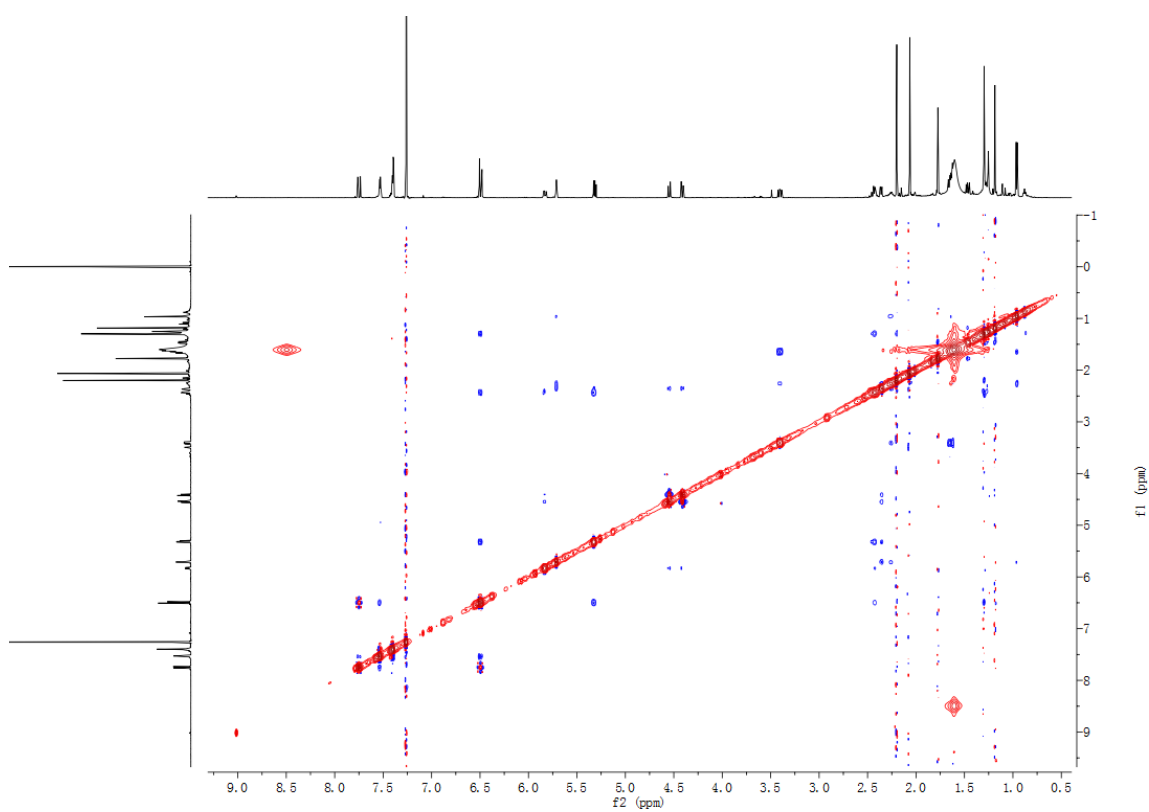
**Figure S14:** HMBC spectrum of **1** (From  $\delta_c$  60 ppm to  $\delta_c$  150 ppm )



