

Supplementary Information for

Unprecedented Polycyclic Polyprenylated Acylphloroglucinols with Anti-Alzheimer's Activity from St. John's Wort

Yi Guo,[‡] Fang Huang,[‡] Weiguang Sun, Yuan Zhou, Chunmei Chen, Changxing Qi, Jing Yang,
Xiao-Nian Li, Zengwei Luo, Hucheng Zhu,* Xiaochuan Wang,* and Yonghui Zhang*

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Table S1. ¹H NMR Data of Hyperforones A–E (1–5)

no.	1 ^a	2 ^a	2 ^b	3 ^c	3 ^d	3 ^e	4 ^b	5 ^f	5 ^b	5 ^e
3	<i>a</i> 3.10 dd (19.6, 4.3) <i>b</i> 1.83 m						<i>a</i> 2.28 br d (15.7) <i>b</i> 2.09 dd (15.7, 8.7)	<i>a</i> 1.60 m <i>b</i> 1.46 t (12.6)	<i>a</i> 1.66 m <i>b</i> 1.61 m	<i>a</i> 1.70 m <i>b</i> 1.59 m
4	2.56 m	2.70 br d (9.5)	2.67 dd (10.0, 3.9)	2.99 m	2.75 dd (9.3, 3.1)	2.74 d (7.5)	2.94 m	1.82 m	1.90 m	1.75 m
6	3.97 br s	<i>a</i> 1.66 m <i>b</i> 1.55 m	<i>a</i> 1.66 m <i>b</i> 1.54 m	<i>a</i> 1.63 m <i>b</i> 1.43 m	<i>a</i> 1.66 m <i>b</i> 1.57 m	<i>a</i> 1.66 m <i>b</i> 1.53 m	<i>a</i> 1.84 m <i>b</i> 1.45 m	<i>a</i> 1.65 m <i>b</i> 1.12 m	<i>a</i> 1.74 m <i>b</i> 1.26 m	<i>a</i> 1.71 m <i>b</i> 1.34 m
7	<i>a</i> 2.26 m <i>b</i> 2.02 m	<i>a</i> 1.72 m <i>b</i> 1.72 m	<i>a</i> 1.72 m <i>b</i> 1.72 m	<i>a</i> 1.61 m <i>b</i> 1.45 m	<i>a</i> 1.67 m <i>b</i> 1.67 m	<i>a</i> 1.65 m <i>b</i> 1.65 m	<i>a</i> 1.91 m <i>b</i> 1.45 m	<i>a</i> 1.90 m <i>b</i> 1.90 m	<i>a</i> 1.94 m <i>b</i> 1.94 m	<i>a</i> 1.82 m <i>b</i> 1.82 m
8	2.80 dd (9.8, 2.9)	2.37 t (6.9)	2.50 t (7.4)	2.35 t (7.9)	2.37 t (7.9)	2.37 m	3.28 dd (8.4, 3.1)	2.32 d (9.6)	2.37 d (10.3)	2.22 m
11	1.24 s	1.54 s	1.58 s	1.63 s	1.40 s	1.40 s	1.76 s	1.80 s	1.87 s	1.92 s
12	1.31 s	1.68 s	1.66 s	1.84 s	1.63 s	1.67 s	1.71 s	1.59 s	1.65 s	1.69 s
14	<i>a</i> 2.65 dd (13.5, 4.9) <i>b</i> 2.78 dd (13.5, 3.2)	<i>a</i> 2.56 t (16.0) <i>b</i> 2.42 br d (16.0)	<i>a</i> 2.59 dd (17.3, 14.7) <i>b</i> 2.45 dd (17.3, 3.6)	<i>a</i> 3.96 br d (19.0) <i>b</i> 3.74 ddd (19.0, 6.0, 2.2)	<i>a</i> 3.33 m <i>b</i> 3.33 m	<i>a</i> 3.39 m <i>b</i> 3.39 m	<i>a</i> 2.99 dd (15.3, 11.9) <i>b</i> 2.52 br d (15.3)	<i>a</i> 2.52 m <i>b</i> 2.08 m	<i>a</i> 2.57 dd (12.3, 5.8) <i>b</i> 2.23 t (12.3)	<i>a</i> 2.40 dd (12.1, 5.6) <i>b</i> 2.23 t (12.1)
15	3.98 dd (4.9, 3.2)	4.25 br d (16.0)	4.26 dd (14.7, 3.6)	4.31 m	4.08 m	4.12 m	4.92 dd (11.9, 1.4)	4.11 dd (10.4, 5.8)	4.13 dd (10.5, 5.8)	4.04 dd (10.6, 5.6)
17	1.44 s	1.29 s	1.28 s	1.31 s	1.30 s	1.30 s	1.21 s	1.14 s	1.27 s	1.33 s
18	1.85 s	1.25 s	1.26 s	1.65 s	1.42 s	1.44 s	1.20 s	1.06 s	1.17 s	1.19 s
19	<i>a</i> 2.02 m <i>b</i> 1.84 m	<i>a</i> 2.63 br d (15.1) <i>b</i> 2.18 m	<i>a</i> 2.55 m <i>b</i> 2.22 m	<i>a</i> 2.76 m <i>b</i> 2.56 m	<i>a</i> 2.44 m <i>b</i> 2.29 m	<i>a</i> 2.42 m <i>b</i> 2.28 m	<i>a</i> 2.23 m <i>b</i> 1.87 m	<i>a</i> 2.14 m <i>b</i> 1.71 m	<i>a</i> 2.22 m <i>b</i> 1.78 m	<i>a</i> 2.17 m <i>b</i> 1.75 m
20	5.07 t (6.5)	5.21 t (6.3)	5.24 t (6.8)	5.49 t (6.8)	5.25 t (6.9)	5.26 t (6.5)	5.06 t (7.7)	5.16 t (6.9)	5.17 t (7.2)	5.04 t (7.2)
22	1.67 s	1.68 s	1.68 s	1.72 s	1.69 s	1.69 s	1.59 s	1.69 s	1.73 s	1.73 s
23	1.58 s	1.62 s	1.63 s	1.72 s	1.63 s	1.63 s	1.63 s	1.57 s	1.63 s	1.60 s
24	1.39 s	0.98 s	0.98 s	1.18 s	1.00 s	1.01 s	1.07 s	0.97 s	1.06 s	1.06 s
26	1.13 s	1.25 s	1.28 s	1.54 s	1.30 s	1.33 s	1.08 s	1.14 s	1.22 s	1.23 s
27	1.31 s	1.29 s	1.28 s	1.27 s	1.26 s	1.28 s	1.30 s	1.23 s	1.29 s	1.30 s

^a Recorded at 600 MHz in CDCl₃; ^b Recorded at 400 MHz in CD₃OD; ^c Recorded at 600 MHz in C₅D₅N; ^d Recorded at 800 MHz in CD₃OD; ^e Recorded at 400 MHz in CDCl₃; ^f Recorded 400MHz in DMSO-*d*₆.

Table S2. ¹H NMR Data of Hyperforones F–J (6–10)

<i>no.</i>	6^a	6^b	6^c	7^b	8^b	9^d	9^b	10^e
3								2.82 m
4	<i>a</i> 2.06 m <i>b</i> 1.90 t (14.1)	<i>a</i> 2.12 m <i>b</i> 1.90 t (13.9)	<i>a</i> 2.01 m <i>b</i> 1.80 t (13.9)	<i>a</i> 2.36 m <i>b</i> 1.53 t (13.2)	<i>a</i> 2.10 dd (14.0, 2.0) <i>b</i> 1.91 t (13.4)	<i>a</i> 2.04 m <i>b</i> 1.71 m	<i>a</i> 2.08 m <i>b</i> 1.78 m	<i>a</i> 2.07 m <i>b</i> 1.10 d (12.8)
5	2.50 m	2.70 m	2.62 m	1.77 m	1.60 m	2.49 m	2.55 m	1.53 m
7	<i>a</i> 1.94 dd (13.1, 6.4) <i>b</i> 1.37 m	<i>a</i> 2.02 dd (12.9, 6.5) <i>b</i> 1.31 m	<i>a</i> 1.93 m <i>b</i> 1.13 m	<i>a</i> 2.06 m <i>b</i> 1.41 m	<i>a</i> 1.97 m <i>b</i> 1.25 m	<i>a</i> 1.88 m <i>b</i> 1.36 m	<i>a</i> 1.95 m <i>b</i> 1.31 m	<i>a</i> 2.46 td (14.5, 4.5) <i>b</i> 1.83 ddd (14.9, 4.3, 2.6)
8	<i>a</i> 2.40 m <i>b</i> 2.09 m	<i>a</i> 2.58 m <i>b</i> 2.11 m	<i>a</i> 2.45 m <i>b</i> 2.03 m	<i>a</i> 2.35 m <i>b</i> 2.35 m	<i>a</i> 2.16 m <i>b</i> 2.16 m	<i>a</i> 1.63 m <i>b</i> 1.39 m	<i>a</i> 1.70 m <i>b</i> 1.46 m	<i>a</i> 1.98 m <i>b</i> 1.73 m
9	4.08 t (9.7)	4.00 t (9.7)	3.81 t (9.6)	3.86 dd (8.6, 5.4)	4.23 dd (12.3, 7.6)	3.51 dd (12.9, 3.4)	3.52 dd (13.0, 3.7)	2.40 dd (12.2, 7.2)
11	<i>a</i> 3.57 t (11.7) <i>b</i> 2.06 m	<i>a</i> 3.64 t (11.8) <i>b</i> 2.06 dd (12.0, 4.9)	<i>a</i> 3.53 t (11.6) <i>b</i> 1.99 m	<i>a</i> 2.77 dd (13.8, 10.9) <i>b</i> 2.45 dd (13.8, 2.1)	<i>a</i> 3.24 dd (13.4, 11.1) <i>b</i> 1.98 m			
12	4.74 dd (11.4, 4.7)	4.79 dd (11.5, 4.9)	4.62 dd (11.3, 5.0)	5.08 dd (10.9, 2.1)	3.85 dd (11.0, 2.5)	2.99 sept (6.4)	3.25 sept (6.4)	2.71 sept (6.6)
13						1.24 d (6.4)	1.19 d (6.4)	1.00 d (6.6)
14						1.02 d (6.4)	1.01 d (6.4)	1.08 d (6.6)
15	2.39 m	2.48 sept (6.4)	2.42 m	2.66 sept (6.4)	2.40 sept (6.4)	<i>a</i> 2.38 dd (18.0, 4.8) <i>b</i> 2.09 m	<i>a</i> 2.39 dd (17.6, 5.0) <i>b</i> 2.02 m	<i>a</i> 2.39 m <i>b</i> 1.94 m
16	1.26 d (6.4)	1.22 d (6.4)	1.12 d (6.3)	1.34 d (6.4)	1.23 d (6.4)	3.66 m	3.66 dd (5.0, 3.5)	5.09 t (7.2)
17	1.12 d (6.3)	1.12 d (6.4)	1.04 d (6.3)	1.21 d (6.4)	1.12 d (6.4)			
18	<i>a</i> 2.98 dd (14.3, 8.7) <i>b</i> 2.30 dd (14.3, 6.8)	<i>a</i> 2.93 dd (14.1, 8.6) <i>b</i> 2.28 m	<i>a</i> 2.80 dd (14.1, 8.6) <i>b</i> 2.18 m	<i>a</i> 2.61 dd (11.7, 5.2) <i>b</i> 2.54 dd (14.1, 7.9)	<i>a</i> 2.64 dd (13.9, 8.3) <i>b</i> 2.23 dd (13.0, 6.1)	1.40 s	1.17 s	1.71 s
19	5.10 t (7.9)	5.15 t (7.7)	5.09 t (7.6)	5.08 m	5.21 t (7.7)	1.17 s	1.34 s	1.61 s
20						<i>a</i> 2.10 m <i>b</i> 1.71 m	<i>a</i> 2.14 m <i>b</i> 1.79 m	<i>a</i> 2.05 m <i>b</i> 1.67 m
21	1.70 s	1.71 s	1.67 s	1.70 s	1.69 s	5.10 t (7.3)	5.14 t (7.3)	5.02 t (7.3)
22	1.68 s	1.69 s	1.63 s	1.64 s	1.66 s			
23	<i>a</i> 2.21 dd (13.9, 6.5) <i>b</i> 1.73 m	<i>a</i> 2.25 m <i>b</i> 1.79 m	<i>a</i> 2.15 m <i>b</i> 1.70 m	<i>a</i> 2.14 m <i>b</i> 1.76 m	<i>a</i> 2.16 m <i>b</i> 1.80 m	1.71 s	1.71 s	1.71 s
24	5.21 t (7.6)	5.30 t (6.8)	5.24 t (7.2)	5.23 t (6.8)	5.12 t (7.0)	1.60 s	1.63 s	1.58 s
25						0.87 s	0.92 s	1.01 s
26	1.73 s	1.73 s	1.67 s	1.77 s	1.75 s			
27	1.65 s	1.66 s	1.61 s	1.66 s	1.66 s	1.42 s	1.42 s	1.19 s
28	0.97 s	1.01 s	0.92 s	1.05 s	0.94 s	1.45 s	1.49 s	1.32 s
30	1.19 s	1.22 s	1.13 s	1.19 s	1.50 s			
31	1.19 s	1.20 s	1.10 s	1.15 s	1.54 s			

