

## **Garynthone A-I, PPAPs with diverse skeletons isolated from *Garcinia yunnanensis* and its immunosuppressive activity**

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Table S1. The  $^1\text{H}$  (600 MHz) and  $^{13}\text{C}$  (150 MHz) NMR data of **1** in pyridine- $d_5$  and MeOH- $d_4$  ( $\delta$  in ppm,  $J$  in Hz)

No.	<b>1<sup>a</sup></b>		<b>1<sup>b</sup></b>	
	$^1\text{H}$	$^{13}\text{C}$	$^1\text{H}$	$^{13}\text{C}$
1	-	92.3, C	-	93.1, C
2	-	70.9, C	-	71.9, C
3	-	206.9, C	-	207.35, C
4	-	72.8, C	-	73.7, C
5	-	48.7, C	-	49.7, C
6	1.73, overlap	48.0, CH	1.92, overlap	49.6 CH
7	2.15, overlap 1.86, d (11.2)	47.1, CH <sub>2</sub>	2.15, overlap 1.83, overlap	48.1, CH <sub>2</sub>
8	-	60.3, C	-	61.2, C
9	-	210.6, C	-	212.0, C
10	-	197.9, C	-	199.2, C
11	-	130.5, C	-	130.8, C
12	7.91, s	119.0, CH	7.15, d (2.2)	118.5, CH
13	-	146.6, C	-	145.9, C
14	-	151.8, C	-	151.0, C
15	7.28, brd (8.5)	115.5, CH	6.73, d (8.5)	114.9, CH
16	7.50, brd (8.5)	124.2, CH	6.91, dd (8.5, 2.2)	125.0, CH
17	2.61, d (11.7) 2.51, d (14.9)	26.6, CH <sub>2</sub>	2.42, dd (13.5, 9.4) 2.25, overlap	27.0, CH <sub>2</sub>
18	5.50, s	121.3, CH	5.06, m	121.3, CH
19	-	134.6, C	-	135.9, C
20	1.88, s	26.3, CH <sub>3</sub>	1.73, s	26.4, CH <sub>3</sub>
21	1.80, s	18.4, CH <sub>3</sub>	1.67, s	18.3, CH <sub>3</sub>
22	0.84, s	25.1, CH <sub>3</sub>	0.90, s	25.4, CH <sub>3</sub>
23	0.93, s	23.3, CH <sub>3</sub>	0.92, s	23.2, CH <sub>3</sub>
24	3.69, d (14.7) 2.45, d (14.5)	36.1, CH <sub>2</sub>	3.26, dd (14.7, 3.2) 2.25, overlap	36.7, CH <sub>2</sub>
29	3.16, t (11.5) 1.12, overlap	31.1, CH <sub>2</sub>	2.86, dd (14.0, 8.7) 0.88, d (8.9)	31.6, CH <sub>2</sub>

30	1.66, overlap	43.2, CH	1.58, dd, (9.3, 4.2)	44.0, CH
31	-	83.8, C	-	85.3, C
32	3.00, d (14.4)	49.5, CH <sub>2</sub>	2.67, d (14.5)	50.0, CH <sub>2</sub>
	2.13, overlap		1.90, d (14.5)	
33	1.08, s	23.4, CH <sub>3</sub>	0.91, s	23.5, CH <sub>3</sub>
34	2.22, d (15.3)	31.8, CH <sub>2</sub>	2.17, dd (12.3, 3.3)	32.4, CH <sub>2</sub>
	1.94, m		1.85, overlap	
35	5.23, s	123.1, CH	5.13, m	123.4, CH
36	-	132.4, C	-	133.5, C
37	1.70, s	25.9, CH <sub>3</sub>	1.71, s	26.0, CH <sub>3</sub>
38	1.57, s	17.9, CH <sub>3</sub>	1.61, s	18.0, CH <sub>3</sub>

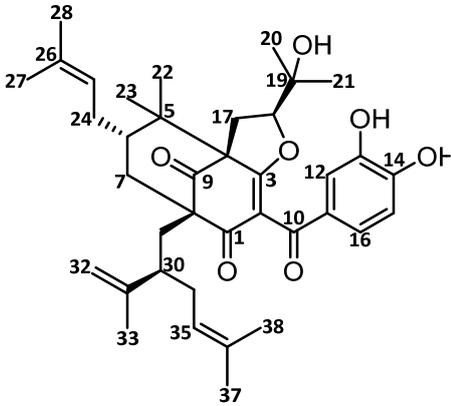
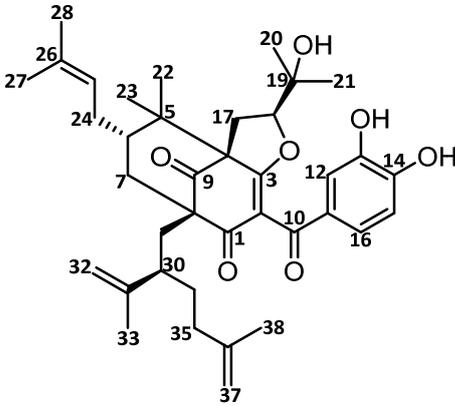
<sup>a</sup> recorded in pyridine-*d*<sub>5</sub>; <sup>b</sup> recorded in MeOH-*d*<sub>4</sub>

Table S2. The <sup>1</sup>H (600 MHz) and <sup>13</sup>C (150 MHz) NMR data of **2** and **3** in pyridine-*d*<sub>5</sub> ( $\delta$  in ppm, *J* in Hz)

No.	<b>2</b>		<b>3</b>	
	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
1	-	201.8, C	-	201.8, C
2	-	89.8, C	-	89.8, C
3	-	202.3, C	-	202.4, C
4	-	73.3, C	-	73.4, C
5	-	47.1, C	-	47.1, C
6	2.12, t (7.7)	42.1, CH	2.12, t (7.7)	42.1, CH
7	2.59, dd (14.6, 6.4)	37.0, CH <sub>2</sub>	2.55, dd (14.6, 6.5)	37.2, CH <sub>2</sub>
	2.41, overlap		2.38, d (15.4)	
8	-	66.5, C	-	66.5, C
9	-	204.8, C	-	204.8, C
10	-	167.0, C	-	167.0, C
11	-	120.2, C	-	120.2, C
12	8.06, d (2.1)	118.1, CH	8.06, d (2.1)	118.1, CH
13	-	147.8, C	-	147.8, C
14	-	154.1, C	-	154.2, C
15	7.21, d (8.3)	116.8, CH	7.21, d (8.3)	116.8, CH
16	7.95, dd (8.3, 2.1)	124.2, CH	7.96, dd (8.3, 2.1)	124.2, CH
17	2.89, dd (14.6, 7.2)	26.6, CH <sub>2</sub>	2.86, dd (14.6, 7.2)	26.6, CH <sub>2</sub>

	2.77, dd (14.6, 5.6)		2.76, dd (14.5, 5.6)	
18	5.56, m	122.4, CH	5.55, m	122.4, CH
19	-	131.3, C	-	131.3, C
20	1.62, s	26.5, CH <sub>3</sub>	1.62, s	26.6, CH <sub>3</sub>
21	1.73, s	18.4, CH <sub>3</sub>	1.70, s	18.3, CH <sub>3</sub>
22	1.14, s	25.6, CH <sub>3</sub>	1.13, s	25.6, CH <sub>3</sub>
23	1.10, s	23.6, CH <sub>3</sub>	1.07, s	23.6, CH <sub>3</sub>
24	2.38, overlap 2.19, dd (15.5, 11.9)	27.1, CH <sub>2</sub>	2.36, overlap 2.19, dd (15.2, 11.2)	27.2, CH <sub>2</sub>
25	2.65, dd (11.6, 7.7)	46.8, CH	2.64, overlap	46.8, CH
26	-	74.6, C	-	74.7, C
27	1.84, s	31.0, CH <sub>3</sub>	1.83, s	31.2, CH <sub>3</sub>
28	1.72, s	29.2, CH <sub>3</sub>	1.71, s	29.2, CH <sub>3</sub>
29	2.36, overlap 2.30, dd (14.9, 3.5)	34.6, CH <sub>2</sub>	2.34, overlap 2.22, dd (14.9, 3.6)	34.9, CH <sub>2</sub>
30	2.71, m	43.8, CH	2.66, overlap	43.3, CH
31	-	150.4, C	-	149.6, C
32	4.85, s 4.83, s	112.2, CH <sub>2</sub>	4.84, s 4.83, s	112.8, CH <sub>2</sub>
33	1.75, s	19.6, CH <sub>3</sub>	1.70, s	18.9, CH <sub>3</sub>
34	2.48, overlap 2.24, m	35.0, CH <sub>2</sub>	1.87, m 1.60, overlap	34.1, CH <sub>2</sub>
35	5.25, m	124.2, CH	1.98, m 1.95, m	36.3, CH <sub>2</sub>
36	-	132.0, C	-	146.6, C
37	1.62, s	26.2, CH <sub>3</sub>	4.82, s 4.78, s	110.5, CH <sub>2</sub>
38	1.63, s	18.3, CH <sub>3</sub>	1.70, s	23.1, CH <sub>3</sub>

Table S3. The <sup>1</sup>H (600 MHz) and <sup>13</sup>C (150 MHz) NMR data of **4** and **5** in MeOH-*d*<sub>4</sub> (δ in ppm, *J* in Hz)

No.				
	<b>4</b>	<b>5</b>	<b>4</b>	<b>5</b>
	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
1	-	196.6, C	-	196.6, C

2	-	120.7, C	-	120.6, C
3	-	176.2, C	-	176.2, C
4	-	68.9, C	-	68.9, C
5	-	50.0, C	-	50.0, C
6	1.64, overlap	46.9, CH	1.64, overlap	46.9, CH
7	2.17, d (13.9) 2.06, overlap	43.4, CH <sub>2</sub>	2.17, d (13.9) 2.06, overlap	43.4, CH <sub>2</sub>
8	-	61.8, C	-	61.8, C
9	-	208.0, C	-	208.0, C
10	-	191.2, C	-	191.2, C
11	-	130.4, C	-	130.3, C
12	7.25, d (2.1)	116.7, CH	7.25, d (2.1)	116.7, CH
13	-	146.5, C	-	146.4, C
14	-	153.1, C	-	152.7, C
15	6.75, d (8.2)	115.6, CH	6.76, d (8.2)	115.5, CH
16	7.11, dd (8.2, 2.1)	124.9, CH	7.11, dd (8.2, 2.1)	124.7, CH
17	2.82, dd (13.3, 8.4) 2.21, dd (13.4, 9.4)	25.1, CH <sub>2</sub>	2.82, dd (13.3, 8.4) 2.21, dd (13.4, 9.4)	25.1, CH <sub>2</sub>
18	3.94, t (8.9)	92.3, CH	3.92, t (8.9)	92.3, CH
19	-	71.2, C	-	71.2, C
20	1.07, s	26.7, CH <sub>3</sub>	1.07, s	26.6, CH <sub>3</sub>
21	1.15, s	25.9, CH <sub>3</sub>	1.15, s	26.0, CH <sub>3</sub>
22	1.02, s	27.4, CH <sub>3</sub>	1.02, s	27.4, CH <sub>3</sub>
23	1.21, s	25.0, CH <sub>3</sub>	1.21, s	25.0, CH <sub>3</sub>
24	2.51, overlap 2.44, overlap	30.8, CH <sub>2</sub>	2.51, m 2.44, m	30.8, CH <sub>2</sub>
25	4.90, m	126.2, CH	4.90, m	126.2, CH
26	-	133.9, C	-	133.2, C
27	1.60, s	26.0, CH <sub>3</sub>	1.60, s	26.0, CH <sub>3</sub>
28	1.67, s	18.4, CH <sub>3</sub>	1.67, s	18.4, CH <sub>3</sub>
29	2.00, overlap 1.75, dd (14.1, 4.6)	37.8, CH <sub>2</sub>	2.03, m 1.74, dd (14.7, 4.1)	38.2, CH <sub>2</sub>
30	2.47, overlap	45.3, CH	2.42, m	44.8, CH
31	-	149.3, C	-	148.7, C
32	4.45, s 4.38, s	113.4, CH <sub>2</sub>	4.67, s 4.63, s	114.1, CH <sub>2</sub>
33	1.45, s	18.0, CH <sub>3</sub>	1.47, s	17.6, CH <sub>3</sub>
34	2.01, overlap 1.97, overlap	34.1, CH <sub>2</sub>	1.44, m 1.40, m	33.2, CH <sub>2</sub>
35	4.98, m	124.3, CH	1.85, m 1.78, m	36.6, CH <sub>2</sub>
36	-	132.5, C	-	147.2, C
37	1.59, s	25.9, CH <sub>3</sub>	4.47, s 4.42, s	110.1, CH <sub>2</sub>

38                      1.65, s                      18.1, CH<sub>3</sub>                      1.70, s                      22.8, CH<sub>3</sub>

Table S4. The <sup>1</sup>H (600 MHz) and <sup>13</sup>C (150 MHz) NMR data of **6** and **7** in MeOH-*d*<sub>4</sub> (δ in ppm, *J* in Hz)

No.	<b>6</b>		<b>7</b>	
	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
1	-	173.0, C	-	173.0, C
2	-	124.0, C	-	125.2, C
3	-	196.5, C	-	196.6, C
4	-	70.3, C	-	70.3, C
5	-	47.8, C	-	47.8, C
6	1.60, m	47.8, CH	1.60, m	47.9, CH
7	2.74, d (14.1) 1.98, dd (14.3, 7.2)	39.6, CH <sub>2</sub>	2.76, d (14.0) 2.01, dd (14.0, 7.2)	39.7, CH <sub>2</sub>
8	-	49.0, C	-	49.4, C
9	-	209.6, C	-	209.5, C
10	-	194.4, C	-	194.7, C
11	-	130.7, C	-	130.4, C
12	7.29, d (2.1)	116.4, CH	7.31, d (2.1)	116.2, CH
13	-	146.7, C	-	146.8, C
14	-	153.2, C	-	153.6, C
15	6.74, d (8.1)	115.8, CH	6.73, d (8.1)	115.8, CH
16	7.12, dd (8.1, 2.1)	124.9, CH	7.11, dd (8.1, 2.1)	124.3, CH
17	2.61, dd (13.5, 8.2) 2.45, m	26.5, CH <sub>2</sub>	2.63, dd (13.5, 8.2) 2.46, dd (14.3, 6.2)	26.3, CH <sub>2</sub>
18	4.89, m	121.2, CH	4.94, m	121.2, CH
19	-	135.4, C	-	135.5, C
20	1.58, s	26.3, CH <sub>3</sub>	1.60, s	26.5, CH <sub>3</sub>
21	1.58, s	18.2, CH <sub>3</sub>	1.62, s	18.3, CH <sub>3</sub>
22	0.99, s	27.0, CH <sub>3</sub>	1.01, s	27.0, CH <sub>3</sub>
23	1.14, s	22.7, CH <sub>3</sub>	1.14, s	22.7, CH <sub>3</sub>
24	2.50, m 2.32, m	31.3, CH <sub>2</sub>	2.47, m 2.31, m	31.3, CH <sub>2</sub>
25	5.07, m	126.7, CH	5.09, m	126.8, CH
26	-	133.4, C	-	133.4, C

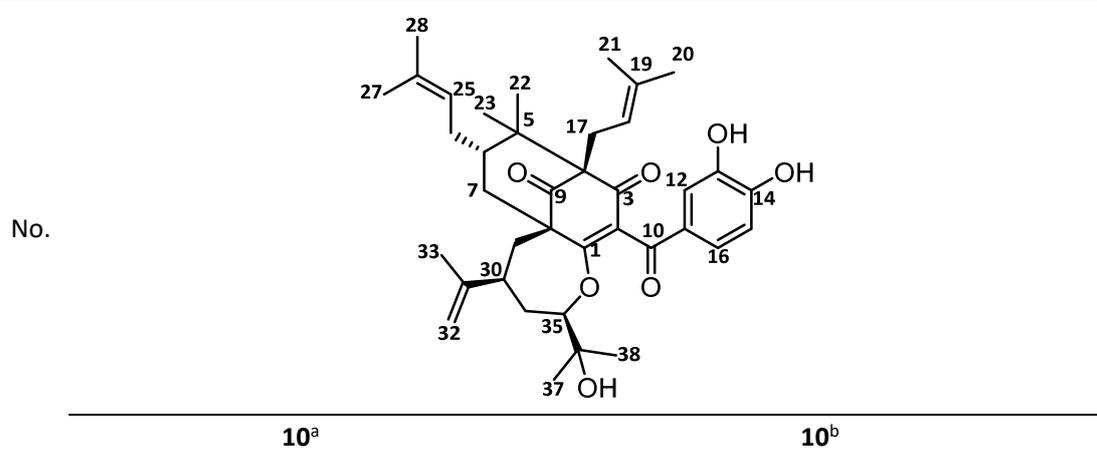
27	1.68, s	26.0, CH <sub>3</sub>	1.69, s	26.0, CH <sub>3</sub>
28	1.69, s	18.4, CH <sub>3</sub>	1.71, s	18.5, CH <sub>3</sub>
29	2.26, t (14.0)	33.6, CH <sub>2</sub>	2.27, t (14.0)	33.4, CH <sub>2</sub>
	1.71, m		1.74, dd (14.0, 3.2)	
30	2.96, overlap	40.0, CH	2.99, ddd (14.0, 11.0, 3.1)	39.8, CH
31	-	146.0, C	-	145.8, C
32	4.94, s	115.1, CH <sub>2</sub>	4.97, s	115.2, CH <sub>2</sub>
	4.94, s		4.96, s	
33	1.74, s	19.8, CH <sub>3</sub>	1.76, s	20.0, CH <sub>3</sub>
34	4.11, d (11.0)	82.6, CH	4.14, d (11.0)	83.1, CH
35	3.38, overlap	74.8, CH	3.34, overlap	76.5, CH
36	-	78.1, C	-	73.4, C
37	0.99, s	22.6, CH <sub>3</sub>	0.78, s	26.8, CH <sub>3</sub>
38	0.67, s	20.3, CH <sub>3</sub>	1.00, s	25.5, CH <sub>3</sub>
-OCH <sub>3</sub>	2.94, s	49.2, CH <sub>3</sub>	-	-

Table S5. The <sup>1</sup>H (600 MHz) and <sup>13</sup>C (150 MHz) NMR data of **8** and **9** in MeOH-*d*<sub>4</sub> ( $\delta$  in ppm, *J* in Hz)

No.	<b>8</b>		<b>9</b>	
	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
1	-	173.8, C	-	173.8, C
2	-	126.7, C	-	127.0, C
3	-	196.6, C	-	196.6, C
4	-	69.4, C	-	69.4, C
5	-	47.1, C	-	47.2, C
6	1.50, m	47.5, CH	1.51, m	47.5, CH
7	2.31, d (14.6)	40.5, CH <sub>2</sub>	2.31, d (14.7)	40.3, CH <sub>2</sub>
	2.05, dd (14.8, 7.4)		2.07, dd (14.7, 7.6)	
8	-	52.4, C	-	52.6, C
9	-	207.8, C	-	207.8, C
10	-	194.4, C	-	194.3, C
11	-	130.8, C	-	130.8, C
12	7.28, d (2.1)	116.1, CH	7.30, d (2.1)	116.0, CH
13	-	146.7, C	-	146.8, C
14	-	152.8, C	-	152.8, C
15	6.73, d (8.2)	115.8, CH	6.71, d (8.2)	115.6, CH

16	7.05, dd (8.2, 2.1)	124.6, CH	7.00, dd (8.2, 2.1)	124.8, CH
17	2.62, m 2.44, dd (13.5, 5.5)	26.5, CH <sub>2</sub>	2.62, dd (13.5, 8.4) 2.46, m	26.6, CH <sub>2</sub>
18	4.91, m	121.1, CH	4.91, m	121.1, CH
19	-	135.4, C	-	135.5, C
20	1.57, s	26.6, CH <sub>3</sub>	1.58, s	26.6, CH <sub>3</sub>
21	1.60, s	18.1, CH <sub>3</sub>	1.60, s	18.3, CH <sub>3</sub>
22	0.98, s	27.0, CH <sub>3</sub>	1.00, s	27.0, CH <sub>3</sub>
23	1.14, s	22.8, CH <sub>3</sub>	1.14, s	22.8, CH <sub>3</sub>
24	2.64, m 2.13, overlap	30.6, CH <sub>2</sub>	2.67, m 2.12, m	30.6, CH <sub>2</sub>
25	4.92, m	126.4, CH	4.94, m	126.4, CH
26	-	134.0, C	-	134.0, C
27	1.68, s	26.1, CH <sub>3</sub>	1.68, s	26.1, CH <sub>3</sub>
28	1.69, s	18.6, CH <sub>3</sub>	1.69, s	18.6, CH <sub>3</sub>
29	3.06, dd (14.2, 3.9) 1.08, t (13.6)	26.6, CH <sub>2</sub>	3.14, m 1.10, t (13.6)	28.3, CH <sub>2</sub>
30	1.68, m	38.7, CH	1.61, m	37.9, CH
31	-	89.9, C	-	90.1, C
32	3.22, d (11.9) 3.16, d (11.9)	69.0, CH <sub>2</sub>	3.17, d (11.9) 3.11, d (11.9)	69.1, CH <sub>2</sub>
33	1.23, s	17.3, CH <sub>3</sub>	1.23, s	17.2, CH <sub>3</sub>
34	2.13, overlap 1.82, m	30.1, CH <sub>2</sub>	1.66, m 1.16, m	29.2, CH <sub>2</sub>
35	5.20, m	122.9, CH	2.26, m 2.12, m	36.2, CH <sub>2</sub>
36	-	134.6, C	-	146.3, C
37	1.63, s	26.0, CH <sub>3</sub>	4.77, s 4.75, s	111.4, CH <sub>2</sub>
38	1.78, s	18.2, CH <sub>3</sub>	1.73, s	22.4, CH <sub>3</sub>

Table S6. The <sup>1</sup>H (600 MHz) and <sup>13</sup>C (150 MHz) NMR data of **10** in MeOH-*d*<sub>4</sub> and CHCl<sub>3</sub>-*d* ( $\delta$  in ppm, *J* in Hz)



	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
1	-	175.8, C	-	175.4, C
2	-	127.6, C	-	126.7, C
3	-	197.0, C	-	195.2, C
4	-	69.2, C	-	68.2, C
5	-	48.5, C	-	47.9, C
6	1.70, m	47.8, CH	1.64, overlap	46.7, CH
7	2.78, d (13.9) 2.05, dd (14.8, 6.8)	37.3, CH <sub>2</sub>	2.74, d (14.5) 1.99, dd (14.6, 6.7)	36.7, CH <sub>2</sub>
8	-	55.2, C	-	54.2, C
9	-	208.4, C	-	207.4, C
10	-	195.1, C	-	195.0, C
11	-	130.9, C	-	130.4, C
12	7.29, d (2.1)	116.1, CH	7.61, d (2.1)	115.0, CH
13	-	146.7, C	-	144.2, C
14	-	153.0, C	-	150.5, C
15	6.74, d (8.2)	115.8, CH	6.79, d (8.3)	114.2, CH
16	7.04, dd (8.2, 2.1) 2.60, dd (13.5, 8.3)	124.8, CH	7.06, dd (8.3, 2.0)	125.2, CH
17	2.45, m	26.8, CH <sub>2</sub>	2.62, overlap 2.49, overlap	25.9 CH <sub>2</sub>
18	4.90, m	121.0, CH	4.96, brt, (7.0)	119.8, CH
19	-	135.7, C	-	135.2, C
20	1.57, s	26.4, CH <sub>3</sub>	1.70, s	26.5, CH <sub>3</sub>
21	1.59, s	18.3, CH <sub>3</sub>	1.61, s	18.4, CH <sub>3</sub>
22	1.00, s	27.0, CH <sub>3</sub>	1.00, s	26.9, CH <sub>3</sub>
23	1.15, s	22.9, CH <sub>3</sub>	1.15, s	22.5, CH <sub>3</sub>
24	2.39, m 2.35, m	31.6, CH <sub>2</sub>	2.34, overlap	30.0, CH <sub>2</sub>
25	5.13, m	126.0, CH	5.09, brt (6.8)	124.0, CH
26	-	134.1, C	-	134.1, C
27	1.68, s	25.9, CH <sub>3</sub>	1.70, s	26.0, CH <sub>3</sub>
28	1.71, s	18.7, CH <sub>3</sub>	1.60, s	18.3, CH <sub>3</sub>
29	2.26, d (15.3) 1.81, dd (15.3, 13.0)	39.1, CH <sub>2</sub>	2.34, overlap 1.91, overlap	37.2, CH <sub>2</sub>
30	2.51, t (12.3)	41.0, CH	2.49, overlap	40.4, CH
31	-	150.9, C	-	149.0, C
32	4.84, s 4.80, s	110.6, CH <sub>2</sub>	4.83, s 4.80, s	110.7, CH <sub>2</sub>
33	1.80, s	20.8, CH <sub>3</sub>	1.78, s	20.5, CH <sub>3</sub>
34	2.13, d (16.5) 1.50, overlap	36.7, CH <sub>2</sub>	1.91, overlap 1.55, m	36.2, CH <sub>2</sub>
35	4.07, d (10.6)	91.0, CH	4.16, d (10.8)	90.6, CH
36	-	73.6, C	-	73.6, C
37	0.91, s	26.5, CH <sub>3</sub>	1.16, s	26.2, CH <sub>3</sub>

Table S7. Immunosuppressive Activities of Compounds **1-17**

Comp.	ConA-induced T-cell proliferation ( $\mu$ M)	Lps-induced B-cell proliferation ( $\mu$ M)
(+)- <b>1</b>	33.52 $\pm$ 4.85	> 40
(-)- <b>1</b>	35.62 $\pm$ 2.78	> 40
(+)- <b>2</b>	10.15 $\pm$ 2.13	16.41 $\pm$ 1.35
(-)- <b>2</b>	33.21 $\pm$ 6.48	> 40
<b>3</b>	5.96 $\pm$ 1.87	36.35 $\pm$ 4.96
(+)- <b>4</b>	18.39 $\pm$ 3.27	31.34 $\pm$ 2.84
(-)- <b>4</b>	36.13 $\pm$ 5.24	> 40
<b>5</b>	3.88 $\pm$ 2.57	35.42 $\pm$ 2.48
(+)- <b>6</b>	10.02 $\pm$ 1.47	20.54 $\pm$ 2.64
(-)- <b>6</b>	16.07 $\pm$ 4.25	32.86 $\pm$ 6.42
(+)- <b>7</b>	17.15 $\pm$ 1.17	19.67 $\pm$ 4.52
(-)- <b>7</b>	20.41 $\pm$ 5.25	20.58 $\pm$ 1.94
(+)- <b>8</b>	> 40	> 40
(-)- <b>8</b>	> 40	> 40
<b>9</b>	11.07 $\pm$ 2.71	35.10 $\pm$ 3.84
(+)- <b>10</b>	34.52 $\pm$ 4.21	37.41 $\pm$ 7.85
(-)- <b>10</b>	31.62 $\pm$ 1.26	> 40
(+)- <b>11</b>	28.12 $\pm$ 6.24	23.87 $\pm$ 3.57
(-)- <b>11</b>	32.04 $\pm$ 5.74	31.84 $\pm$ 1.70
<b>12</b>	15.81 $\pm$ 2.81	18.22 $\pm$ 4.25
(+)- <b>13</b>	> 40	> 40
(-)- <b>13</b>	> 40	> 40
<b>14</b>	> 40	13.13 $\pm$ 3.54
(+)- <b>15</b>	23.05 $\pm$ 1.01	> 40
(-)- <b>15</b>	25.52 $\pm$ 3.77	> 40
<b>16</b>	10.23 $\pm$ 1.84	15.25 $\pm$ 2.11
<b>17</b>	2.02 $\pm$ 1.02	16.18 $\pm$ 0.84
CsA	0.04 $\pm$ 0.008	0.2 $\pm$ 0.1

Data are expressed as Mean  $\pm$  SD, three independent experiments were performed with similar results.