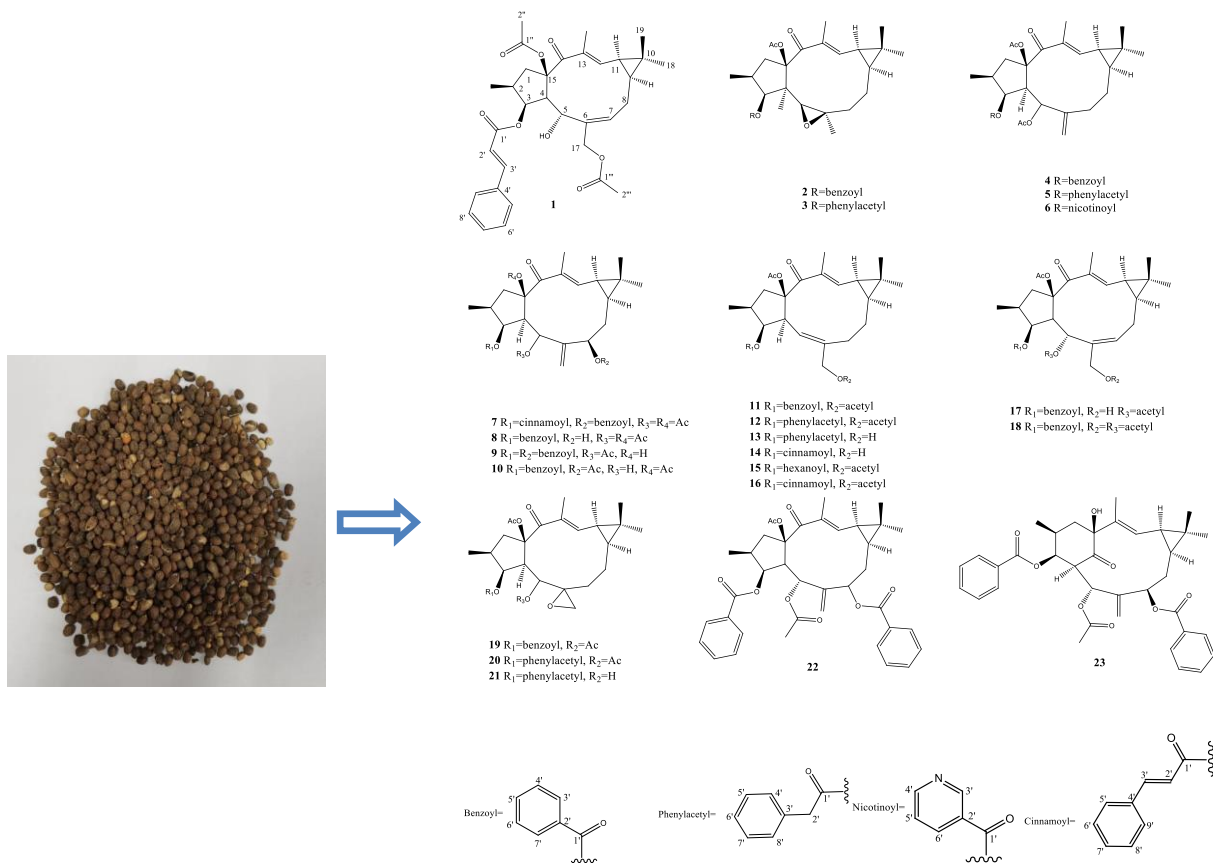
**Figure S15:** HMBC spectrum of **1** (From  $\delta_c$  110 ppm to  $\delta_c$  210 ppm )



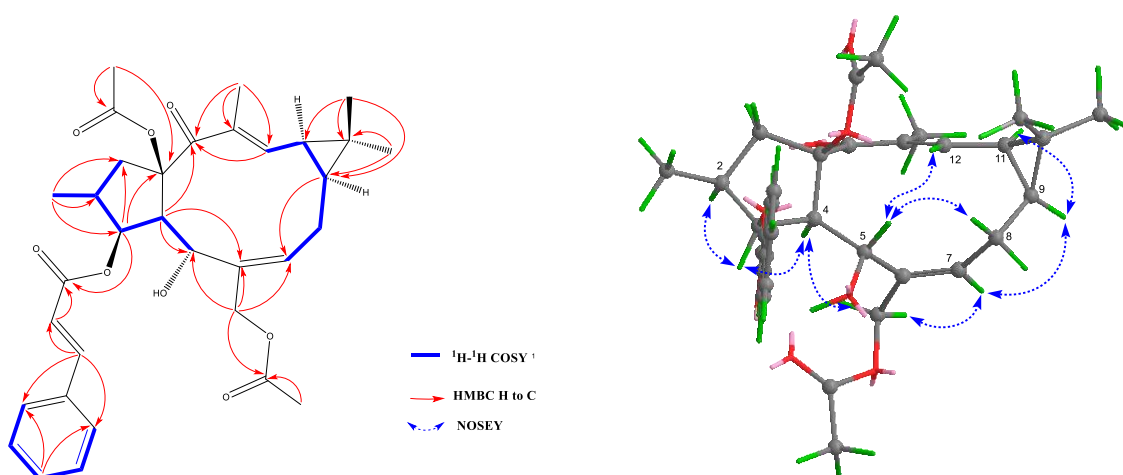
**Figure S16:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**