^a Recorded at 600 MHz in CDCl₃; ^b Recorded at 400 MHz in CD₃OD; ^c Recorded 400MHz in DMSO-*d*₆; ^d Recorded at 400 MHz in CDCl₃; ^e Recorded at 800 MHz in CDCl₃;

Table S3. ^{13}C NMR Data of Hyperforones A–E (1–5)

no.	1 ^a	2 ^a	2 ^b	3 ^c	3 ^d	3 ^e	4 ^b	5 ^f	5 ^b	5 ^e
1	73.5	71.3	72.7	75.0	76.2	74.8	70.7	96.4	98.3	97.1
2	176.5	176.4	179.7	205.7	208.6	206.9	175.8	176.5	178.9	176.6
3	43.5	116.2	117.1	113.0	114.2	113.5	49.4	29.2	30.8	29.4
4	35.9	48.3	49.8	47.8	48.7	47.1	40.6	33.4	35.7	34.7
5	64.9	55.6	56.6	53.5	54.5	53.3	61.4	46.9	48.7	47.5
6	80.7	44.2	45.7	45.7	46.5	45.2	39.8	34.4	35.9	34.8
7	31.1	27.6	28.5	27.4	28.1	27.1	25.7	21.7	23.1	22.4
8	50.0	61.7	62.8	62.8	64.1	62.4	60.8	50.0	54.3	53.4
9	117.5	145.1	146.9	150.2	150.0	148.6	146.9	149.3	150.3	148.6
10	73.9	108.0	108.9	105.1	107.1	106.2	111.0	108.3	111.5	110.9
11	27.7	19.1	19.7	21.4	21.4	20.9	23.4	19.8	20.6	20.0
12	24.9	18.3	18.6	18.7	18.5	18.3	20.3	19.4	19.7	19.5
13	208.8	190.3	193.4	169.6	171.6	167.6	212.3	77.8	79.9	78.3
14	47.6	36.7	37.0	41.5	41.7	40.7	42.9	34.5	36.3	35.1
15	77.3	86.1	87.5	74.1	74.9	74.7	79.4	82.0	84.0	82.1
16	89.6	71.3	71.5	91.1	92.3	89.7	72.4	68.8	70.9	70.4
17	26.0	25.6	27.2	25.7	26.0	25.8	27.2	25.3	25.7	26.3
18	23.4	25.0	24.6	21.5	21.3	20.8	25.3	25.3	25.1	24.0
19	31.2	28.9	30.2	30.6	31.0	29.7	31.3	28.4	29.8	28.7
20	121.8	124.7	126.1	126.6	126.8	125.8	123.9	122.9	124.0	122.5
21	133.8	131.2	132.0	130.5	131.6	130.6	134.8	132.3	134.6	134.1
22	25.9	25.8	25.9	26.0	26.1	25.9	25.8	25.6	26.0	25.9
23	18.1	18.0	18.2	18.0	18.1	17.9	17.9	17.7	18.0	17.9
24	12.0	18.6	19.2	19.3	19.5	18.8	19.7	17.0	17.7	17.2
25	80.1	80.7	82.2	81.3	82.5	81.1	81.5	81.4	83.1	81.6
26	29.1	28.8	29.2	29.0	29.2	28.5	29.5	27.4	28.0	27.8
27	26.0	23.2	23.4	23.8	23.9	23.6	24.1	24.4	24.8	24.5

^a Recorded at 150 MHz in CDCl_3 ; ^b Recorded at 100 MHz in CD_3OD ; ^c Recorded at 150 MHz in $\text{C}_5\text{D}_5\text{N}$; ^d Recorded at 200 MHz in CD_3OD ; ^e Recorded at 100 MHz in CDCl_3 ; ^f Recorded 100MHz in $\text{DMSO}-d_6$.

Table S4. ^{13}C NMR Data of Hyperforones F–J (6–10)

no.	6 ^a	6 ^b	6 ^c	7 ^b	8 ^b	9 ^d	9 ^b	10 ^e
1	81.7	83.5	81.4	85.7	81.4	66.8	68.0	87.6
2	203.8	205.9	203.5	207.9	205.5	140.3	141.2	210.5
3	60.9	62.3	60.3	64.2	63.7	109.4	110.1	48.8
4	30.7	32.0	30.2	33.3	33.4	31.2	32.5	34.1
5	36.6	37.4	35.5	37.6	40.6	35.5	37.1	40.2
6	51.4	52.6	51.0	55.0	53.9	42.6	43.8	49.4
7	35.0	36.2	34.8	37.1	36.7	33.4	34.7	29.2
8	27.1	28.0	26.4	25.8	28.6	14.6	15.8	23.4
9	61.1	62.2	60.1	63.0	60.4	51.6	53.2	58.4
10	208.9	212.4	209.5	212.8	208.2	78.6	80.0	211.9
11	37.8	38.9	37.5	45.9	43.8	218.3	221.4	209.9
12	84.0	83.8	81.8	84.5	76.5	40.5	41.0	39.9
13	170.8	171.0	168.9	171.4	173.0	23.4	24.6	22.3
14	214.1	215.8	214.0	214.7	215.0	20.2	20.8	20.4
15	42.2	43.1	41.0	42.6	43.1	33.3	33.9	27.7
16	23.6	24.0	23.3	24.3	24.1	69.3	69.8	121.3
17	20.5	21.0	20.5	21.6	21.1	76.4	77.7	133.3
18	33.2	34.6	33.0	35.8	35.9	23.3	23.9	25.8
19	118.3	120.1	119.0	119.4	120.3	22.6	23.1	17.9
20	137.0	137.5	135.6	137.2	136.8	27.6	28.8	26.1
21	26.1	26.0	25.6	26.2	26.2	123.1	124.7	122.3
22	18.3	18.4	18.0	18.2	18.2	132.5	133.1	133.6
23	29.3	30.6	29.0	29.4	30.1	25.8	26.1	25.8
24	122.9	124.6	123.6	124.2	123.8	17.8	18.0	17.9
25	133.9	134.2	132.2	133.7	134.6	20.3	21.1	16.2
26	25.9	26.0	25.8	26.0	26.0	83.9	85.8	72.1
27	17.8	18.0	17.6	18.1	18.1	29.5	29.8	28.3
28	18.5	19.0	18.2	18.5	21.2	23.3	23.6	24.9
29	71.6	72.2	70.1	71.3	87.2	172.0	174.9	
30	26.7	26.3	26.0	26.5	25.0			
31	24.2	25.6	24.9	24.7	17.4			

^a Recorded at 150 MHz in CDCl_3 ; ^b Recorded at 100 MHz in CD_3OD ; ^c Recorded 100MHz in $\text{DMSO}-d_6$; ^d Recorded at 100 MHz in CDCl_3 ; ^e Recorded at 200 MHz in CDCl_3 ;

Table S5. The Computed ^{13}C NMR Data for **2a** and **2b**.

no.	2a			2b			
	exptl	calcd	$\Delta\delta$	exptl	calcd	$\Delta\delta$	
1	72.7	75.2	2.5	72.7	76.3	3.6	
2	179.7	174.1	-5.6	179.7	172.5	-7.2	
3	117.1	114.8	-2.3	117.1	120.3	3.2	
4	49.8	51.4	1.6	49.8	57.1	7.3	
5	56.6	61.4	4.8	56.6	53.7	-2.9	
6	45.7	43.3	-2.4	45.7	56.5	10.8	
7	28.5	30.3	1.8	28.5	24.0	-4.5	
8	62.8	64.2	1.4	62.8	65.0	2.2	
9	146.9	145.5	-1.4	146.9	146.1	-0.8	
10	108.9	108.8	-0.1	108.9	103.8	-5.1	
11	19.7	20.8	1.1	19.7	21.4	1.7	
12	18.6	19.6	1.0	18.6	19.5	0.9	
13	193.4	185.5	-7.9	193.4	185.8	-7.6	
14	37.0	38.2	1.2	37.0	38.6	1.6	
15	87.5	87.8	0.3	87.5	90.8	3.3	
16	71.4	72.9	1.5	71.4	72.9	1.5	
17	29.2	26.1	-3.1	29.2	26.2	-3.0	
18	24.6	24.1	-0.5	24.6	24.8	0.2	
19	30.2	31.1	0.9	30.2	32.8	2.6	
20	126.1	125.7	-0.4	126.1	125.7	-0.4	
21	132.0	130.3	-1.7	132.0	131.7	-0.3	
22	25.9	26.8	0.9	25.9	26.8	0.9	
23	18.2	19.2	1.0	18.2	19.1	0.9	
24	19.2	20.7	1.5	19.2	23.4	4.2	
25	82.2	83.2	1.0	82.2	78.1	-4.1	
26	27.2	30.4	3.2	27.2	31.3	-4.1	
27	23.4	24.0	0.6	23.4	24.1	0.7	
		AveDev	1.91			AveDev	3.2
		MaxDev	7.9			MaxDev	10.8

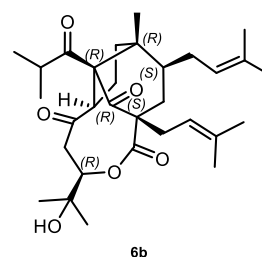
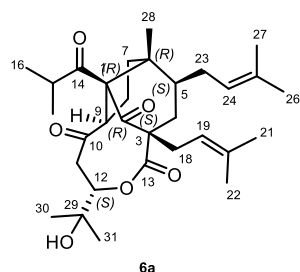
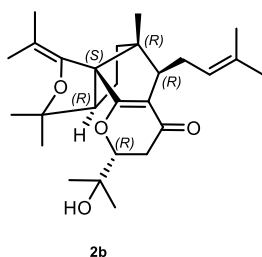
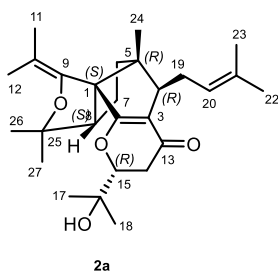


Table S6. The Computed ^{13}C NMR Data for **6a** and **6b**.

no.	6a			6b		
	exptl	calcd	$\Delta\delta$	exptl	calcd	$\Delta\delta$
1	81.7	80.8	-0.9	81.7	77.5	-4.2
2	203.8	203.3	-0.5	203.8	201.6	-2.2
3	60.9	64.5	3.6	60.9	62.8	1.9
4	30.7	31.8	1.1	30.7	32.1	1.4
5	36.6	38.4	1.8	36.6	42.2	5.6
6	51.4	56.3	4.9	51.4	56.2	4.8
7	35	37.3	2.3	35	38.6	3.6
8	27.1	29.3	2.2	27.1	28.4	1.3
9	61.1	66.1	5.0	61.1	64.5	3.4
10	208.9	208.0	-0.9	208.9	200.3	-8.6
11	37.8	36.0	-1.8	37.8	44.7	6.9
12	84	90.1	6.1	84	79.8	-4.2
13	170.7	169.4	-1.3	170.7	169.2	-1.5
14	214.1	214.0	-0.1	214.1	213.3	-0.8
15	42.2	42.1	-0.1	42.2	42.4	0.2
16	23.6	20.7	-2.9	23.6	20.9	-2.7
17	20.5	19.5	-1.0	20.5	19.6	-0.9
18	33.2	38.9	5.7	33.2	36.6	3.4
19	118.3	118.3	0.0	118.3	118.3	0.0
20	137	135.9	-1.1	137	135.1	-1.9
21	18.3	18.9	0.6	18.3	18.7	0.4
22	26.1	27.2	1.1	26.1	27.0	0.9
23	29.3	32.9	3.6	29.3	32.1	2.8
24	122.8	123.6	0.8	122.8	121.5	-1.3
25	133.9	133.0	-0.9	133.9	134.0	0.1
26	25.9	27.1	1.2	25.9	26.8	0.9
27	17.8	18.9	1.1	17.8	18.4	0.6
28	18.5	20.4	1.9	18.5	21.1	2.6
29	71.6	69.3	-2.3	71.6	72.1	0.5
30	26.7	27.8	1.1	26.7	22.1	-4.6
31	24.2	27.4	3.2	24.2	27.4	3.2
		AveDev	1.98		AveDev	2.49
		MaxDev	6.1		MaxDev	8.6

Table S7. The virtual docking^a of BACE1 and PP2Ac for **1–10** and the total-score values.

Compound	BACE1 (4YBI)	PP2Ac (2IE4)
1	5.32	5.97
2	5.84	4.11
3	5.78	5.21
4	7.62	4.59
5	4.52	3.59
6	7.85	5.69
7	6.16	3.12
8	6.21	3.89
9	3.96	4.94
10	3.83	4.65

^a The X-ray crystallographic structure of the PP2Ac and BACE1 were implemented in the Surflex-Dock module of the Sybyl software.

Table S8. IC₅₀ for BACE1 and EC₅₀ for PP2A of compounds **1–10**.