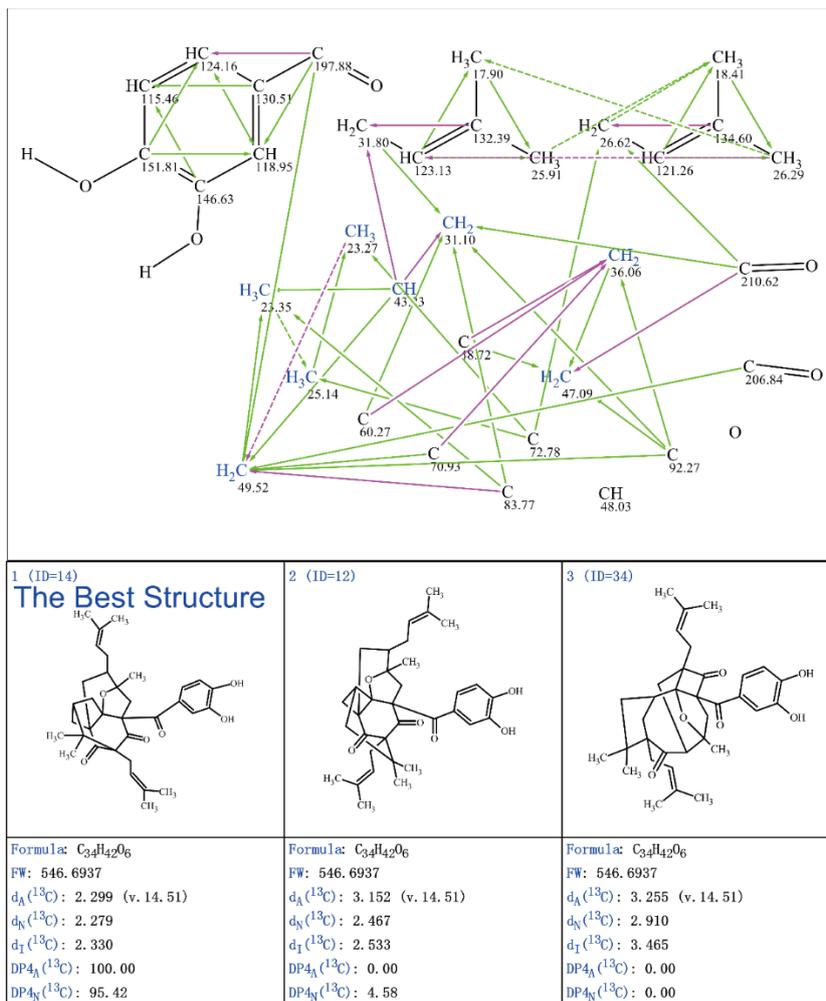


Figure S1. Edited molecular connectivity diagram (MCD) and top 3 ranked structures for **1**

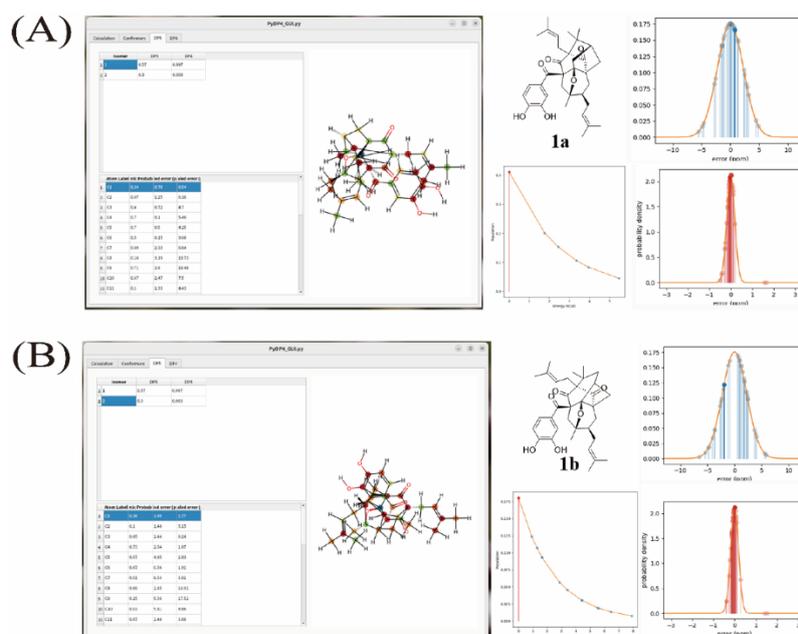


Figure S2. The DP5 GUI, conformer energy distributions, and DP4 statistics of **1a** (A) and **1b** (B)



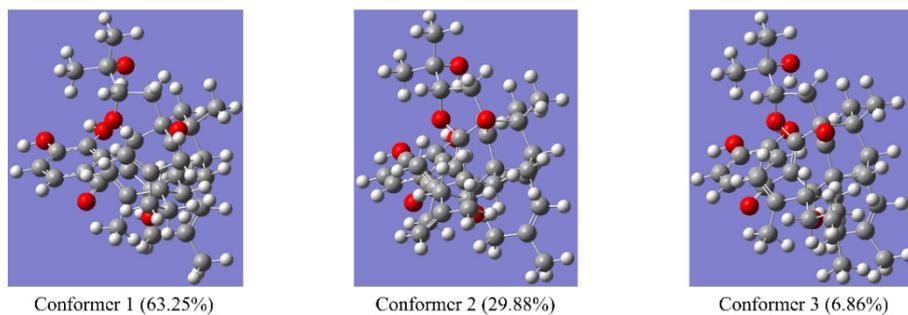


Figure S6. The low-energy conformers and equilibrium populations of compound **4**

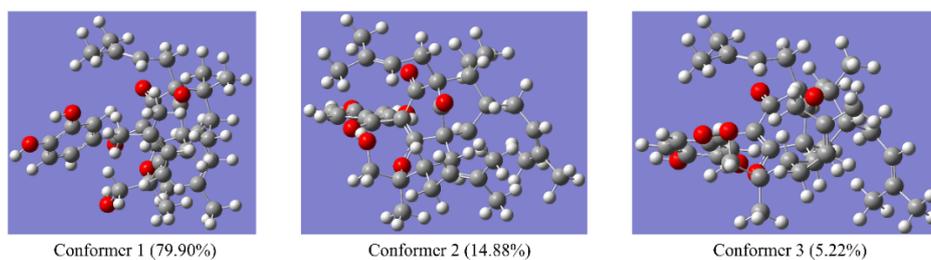


Figure S7. The low-energy conformers and equilibrium populations of compound **8**

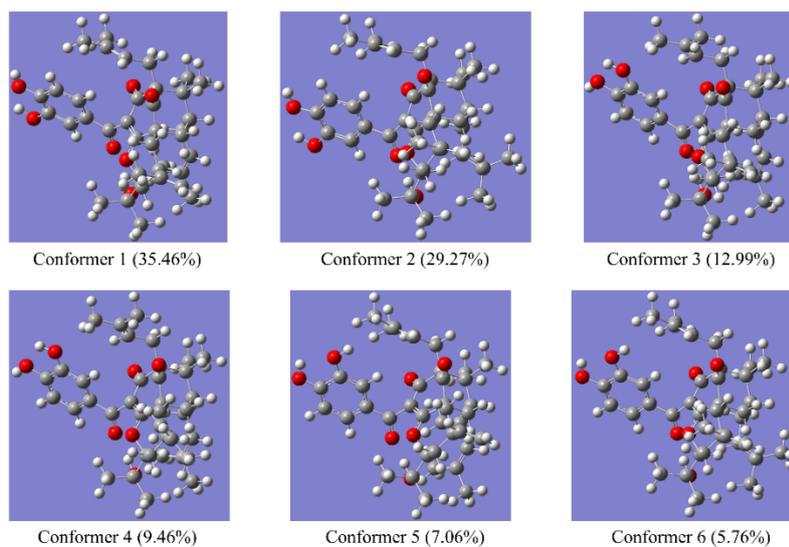
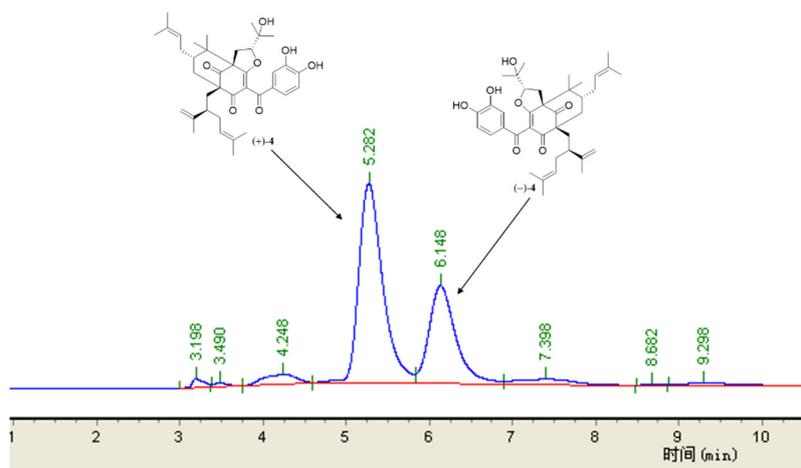
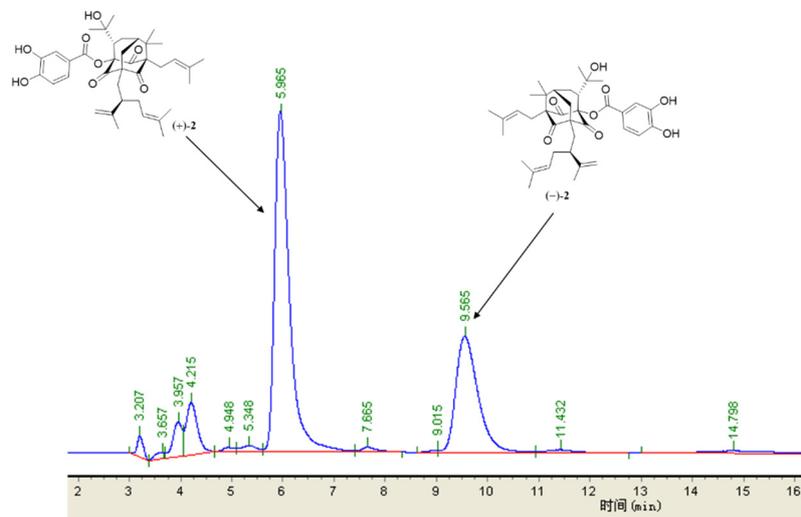
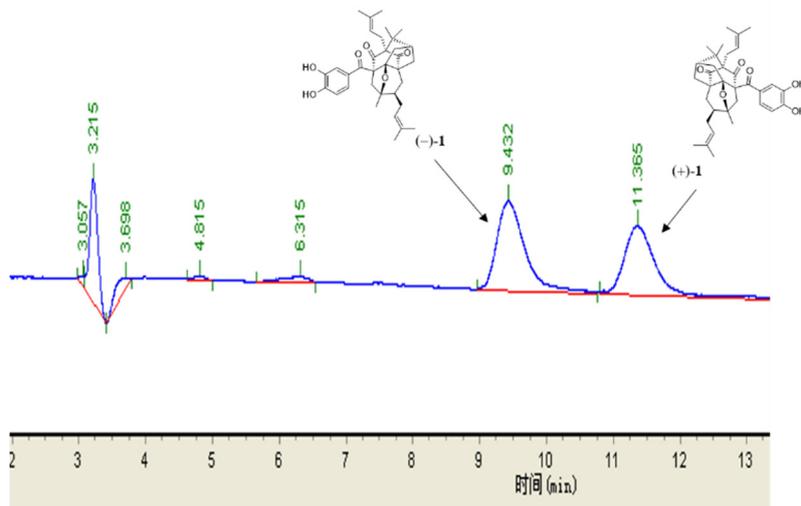
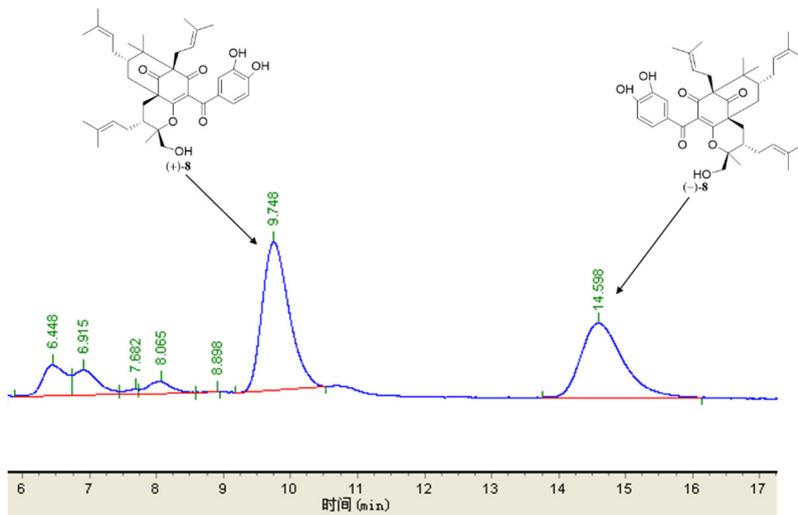
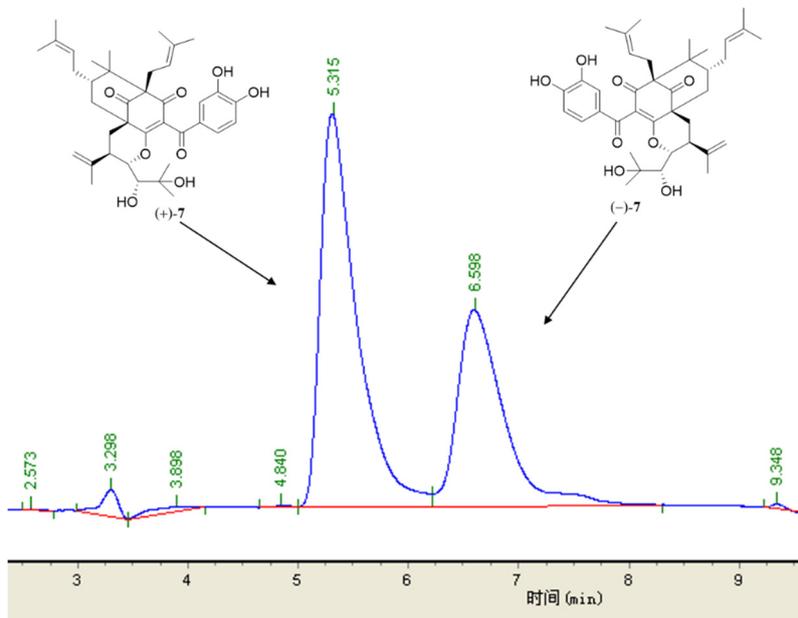
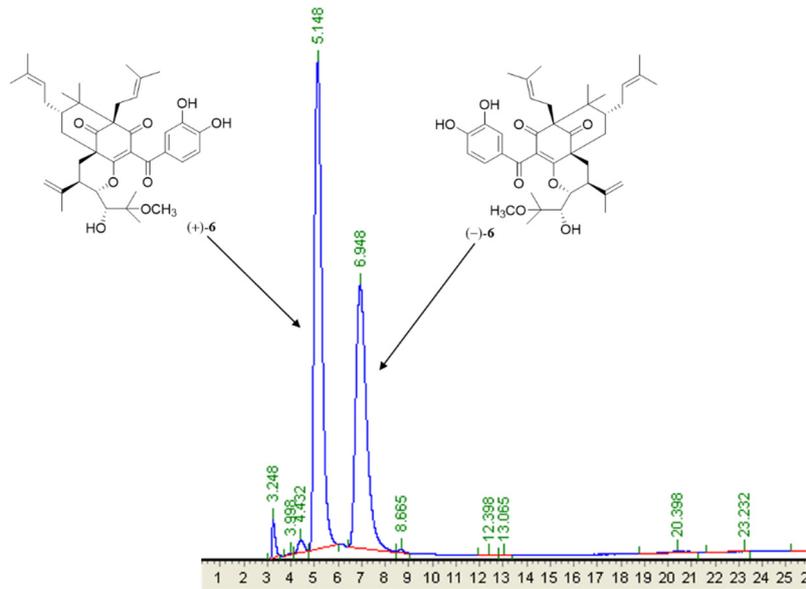
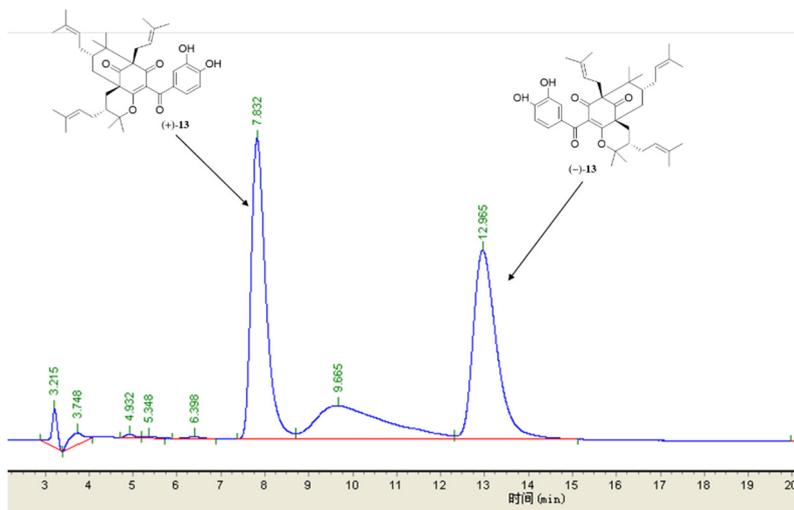
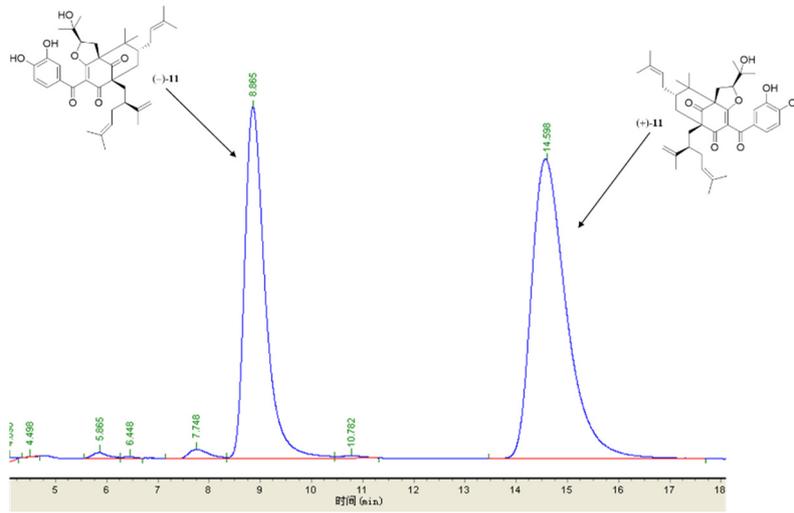
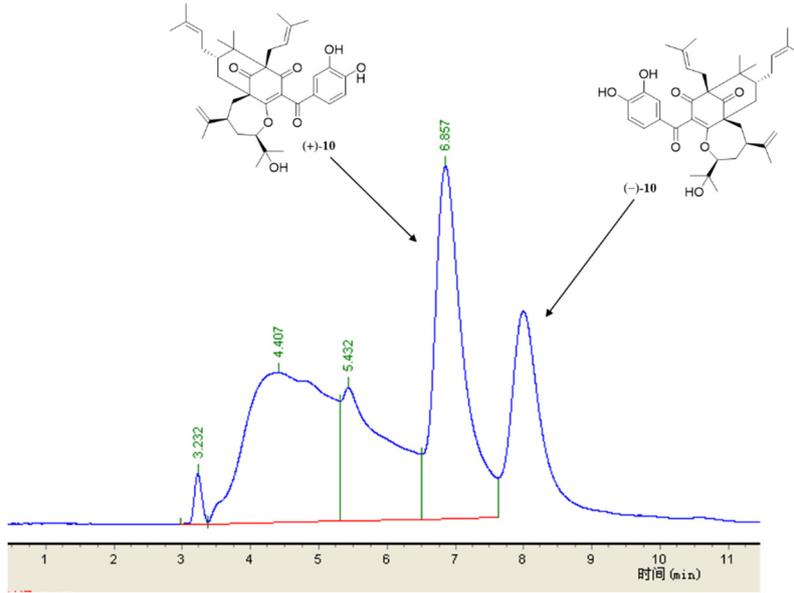


Figure S8. The low-energy conformers and equilibrium populations of compound **10**







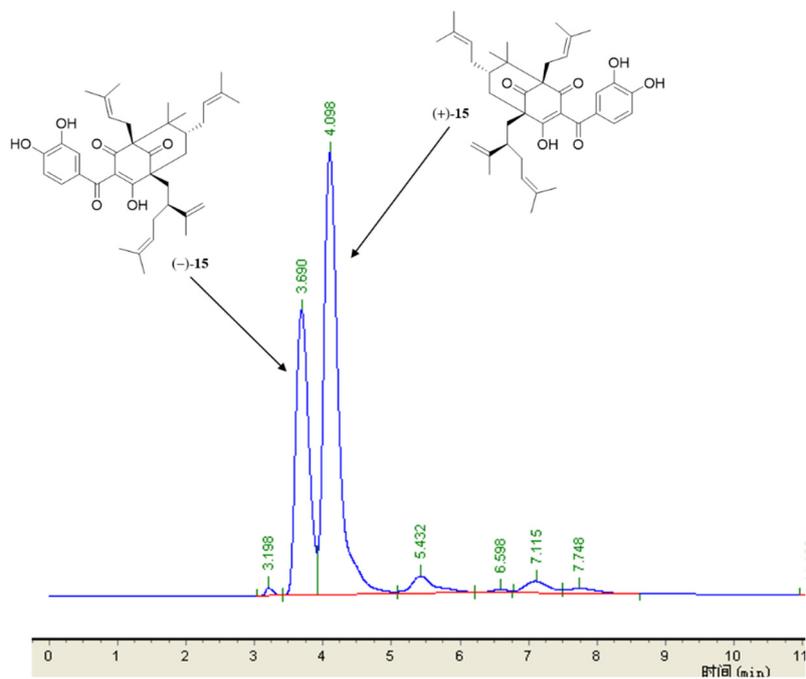


Figure S9. HPLC chromatograms of Chiral separation using *n*-hexane-2-propanol (10:1) for **1**, **2**, **4**, **6**, **7**, **8**, **10**, **11**, **13**, **15**

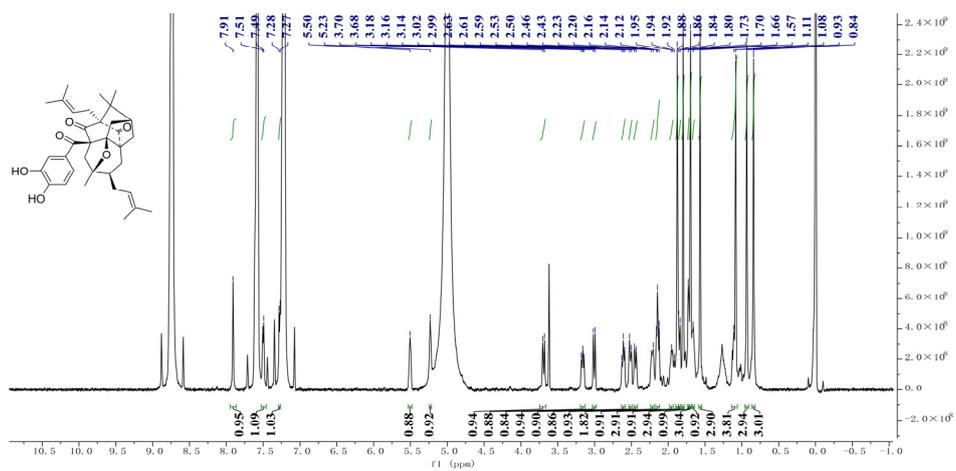


Figure S10. <sup>1</sup>H NMR spectrum of compound **1** (recorded in Pyridine-*d*<sub>5</sub>)

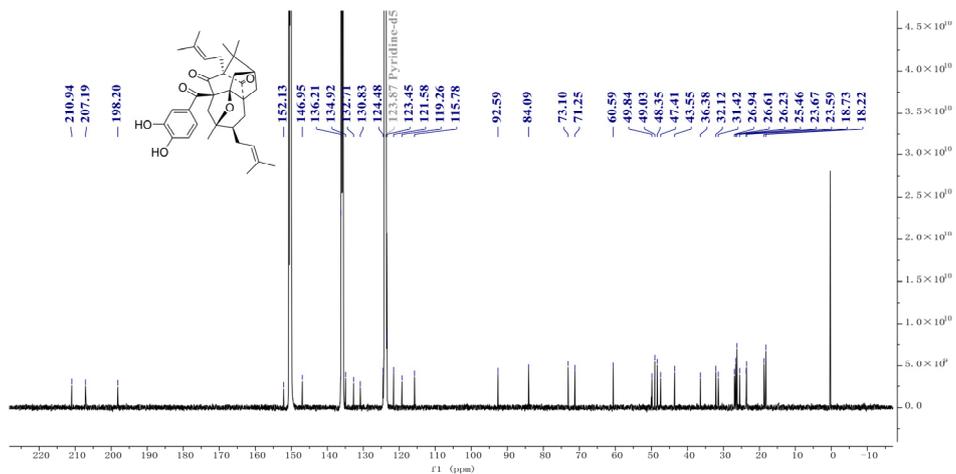


Figure S11.  $^{13}\text{C}$  NMR spectrum of compound 1 (recorded in Pyridine- $d_5$ )

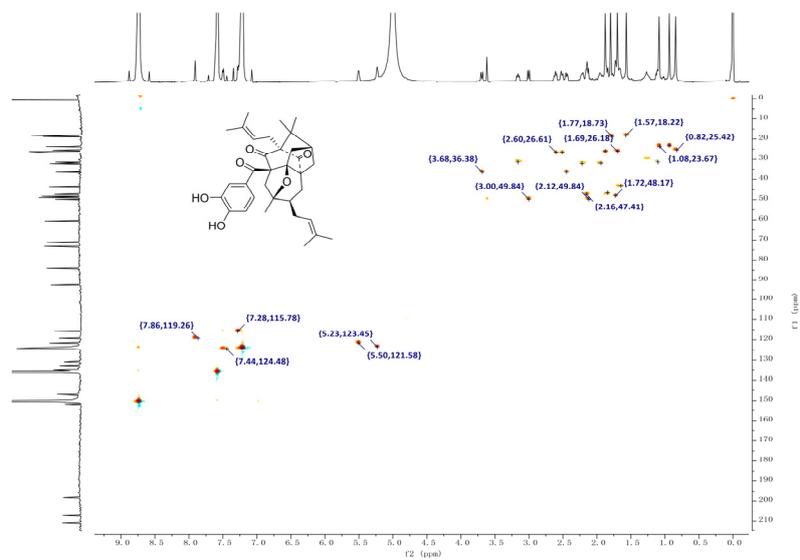


Figure S12. HSQC spectrum of compound 1 (recorded in Pyridine- $d_5$ )

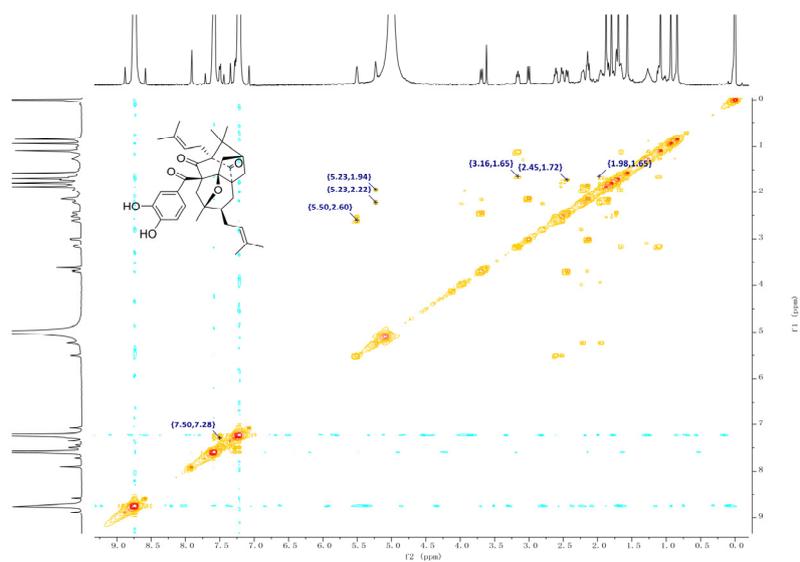


Figure S13.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** (recorded in Pyridine- $d_5$ )

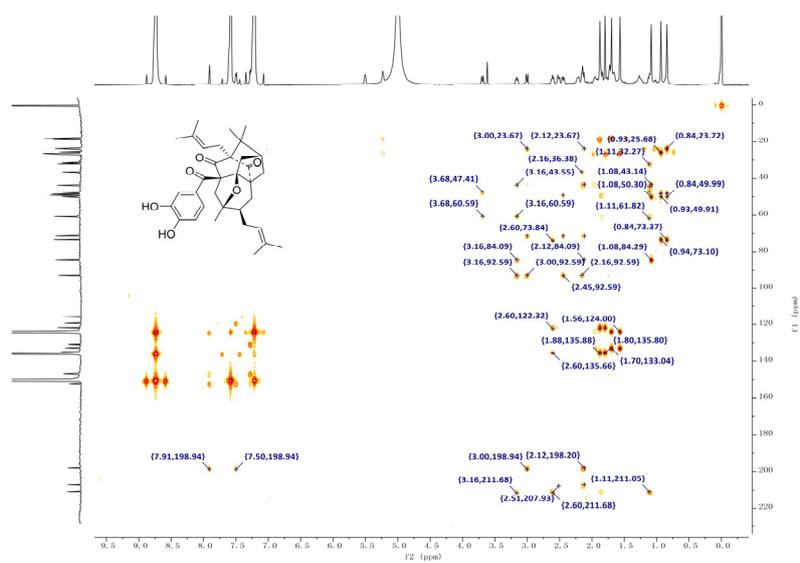


Figure S14. HMBC spectrum of compound **1** (recorded in pyridine- $d_5$ )

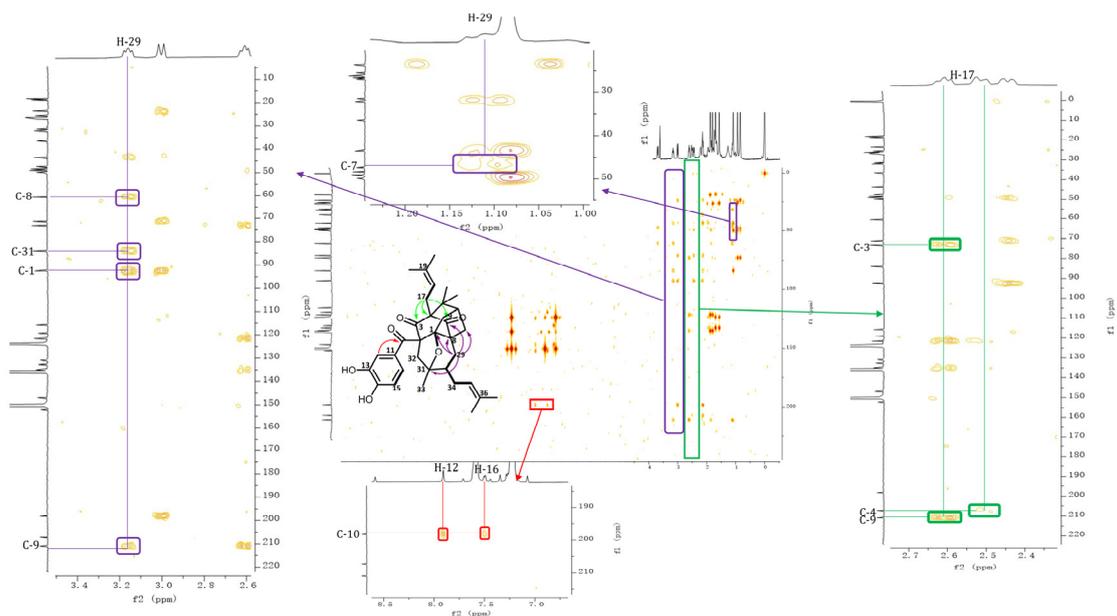


Figure S15. Detailed HMBC spectrum of compound **1** (recorded in pyridine-*d*<sub>5</sub>)

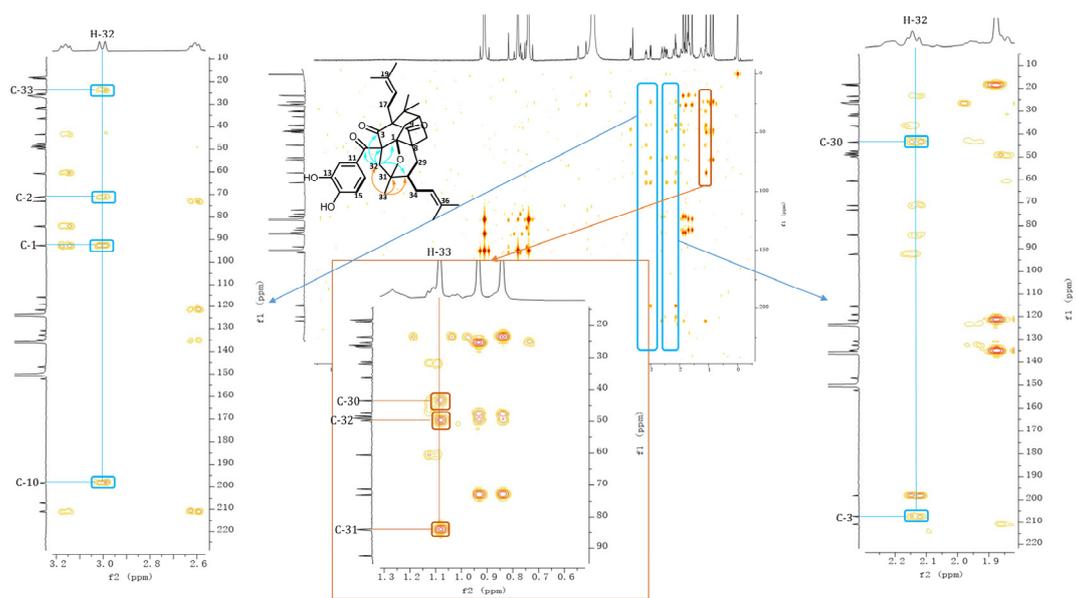


Figure S16. Detailed HMBC spectrum of compound **1** (recorded in pyridine-*d*<sub>5</sub>)