**Figure S17:** NOESY spectrum of **1**



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

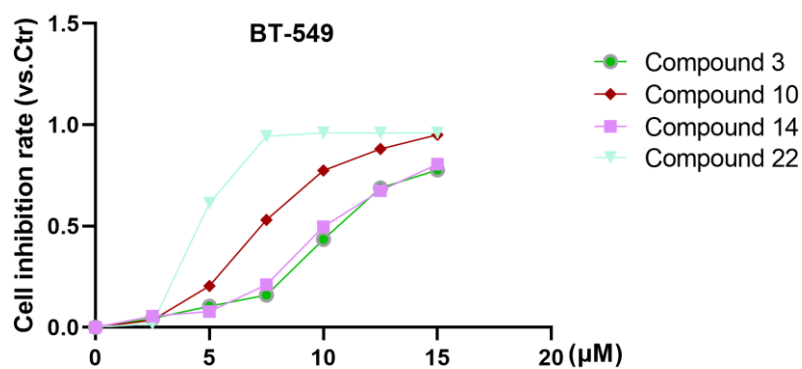


**Figure S19:** Selected HMBC, <sup>1</sup>H–<sup>1</sup>H COSY and NOESY correlations of compound 1.

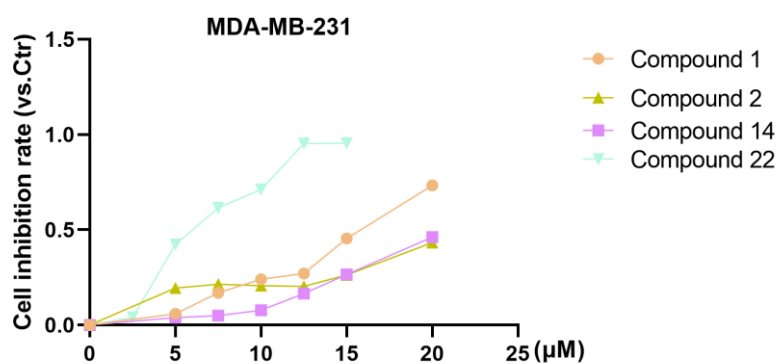
**Table S1:**  $^1\text{H}$  (600 MHz) and  $^{13}\text{C}$  (150 MHz) NMR data for compound **1** ( $\text{CDCl}_3$ ,  $\delta$  in ppm,  $J$  in Hz)

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

<sup>a, b</sup> 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  $\mu M$ )

Compound	$IC_{50}$ ( $\mu M$ )	
	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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<input type="checkbox"/> 95-98	7
<input type="checkbox"/> 90-94	7
<input type="checkbox"/> 85-89	60
<input type="checkbox"/> 80-84	664
<input type="checkbox"/> 75-79	1511
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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

Show More

Score: 97

1. 93550-94-8

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

$C_{33}H_{46}O_7$   
2-Propenoic acid, 3-phenyl-, (1aR,2E,4aR,6S,7S,7aS,8Z,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.

$C_{33}H_{46}O_7$   
INDEX NAME NOT YET ASSIGNED

Key Physical Properties

Score: 97

3. 2508024-12-0

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

$C_{33}H_{46}O_7$   
2-Propenoic acid, 3-phenyl-, (1aR,4aR,6S,7S,7aS,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.

$C_{33}H_{46}O_7$   
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

5. 2699621-48-0

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

$C_{33}H_{46}O_7$   
2-Propenoic acid, 3-phenyl-, (1aR,2Z,4aS,6S,7R,7aS,8E,11aR)-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

Key Physical Properties

Score: 97

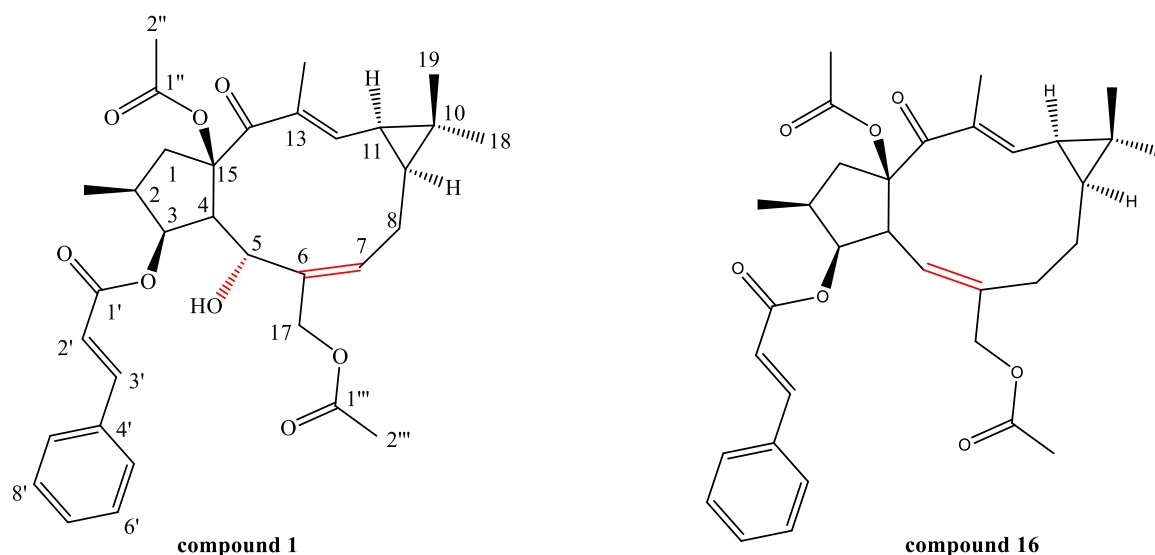
6. 2727249-93-4

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

$C_{33}H_{46}O_7$   
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  $^1\text{H}$  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) <sup>b</sup>	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> ) <sup>a</sup>	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) <sup>b</sup>	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> ) <sup>a</sup>	6.49 (1H, <i>d</i> ) <sup>a</sup>
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> )

<sup>a, b</sup> Overlapping signals

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

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