Compound	Inhibitory activities	Increased PP2A		Inhibitory activities	Increased PP2A
	against BACE1 ^b	activities ^c		against BACE1 ^b	activities ^c
	IC ₅₀ ± SD (nM)	EC ₅₀ ± SD (nM)		IC ₅₀ ± SD (nM)	EC ₅₀ ± SD (nM)
1	275.0 ± 23.0	897.0 ± 97.0	6	98.6 ± 2.0	199.0 ± 36.6
2	739.9 ± 44.6	655.7 ± 66.4	7	270.5 ± 16.7	897.0 ± 193.1
3	433.8 ± 35.1	385.1 ± 22.6	8	398.7 ± 49.8	325.7 ± 30.1
4	136.2 ± 22.8	258.8 ± 24.0	9	1028.0 ± 17.6	786.0 ± 45.7
5	660.1 ± 9.8	7761.0 ± 318.8	10	9553.0 ± 969.2	248.1 ± 100.1
Positive Control ^a	260.2 ± 32.0	413.9 ± 73.5			

^a LY2811376, a BACE1 inhibitor, as a positive control; SCR1693, which increased PP2A activities, as a positive control. ^b BACE1 activity tested in N2a/APP cells. ^c PP2A activity tested in HEK293/tau cells.

Table S9. Antibodies employed in this study.

Antibody	Specific	Type	Dilution	Source
pS199	Phosphorylated tau at Ser199	Poly-	1:1000 for WB	Signalway Antibody
pT231	Phosphorylated tau at Thr231	Poly-	1:1000 for WB	Signalway Antibody
pS396	Phosphorylated tau at Ser396	Poly-	1:1000 for WB	Signalway Antibody
pS404	Phosphorylated tau at Ser404	Poly-	1:1000 for WB	Signalway Antibody
Tau-1	Nonphosphorylated tau at Ser198/199/202	Mono-	1:1000 for WB	Millipore
Tau-5	Total tau	Mono-	1:1000 for WB	Millipore
Synapsin-1	Synapsin-1 C-term	Poly-	1:1000 for WB	Millipore
Synaptophysin	Synaptophysin aa 250-350 (C terminal).	Poly-	1:1000 for WB	Millipore
PP2Ac-mL309	Methylated PP2Ac at Leu309	Mono-	1:1000 for WB	Millipore
PSD93	Post Synaptic Density 93 aa 352-366.	Poly-	1:1000 for WB	Abcam
PSD95	PSD95 N-term	Poly-	1:1000 for WB	Abcam
β-actin	Total β -actin	Mono-	1:1000 for WB	Abcam
PP2Ac-pY307	Phosphorylated PP2Ac at Tyr307	Poly-	1:1000 for WB	Abcam
PP2Ac	PP2A catalytic subunit (both α and β isoforms)	Poly-	1:1000 for WB	Cell Signaling
GSK-3β	Total GSK-3 β	Mono-	1:1000 for WB	Cell Signaling
GSK-3β-pS9	Phosphorylated GSK-3 β at Ser9	Poly-	1:1000 for WB	Cell Signaling
BACE1	Total BACE1	Poly-	1:1000 for WB	Cell Signaling
APP	Full length of total APP	Poly-	1:1000 for WB	Cell Signaling
APP-β	Anti-human sAPP- β antibodies	Poly-	1:1000 for WB	IBL

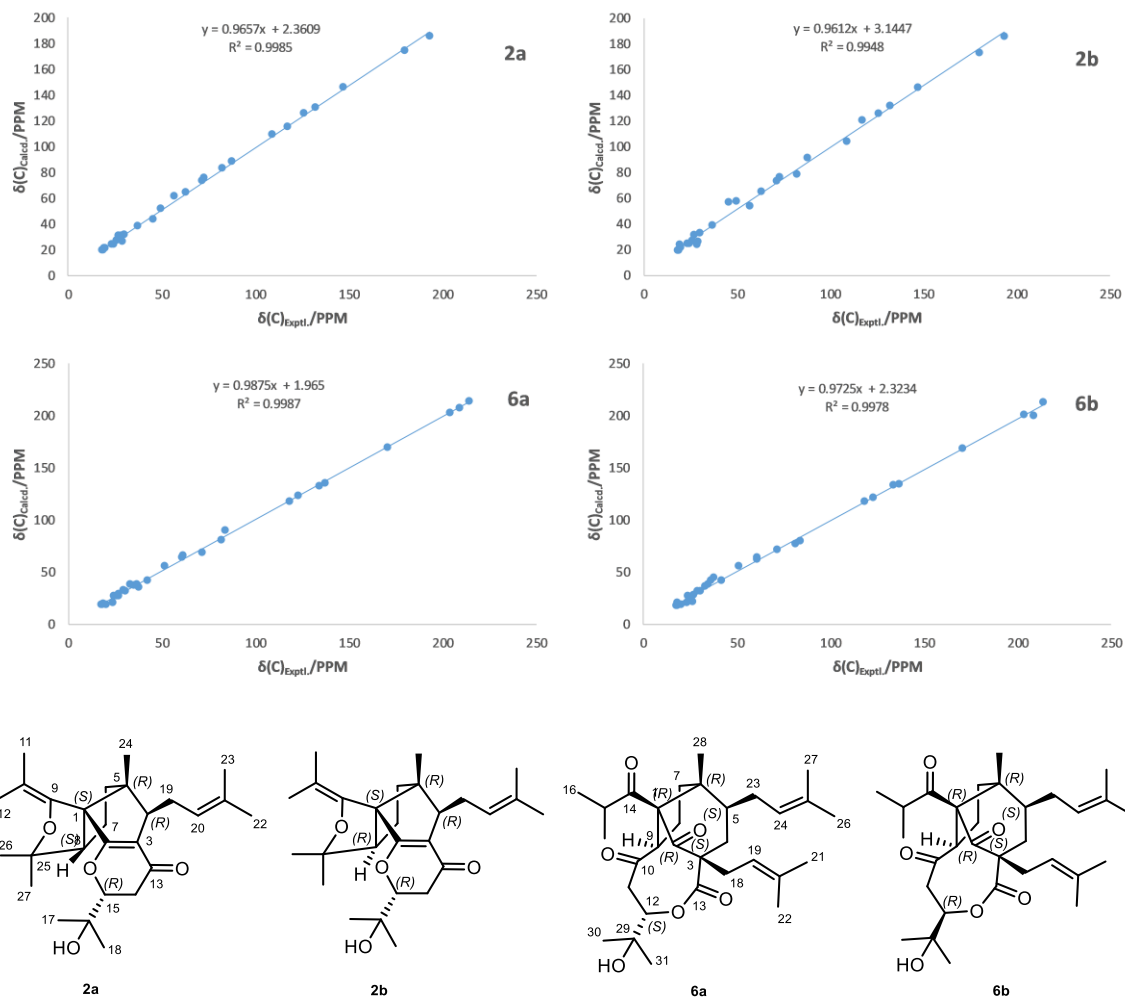


Figure S1. Correlation between experimental and calculated ^{13}C NMR of **2a**, **2b**, **6a**, and **6b**.

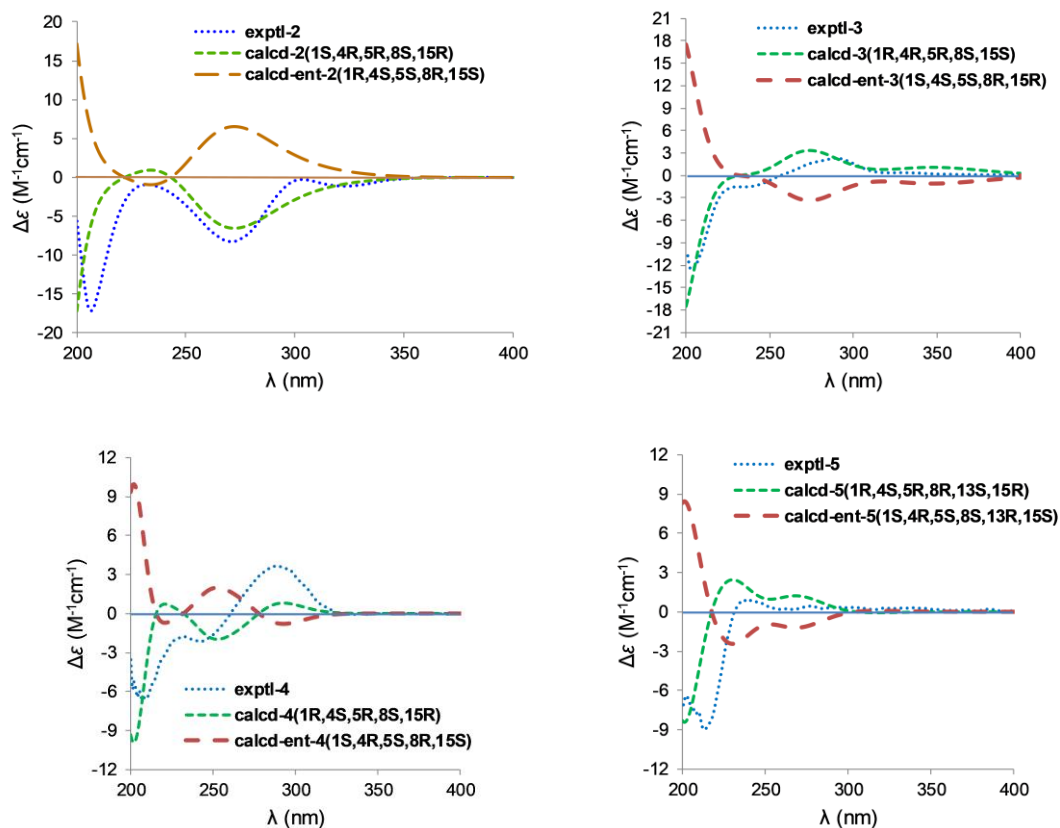


Figure S2. Experimental and calculated ECD spectra of 2–5.

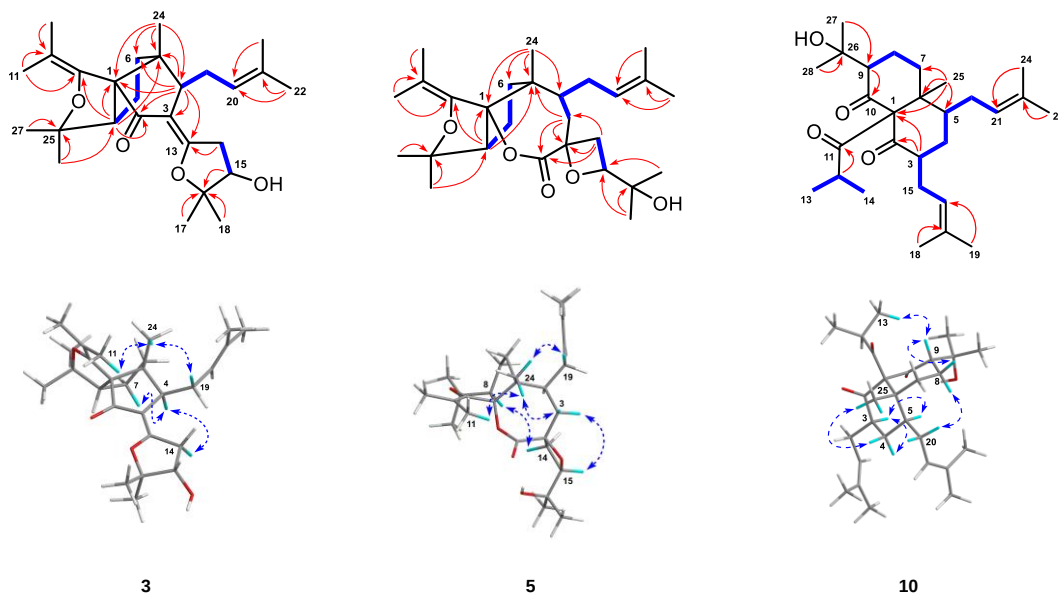


Figure S3. Key ^1H – ^1H COSY (bold), HMBC (arrows), and NOESY (double-headed arrows) correlations of 3, 5, and 10.

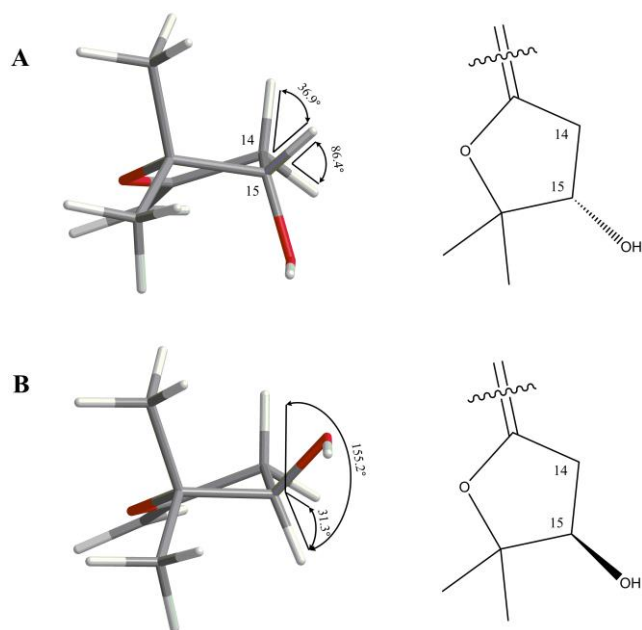


Figure S4. The dihedral angles of H-C(14)-C(15)-H in the optimized 3D structures (A: The β -oriented H-15 in **3**; B: The α -oriented H-15 in **3**).