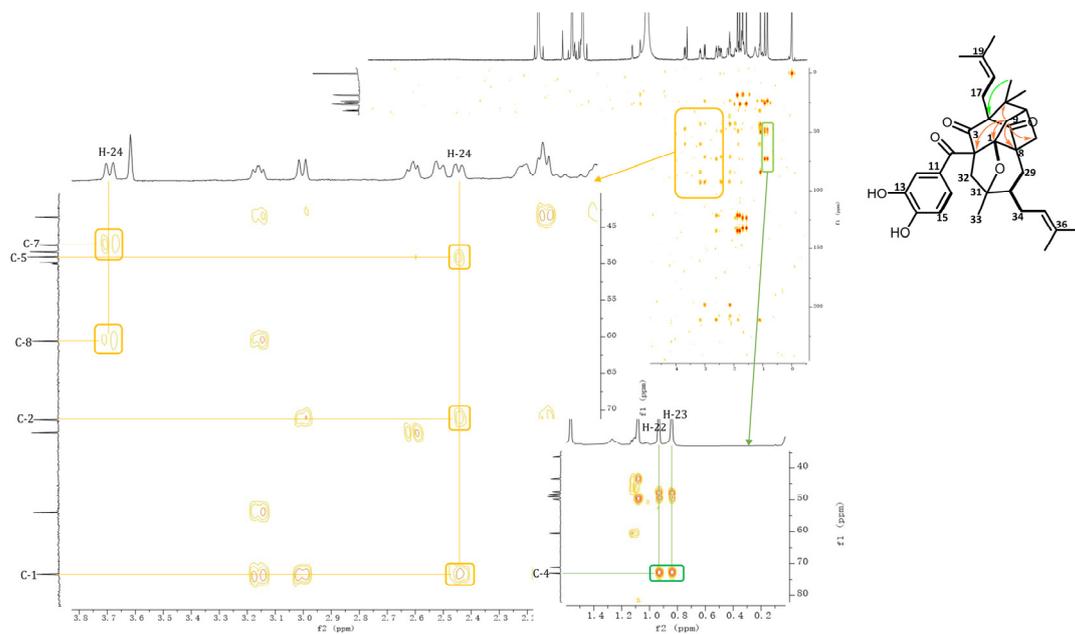


Figure S17. Detailed HMBC spectrum of compound **1** (recorded in pyridine- $d_5$ )

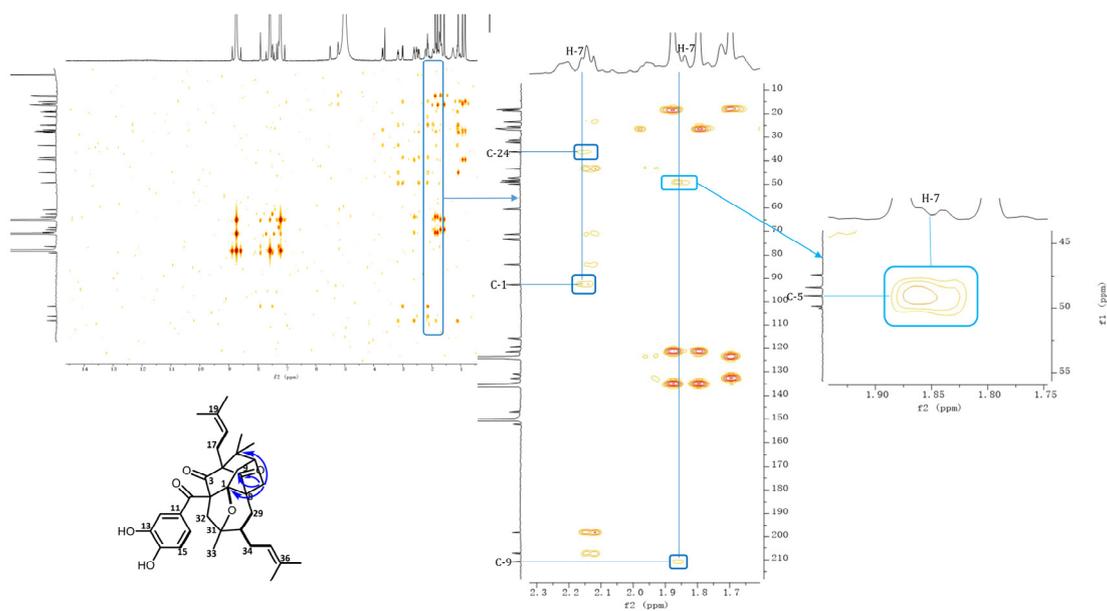


Figure S18. Detailed HMBC spectrum of compound **1** (recorded in pyridine- $d_5$ )



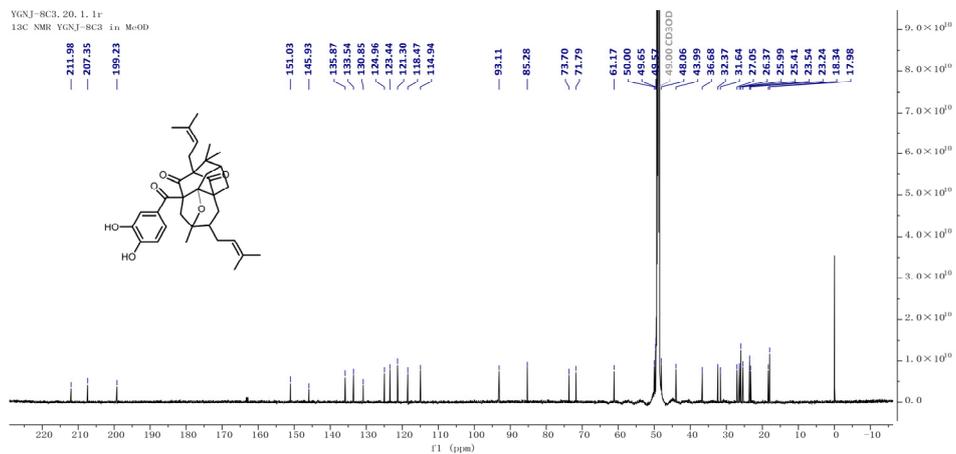


Figure S21. <sup>13</sup>C NMR spectrum of compound 1 (recorded in MeOH-*d*<sub>4</sub>)

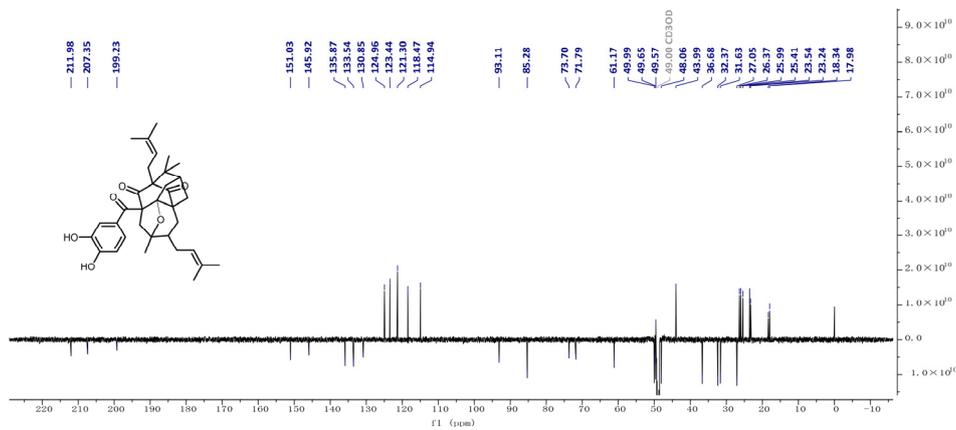


Figure S22. APT spectrum of compound 1 (recorded in MeOH-*d*<sub>4</sub>)

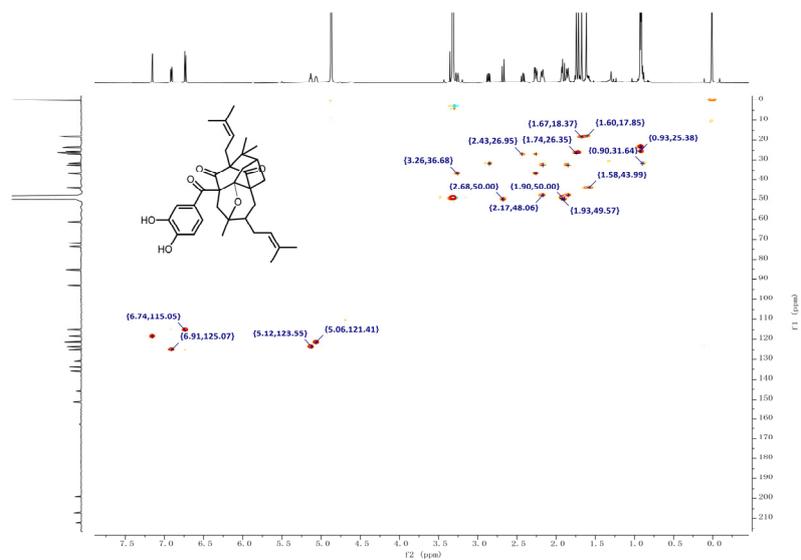


Figure S23. HSQC spectrum of compound **1** (recorded in MeOH-*d*<sub>4</sub>)

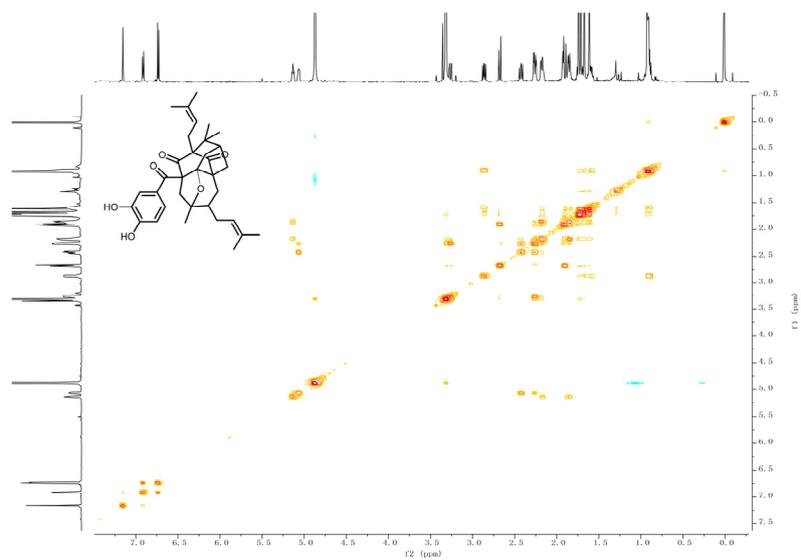


Figure S24. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **1** (recorded in MeOH-*d*<sub>4</sub>)

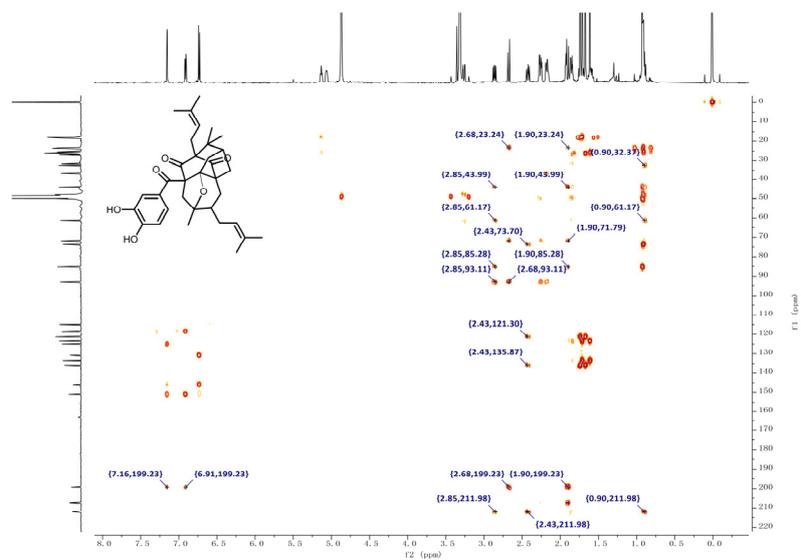


Figure S25. HMBC spectrum of compound **1** (recorded in  $\text{MeOH-}d_4$ )

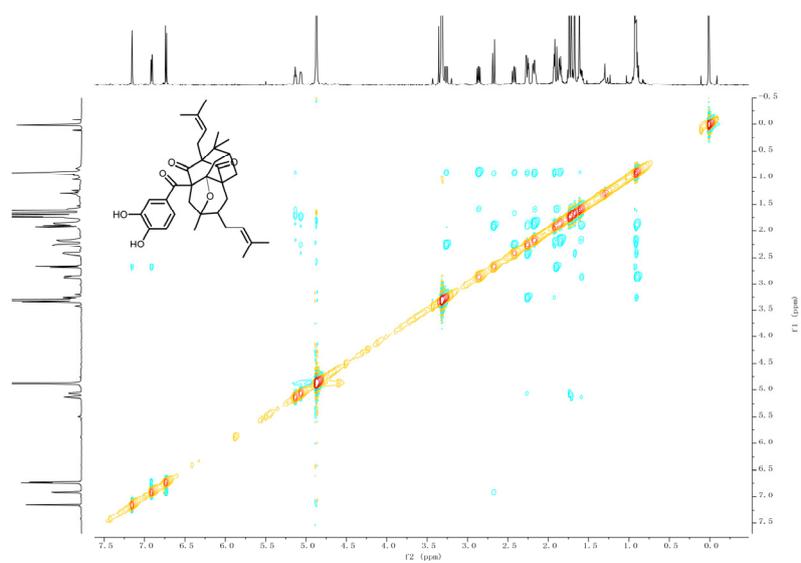


Figure S26. NOESY spectrum of compound **1** (recorded in  $\text{MeOH-}d_4$ )

## Compound Spectrum SmartFormula Report

### Analysis Info

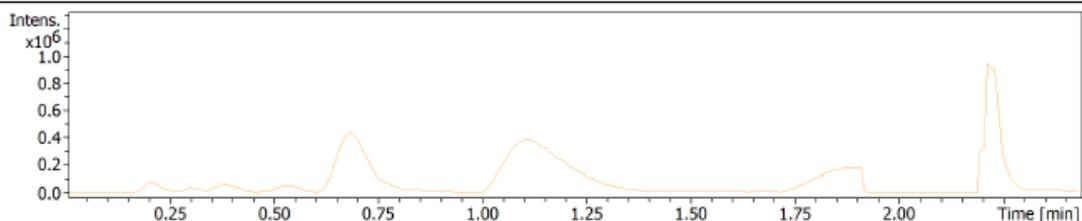
Analysis Name D:\Data\YIJ\20240318\8C3\_9\_1\_6362.d  
Method HPLC\_MS\_pos\_without\_column.m  
Sample Name 8C3  
Comment

Acquisition Date 3/18/2024 2:26:42 PM

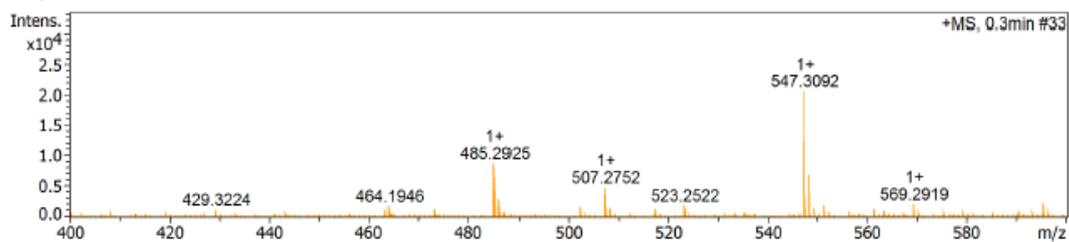
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #33



### C<sub>34</sub>H<sub>42</sub>O<sub>6</sub>, M+nH, 547.3054

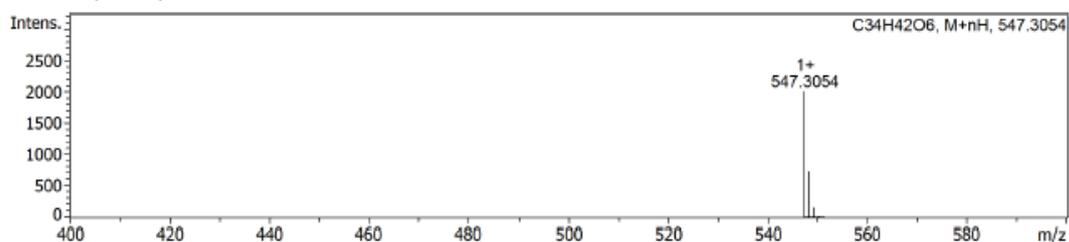


Figure S27. HRESIMS spectrum of compound 1

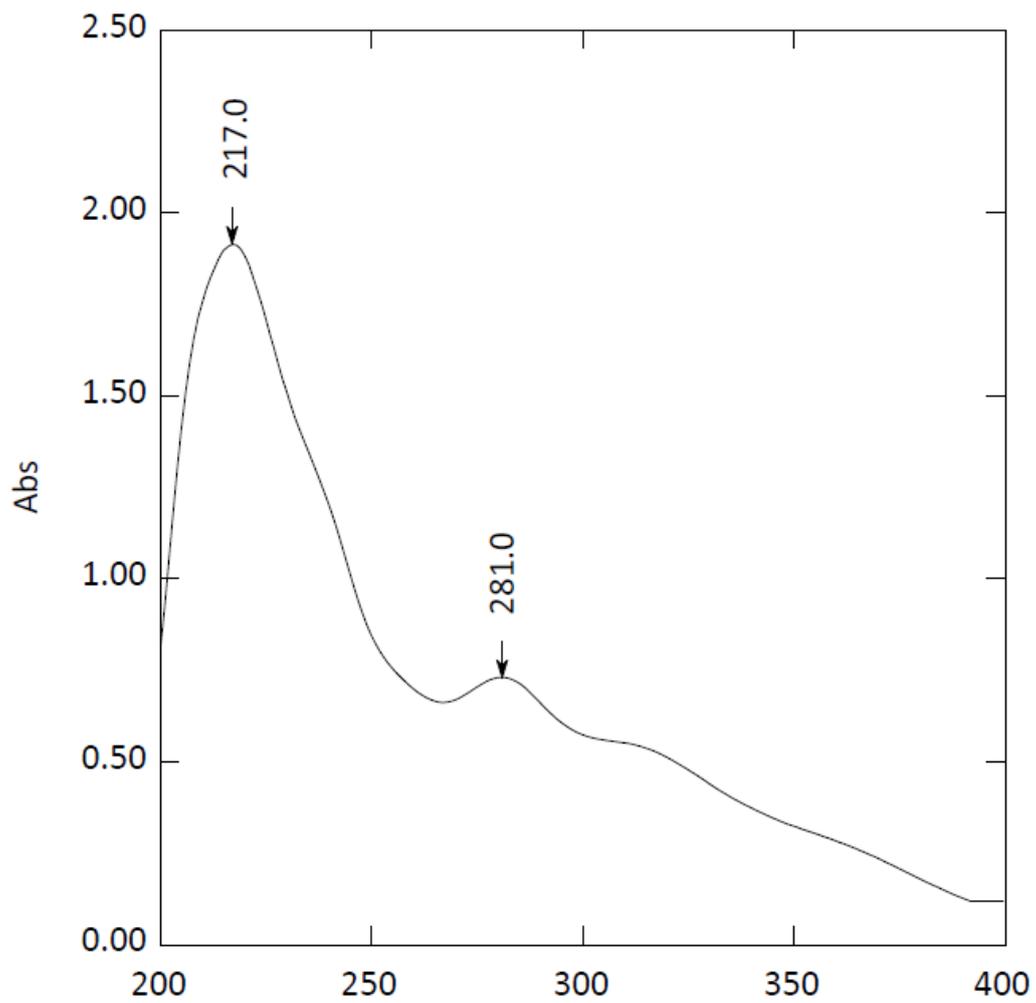


Figure S28. UV spectrum of compound 1

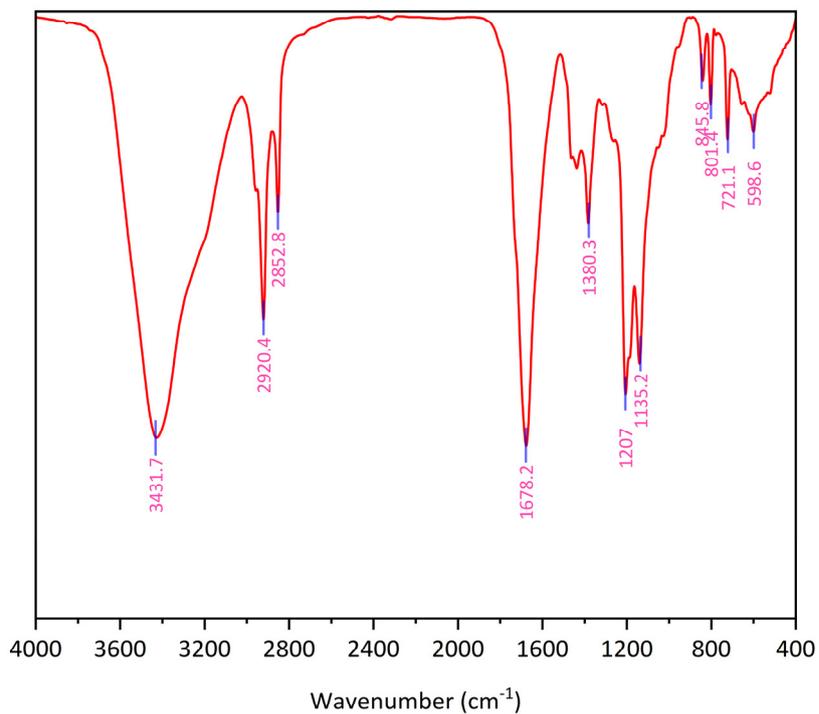


Figure S29. IR spectrum of compound **1**

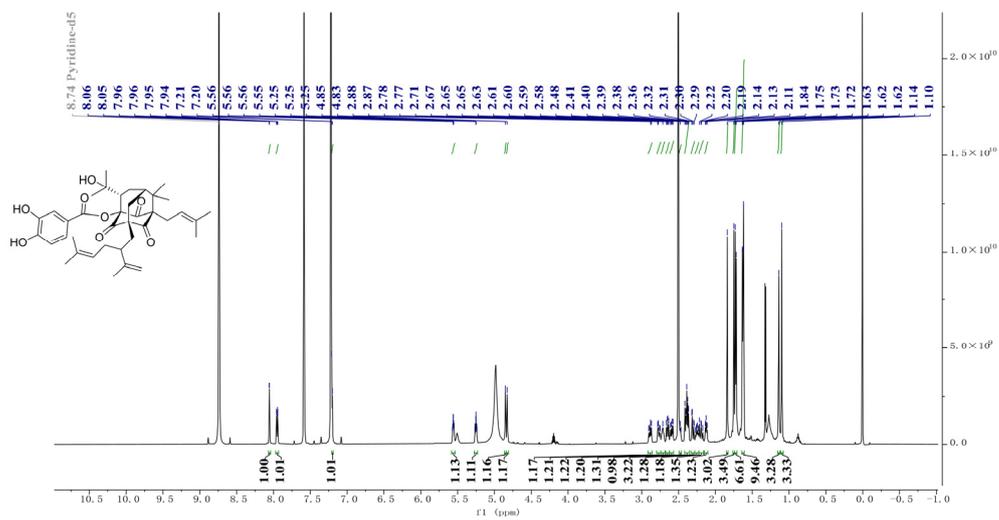


Figure S30. <sup>1</sup>H NMR spectrum of compound **2** (recorded in Pyridine-*d*<sub>5</sub>)

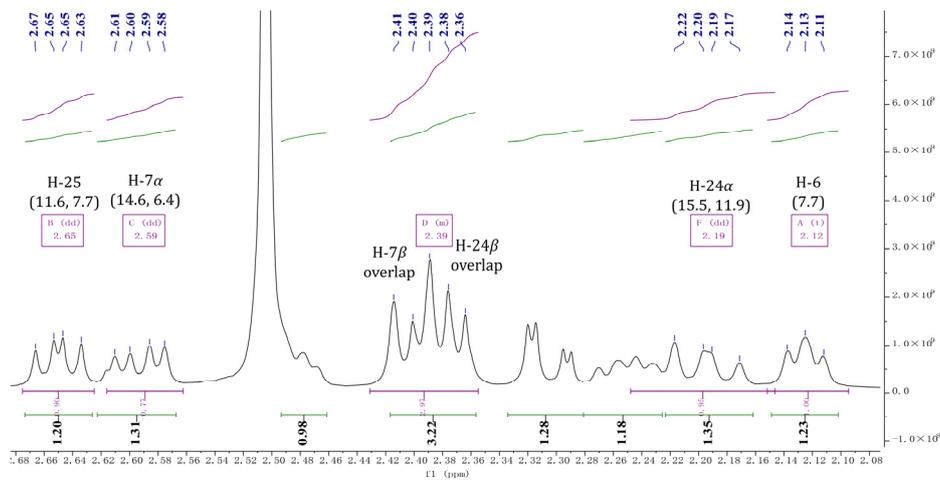


Figure S31. Zoomed-in  $^1\text{H}$  NMR spectrum ( $\delta$  2.10-2.70 ppm) of compound **2**

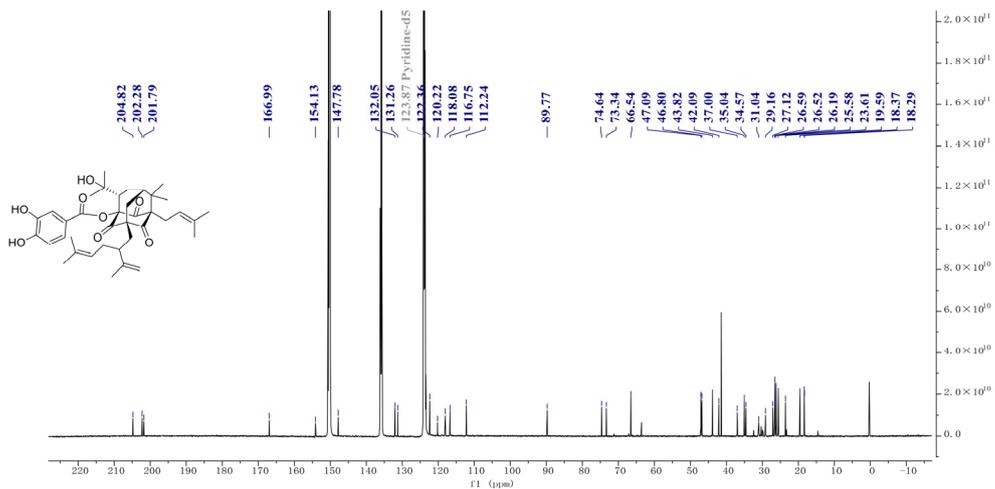


Figure S32.  $^{13}\text{C}$  NMR spectrum of compound **2** (recorded in Pyridine- $d_5$ )

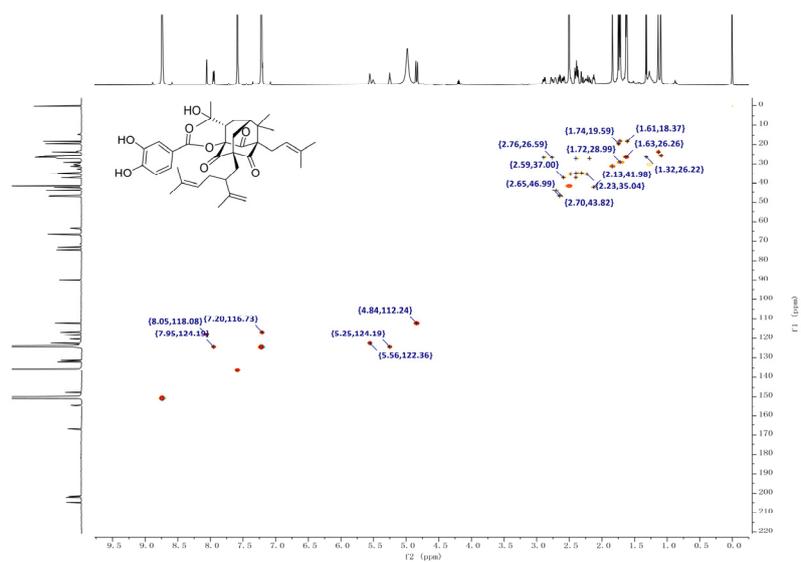


Figure S33. HSQC spectrum of compound **2** (recorded in Pyridine-*d*<sub>5</sub>)

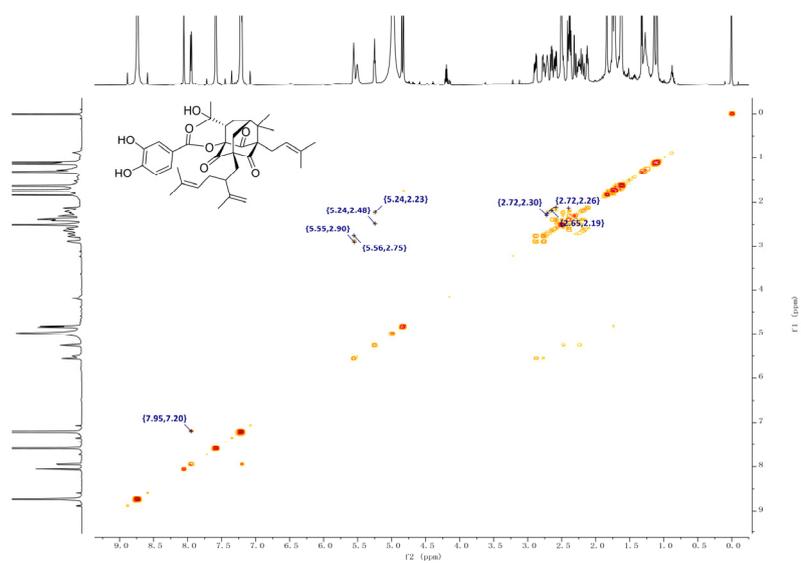


Figure S34. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **2** (recorded in Pyridine-*d*<sub>5</sub>)

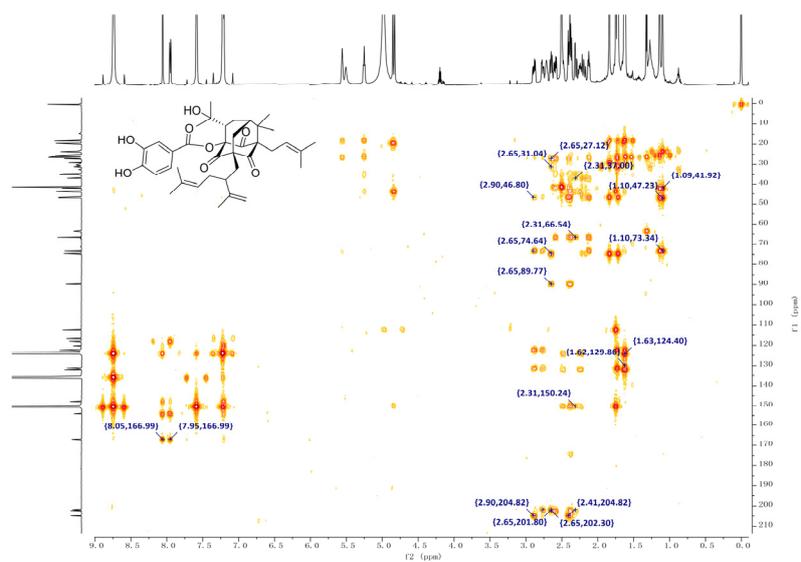


Figure S35. HMBC spectrum of compound **2** (recorded in Pyridine-*d*<sub>5</sub>)