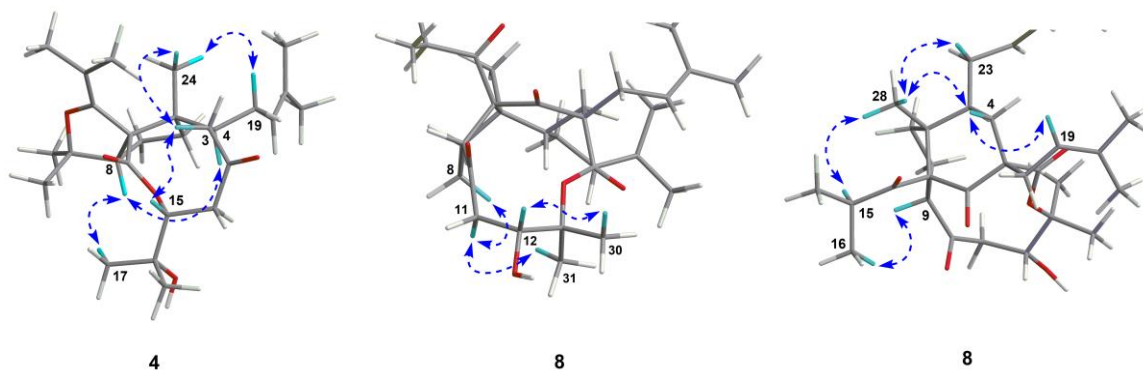


Figure S5. Key NOESY correlations of **4** and **8** (in different angles).

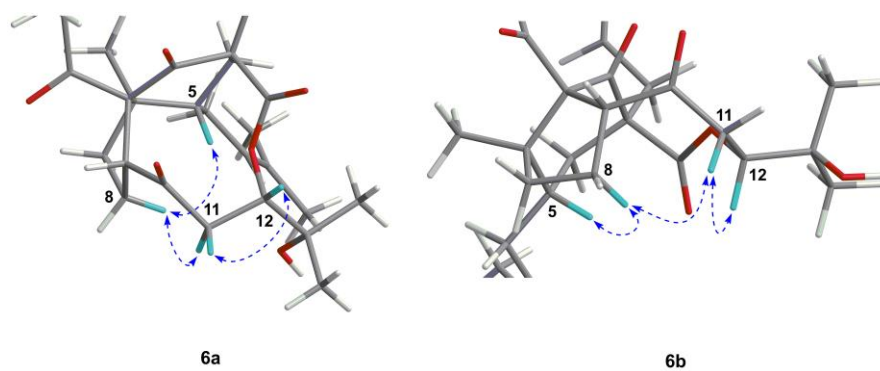


Figure S6. NOESY correlations of **6a** (12S*) and **6b** (12R*). The NOESY interactions of H-5/H-8 α , H-8 α /H-11 α , and H-11 β /H-12 were anticipated for **6a**.

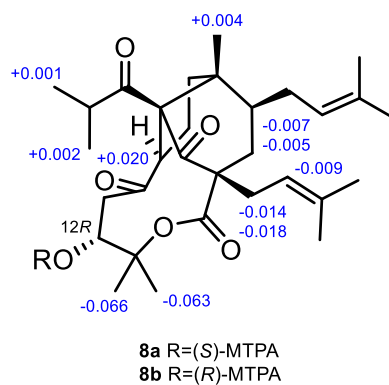


Figure S7. Values of $\delta_S - \delta_R$ for Mosher's MTPA esters of **8**.

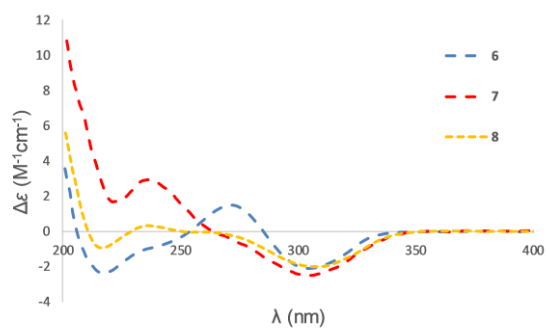


Figure S8. Experimental ECD (in MeOH) spectra of **6–8**.

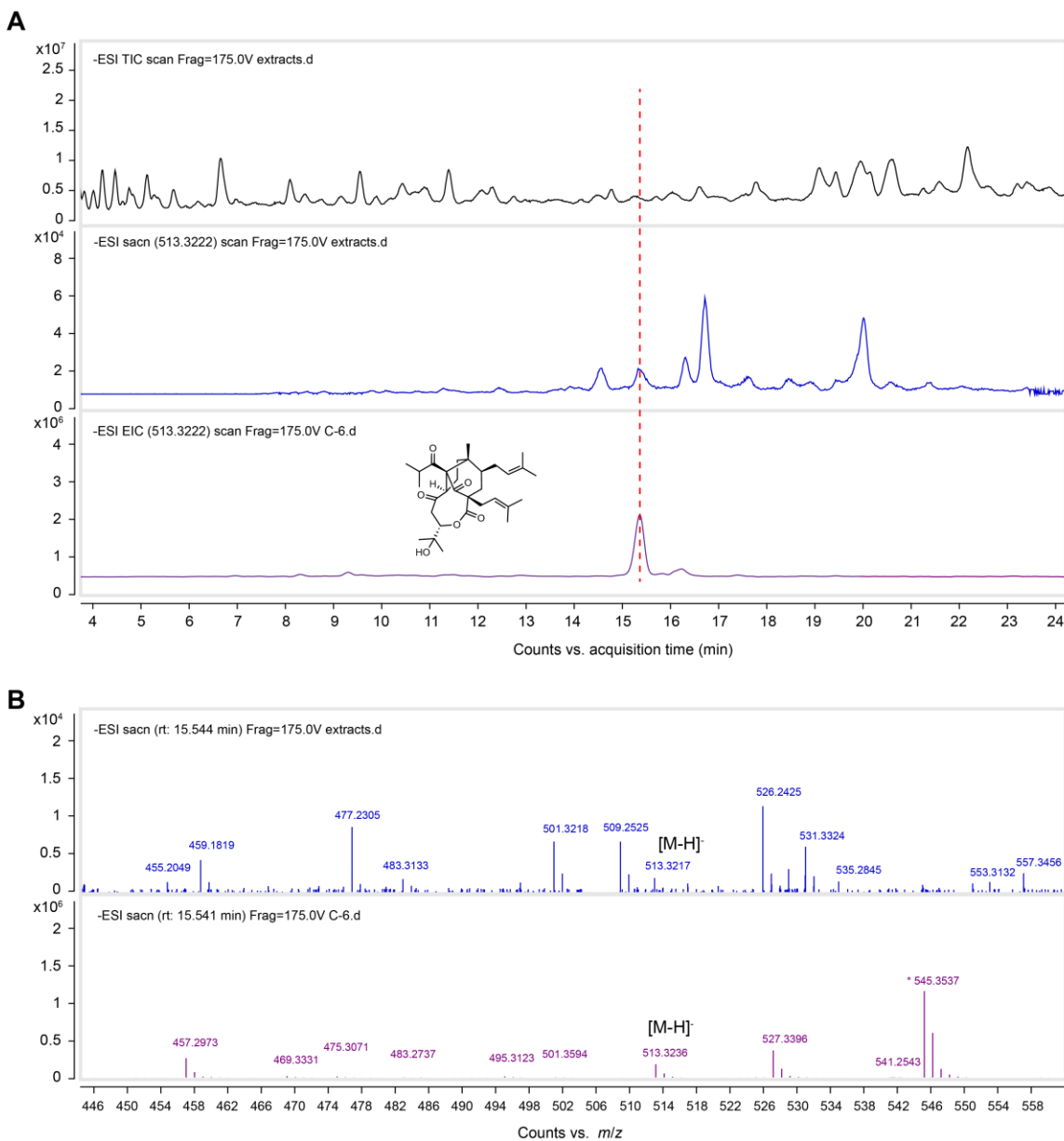


Figure S9. UPLC-ESI-QTOF-MS monitored compound **6** in the ethanolic crude extracts of fresh plant in negative ion source module. (A) Total ion current (TIC) of the crude extracts and extracted ion chromatogram (EIC) of the crude extracts and compound **6** at m/z 513.3222. (B) Mass spectra of peak at 15.5 min in the extracts and compound **6**.

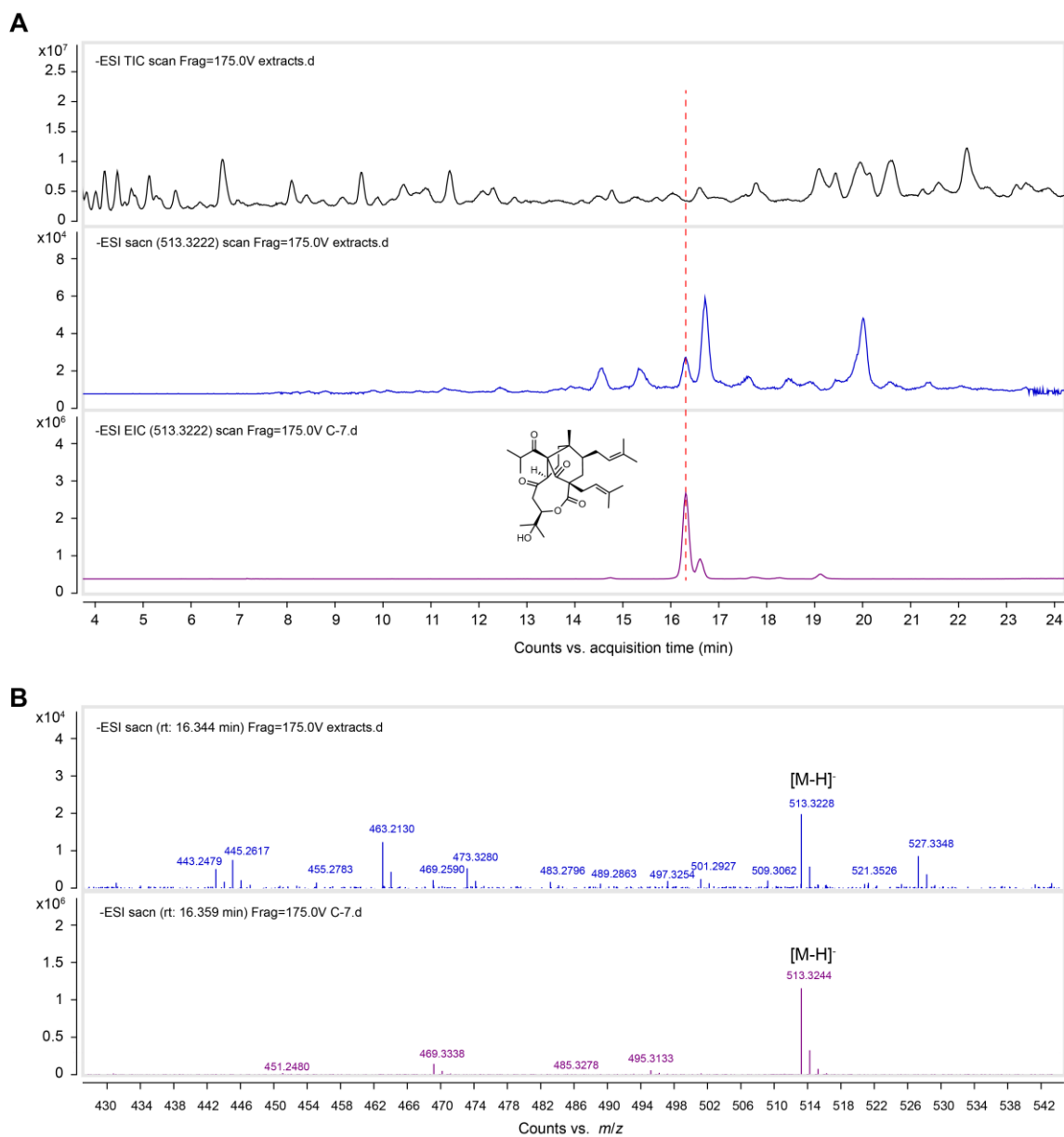


Figure S10. UPLC-ESI-QTOF-MS monitored compound **7** in the ethanolic crude extracts of fresh plant in negative ion source module. (A) TIC of the crude extracts and EIC of the crude extracts and compound **7** at m/z 513.3222. (B) Mass spectra of peak at 16.3 min in the extracts and compound **7**.

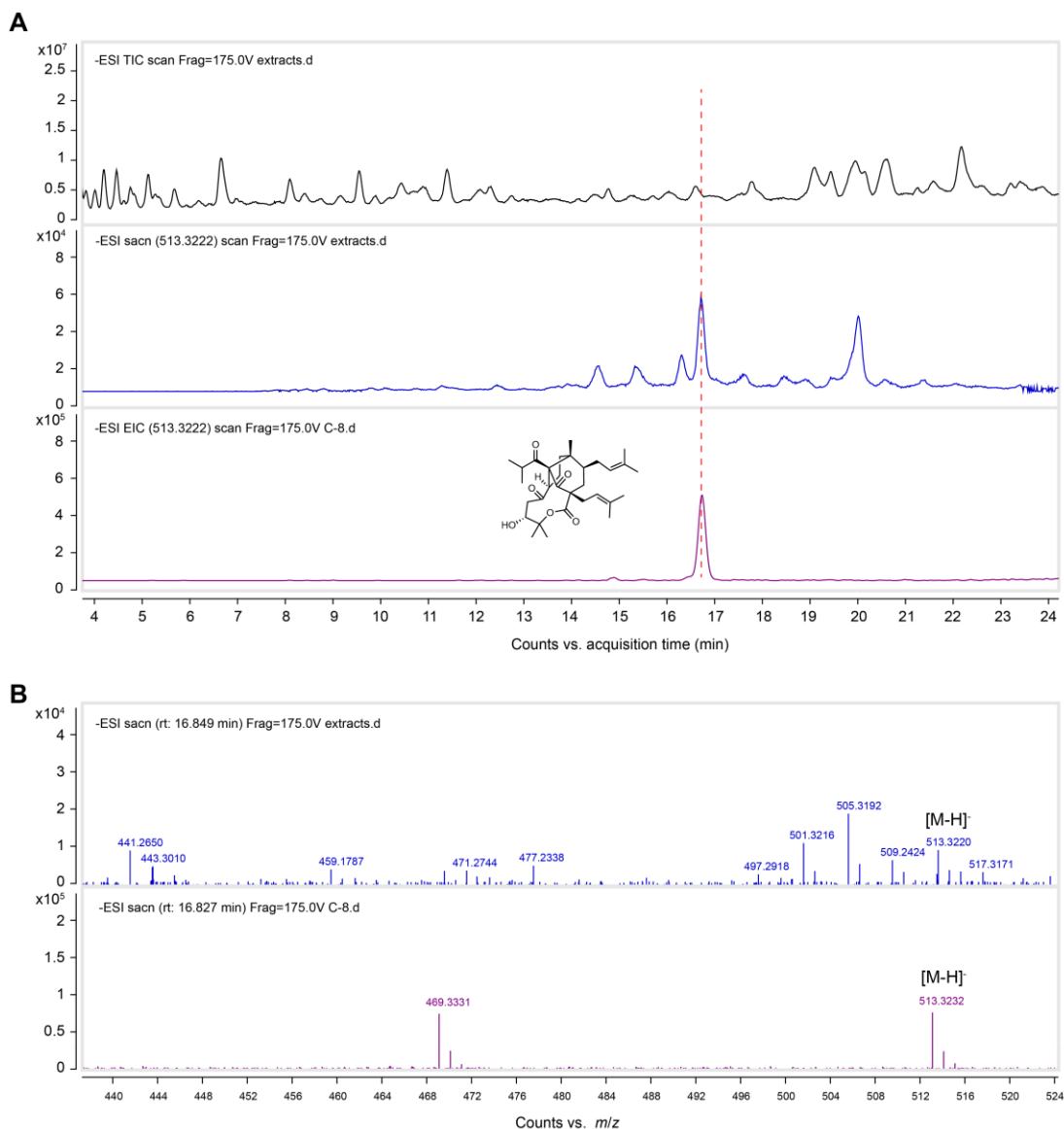


Figure S11. UPLC-ESI-QTOF-MS monitored compound **8** in the ethanolic crude extracts of fresh plant in negative ion source module. (A) TIC of the crude extracts and EIC of the crude extracts and compound **8** at m/z 513.3222. (B) Mass spectra of peak at 16.8 min in the extracts and compound **8**.

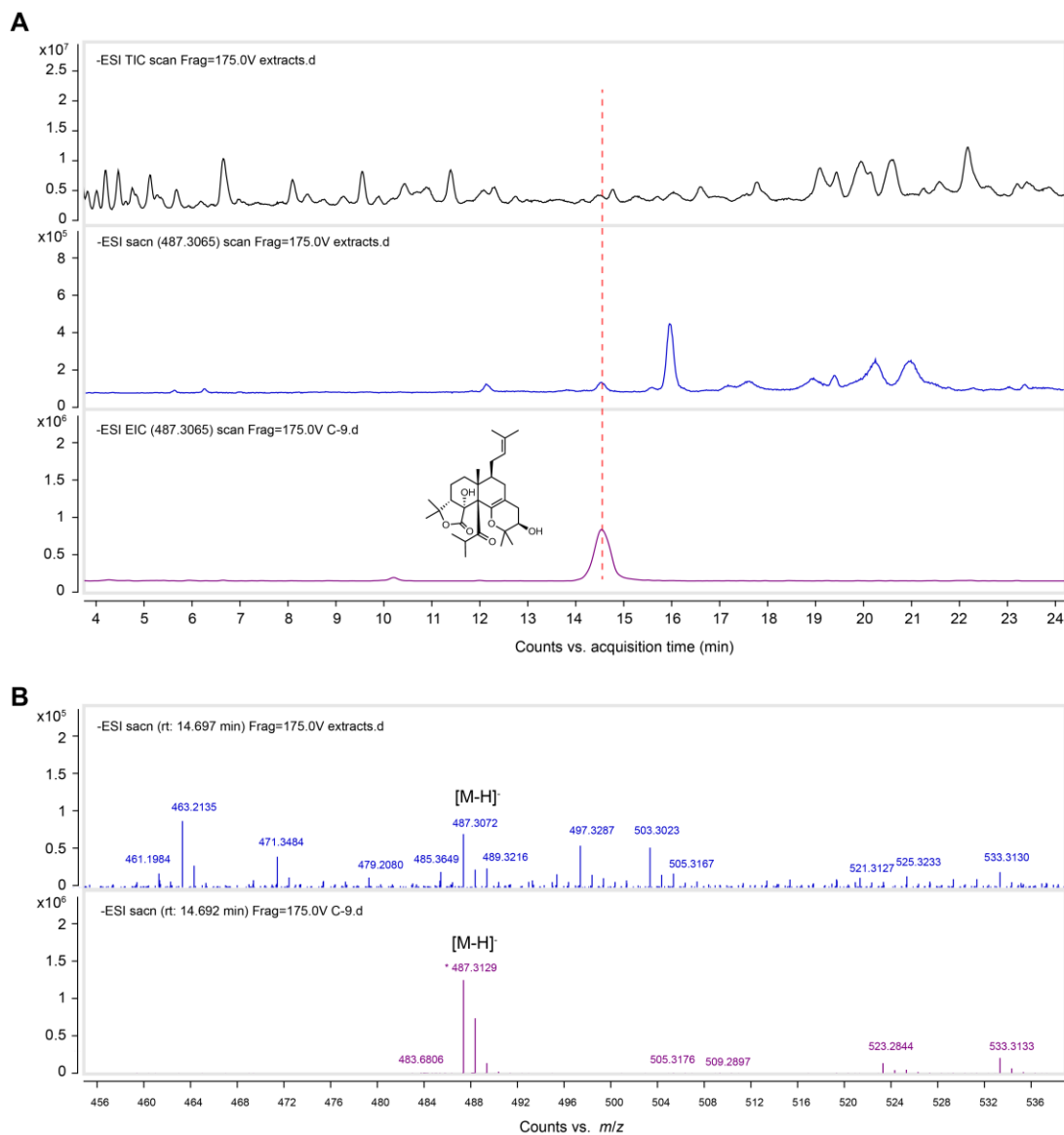


Figure S12. UPLC-ESI-QTOF-MS monitored compound **9** in the ethanolic crude extracts of fresh plant in negative ion source module. (A) TIC of the crude extracts and EIC of the crude extracts and compound **9** at m/z 487.3065. (B) Mass spectra of peak at 14.7 min in the extracts and compound **9**.

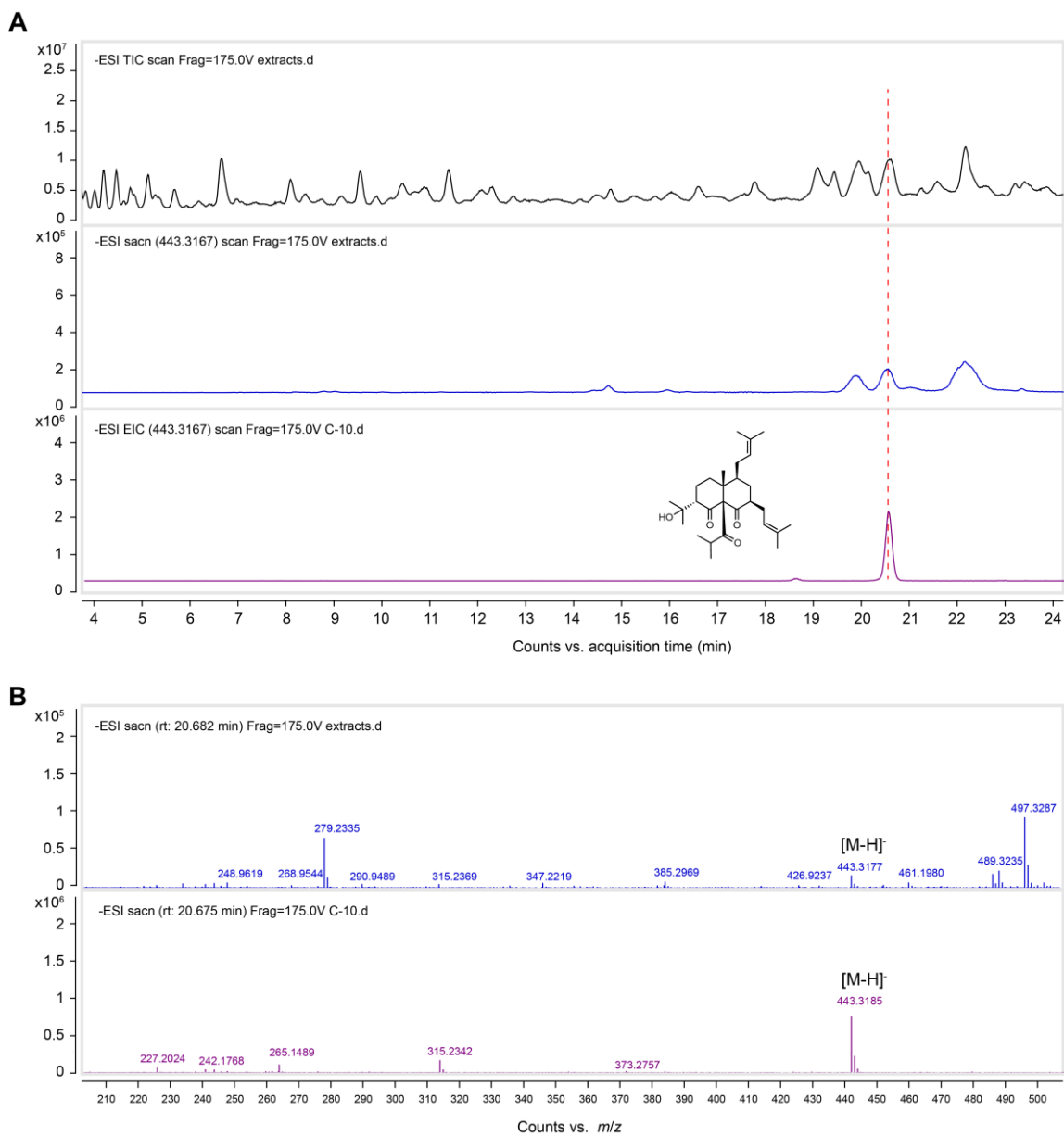


Figure S13. UPLC-ESI-QTOF-MS monitored compound **10** in the ethanolic crude extracts of fresh plant in negative ion source module. (A) TIC of the crude extracts and EIC of the crude extracts and compound **10** at m/z 443.3167. (B) Mass spectra of peak at 20.7 min in the extracts and compound **10**.