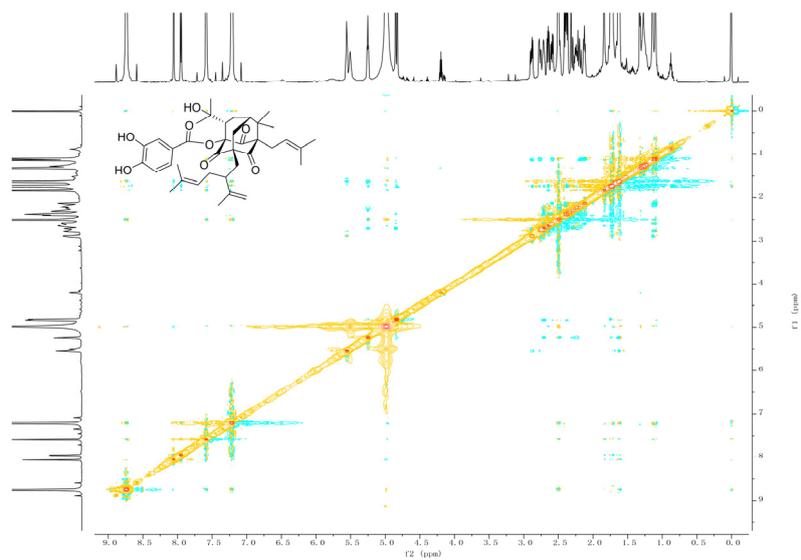


Figure S36. NOESY spectrum of compound **2** (recorded in Pyridine-*d*<sub>5</sub>)

## Compound Spectrum SmartFormula Report

### Analysis Info

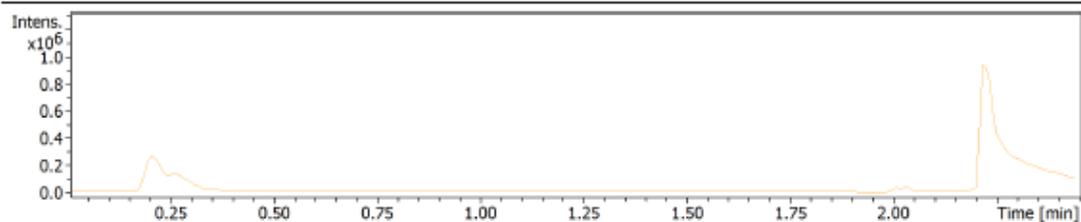
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Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH5  
Comment

Acquisition Date 7/1/2024 2:32:03 PM

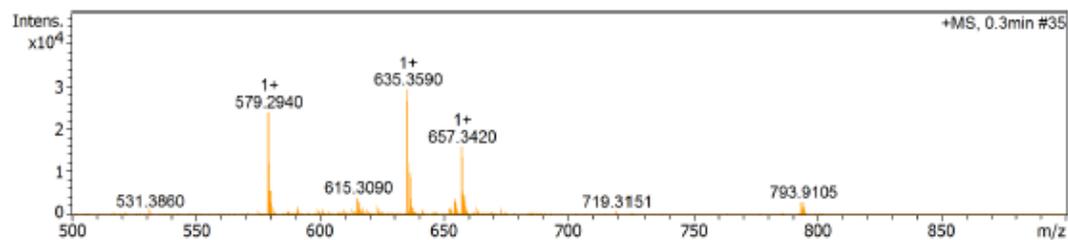
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #35



### C38H50O8, M+nH, 635.3578

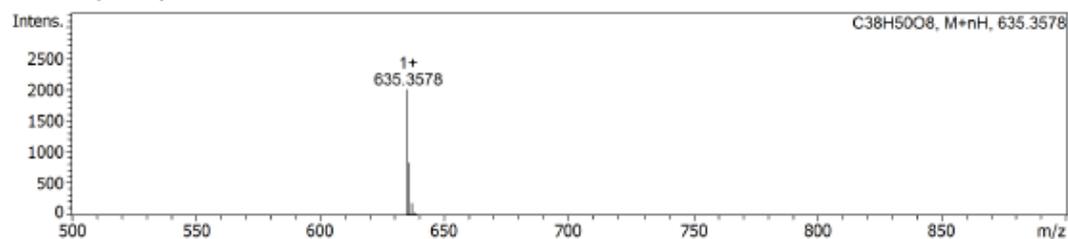


Figure S37. HRESIMS spectrum of compound 2

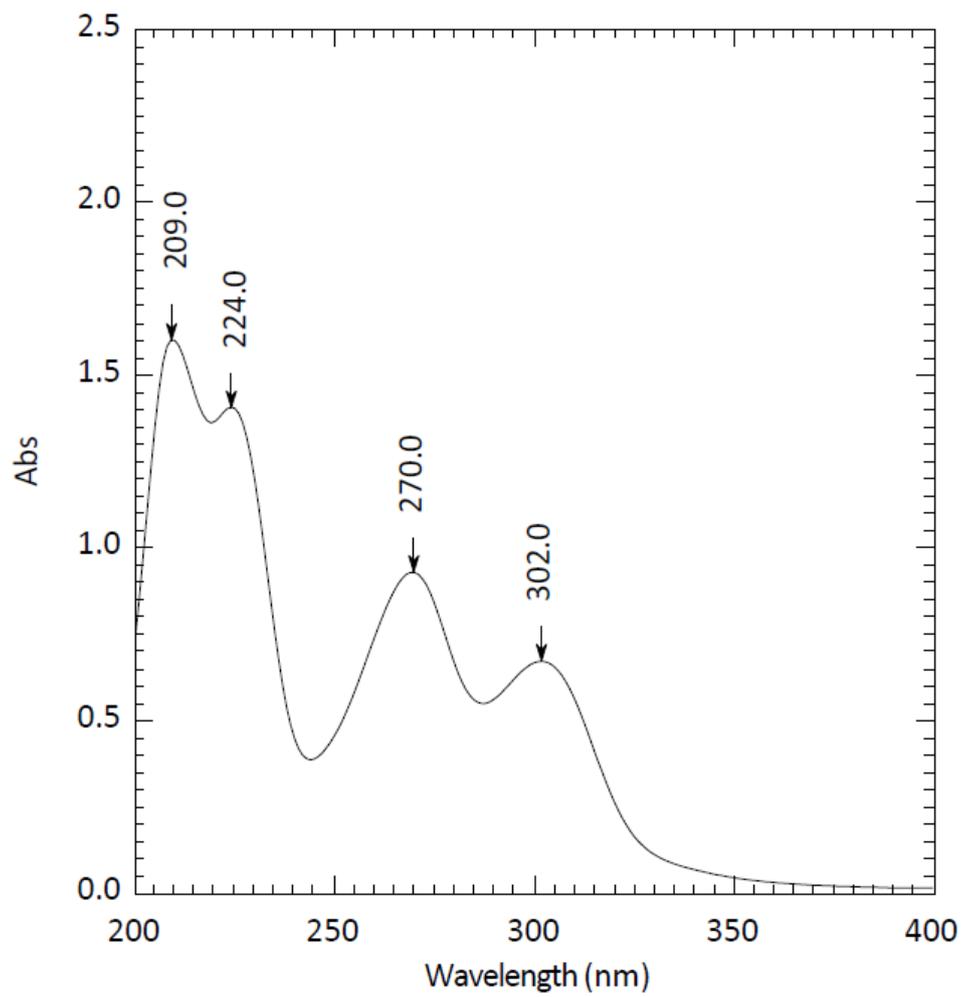


Figure S38. UV spectrum of compound 2

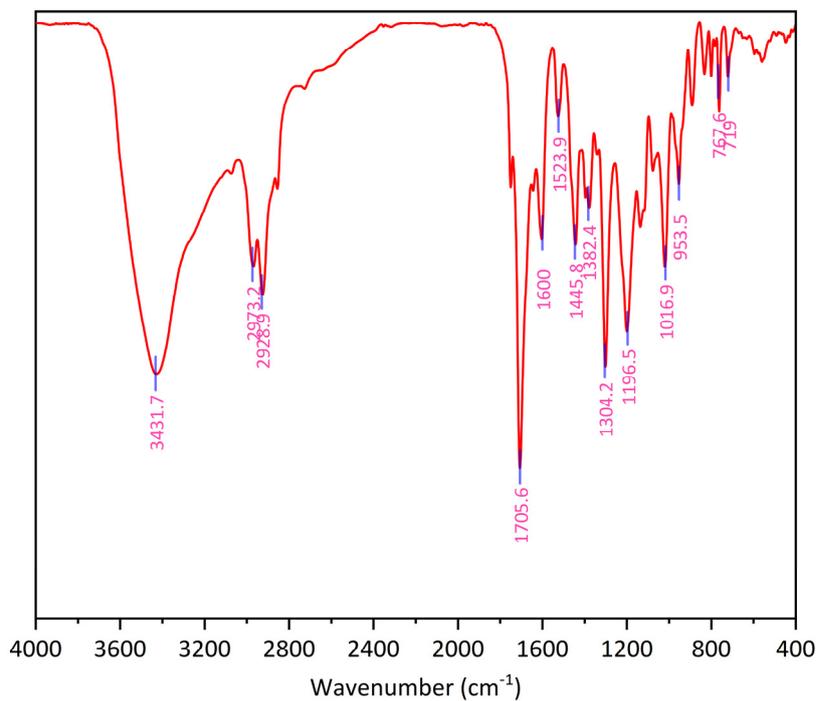


Figure S39. IR spectrum of compound 2

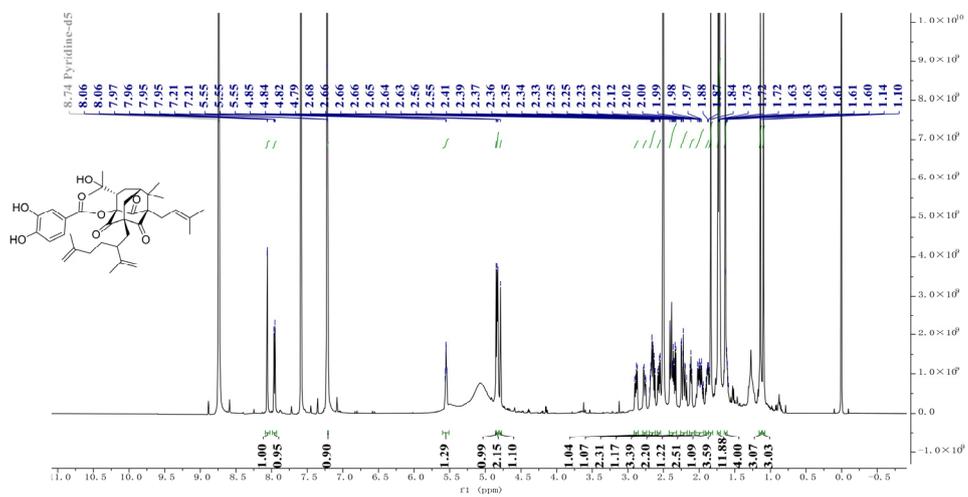


Figure S40. <sup>1</sup>H NMR spectrum of compound 3 (recorded in Pyridine-d<sub>5</sub>)

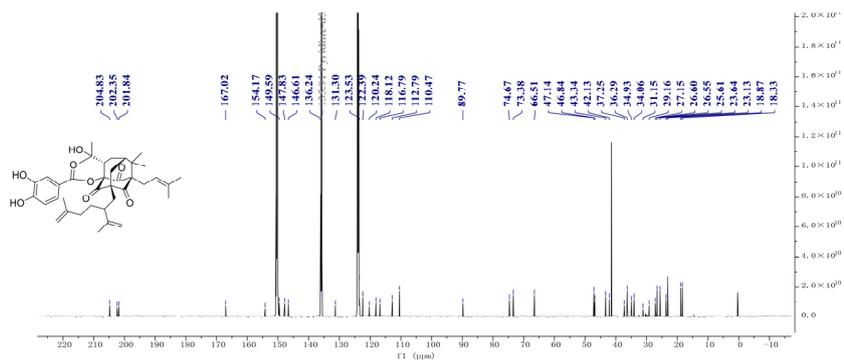


Figure S41.  $^{13}\text{C}$  NMR spectrum of compound **3** (recorded in Pyridine- $d_5$ )

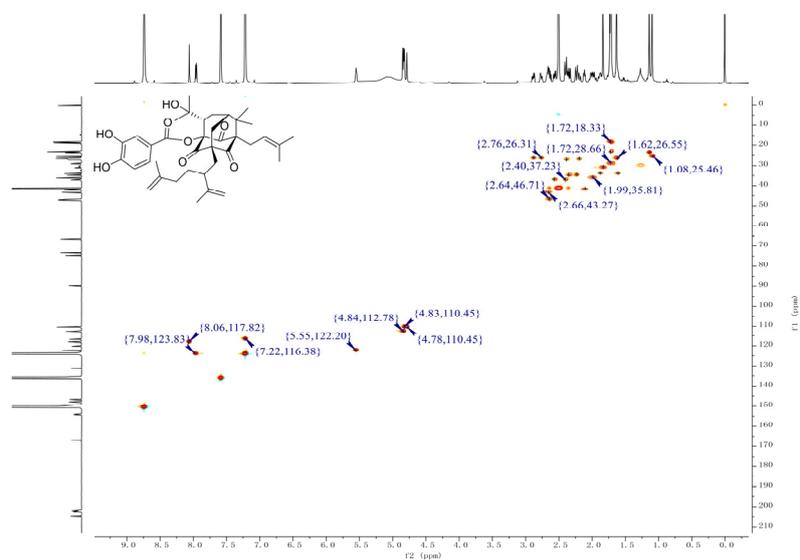


Figure S42. HSQC spectrum of compound **3** (recorded in Pyridine- $d_5$ )

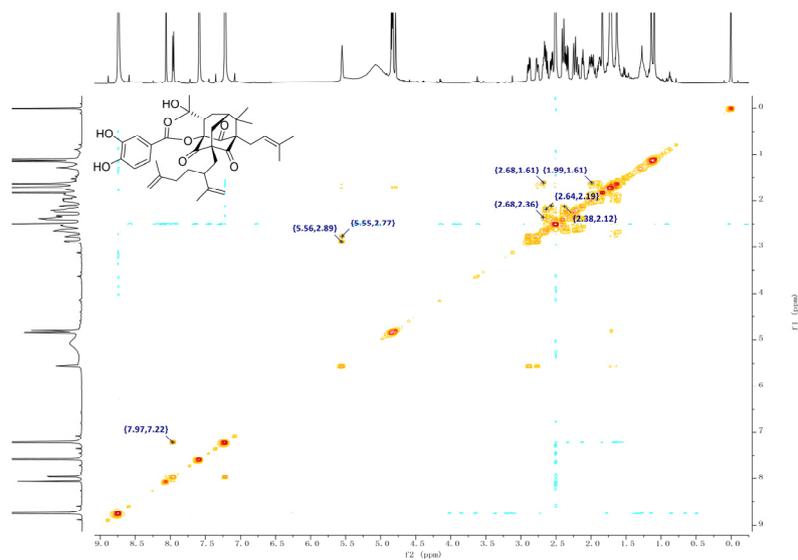


Figure S43.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3** (recorded in Pyridine- $d_5$ )

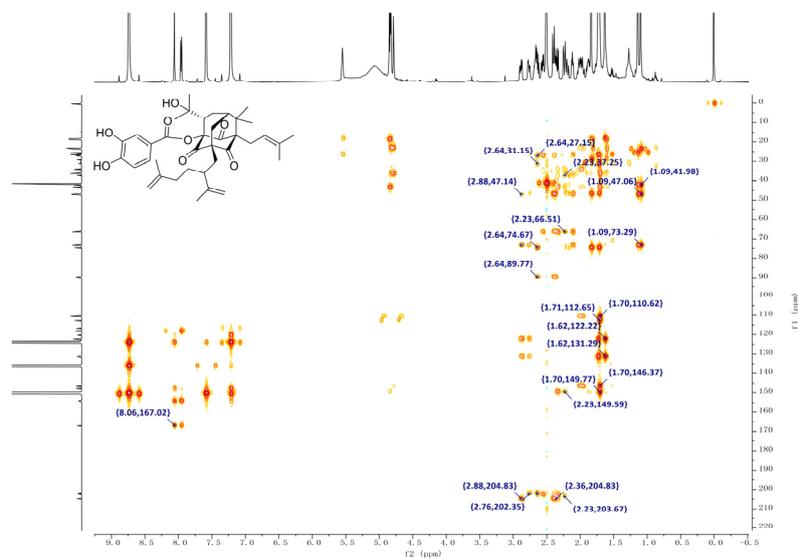


Figure S44. HMBC spectrum of compound **3** (recorded in Pyridine- $d_5$ )

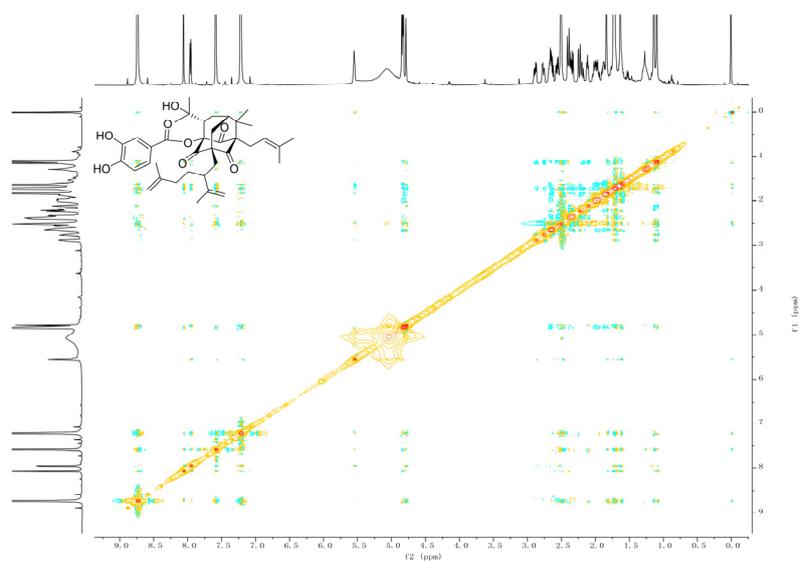


Figure S45. NOESY spectrum of compound **3** (recorded in Pyridine- $d_5$ )

## Compound Spectrum SmartFormula Report

### Analysis Info

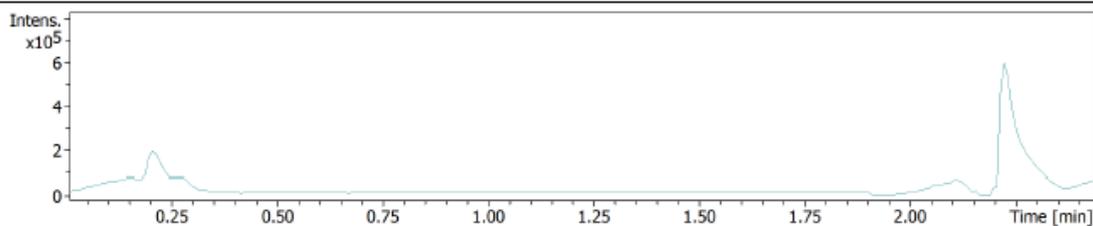
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Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH6  
Comment

Acquisition Date 7/1/2024 2:35:06 PM

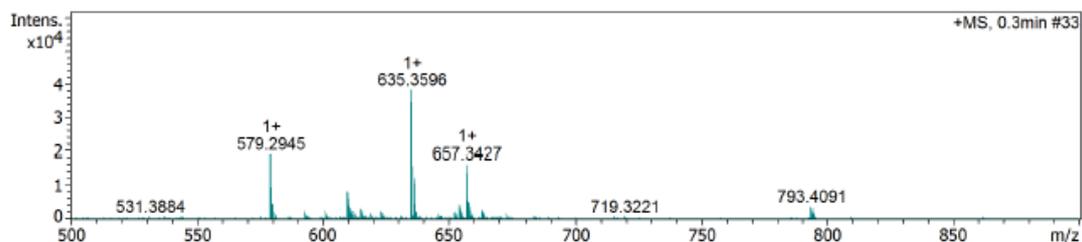
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #33



### C38H50O8, M+nH, 635.3578

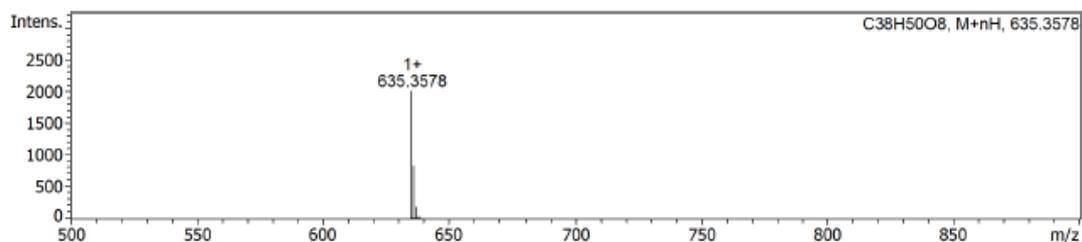


Figure S46. HRESIMS spectrum of compound 3

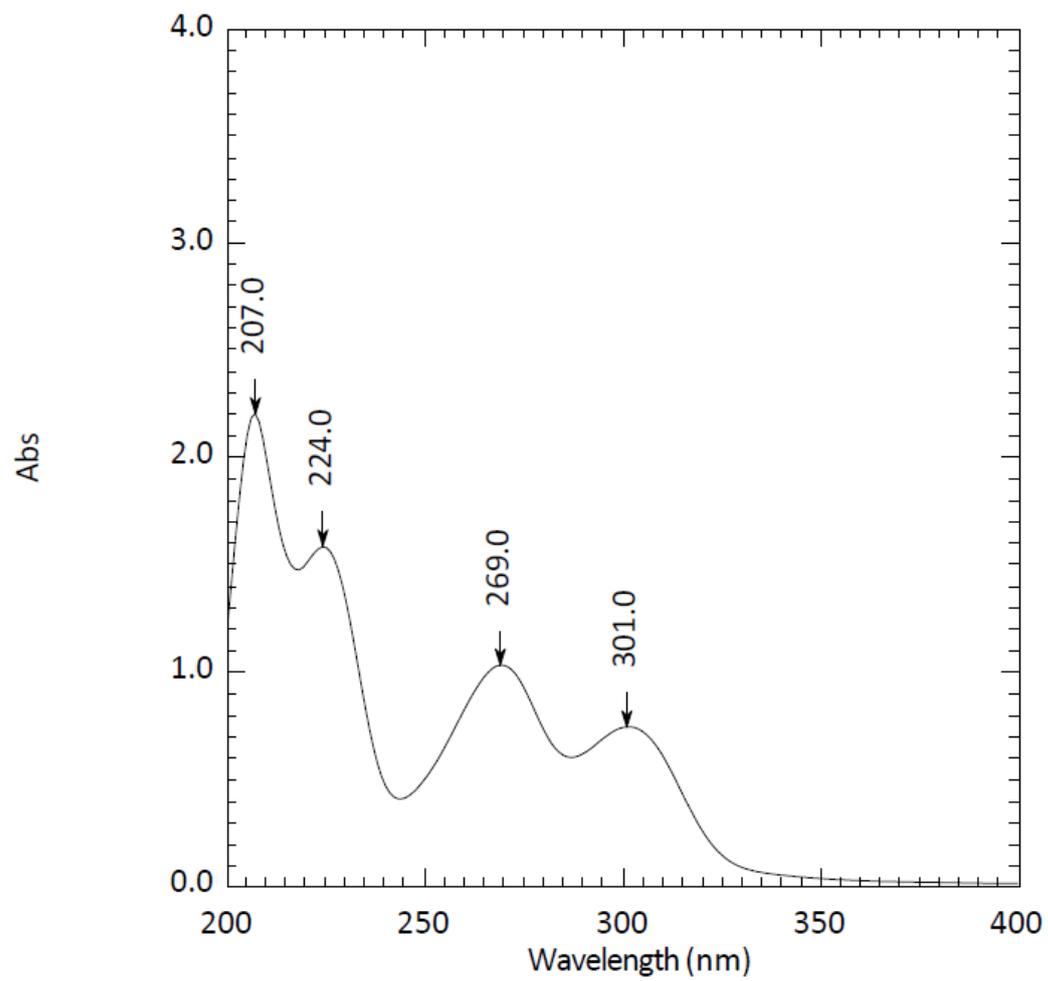


Figure S47. UV spectrum of compound **3**

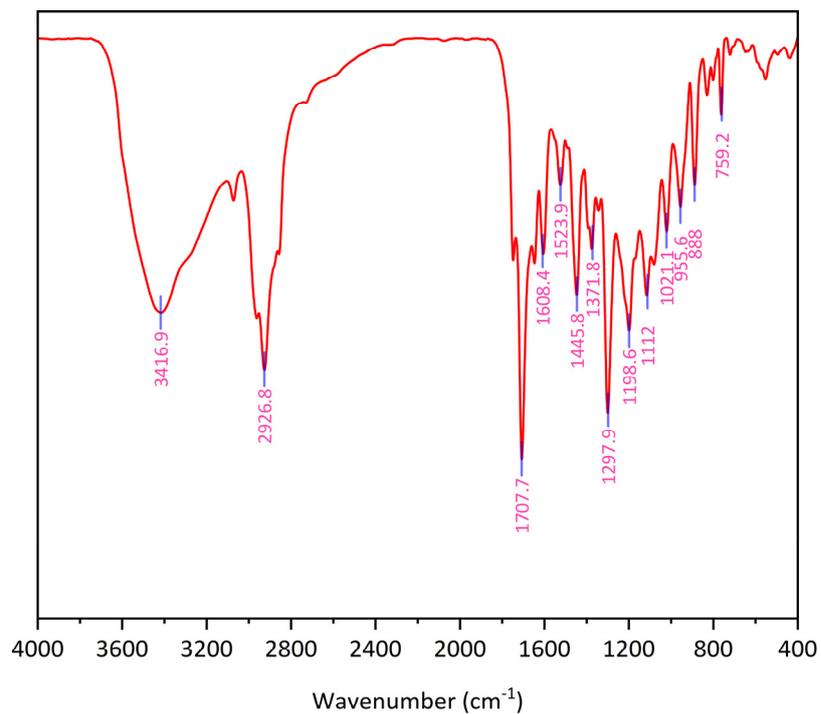


Figure S48. IR spectrum of compound 3

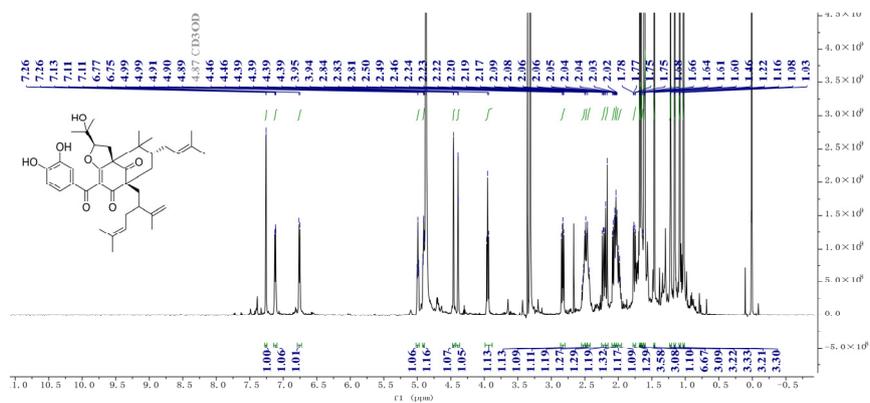


Figure S49. <sup>1</sup>H NMR spectrum of compound 4 (recorded in MeOH-*d*<sub>4</sub>)

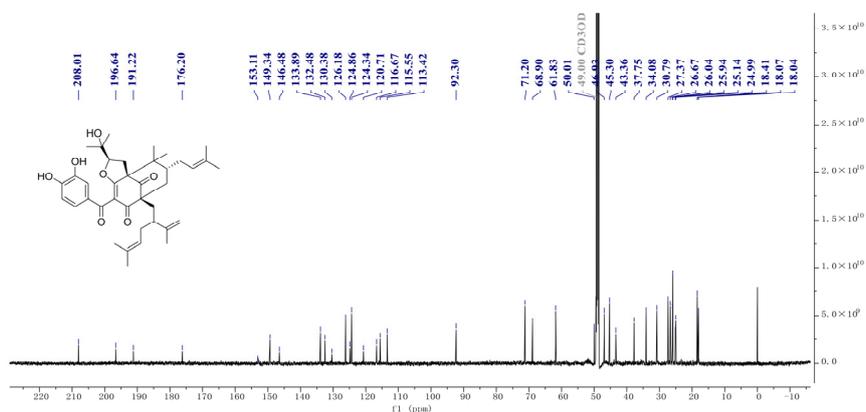


Figure S50.  $^{13}\text{C}$  NMR spectrum of compound **4** (recorded in  $\text{MeOH-}d_4$ )

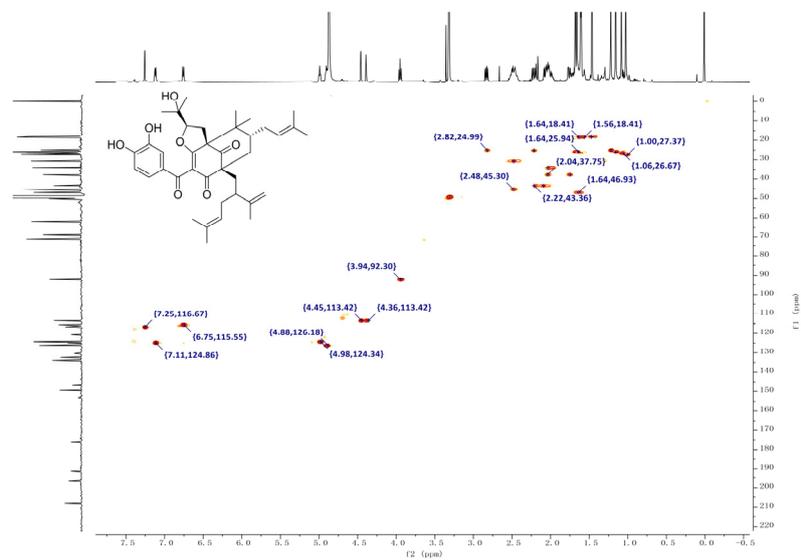


Figure S51. HSQC spectrum of compound **4** (recorded in  $\text{MeOH-}d_4$ )

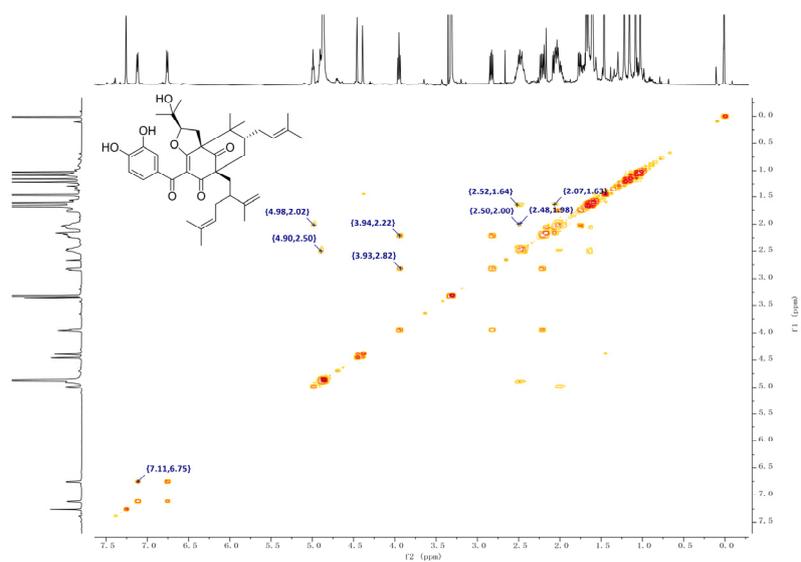


Figure S52.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4** (recorded in  $\text{MeOH-}d_4$ )