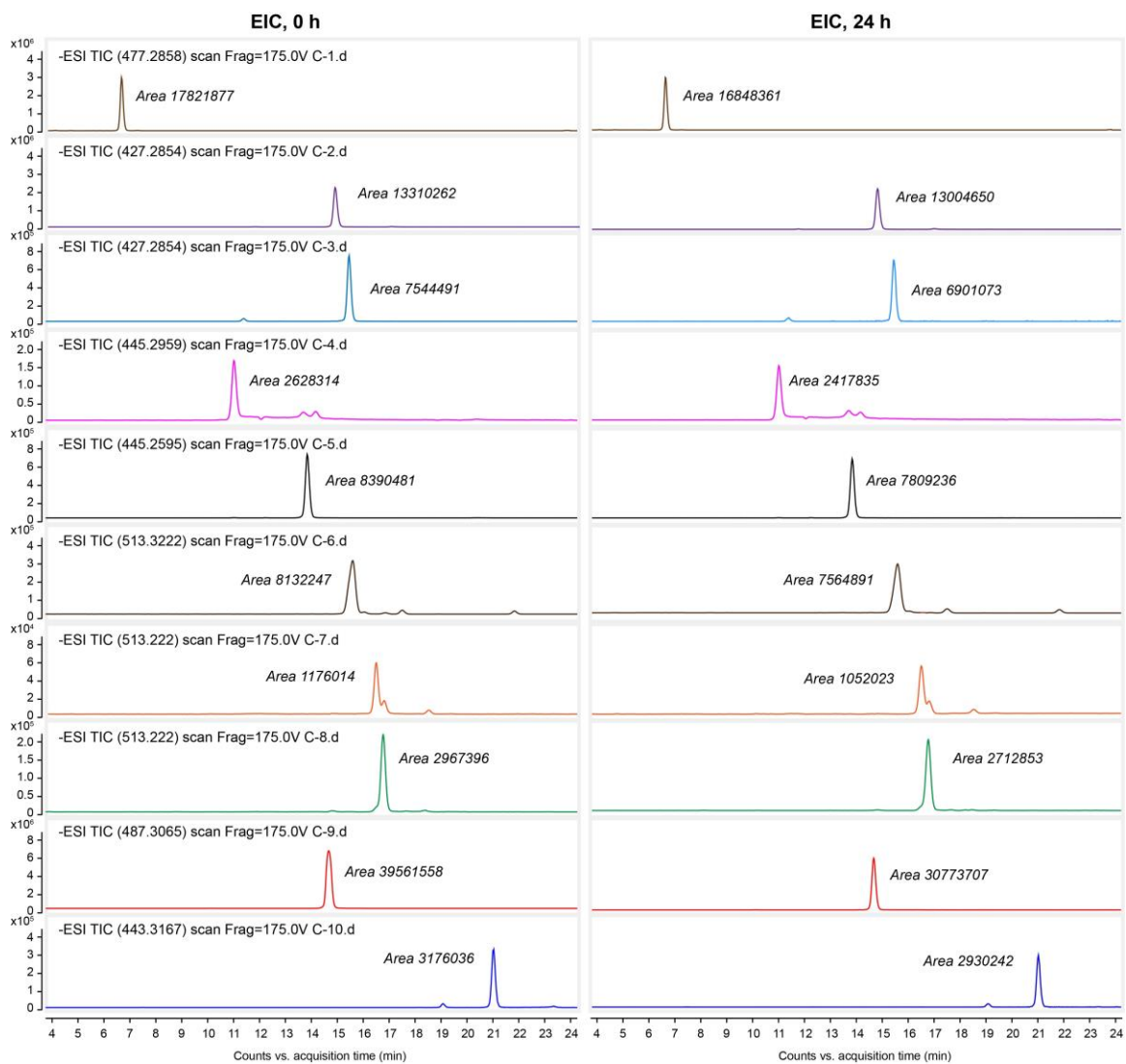


Figure S14. Detect the degradation of compounds **1–10** in aqueous solution by UPLC-ESI-QTOF-MS in negative ion source module. (A) EIC of the standard groups of **1–10** (0 h). (B) EIC of experimental groups of **1–10** (37 °C, 24 h). Italicized numbers in the graph indicate the peak areas of these compounds in EIC mode.

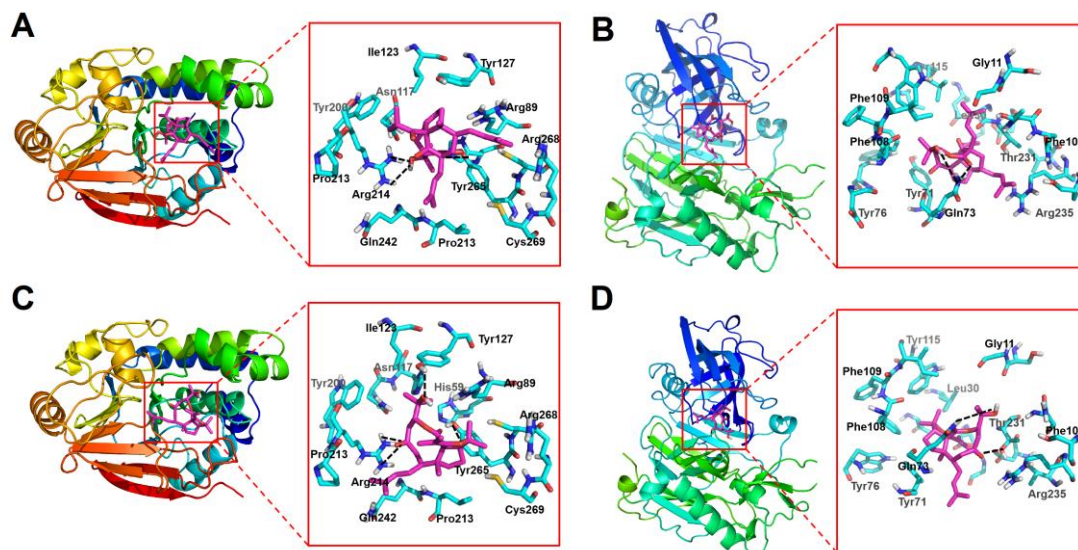


Figure S15. The molecular docking of PP2Ac and BACE1 for **6** and **4**. Low-energy binding conformations of compounds **6** and **4** bound to PP2Ac (A, C) and BACE1 (B, D) generated by virtual ligand docking. Compound was exhibited as the ball-and-stick model showing carbon (purple), hydrogen (grey) and oxygen (red). The key hydrogen bonding interactions with the enzymes were shown with the black line.

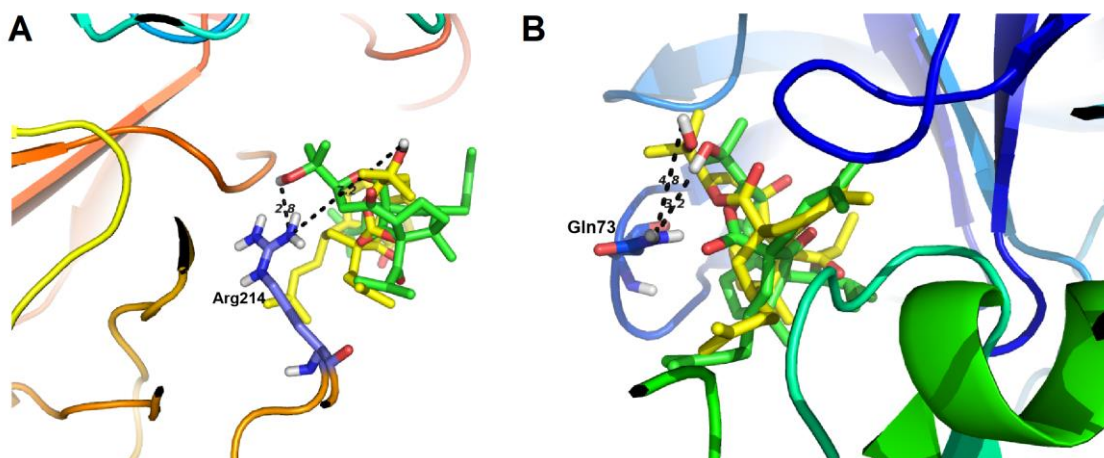


Figure S16. Key hydrogen bonds of compounds **6** (green) and **7** (yellow) with the residue Arg214 of PP2Ac (A) and Gln73 of BACE1 (B). The molecular docking showed the hydrogen bond distances as follows: **6** and Arg214, 2.8 Å; **7** and Arg214, 7.2 Å; **6** and Gln73, 3.2 Å; **7** and Gln73, 4.8 Å.

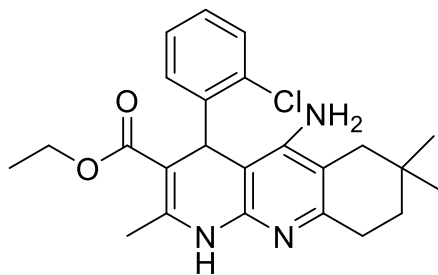


Figure S17. The structure of SCR1693.

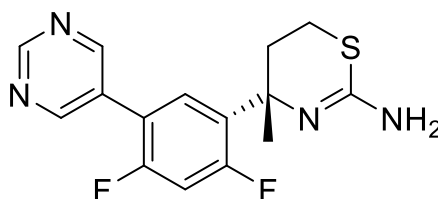


Figure S18. The structure of LY2811376.

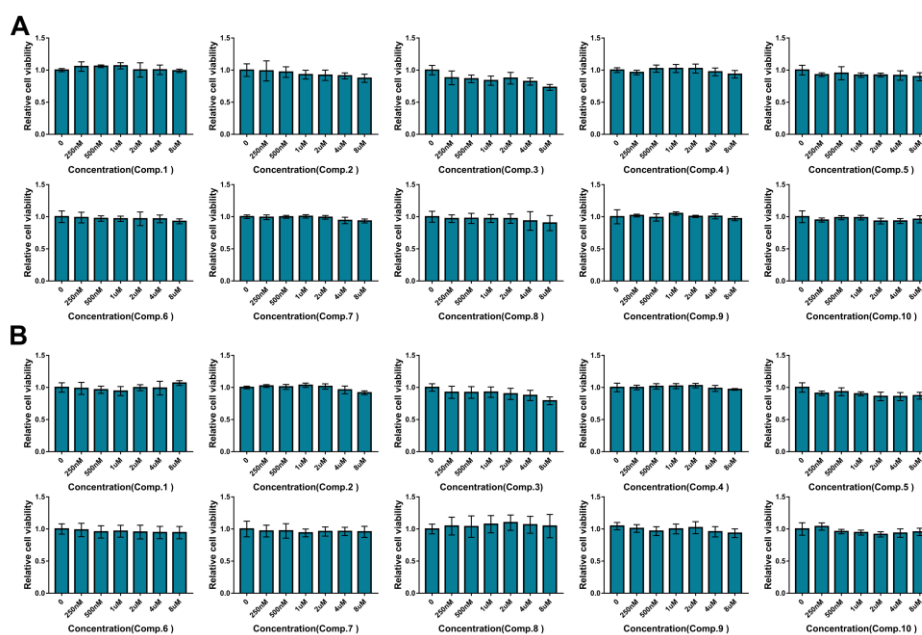


Figure S19. Cell viability after compounds treatment was assessed through CCK8 assay. (A) HEK293/tau cells were treated with 0, 0.25, 0.5, 1, 2, 4 and 8 μ M compounds **1–10** respectively. (B)

N2a/APP cells were treated with 0, 0.25, 0.5, 1, 2, 4 and 8 μ M compounds **1–10** respectively. Data is represented as mean $\pm$ S.E.M. Student t-test compared to cell treated with vehicle alone.

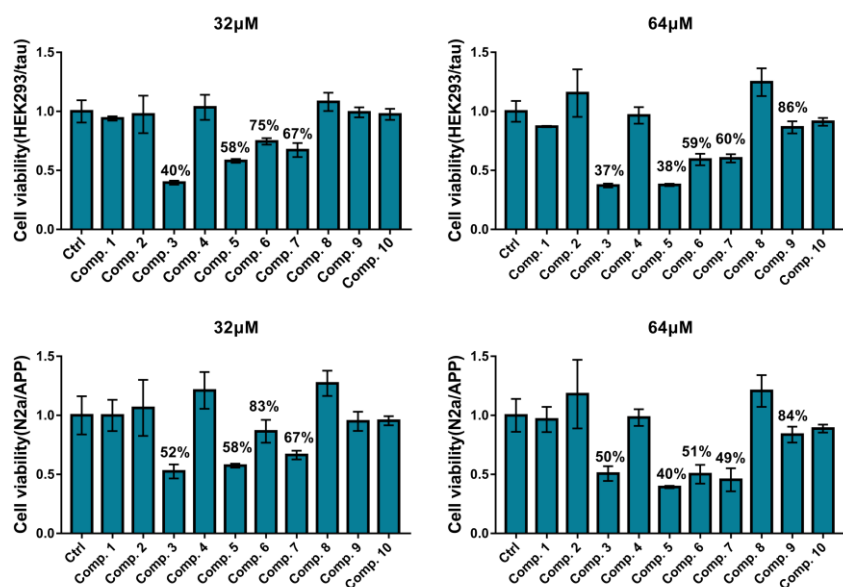


Figure S20. Cell viability after compounds treatment was assessed through CCK8 assay. HEK293/tau and N2a/APP cells were treated with 32 μ M and 64 μ M compounds **1–10**, respectively.

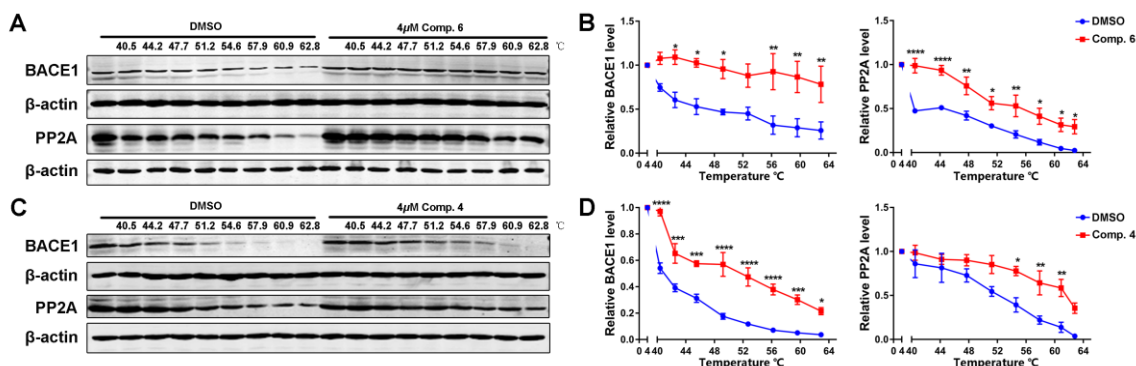


Figure S21. The CETSA confirmed the interaction between compounds and their targets in N2a/APP cell and HEK293/tau cell lysates. (A) Western blot and (B) CETSA curves for BACE1 and PP2A, with compound **6** measured in cell lysates. (C) Western blot and (D) CETSA curves for BACE1 and PP2A, with compound **4** measured in cell lysates. Data are represented as the mean $\pm$ S.E.M. **** p < 0.0001, *** p < 0.001, ** p < 0.01, * p < 0.05 versus the vehicle DMSO group.

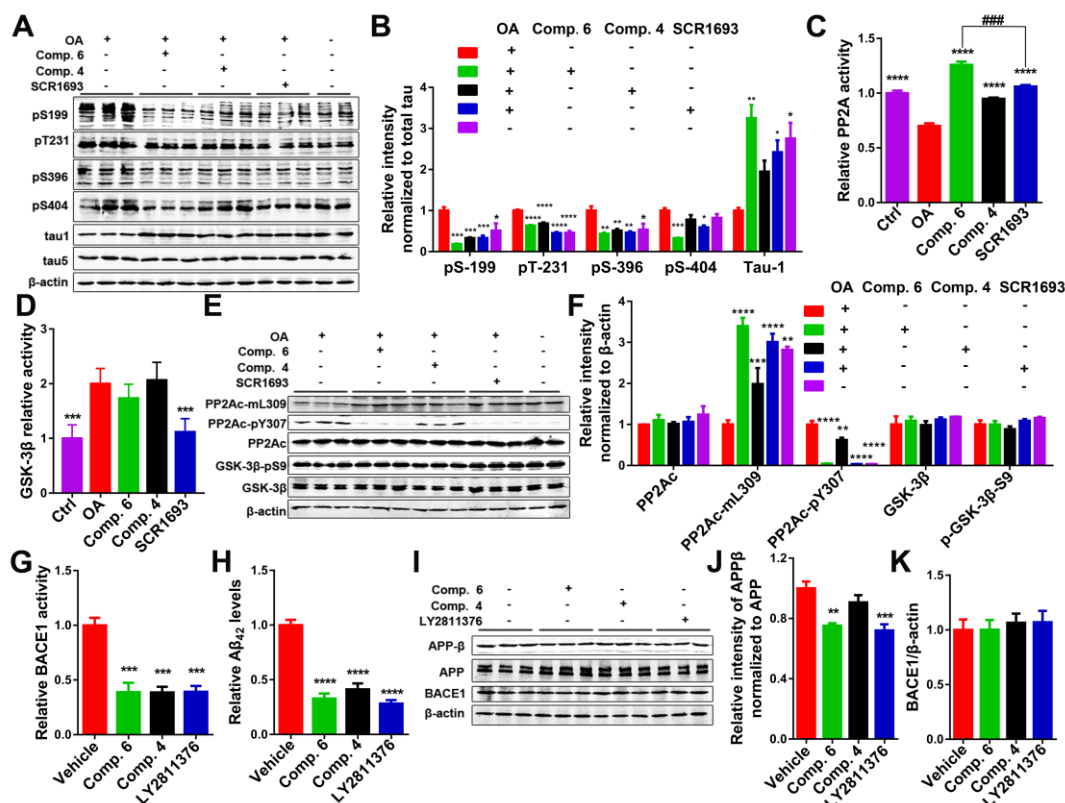


Figure S22. Compound treatment involving the regulation of tau phosphorylation and A β ₄₂ production *in vitro*. (A) Western blot and (B) quantitative analyses showing tau phosphorylation levels at Ser199, Thr231, Ser396 and Ser404, unphosphorylated tau recognized by tau1, and total tau recognized by tau5 in OA-induced HEK293/tau cells treated with compounds 6 (100 nM) and 4 (140 nM). (C) PP2A activity and (D) GSK-3 β activity were determined using an activity assay kit. (E) Western blot showing the inhibitory phosphorylation (PP2Ac-pY307), activated methylation (PP2Ac-mL309) and total levels of PP2Ac, the inhibitory phosphorylation (GSK-3 β -pS9) and total levels of GSK-3 β , and (F) their quantitative analysis normalized to β -actin. (G) BACE1 activity was determined using a β -secretase activity assay kit. (H) A β ₄₂ protein level was determined using a mouse A β ₁₋₄₂ ELISA kit. (I) Western blot showing β -cleavage of APP (APP- β), the total level of APP and BACE1 in N2a/APP cells treated with 6 and 4, and LY2811376 as the positive control. (J) Statistical analyses of APP- β normalized to APP. and (K) BACE1 normalized to β -actin. Data are represented as the mean $\pm$ S.E.M. **** p < 0.0001, *** p < 0.001, ** p < 0.01, * p < 0.05 versus the vehicle or OA group, ### p < 0.001, Comp. 6 group versus the positive control group.

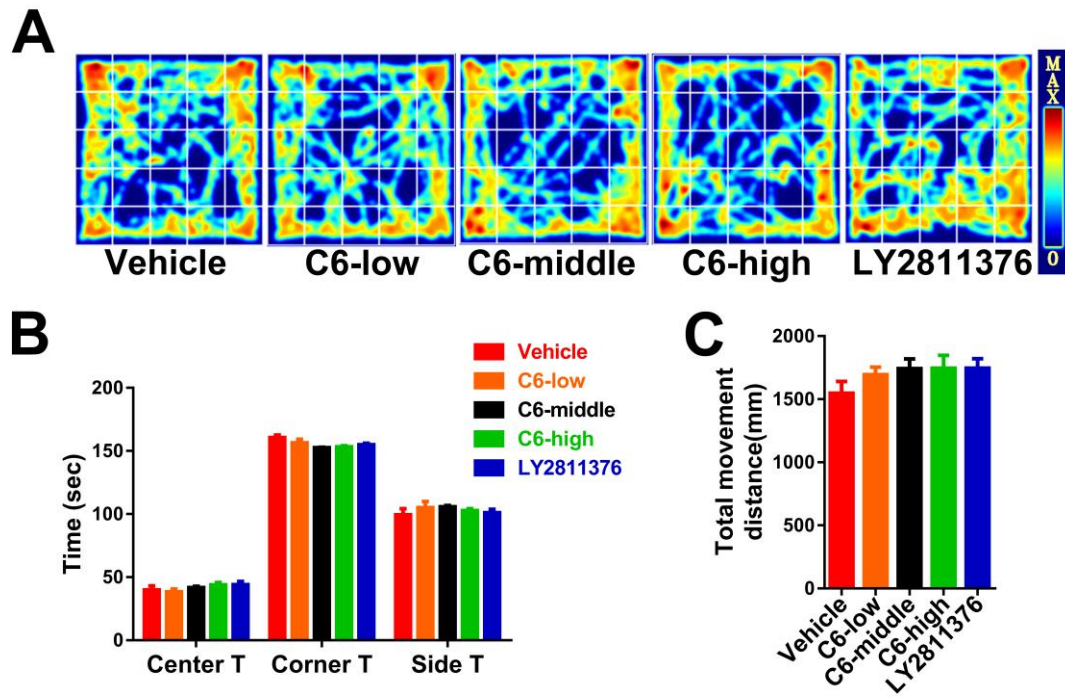


Figure S23. Compound treatment didn't affect anxiety and exploratory activity. (A) Walking tracks of the open field (OF) test. (B) Statistical analyses of the OF test, total moving distance was recorded to assess the motor function of animals. (C) Time spent in the center (Center T), corner (Corner T) and side (Side T) were recorded to assess the anxiety and exploratory activity of animals.

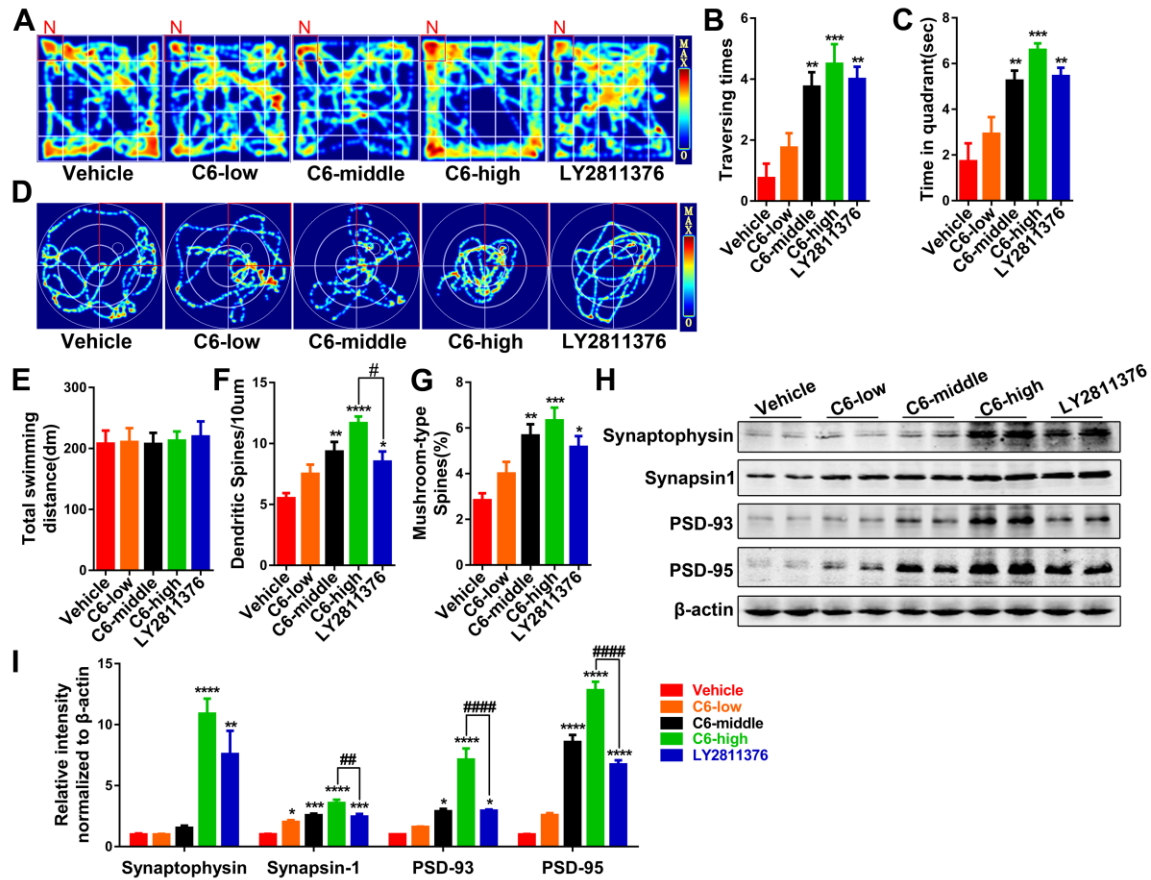


Figure S24. 3 × Tg AD mice treated with compound 6 [C6-low (0.725 μg/μL × 5 μL), C6-middle (2.9 μg/μL × 5 μL), C6-high (11.6 μg/μL × 5 μL)] and LY2811376 (2 μg/μL × 5 μL) improved learning and memory. (A) Walking tracks of the NOR test (N: region for novel object). (B) Times to cross the platform region, (C) time spent in the target quadrant, (D) swimming tracks and (E) total swimming distance during the MWM testing were recorded. (F and G) Quantification of primary dendrites in the hippocampal CA3 region. (H) Western blot and (I) quantitative analyses showing the levels of synaptic associated proteins. Data are represented as the mean ± S.E.M. *****p* < 0.0001, ****p* < 0.001, ***p* < 0.01, **p* < 0.05 versus the vehicle group, #####*p* < 0.0001, ###*p* < 0.01, #*p* < 0.05 C6-high group versus the positive control group.

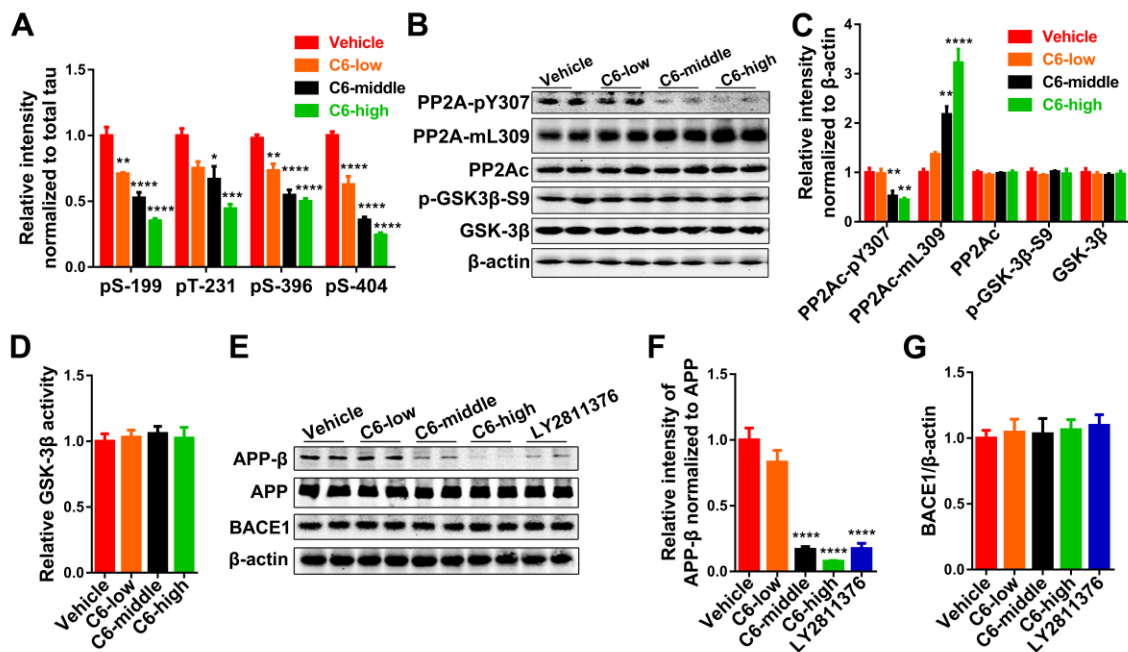


Figure S25. Compound treatment regulated PP2A and BACE1 activity *in vivo*. (A) The quantitative analysis of tau phosphorylation levels normalized to tau5. (B) Western blot showing the inhibitory phosphorylation (PP2Ac-pY307), activated methylation (PP2Ac-mL309) and total levels of PP2Ac, the inhibitory phosphorylation (GSK-3β-pS9) and total levels of GSK-3β, and (C) their quantitative analysis normalized to β-actin. (D) GSK-3β activity was determined using the Activity Assay Kit. (E) Western blot analysis of protein levels of APP-β, APP, and BACE1. (F) Statistical analyses of APP-β normalized to APP and (G) BACE1 normalized to β-actin. Data are represented as the mean ± S.E.M. **** $p < 0.0001$, *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$ versus the vehicle group.