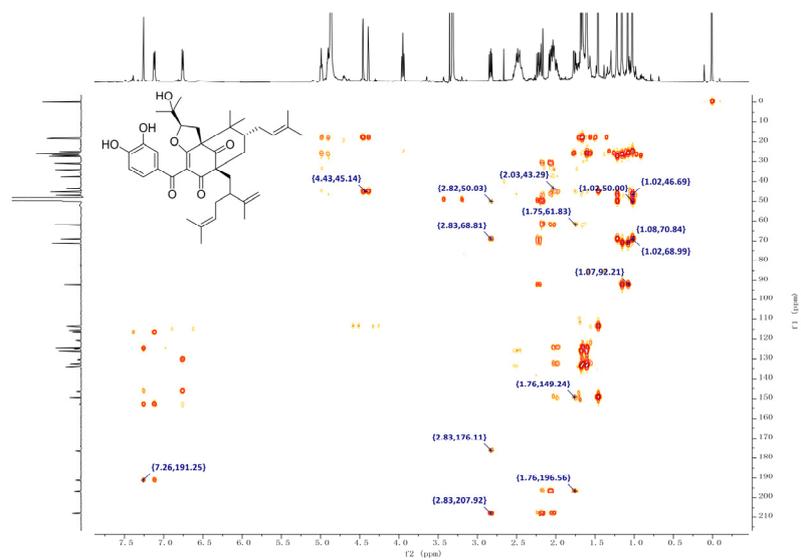


Figure S53. HMBC spectrum of compound **4** (recorded in  $\text{MeOH-}d_4$ )

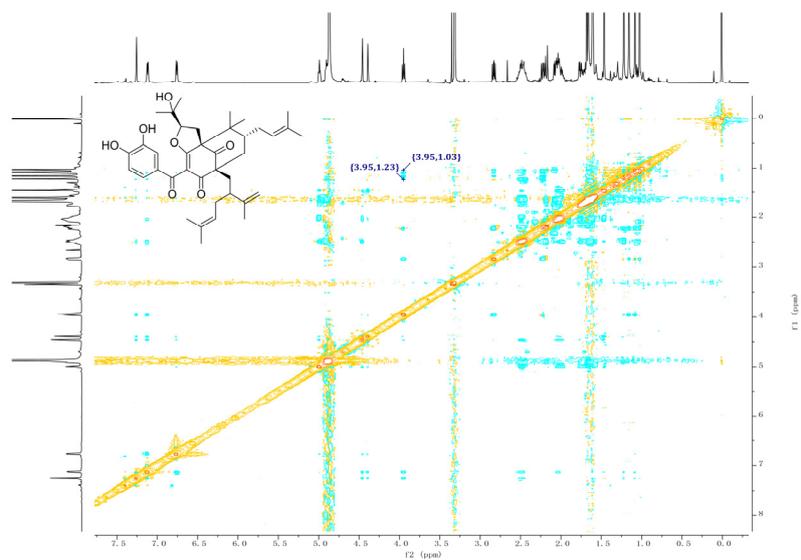


Figure S54. NOESY spectrum of compound **4** (recorded in MeOH-*d*<sub>4</sub>)

## Compound Spectrum SmartFormula Report

### Analysis Info

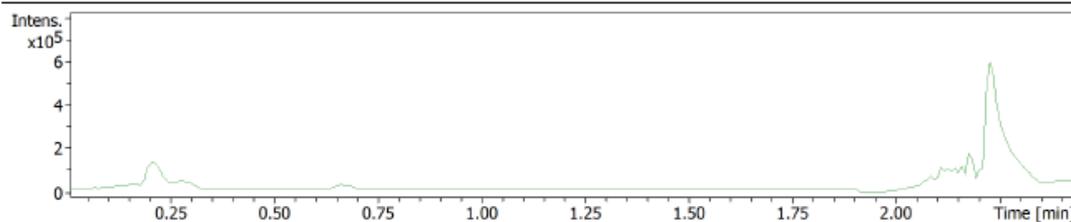
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Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH10  
Comment

Acquisition Date 7/1/2024 2:44:25 PM

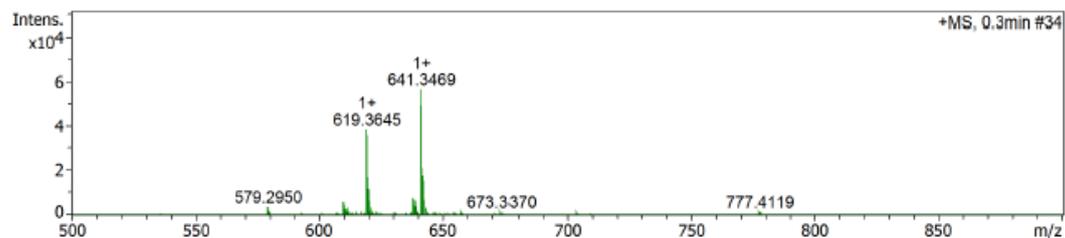
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #34



### C38H50O7, M+nNa, 641.3449

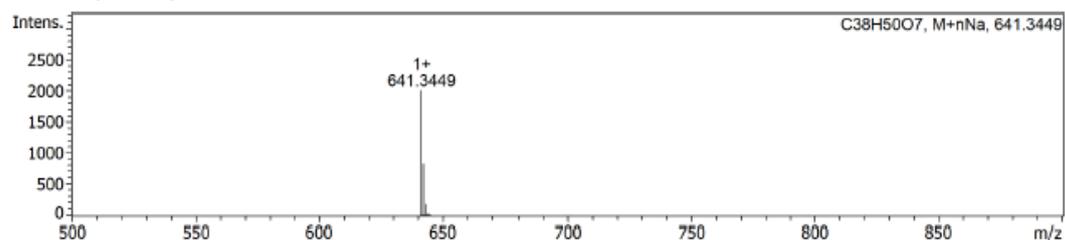


Figure S55. HRESIMS spectrum of compound 4

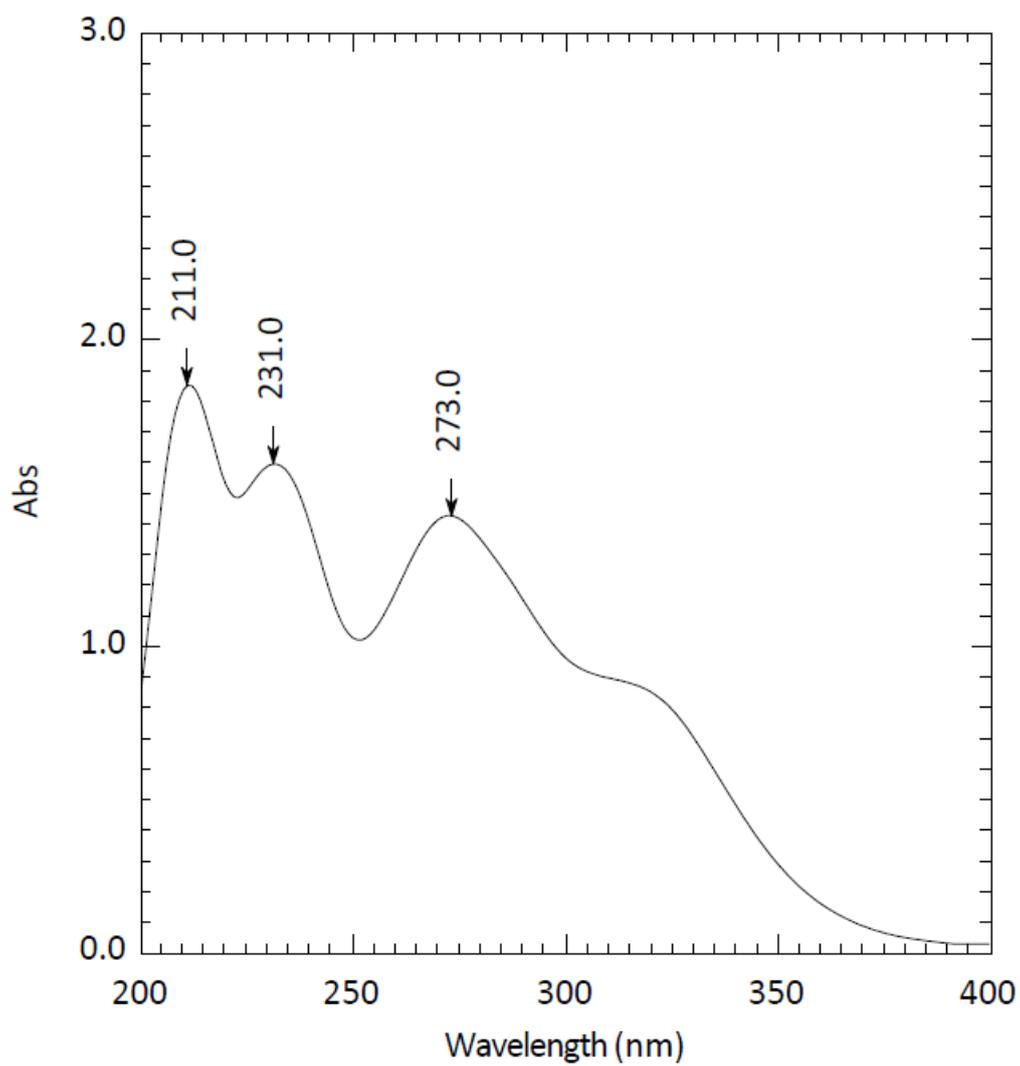


Figure S56. UV spectrum of compound 4

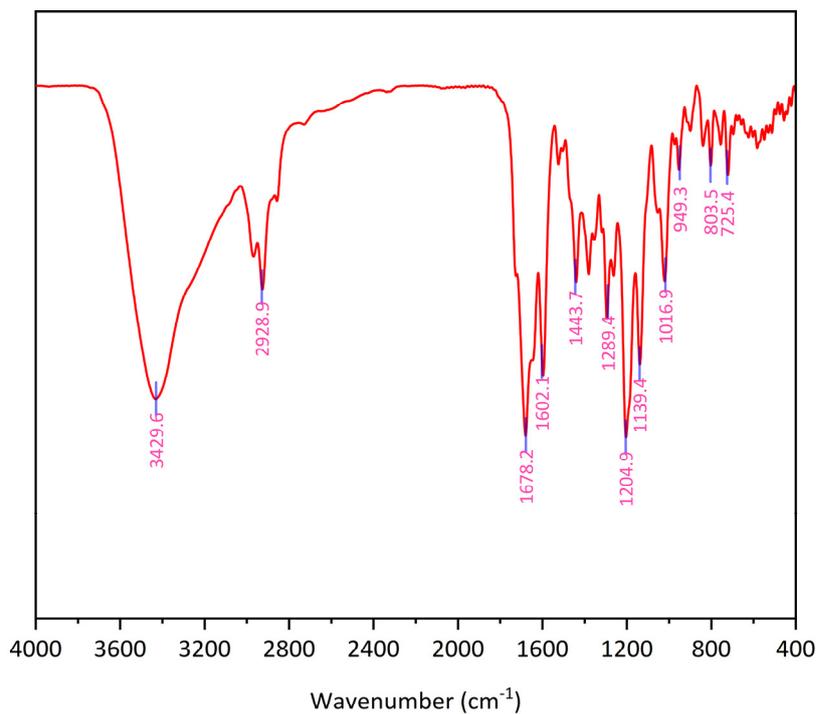


Figure S57. IR spectrum of compound 4

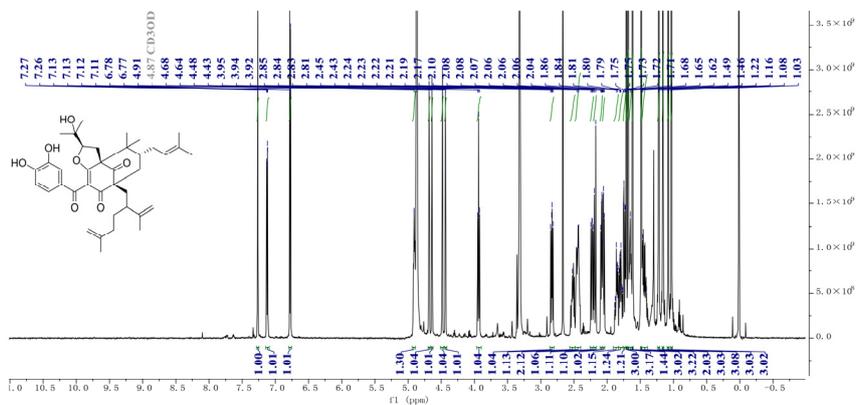


Figure S58. <sup>1</sup>H NMR spectrum of compound 5 (recorded in MeOH-d<sub>4</sub>)

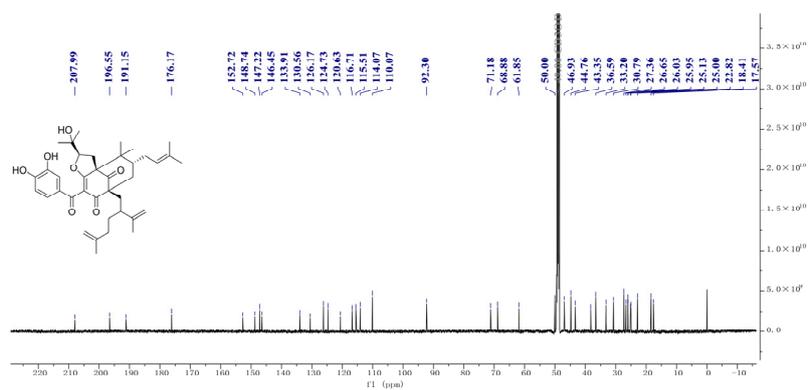


Figure S59.  $^{13}\text{C}$  NMR spectrum of compound **5** (recorded in  $\text{MeOH-}d_4$ )

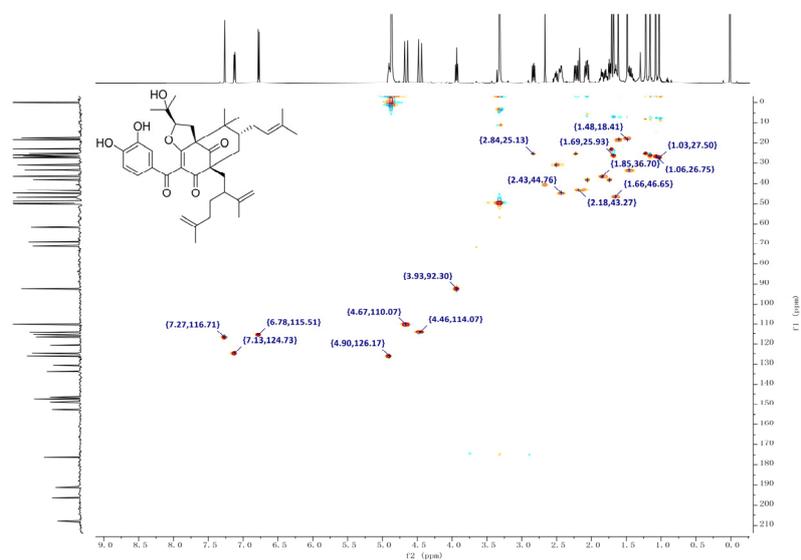


Figure S60. HSQC spectrum of compound **5** (recorded in  $\text{MeOH-}d_4$ )

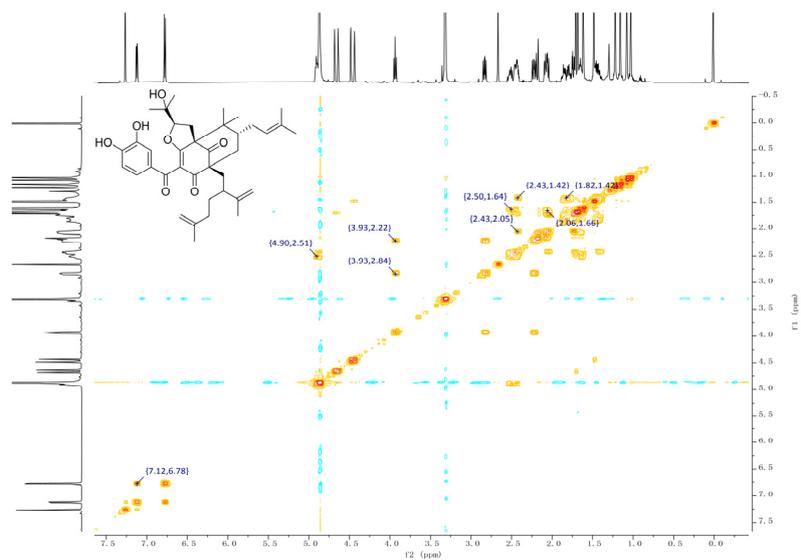


Figure S61.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **5** (recorded in  $\text{MeOH-}d_4$ )

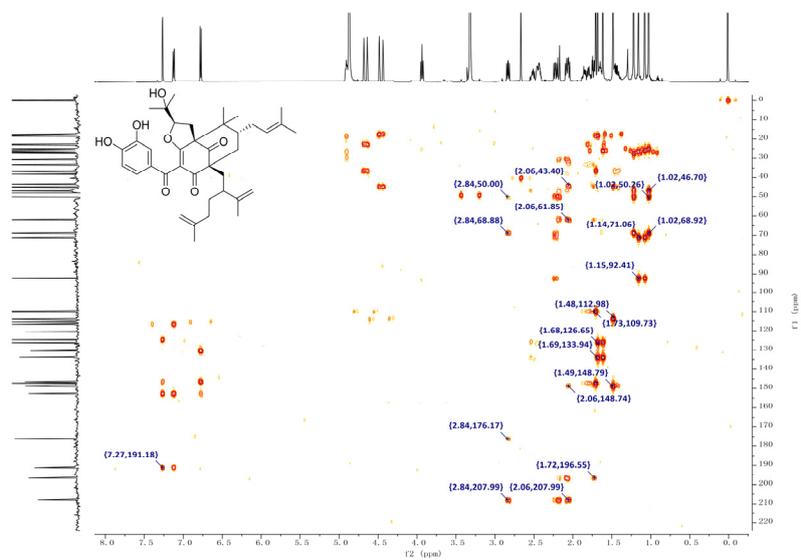


Figure S62. HMBC spectrum of compound **5** (recorded in  $\text{MeOH-}d_4$ )

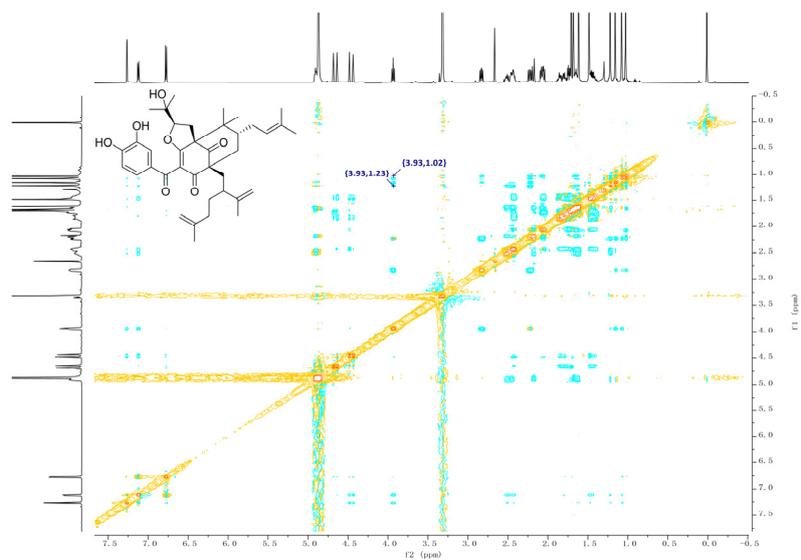


Figure S63. NOESY spectrum of compound **5** (recorded in MeOH- $d_4$ )

## Compound Spectrum SmartFormula Report

### Analysis Info

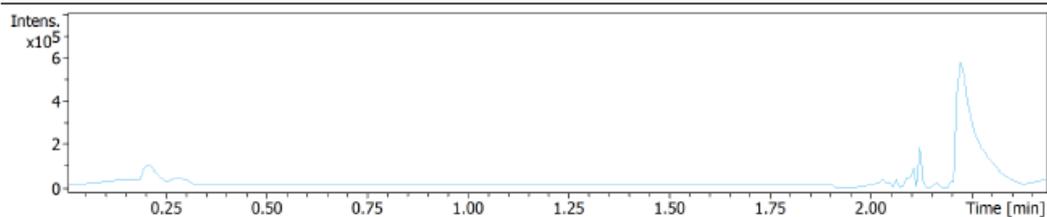
Analysis Name D:\Data\YIJR\20240701\YNTH11\_10\_1\_7037.d  
Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH11  
Comment

Acquisition Date 7/1/2024 2:47:28 PM

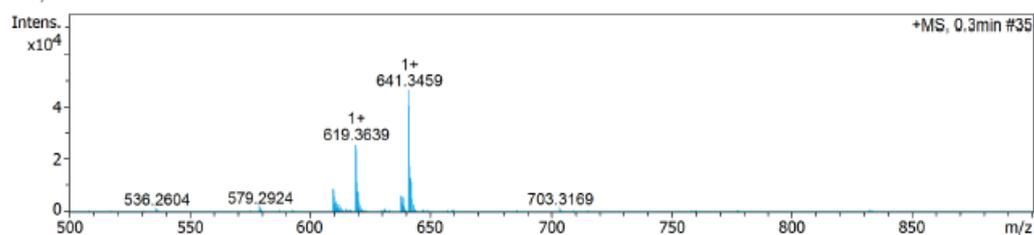
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #35



### C38H50O7, M+nNa, 641.3449

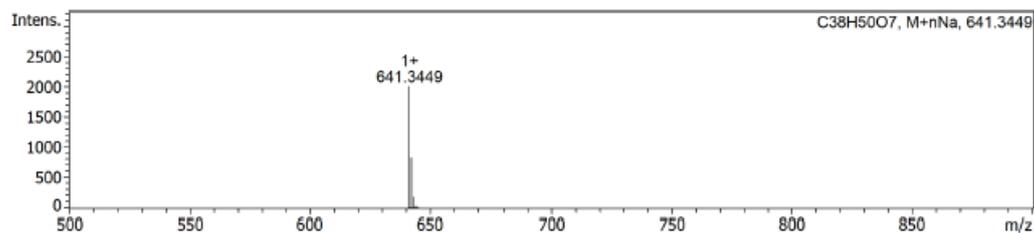


Figure S64. HRESIMS spectrum of compound 5

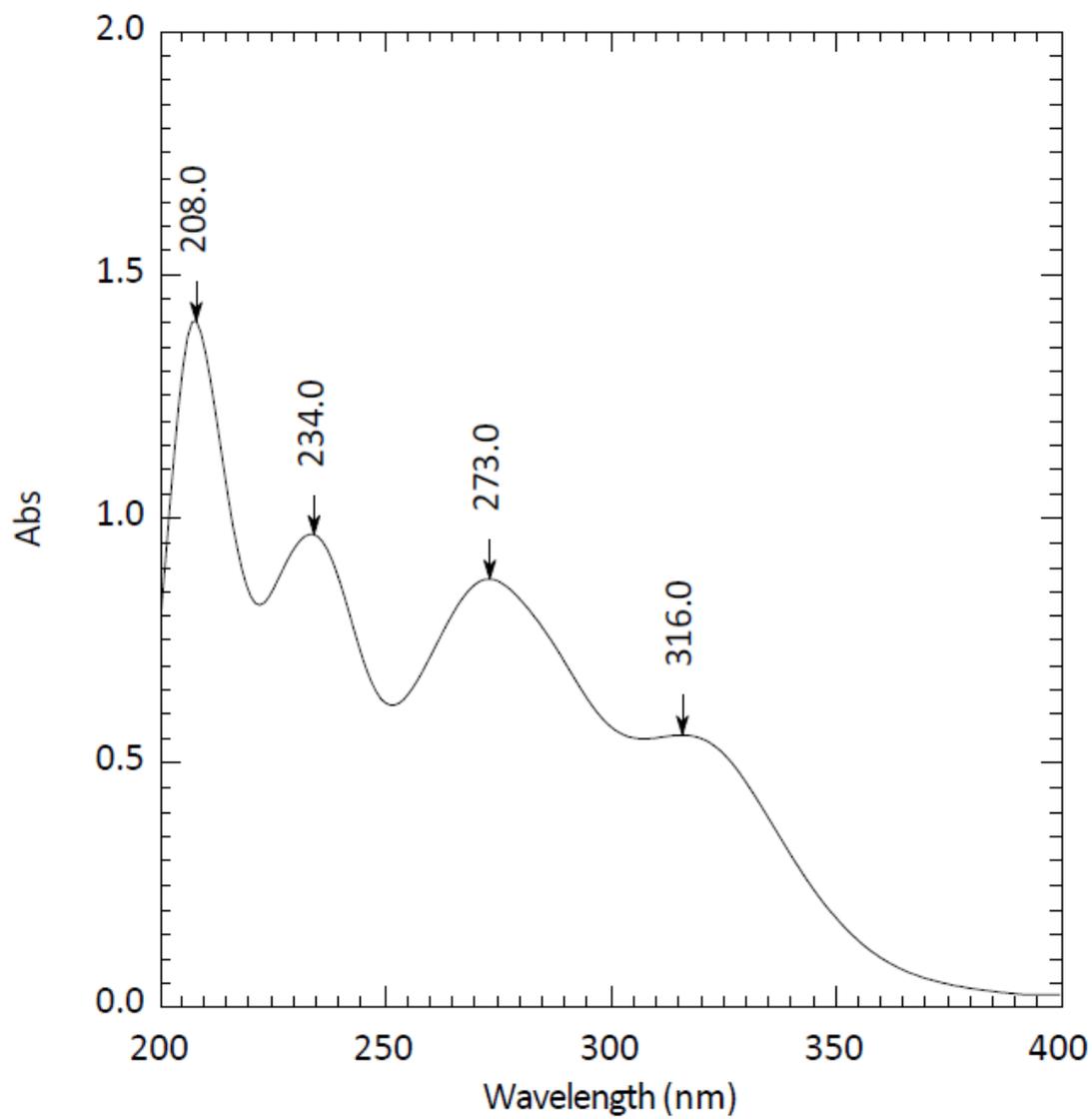


Figure S65. UV spectrum of compound 5

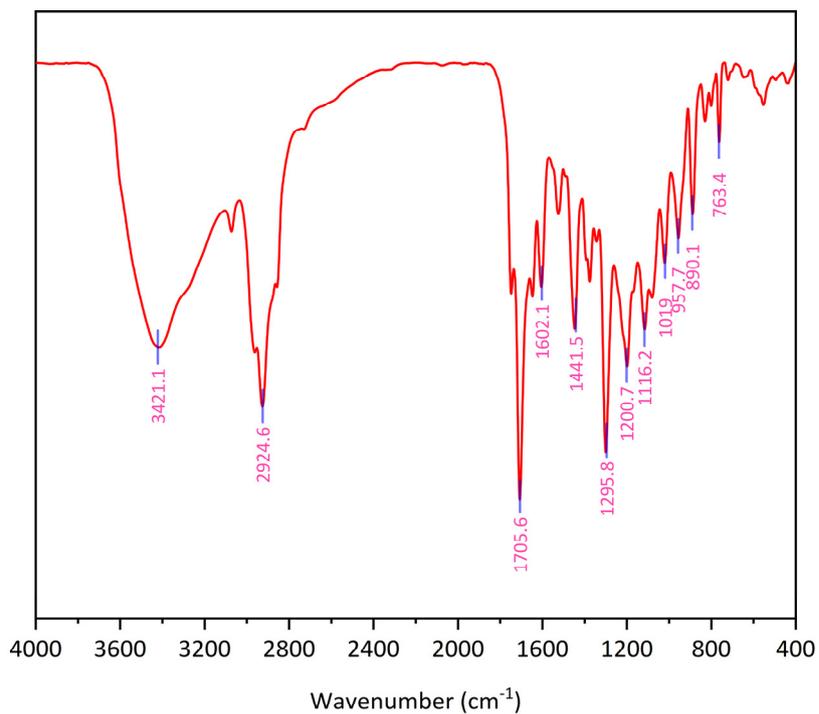


Figure S66. IR spectrum of compound 5

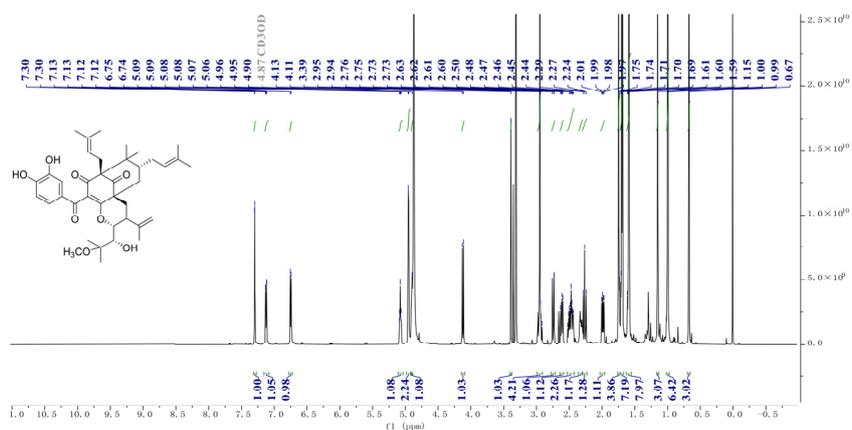


Figure S67. <sup>1</sup>H NMR spectrum of compound 6 (recorded in MeOH-d<sub>4</sub>)

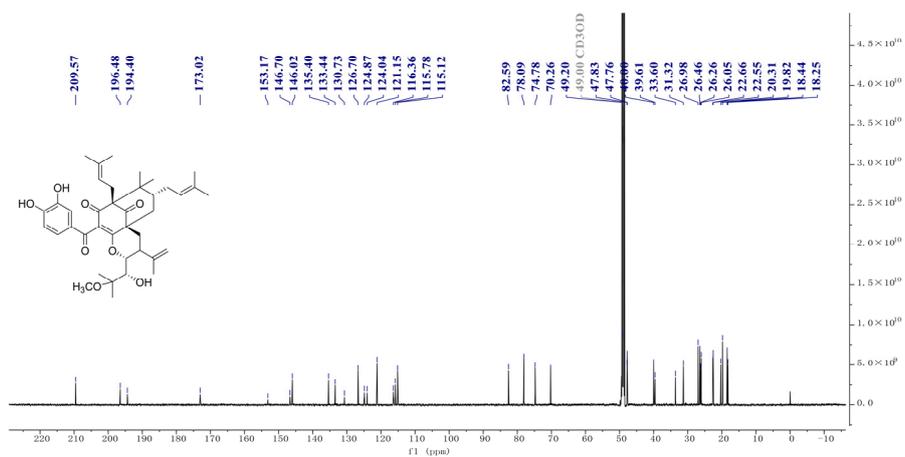


Figure S68.  $^{13}\text{C}$  NMR spectrum of compound 6 (recorded in  $\text{MeOH-}d_4$ )

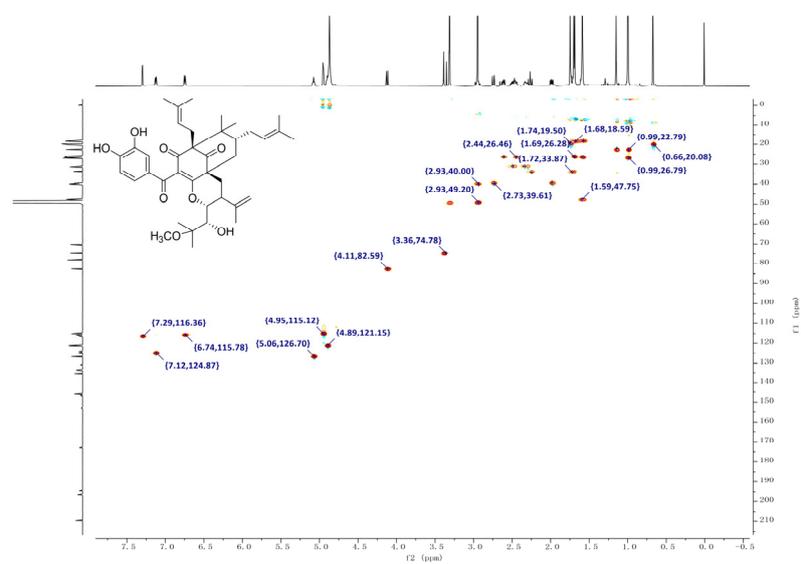


Figure S69. HSQC spectrum of compound 6 (recorded in  $\text{MeOH-}d_4$ )

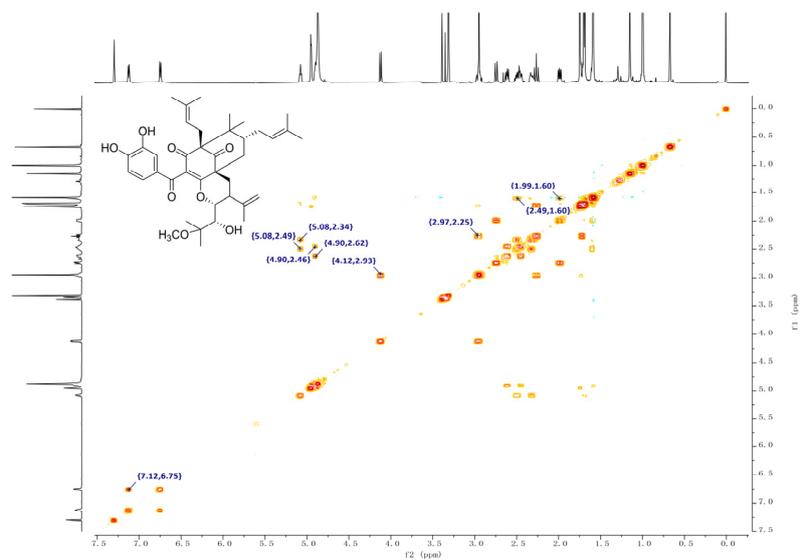


Figure S70.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **6** (recorded in  $\text{MeOH-}d_4$ )

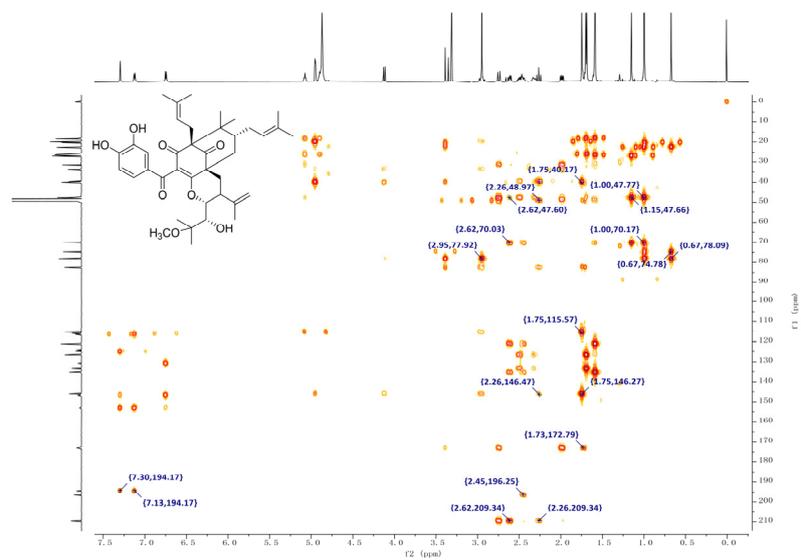


Figure S71. HMBC spectrum of compound **6** (recorded in  $\text{MeOH-}d_4$ )

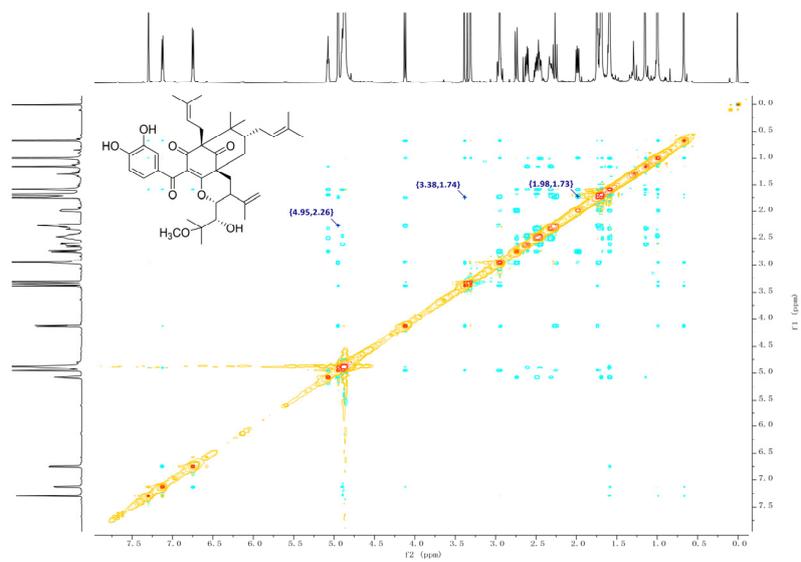


Figure S72. NOESY spectrum of compound **6** (recorded in MeOH-*d*<sub>4</sub>)

## Compound Spectrum SmartFormula Report

### Analysis Info

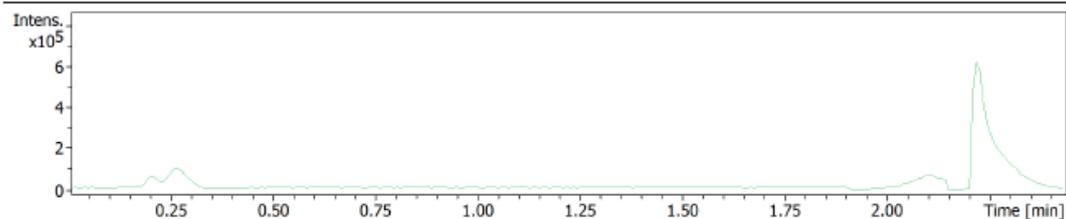
Analysis Name D:\Data\YJ\20240701\YNTH2\_2\_1\_7029.d  
Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH2  
Comment

Acquisition Date 7/1/2024 2:22:49 PM

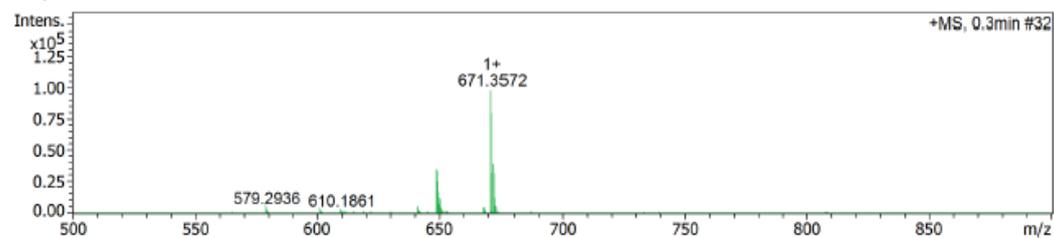
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #32



### C39H52O8, M+nNa, 671.3554

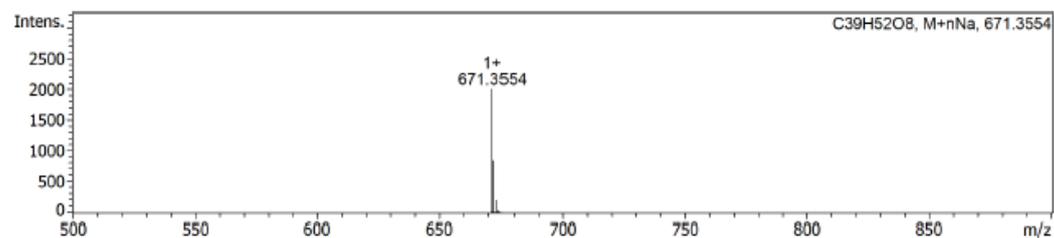


Figure S73. HRESIMS spectrum of compound 6

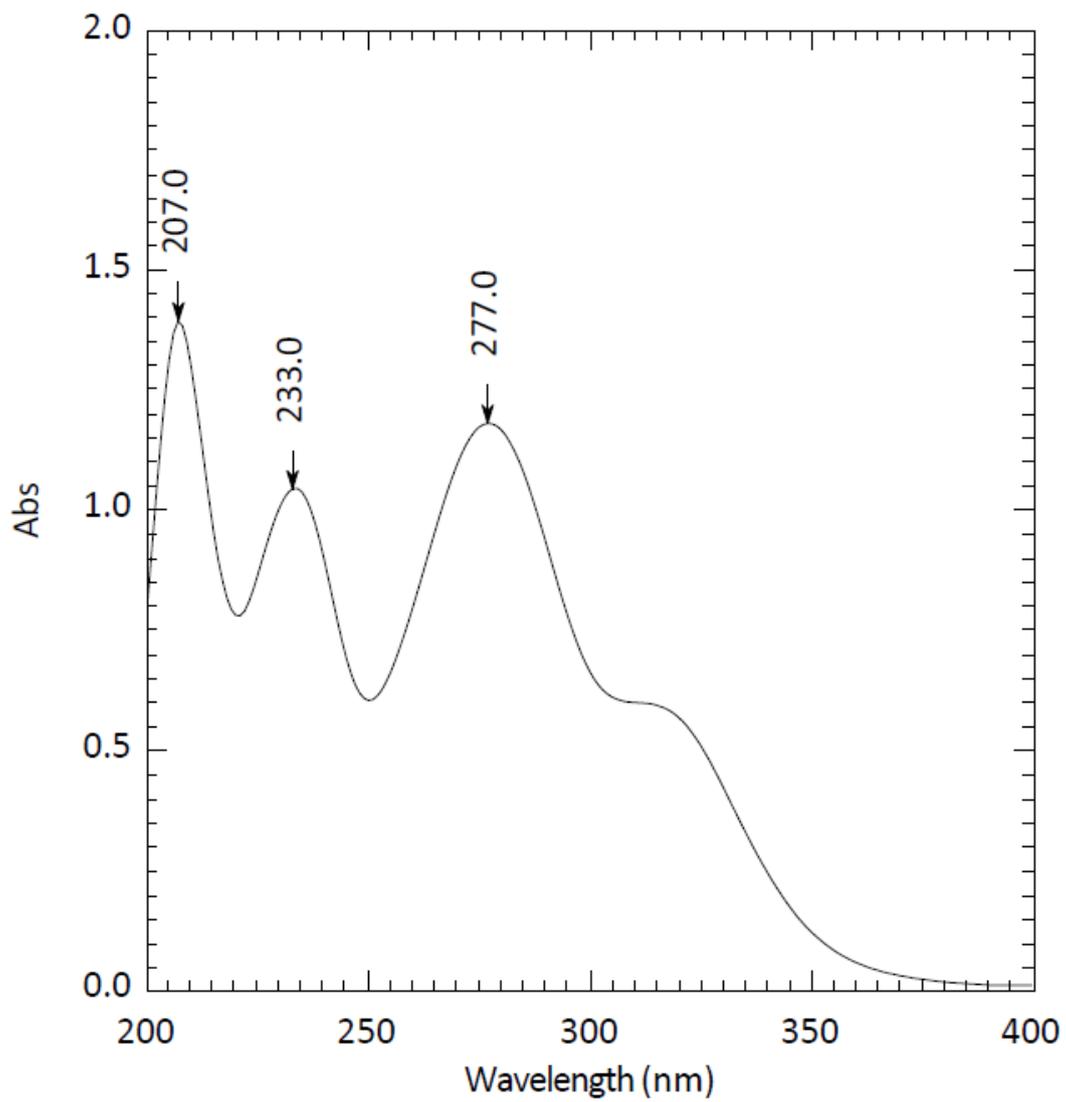


Figure S74. UV spectrum of compound 6



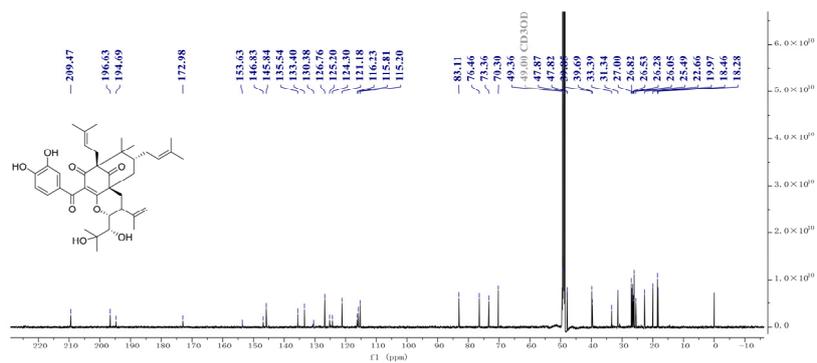


Figure S77.  $^{13}\text{C}$  NMR spectrum of compound 7 (recorded in  $\text{MeOH-}d_4$ )

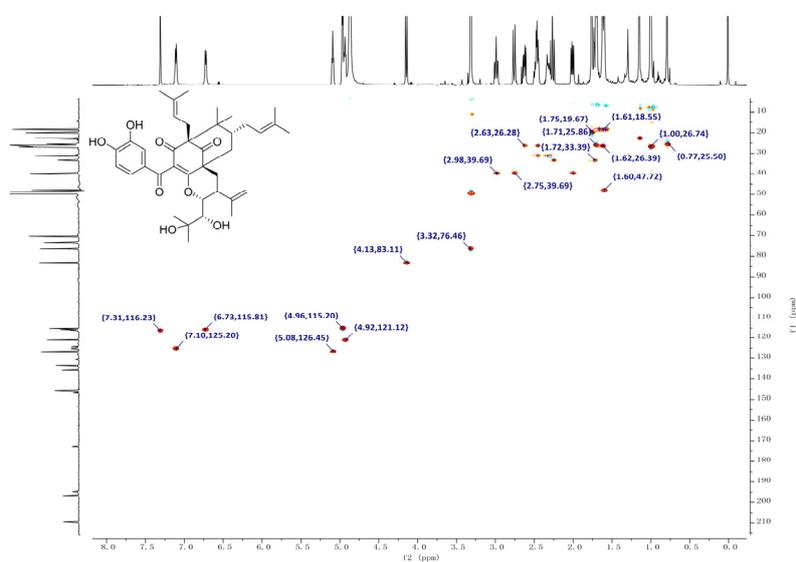


Figure S78.  $^1\text{H}/^{13}\text{C}$  HSQC spectrum of compound 7 (recorded in  $\text{MeOH-}d_4$ )

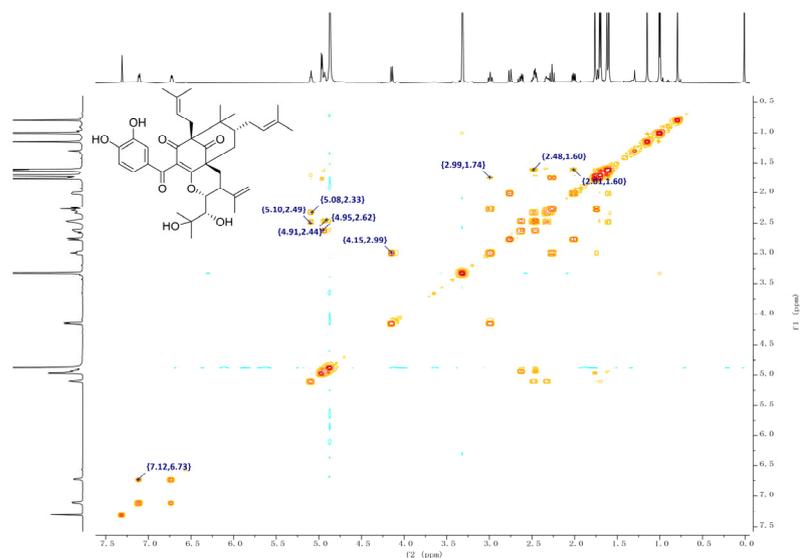


Figure S79.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7** (recorded in  $\text{MeOH-}d_4$ )

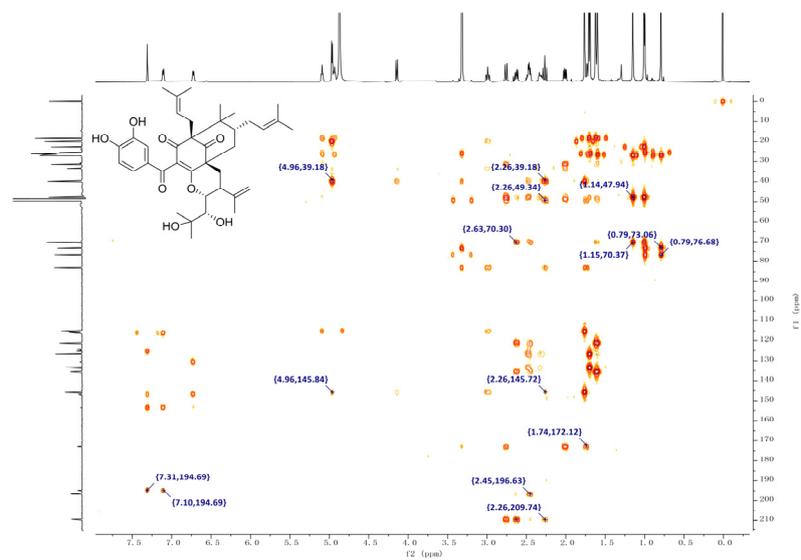


Figure S80. HMBC spectrum of compound **7** (recorded in  $\text{MeOH-}d_4$ )

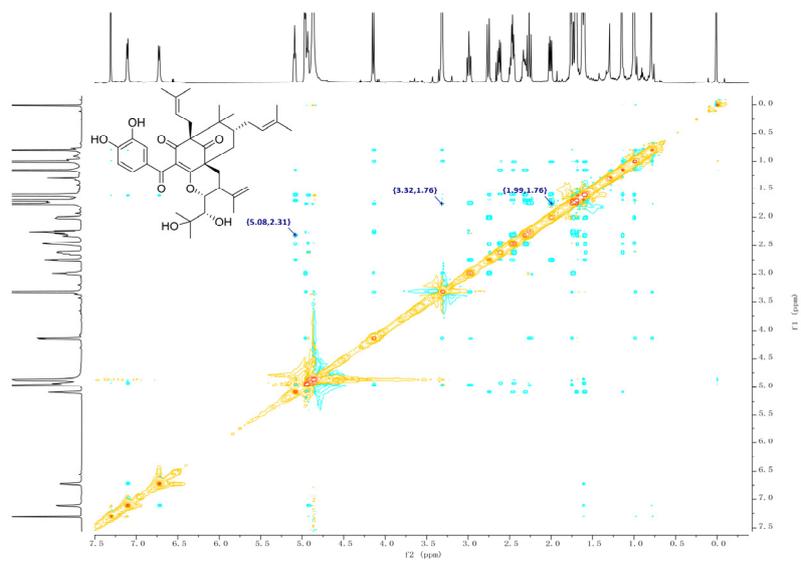


Figure S81. NOESY spectrum of compound **7** (recorded in MeOH-*d*<sub>4</sub>)

## Compound Spectrum SmartFormula Report

### Analysis Info

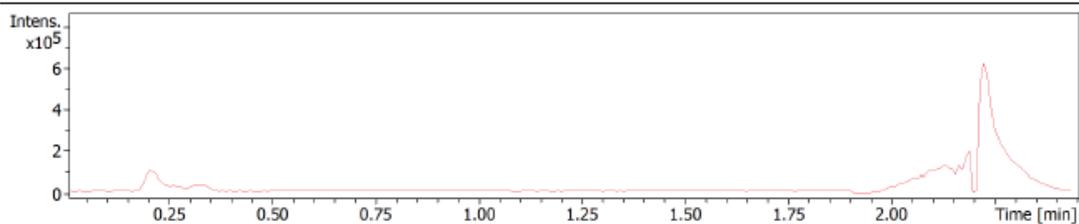
Analysis Name D:\Data\YIJ\20240701\YNTH1\_1\_1\_7028.d  
Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH1  
Comment

Acquisition Date 7/1/2024 2:19:44 PM

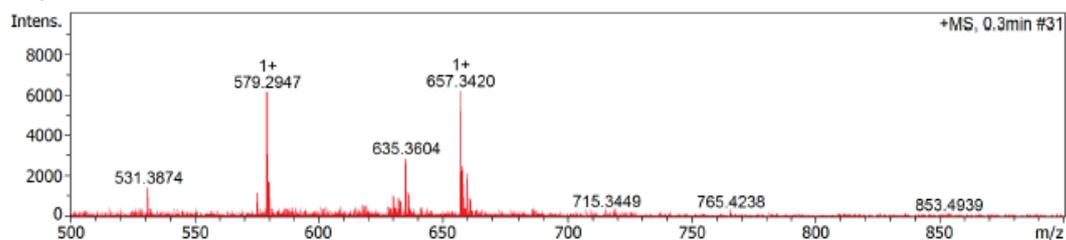
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #31



### C38H50O8, M+nNa, 657.3398

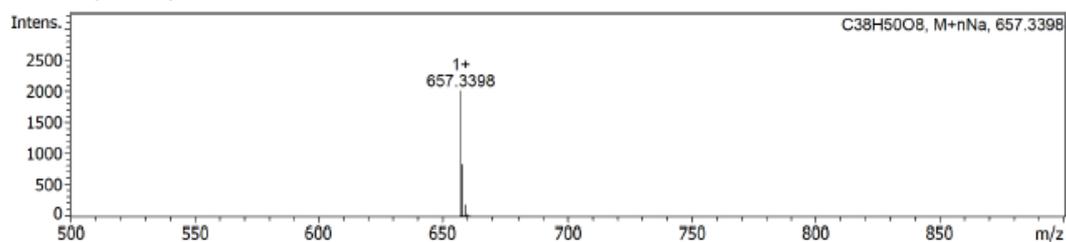


Figure S82. HRESIMS spectrum of compound 7

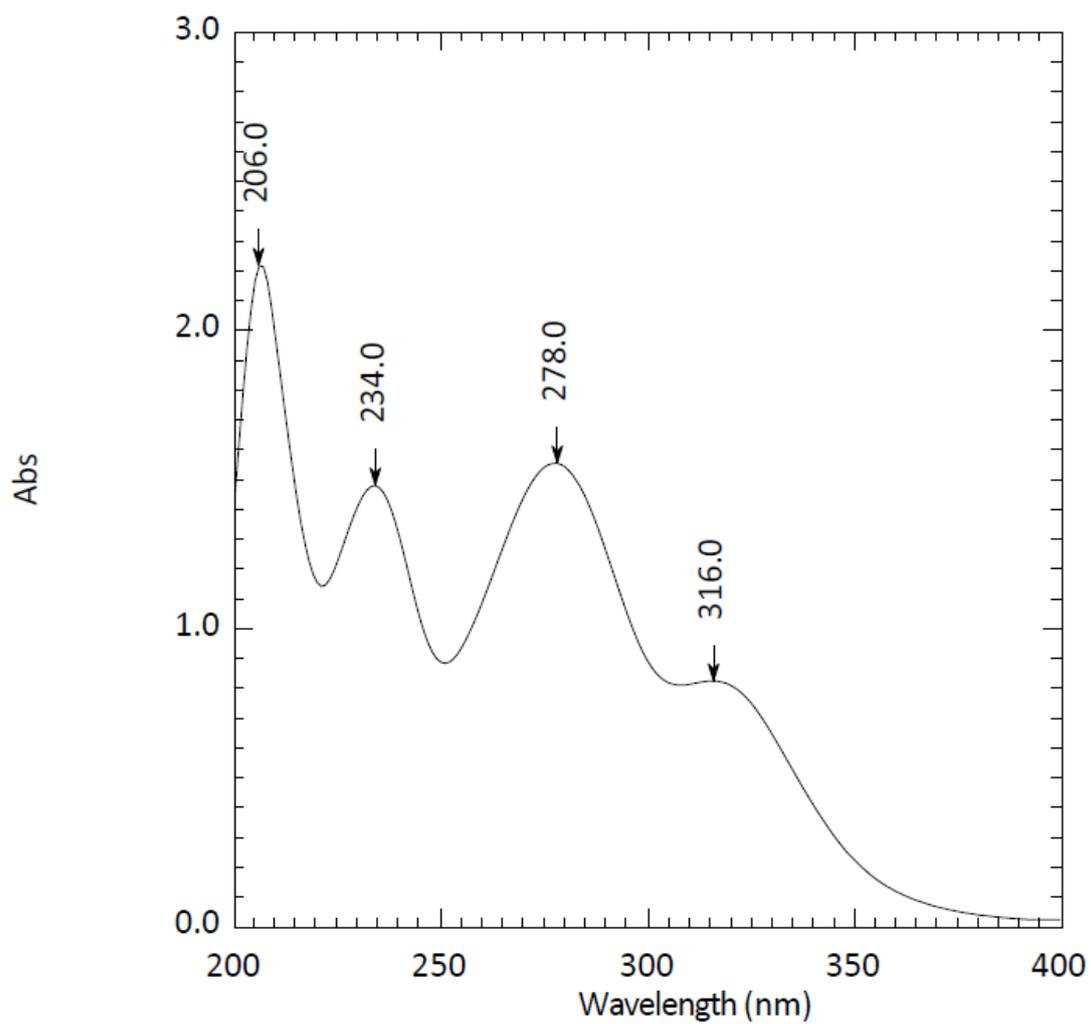


Figure S83. UV spectrum of compound 7

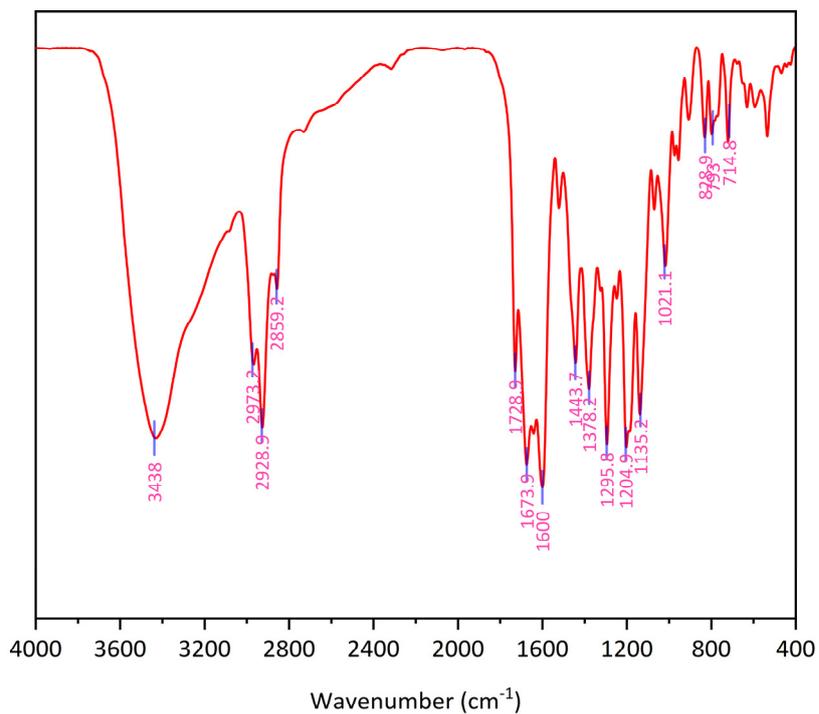


Figure S84. IR spectrum of compound 7

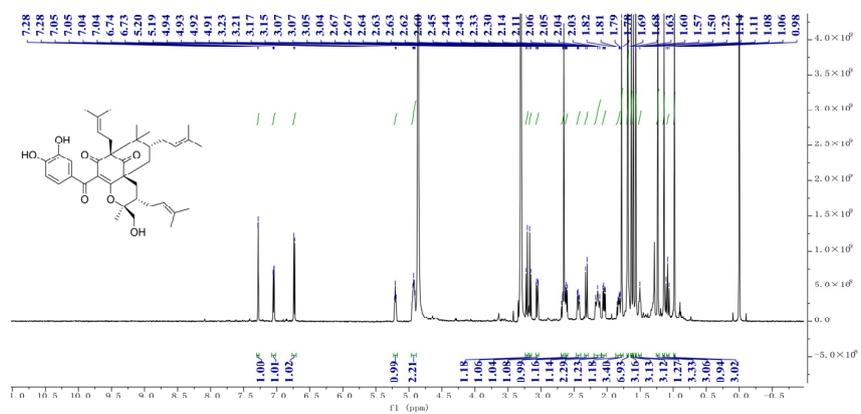


Figure S85. <sup>1</sup>H NMR spectrum of compound 8 (recorded in MeOH-*d*<sub>4</sub>)

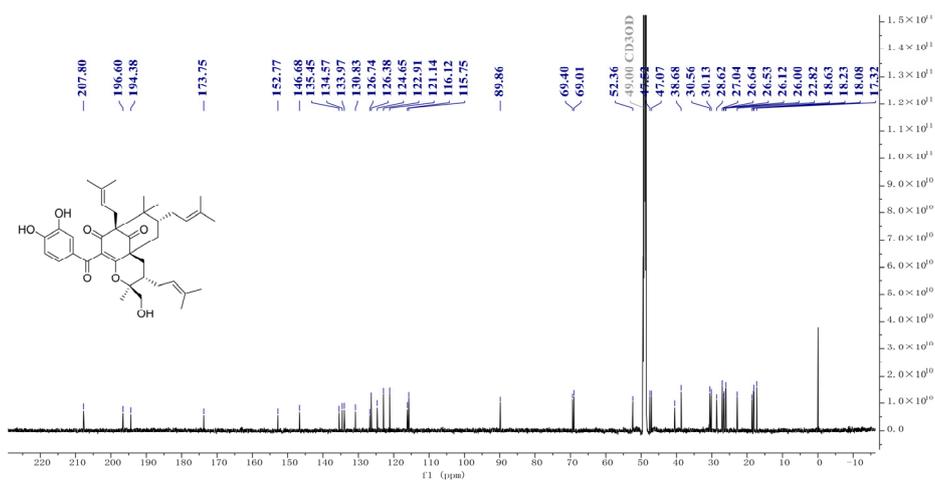


Figure S86.  $^{13}\text{C}$  NMR spectrum of compound **8** (recorded in  $\text{MeOH-}d_4$ )

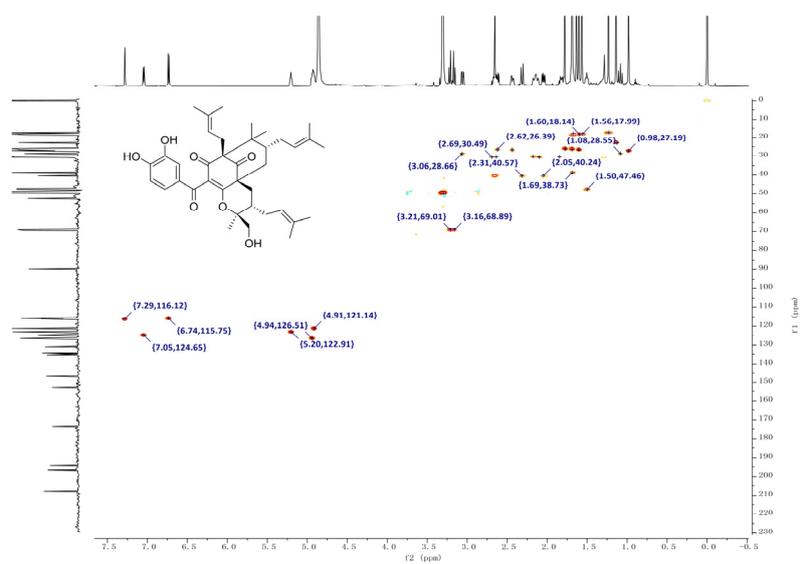


Figure S87. HSQC spectrum of compound **8** (recorded in  $\text{MeOH-}d_4$ )

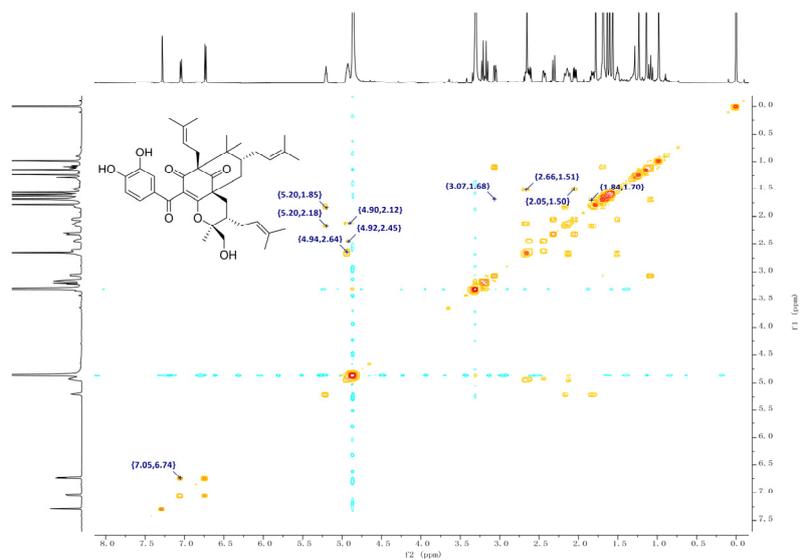


Figure S88.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **8** (recorded in  $\text{MeOH-}d_4$ )

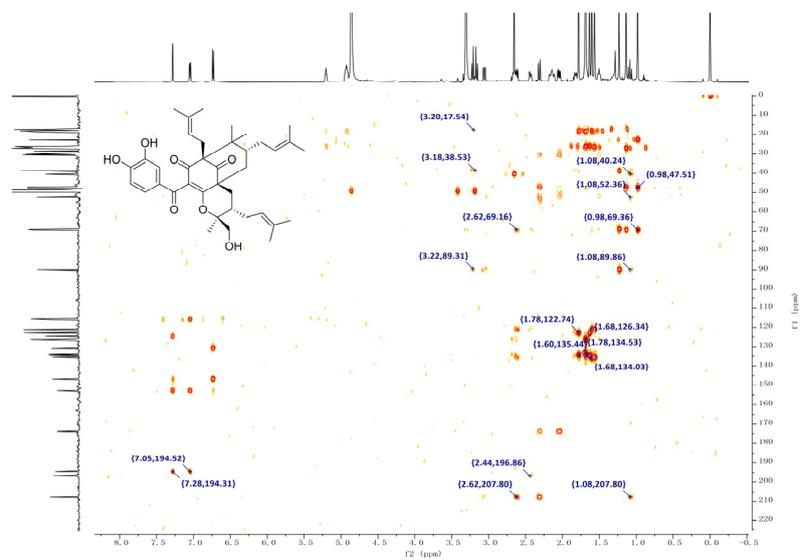


Figure S89. HMBC spectrum of compound **8** (recorded in  $\text{MeOH-}d_4$ )

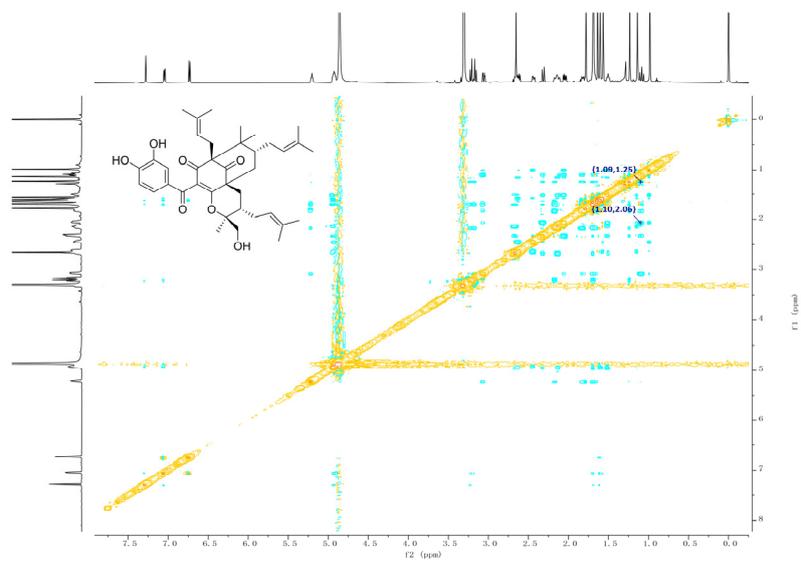


Figure S90. NOESY spectrum of compound **8** (recorded in MeOH-*d*<sub>4</sub>)

## Compound Spectrum SmartFormula Report

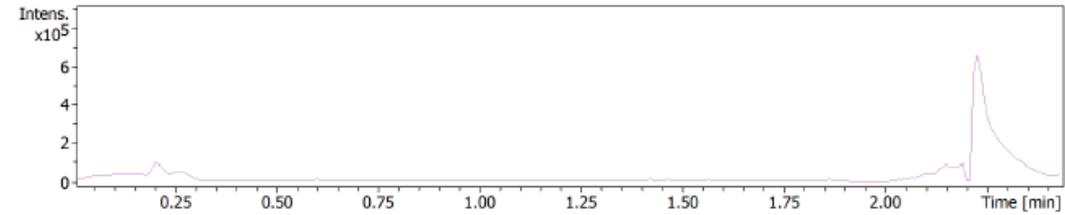
### Analysis Info

Analysis Name D:\Data\YIJ\20240701\YNTH3\_3\_1\_7030.d  
Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH3  
Comment

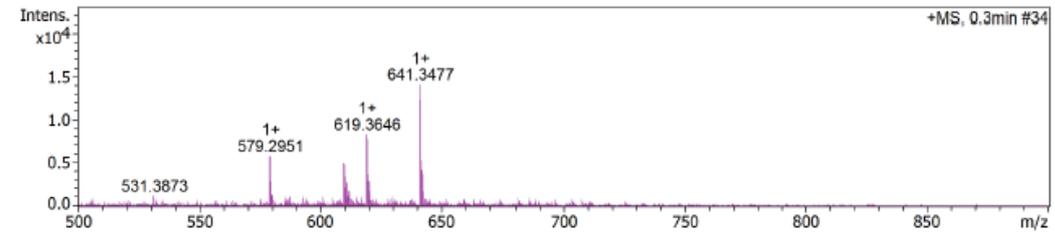
Acquisition Date 7/1/2024 2:25:55 PM  
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #34



### C38H50O7, M+nNa, 641.3449

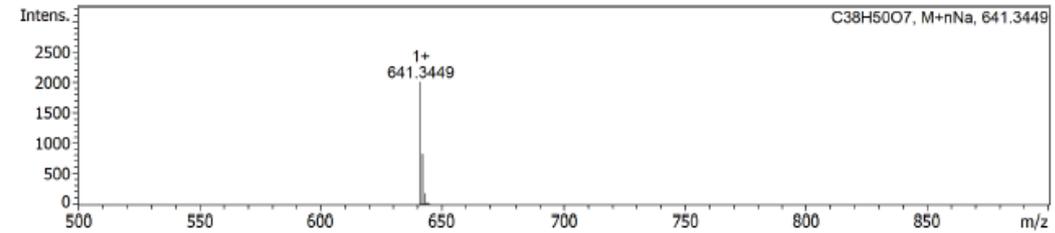


Figure S91. HRESIMS spectrum of compound **8**

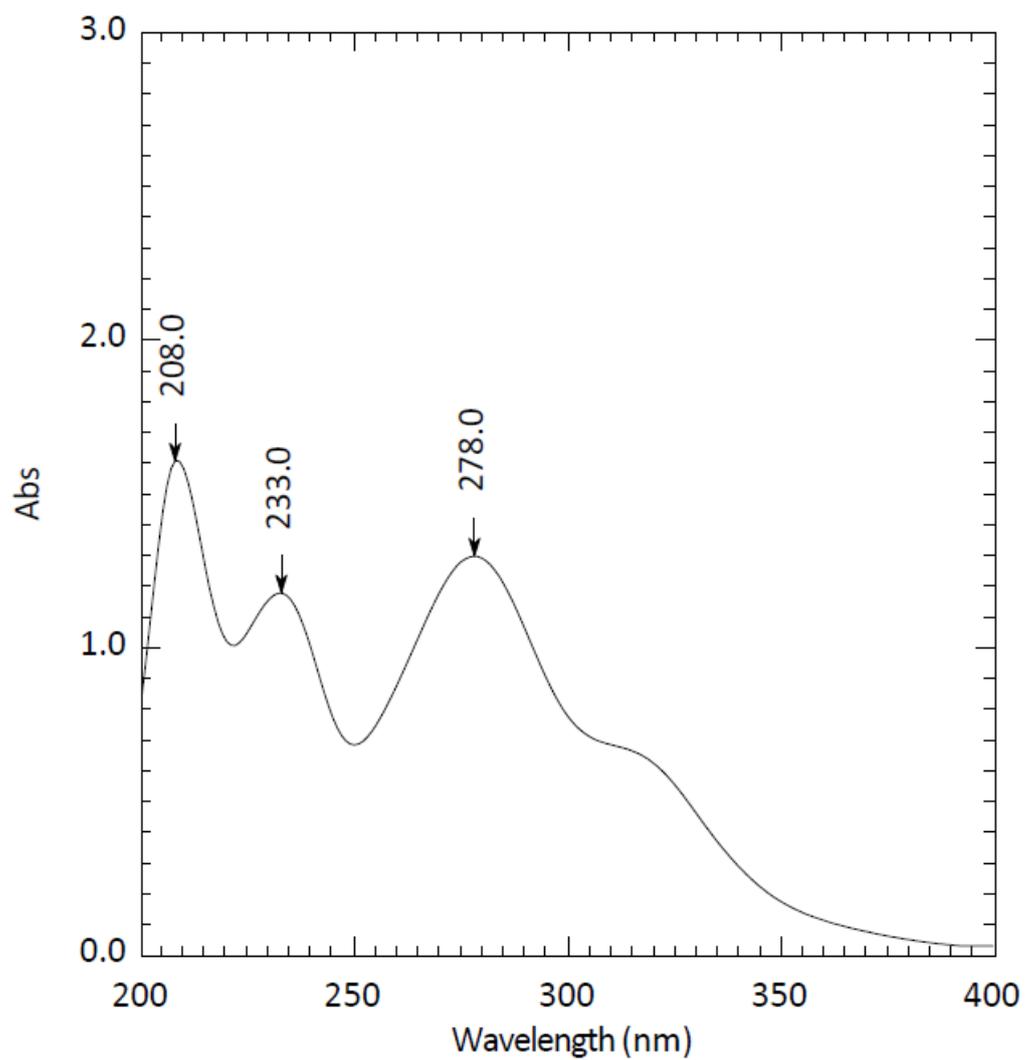


Figure S92. UV spectrum of compound **8**

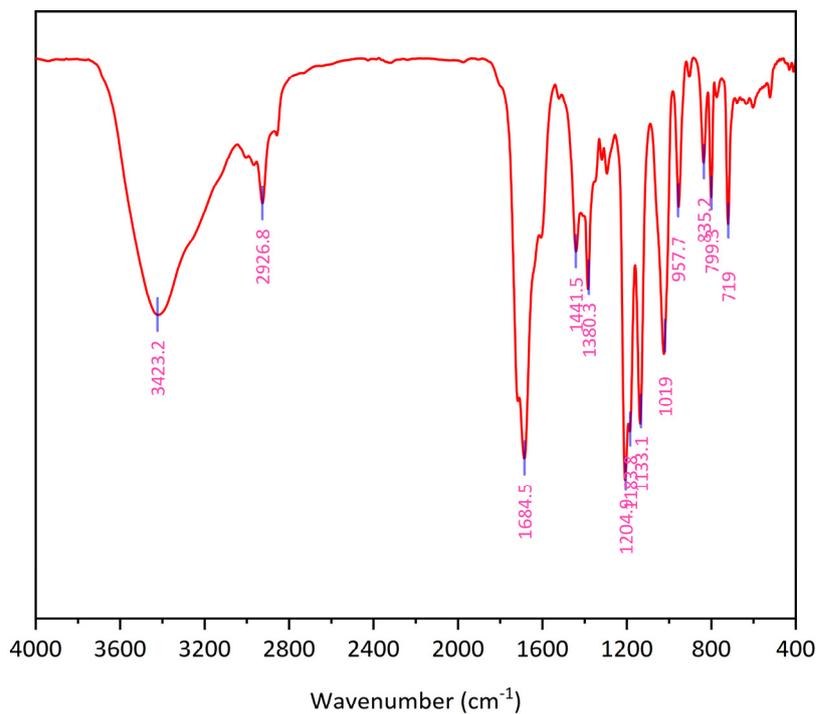


Figure S93. IR spectrum of compound **8**

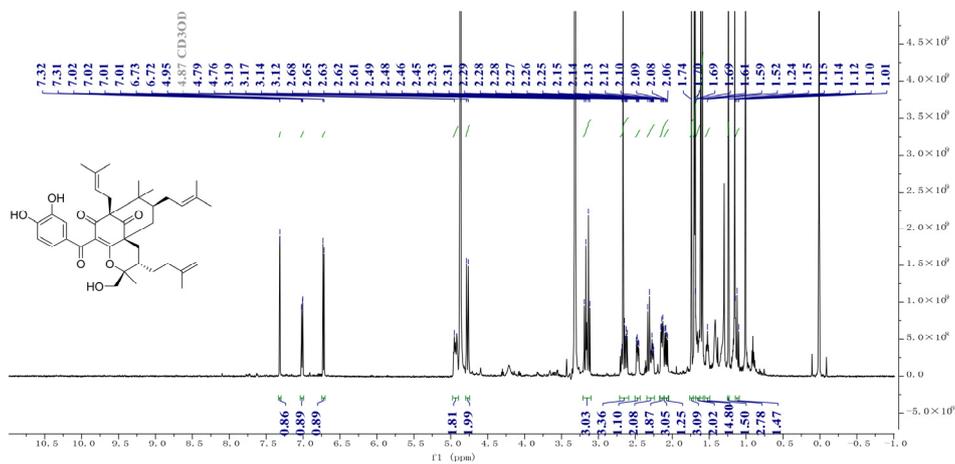


Figure S94. <sup>1</sup>H NMR spectrum of compound **9** (recorded in MeOH-*d*<sub>4</sub>)

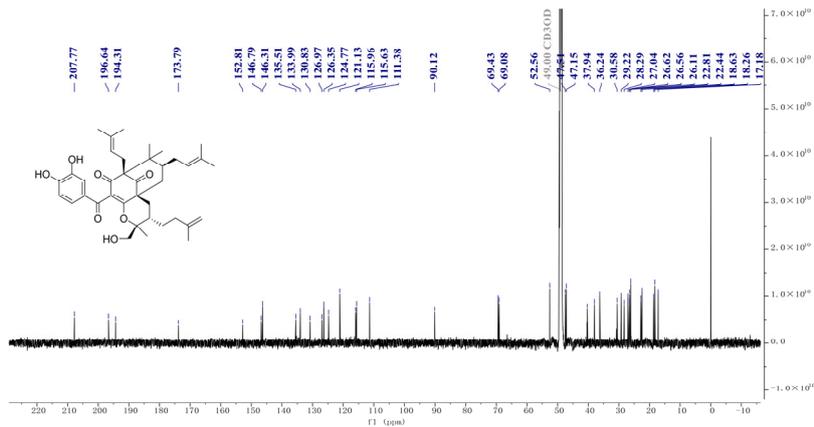


Figure S95.  $^{13}\text{C}$  NMR spectrum of compound **9** (recorded in  $\text{MeOH-}d_4$ )

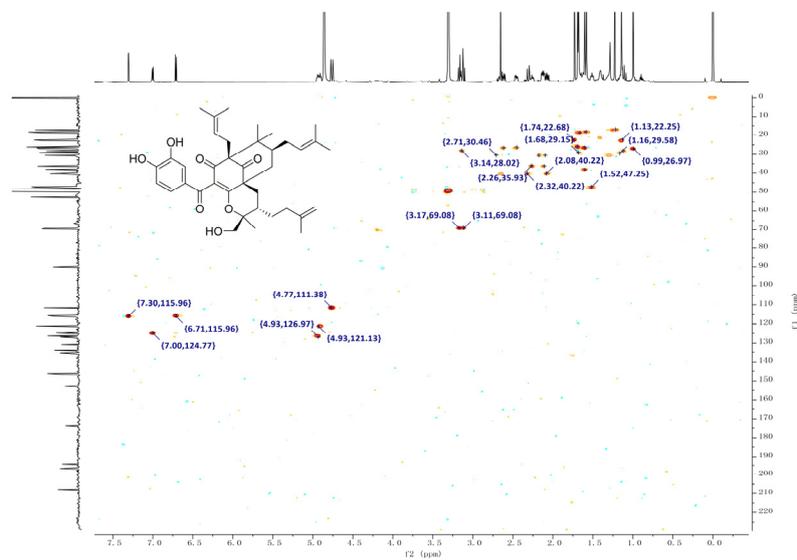


Figure S96. HSQC spectrum of compound **9** (recorded in  $\text{MeOH-}d_4$ )

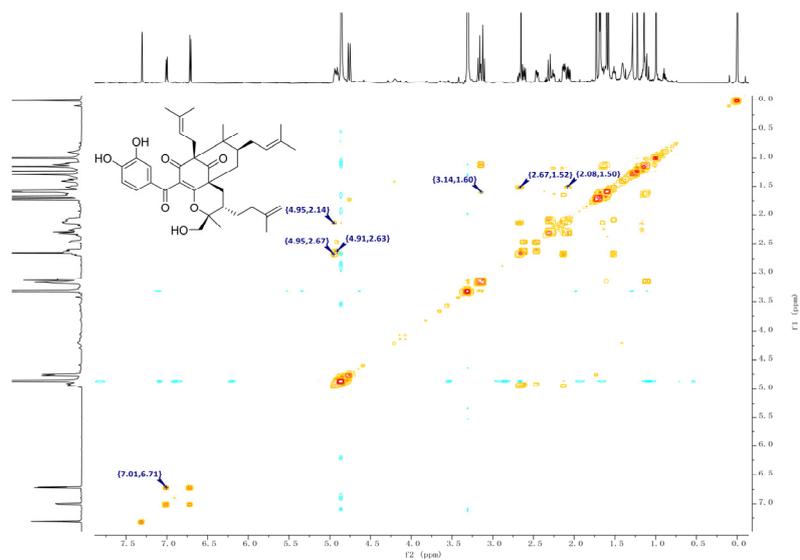


Figure S97.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **9** (recorded in  $\text{MeOH-}d_4$ )

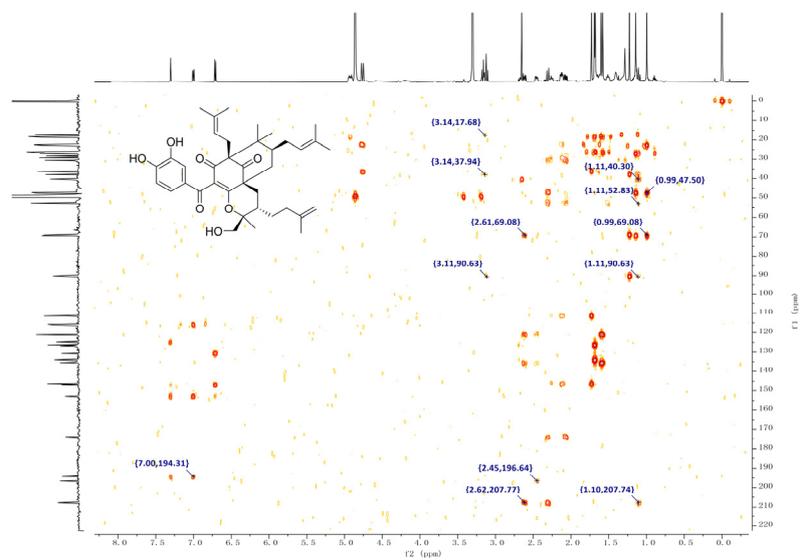


Figure S98. HMBC spectrum of compound **9** (recorded in  $\text{MeOH-}d_4$ )

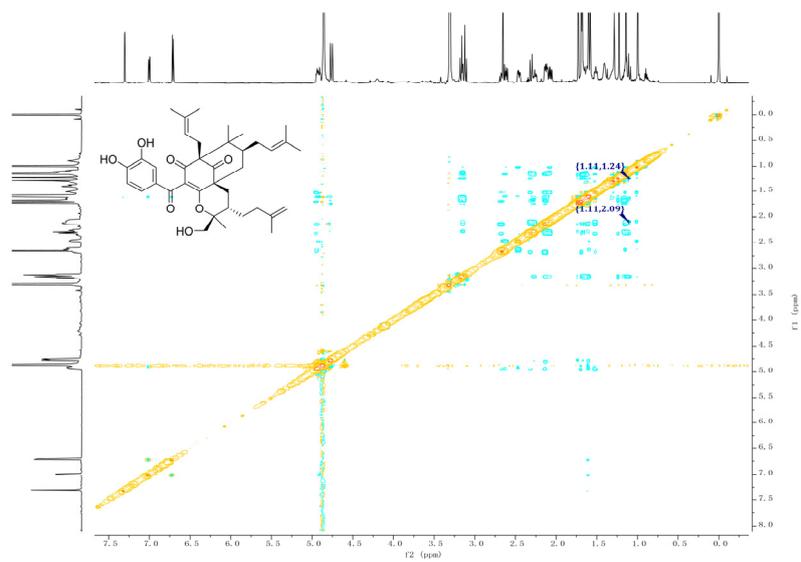


Figure S99. NOESY spectrum of compound **9** (recorded in MeOH-*d*<sub>4</sub>)

## Compound Spectrum SmartFormula Report

### Analysis Info

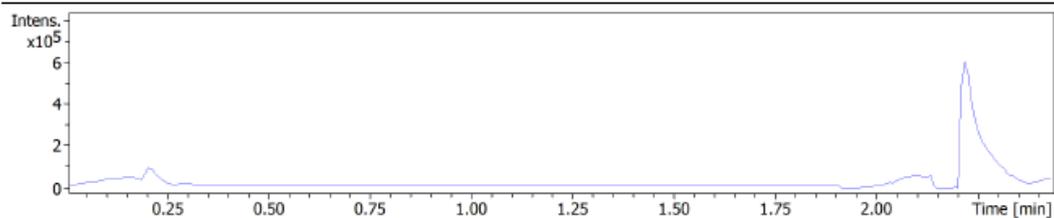
Analysis Name D:\Data\YIJR\20240701\YNTH4\_4\_1\_7031.d  
Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH4  
Comment

Acquisition Date 7/1/2024 2:28:59 PM

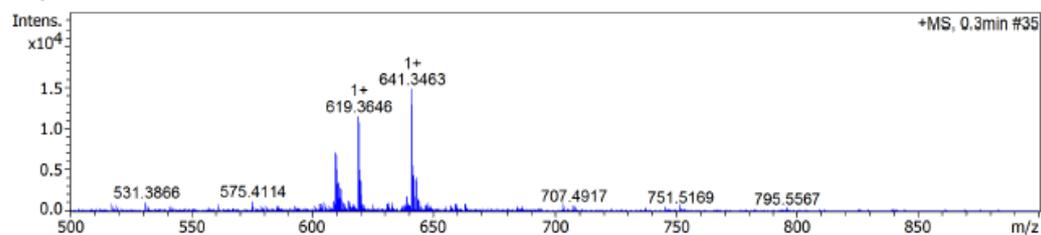
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #35



### C38H50O7, M+nNa, 641.3449

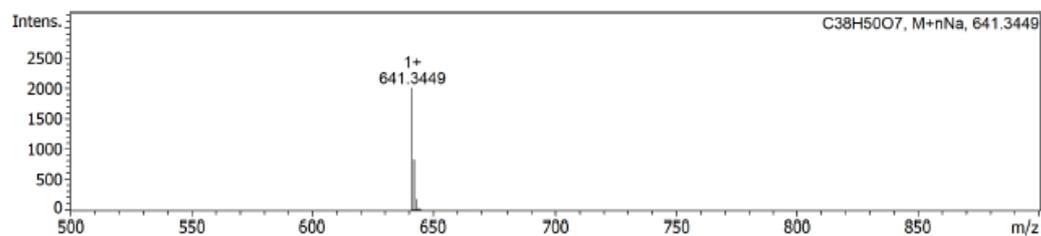


Figure S100. HRESIMS spectrum of compound 9

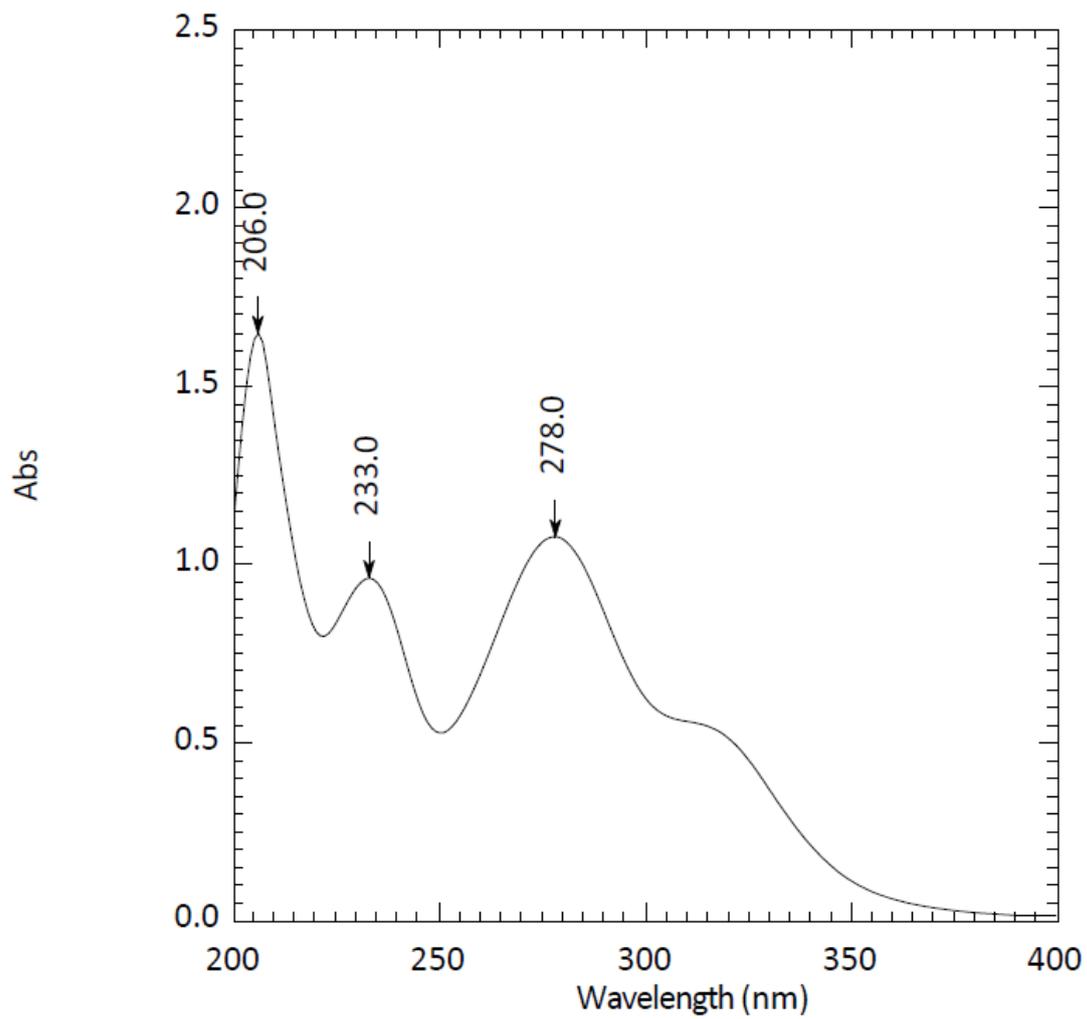


Figure S101. UV spectrum of compound 9

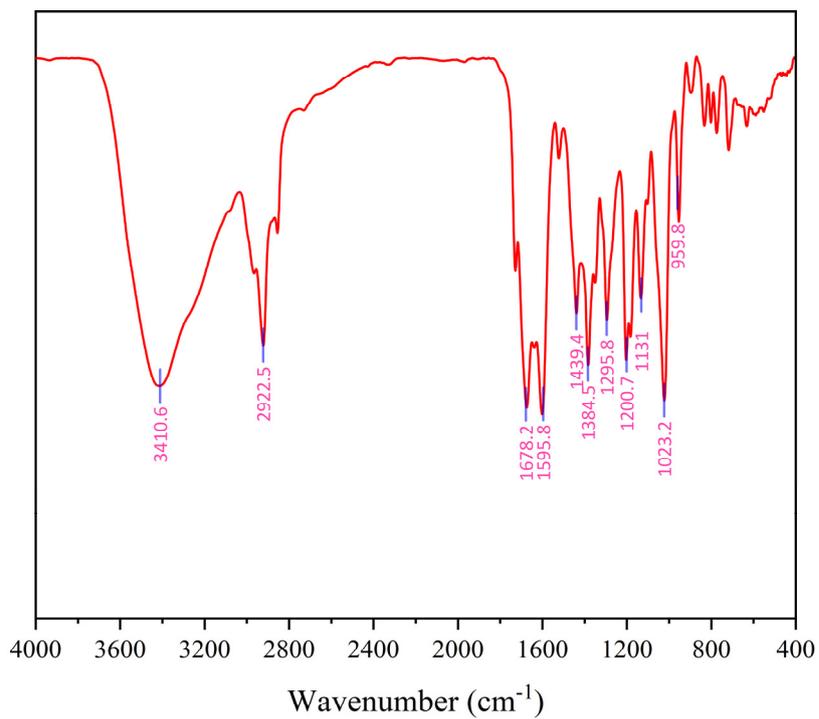


Figure S102. IR spectrum of compound 9

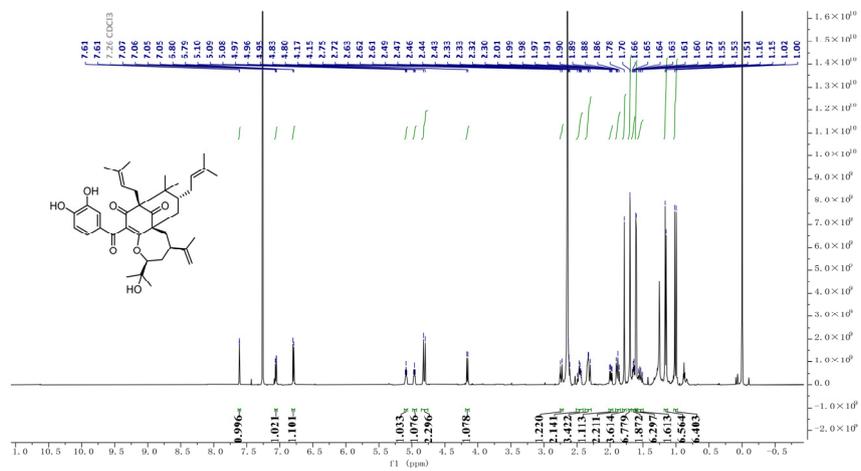


Figure S103.  $^1\text{H}$  NMR spectrum of compound 10 (recorded in  $\text{CDCl}_3$ )

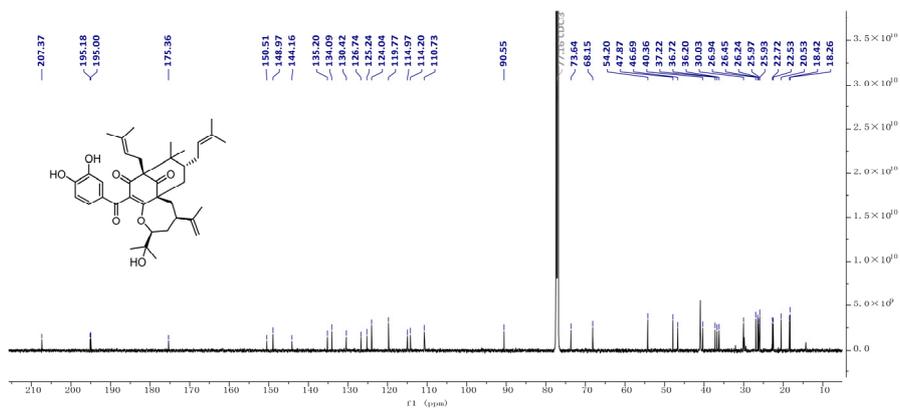


Figure S104.  $^{13}\text{C}$  NMR spectrum of compound **10** (recorded in  $\text{CDCl}_3$ )

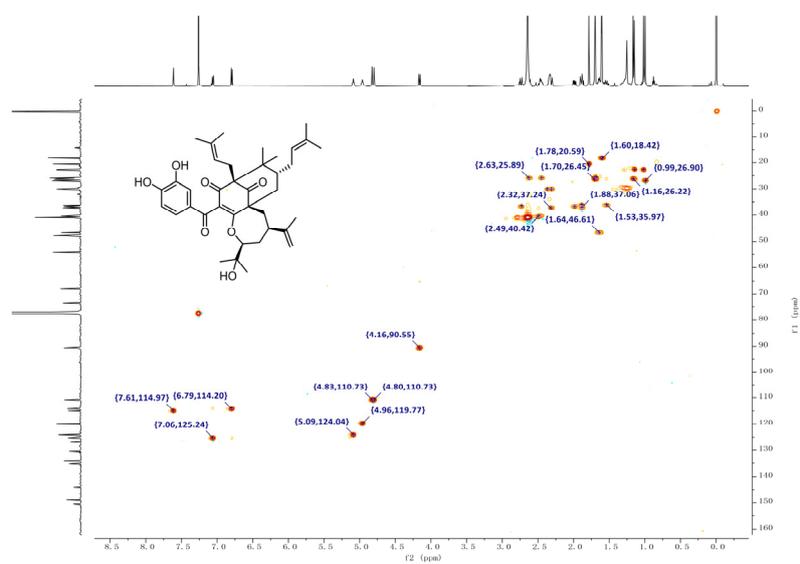


Figure S105. HSQC spectrum of compound **10** (recorded in  $\text{CDCl}_3$ )

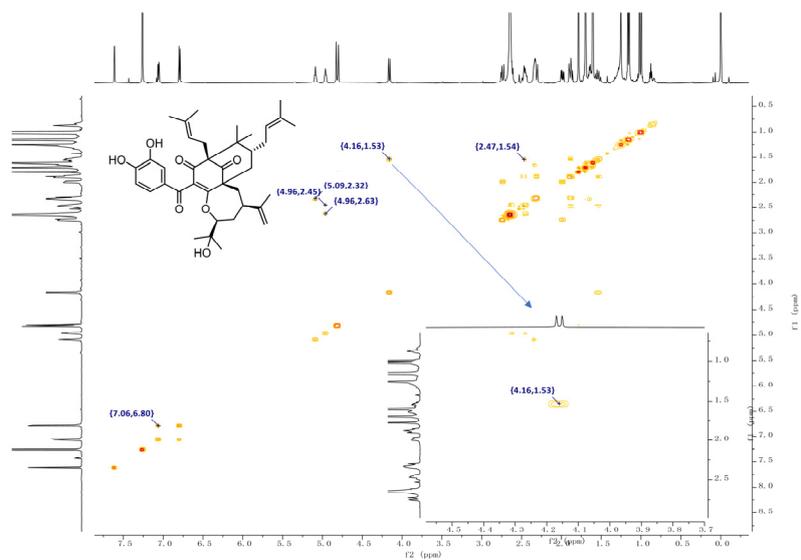


Figure S106.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **10** (recorded in  $\text{CDCl}_3$ )

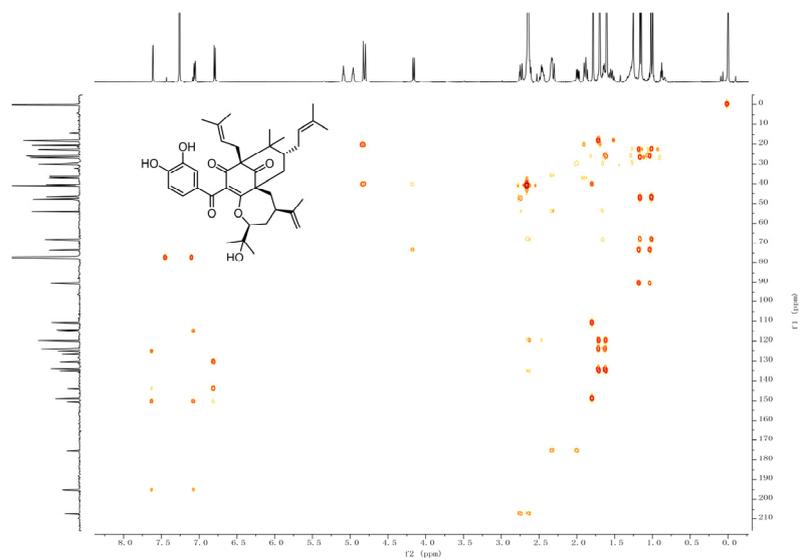


Figure S107. HMBC spectrum of compound **10** (recorded in  $\text{CDCl}_3$ )

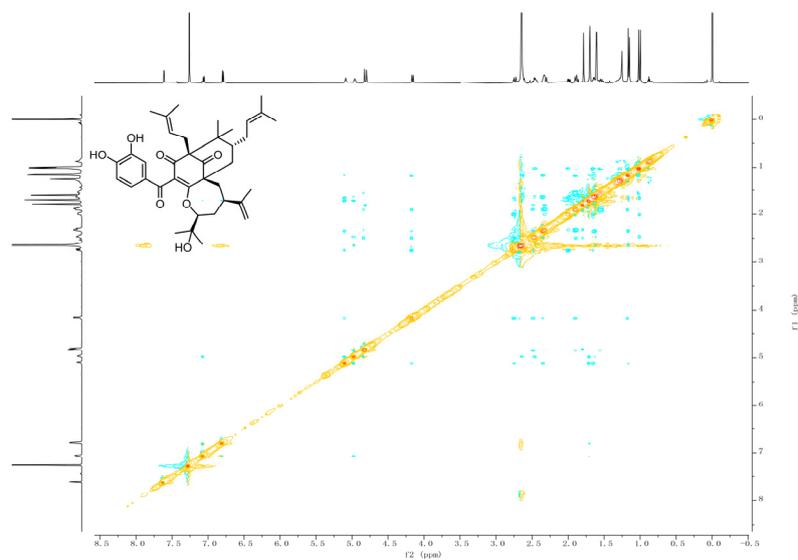


Figure S108. NOESY spectrum of compound **10** (recorded in CDCl<sub>3</sub>)

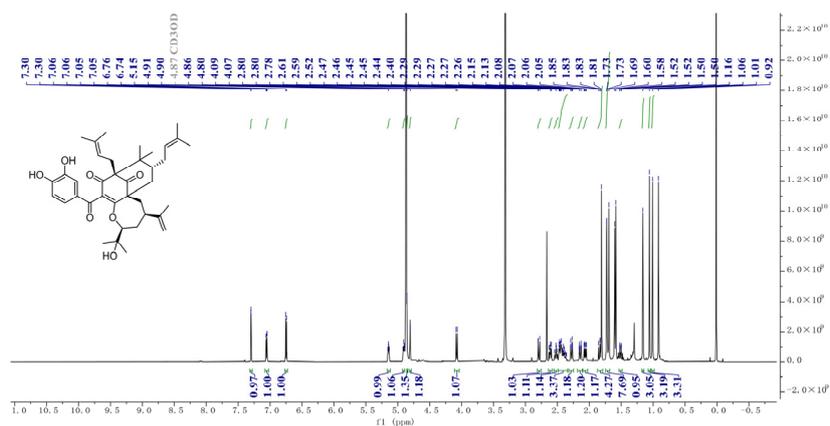


Figure S109. <sup>1</sup>H NMR spectrum of compound **10** (recorded in MeOH-*d*<sub>4</sub>)

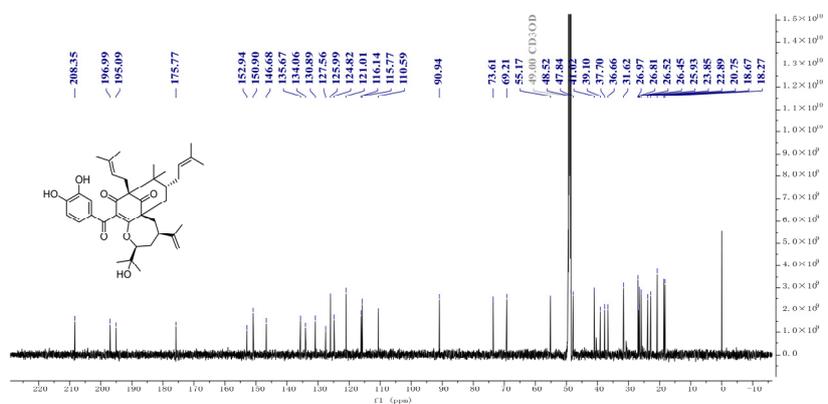


Figure S110.  $^{13}\text{C}$  NMR spectrum of compound **10** (recorded in  $\text{MeOH-}d_4$ )

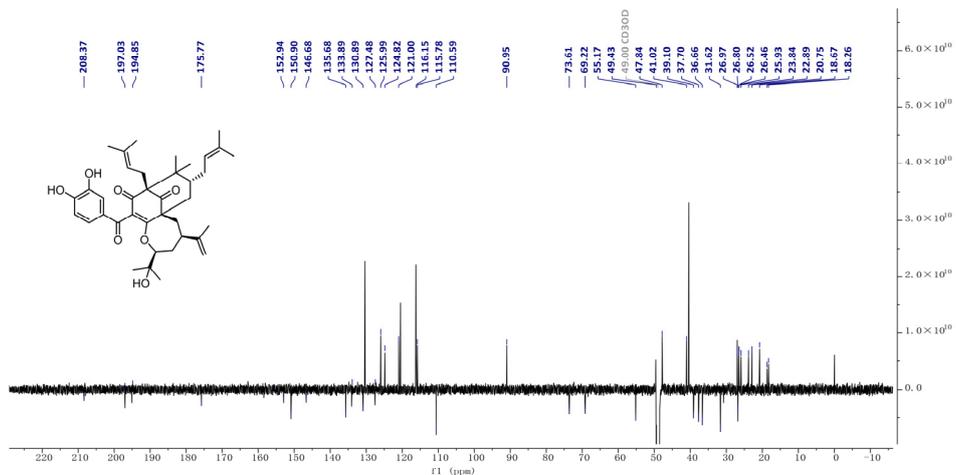


Figure S111. APT spectrum of compound **10** (recorded in  $\text{MeOH-}d_4$ )

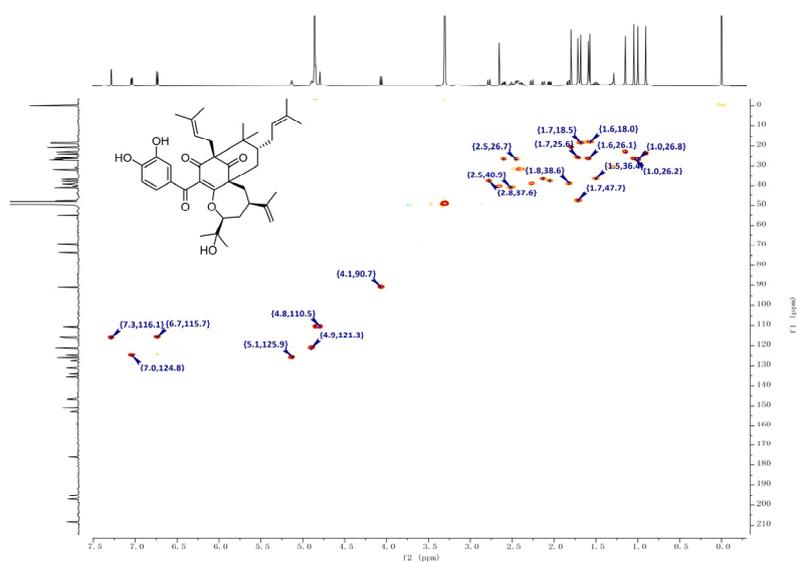


Figure S112. HSQC spectrum of compound **10** (recorded in  $\text{MeOH-}d_4$ )

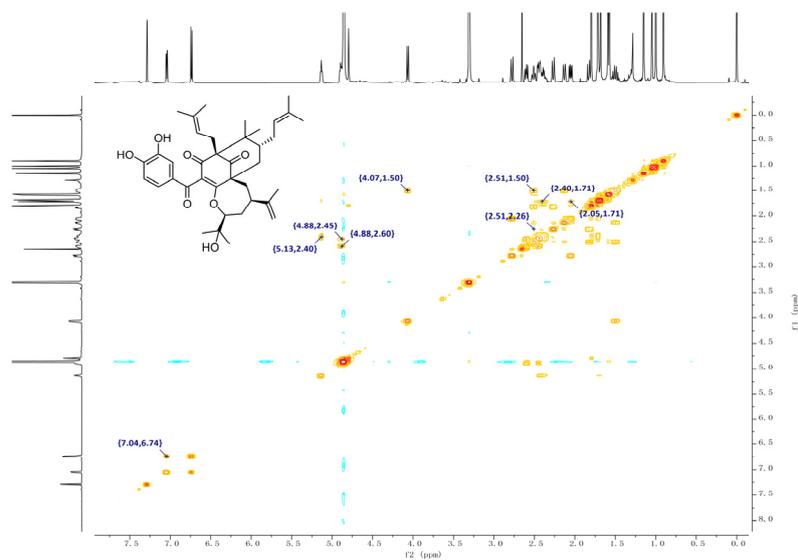


Figure S113.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **10** (recorded in  $\text{MeOH-}d_4$ )

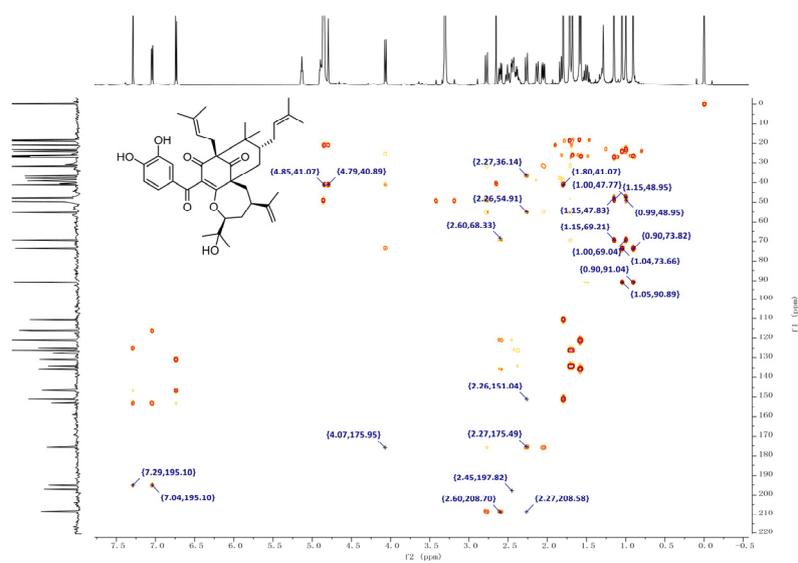


Figure S114. HMBC spectrum of compound **10** (recorded in  $\text{MeOH-}d_4$ )

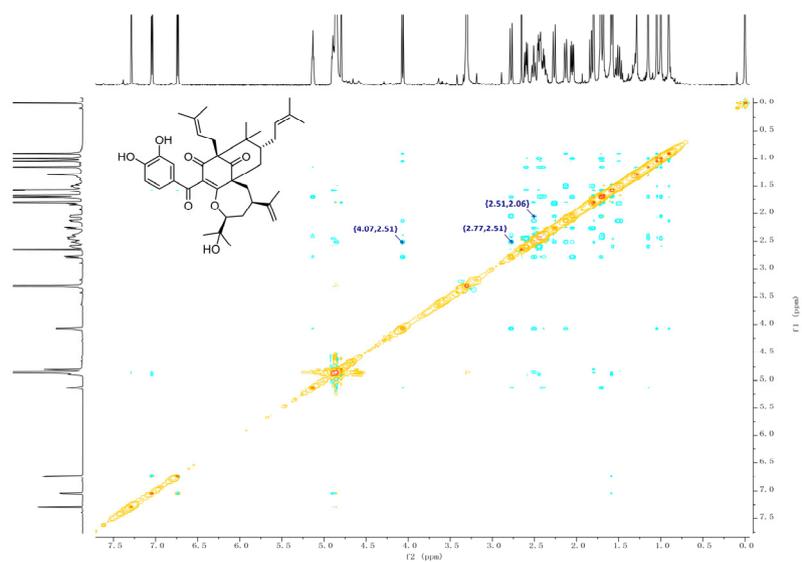


Figure S115. NOESY spectrum of compound **10** (recorded in MeOH-*d*<sub>4</sub>)

## Compound Spectrum SmartFormula Report

### Analysis Info

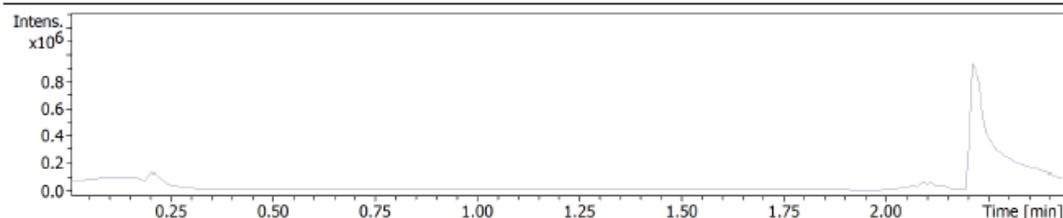
Analysis Name D:\Data\YIJI\20240701\YNTH7\_7\_1\_7034.d  
Method HPLC\_MS\_pos\_without\_column.m  
Sample Name YNTH7  
Comment

Acquisition Date 7/1/2024 2:38:14 PM

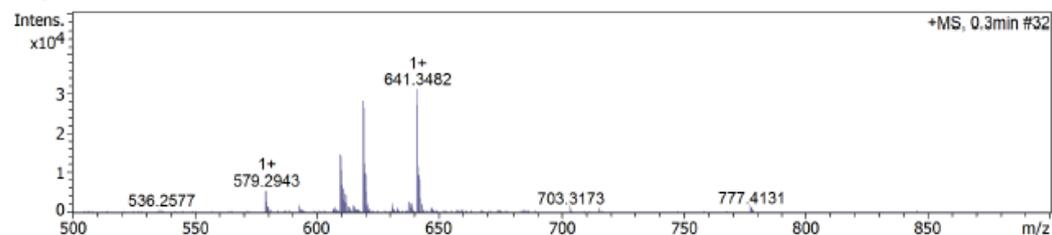
Operator Demo User  
Instrument compact 8255754.20225

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



### +MS, 0.3min #32



### C38H50O7, M+nNa, 641.3449

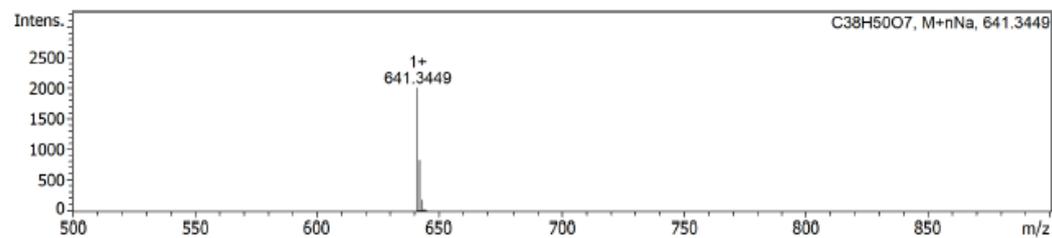


Figure S116. HRESIMS spectrum of compound **10**

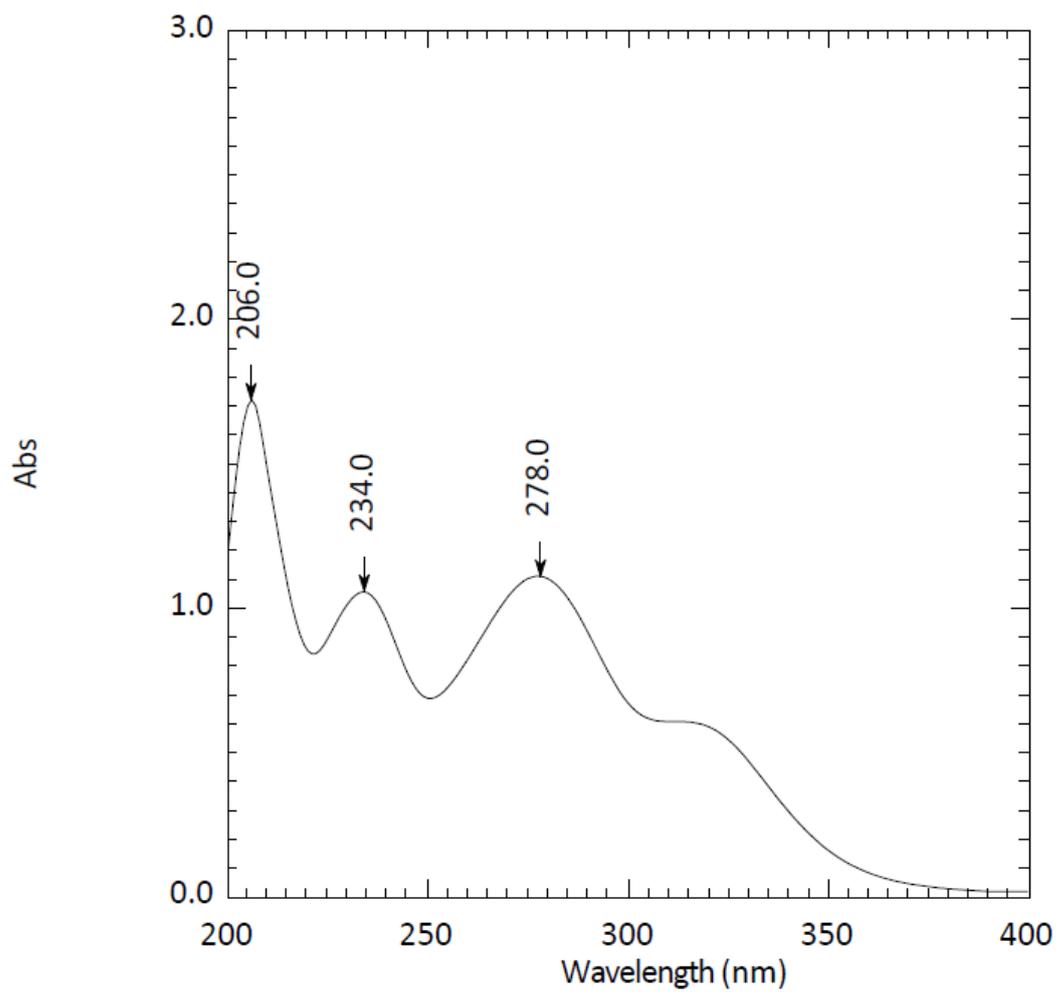


Figure S117. UV spectrum of compound **10**

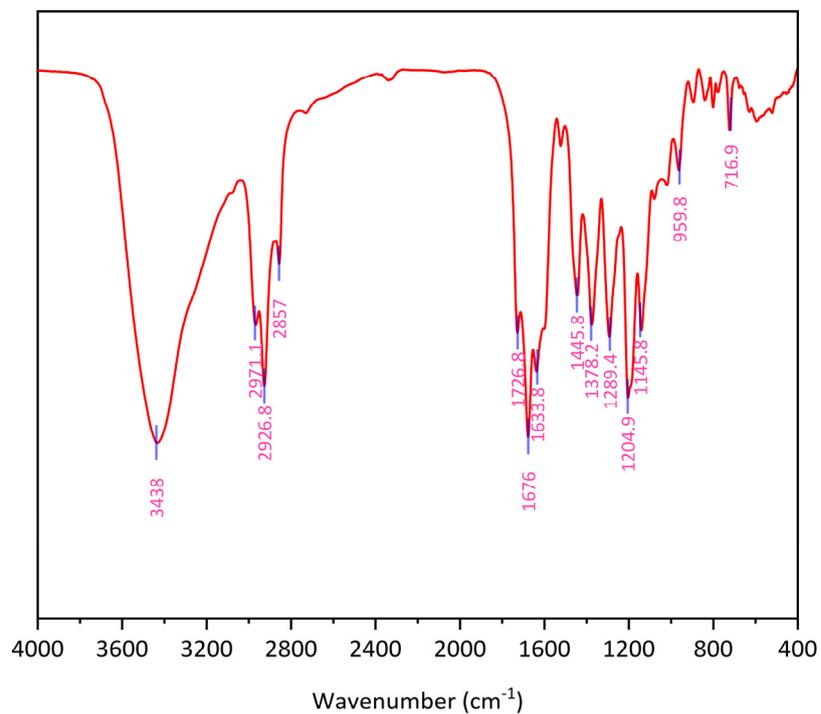


Figure S118. IR spectrum of compound **10**

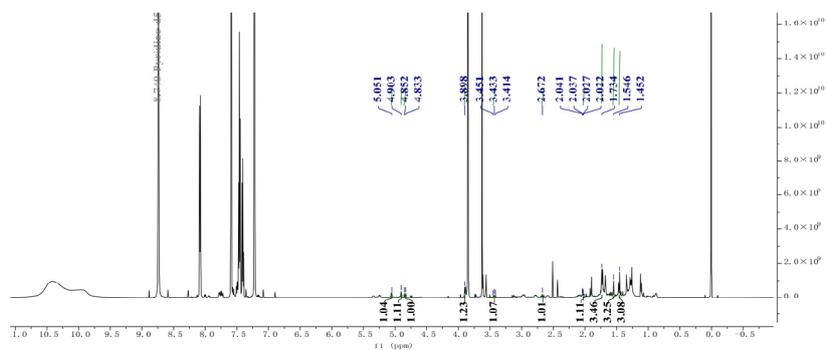


Figure S119. <sup>1</sup>H NMR spectrum of (+)-**7-S-MTPA** ester (recorded in Pyridine-*d*<sub>5</sub>)

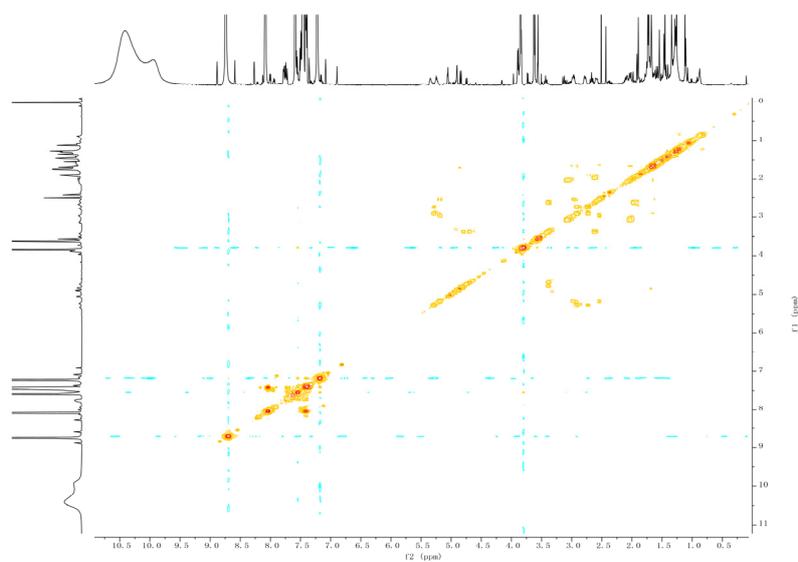


Figure S120.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of (+)-7-S-MTPA ester (recorded in Pyridine- $d_5$ )

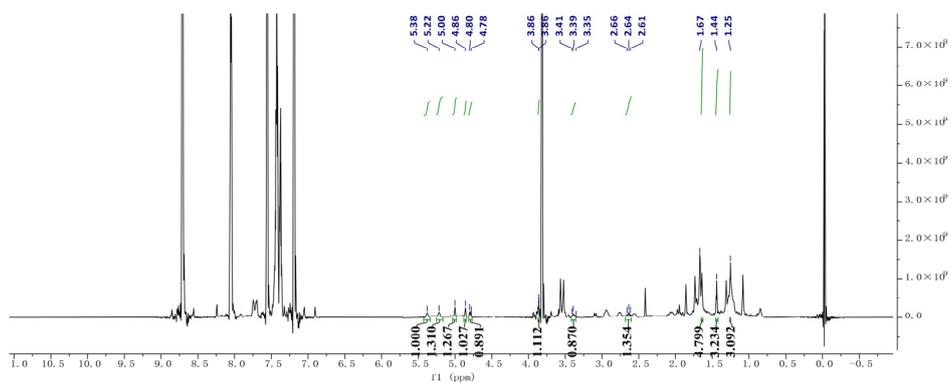


Figure S121.  $^1\text{H}$  NMR spectrum of (+)-7-R-MTPA ester (recorded in Pyridine- $d_5$ )

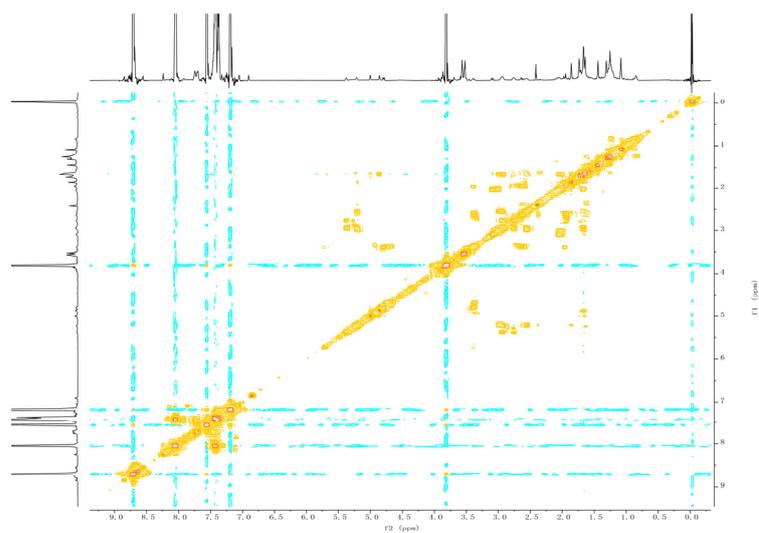


Figure S122.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of (+)-7-R-MTPA ester (recorded in Pyridine- $d_5$ )