METHODS AND MATERIALS

General: Optical rotations were determined with a PerkinElmer 341 polarimeter (PerkinElmer Inc., Fremont, California, USA) and melting points were recorded on an X-5 microscopic melting point apparatus. The UV, ECD, and IR spectra were measured using a Lambda 35 instrument (PerkinElmer Inc., Fremont, California, USA), a JASCO-810 ECD spectrometer (JASCO, Tokyo, Japan), and a Bruker Vertex 70 (Bruker, Karlsruhe, Germany) instrument, respectively. The NMR spectra were recorded on a Bruker AM-400, AV-600, and AV-800 spectrometers. The ^1H and ^{13}C NMR chemical shifts were referenced to the solvent or solvent impurity peaks for CD_3OD (δ_{H} 3.31 and δ_{C} 49.0), CDCl_3 (δ_{C} 77.0 and δ_{H} 7.26), $\text{C}_5\text{D}_5\text{N}$ (δ_{H} 7.19 and δ_{C} 123.5), and $\text{DMSO}-d_6$ (δ_{H} 2.50 and δ_{C} 39.5). HRESIMS data were obtained in the positive ion mode on a Bruker MicrOTOF II and Solarix 7.0 (Bruker, Karlsruhe, Germany) spectrometers. Semipreparative HPLC was carried out using a Dionex HPLC system equipped with an Ultimate 3000 pump, an Ultimate 3000 autosampler injector, and an Ultimate 3000 DAD detector controlled by Chromeleon software (version 6.80), using a reversed-phase C_{18} column (5 μm , 10 $\times$ 250 mm, Welch Ultimate XB- C_{18}) and an Ultimate SiO_2 column (5 μm , 10 $\times$ 250 mm, Welch Ultimate). Column chromatography (CC) was performed using silica gel (100–200 and 200–300 mesh; Qingdao Marine Chemical Inc., China), ODS (50 μm , YMC Co. Ltd., Japan), MCI gel (75–150 μm , Merck, Germany), and Sephadex LH-20 (GE Healthcare Bio-Sciences AB, Sweden).

Plant Material. The aerial parts of *H. perforatum* L were collected from the Shennongjia Forestry District, Hubei province, People's Republic of China, in August 2014. The plants were identified by Professor C. G. Zhang at the School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology (TJMU). A voucher specimen (no. HP20140826) was deposited in the herbarium of Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, TJMU.

Extraction and Isolation. The air-dried aerial parts of *H. perforatum* L (105 kg) were powdered and extracted with 95% EtOH (3 $\times$ 105 L) to afford a residue under vacuum, and the crude extract was sequentially suspended in H_2O and partitioned with CH_2Cl_2 . The CH_2Cl_2 fraction (3.8 kg) was fractionated to seven fractions (A–G) by silica gel column chromatography (CC, 100–200 mesh; 5kg;

20.0 × 120.0 cm) eluting with a gradient of petroleum ether–acetone (50:1–0:1). Fr. C (203.04 g) was subjected to MCI gel column (MeOH–H₂O from 90:10 to 100:0) to remove pigment, and subsequently loaded onto a RP C₋₁₈ column (MeOH–H₂O, from 50: 50 to 100: 0) to yield eight subfractions, C1–C8.

Fr. C5 (13.13 g) was chromatographed on a silica gel column, eluted with petroleum ether–acetone (from 30:1 to 0:1) to yield eleven fractions (Fr. C5a–C5k). Fr. C5e (0.89 g) was subjected to Sephadex LH-20 (MeOH) and was further purified repeatedly by semi-preparative HPLC (CH₃CN–H₂O, 80%, 2 mL/min) to afford **2** (4.5 mg, *t_R* 47.0 min) and **6** (9.4 mg, *t_R* 54.5 min). Fr. C5d (1.45 g) was separated with Sephadex LH-20 (MeOH) and then separated on an ODS RP C₋₁₈ column (MeOH–H₂O, from 50: 50 to 100: 0) to afford five fractions. C5d2 was further purified repeatedly by semi-preparative HPLC to afford **4** (CH₃CN–H₂O, 80%, 2 mL/min, 22.8 mg, *t_R* 13.2 min), **3** (CH₃OH–H₂O, 90%, 2 mL/min, 3.5 mg, *t_R* 14.1 min), **5** (CH₃CN–H₂O, 95%, 2 mL/min, 4.5 mg, *t_R* 5.6 min), and **9** (CH₃OH–H₂O, 100%, 2 mL/min, 13.1 mg, *t_R* 9.4 min).

Fr. C6 (19.23 g) was separated with a silica gel column and eluted with petroleum ether–EtOAc (from 30:1 to 0:1) to give eight subfractions, Fr. C6a–Fr. C6h. Fr. C6c (3.56 g) was subjected to an ODS RP-C₁₈ column (MeOH–H₂O, 60%–90%) and further purified by semipreparative HPLC (hexane–EtOH, 98%, 2 mL/min) to afford **7** (5.6 mg, *t_R* 22.1 min). Fr. C6d (2.74 g) was subjected to an ODS RP-C₁₈ column (MeOH–H₂O, 60%–80%) to yield nine fractions (Fr. C6d1–C6d9). Fr. C6d2 was further purified by semipreparative HPLC (CH₃OH–H₂O, 89%, 2 mL/min) to afford **1** (1.4 mg, *t_R* 23.4 min). Fr. C6d5 was further purified by semipreparative HPLC (CH₃CN–H₂O, 85%, 2 mL/min) to afford **8** (15.3mg, *t_R* 18.1 min).

Fr. C7 (19.13 g) was separated on an ODS RP C₋₁₈ column (MeOH–H₂O, from 60: 40 to 100: 0) to afford six fractions (Fr. C7a–C7f). Fr. C7d (12.38 g) was chromatographed on a silica gel column, eluted with petroleum ether–EtOAc (from 80:1 to 0:1) to yield four fractions (Fr. C7d1–C7d4). Fr. C7d2 was subjected to an ODS RP C₋₁₈ column (MeOH–H₂O, from 70: 30 to 100: 0) and was further purified repeatedly by semi-preparative HPLC (*n*-hexane–EtOH, 98%, 2 mL/min) to afford **10** (2.6 mg, *t_R* 9.3 min).

Compound 1: Colorless crystals, mp 190–192 °C; $[\alpha]_{\text{D}}^{27}$ –10.1 ($c = 0.1$, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$) = 202 (3.87) nm; ECD (MeOH) λ_{max} ($\Delta\epsilon$) 219 (+0.45), 276 (–1.01) nm; IR (KBr) ν_{max} = 3424, 2927, 1699, 1612, 1382, 1129 cm^{-1} ; for ^1H and ^{13}C NMR data see Tables S1 and S3; HRESIMS $[\text{M} + \text{Na}]^+$ m/z 501.2824 (calcd for $\text{C}_{27}\text{H}_{42}\text{O}_7\text{Na}$, 501.2823)

Compound 2: Colorless gum, $[\alpha]_{\text{D}}^{26}$ –144.4 ($c = 0.5$, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$) = 203 (4.23) and 278 (4.01) nm; ECD (MeOH) λ_{max} ($\Delta\epsilon$) 207 (–17.08), 270 (–8.24), 323 (–1.13) nm; IR (KBr) ν_{max} = 3438, 1649, 1605, 1420, 1136 cm^{-1} ; for ^1H and ^{13}C NMR data see Tables S1 and S3; HRESIMS $[\text{M} + \text{H}]^+$ m/z 429.2982 (calcd for $\text{C}_{27}\text{H}_{41}\text{O}_4$, 429.2999)

Compound 3: Colorless oil, $[\alpha]_{\text{D}}^{26}$ –29.2 ($c = 0.3$, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$) = 203 (4.27) and 286 (4.24) nm; ECD (MeOH) λ_{max} ($\Delta\epsilon$) 203 (–12.58), 290 (+2.31) nm; IR (KBr) ν_{max} = 3436, 2972, 2925, 1680, 1596, 1454, 1303, 1134 cm^{-1} ; for ^1H and ^{13}C NMR data see Tables S1 and S3; HRESIMS $[\text{M} + \text{H}]^+$ m/z 429.3009 (calcd for $\text{C}_{27}\text{H}_{41}\text{O}_4$, 429.2999)

Compound 4: Colorless oil, $[\alpha]_{\text{D}}^{21}$ +68.9 ($c = 0.9$, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$) = 204 (4.22) nm; ECD (MeOH) λ_{max} ($\Delta\epsilon$) 207 (–6.68), 242 (–2.16), 289 (+3.65) nm; IR (KBr) ν_{max} = 3450, 2976, 1734, 1696, 1462, 1158 cm^{-1} ; for ^1H and ^{13}C NMR data see Tables S1 and S3; HRESIMS $[\text{M} + \text{H}]^+$ m/z 447.3113 (calcd for $\text{C}_{27}\text{H}_{43}\text{O}_5$, 447.3105)

Compound 5: Colorless oil, $[\alpha]_{\text{D}}^{26}$ –66.4 ($c = 0.3$, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$) = 205 (3.98) nm; ECD (MeOH) λ_{max} ($\Delta\epsilon$) 213 (–9.00), 237 (+0.89) nm; IR (KBr) ν_{max} = 3350, 2976, 2927, 1784, 1682, 1457, 1378, 1139 cm^{-1} ; for ^1H and ^{13}C NMR data see Tables S1 and S3; HRESIMS $[\text{M} + \text{Na}]^+$ m/z 469.2935 (calcd for $\text{C}_{27}\text{H}_{42}\text{O}_5\text{Na}$, 469.2924)

Compound 6: Colorless crystals, mp 155–157 °C; $[\alpha]_{\text{D}}^{26}$ –30.0 ($c = 0.8$, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$) = 202 (4.19) nm; ECD (MeOH) λ_{max} ($\Delta\epsilon$) 217 (–2.37), 272 (+1.49), 304 (–2.11) nm; IR (KBr) ν_{max} = 3436, 1737, 1703, 1626, 1452, 1383 cm^{-1} ; for ^1H and ^{13}C NMR data see Tables S2 and S4; HRESIMS $[\text{M} + \text{Na}]^+$ m/z 537.3182 (calcd for $\text{C}_{31}\text{H}_{46}\text{O}_6\text{Na}$, 537.3187)

Compound 7: Colorless oil, $[\alpha]_{\text{D}}^{22}$ –15.2 ($c = 0.4$, MeOH); UV (MeOH) λ_{max} ($\log \epsilon$) = 202 (4.11) nm; ECD (MeOH) λ_{max} ($\Delta\epsilon$) 237 (+2.93), 306 (–2.51) nm; IR (KBr) ν_{max} = 3449, 2974, 2927, 1749, 1698, 1629, 1451, 1382 cm^{-1} ; for ^1H and ^{13}C NMR data see Tables S2 and S4; HRESIMS $[\text{M} + \text{Na}]^+$ m/z

537.3196 (calcd for C₃₁H₄₆O₆Na, 537.3187)

Compound 8: Colorless oil, $[\alpha]_D^{24}$ -22.3 ($c = 0.9$, MeOH); UV (MeOH) $\lambda_{\max}$ ($\log \epsilon$) = 203 (3.96) nm; ECD (MeOH) $\lambda_{\max}$ ($\Delta\epsilon$) 217 (-0.94), 308 (-2.02) nm; IR (KBr) $\nu_{\max} = 3439, 2968, 2927, 1739, 1706, 1628, 1453, 1382$ cm⁻¹; for ¹H and ¹³C NMR data see Tables S2 and S4; HRESIMS $[M + H]^+$ m/z 515.3375 (calcd for C₃₁H₄₇O₆, 515.3367)

Compound 9: Colorless crystals; mp 175–176 °C; $[\alpha]_D^{14}$ $+60.9$ (c 0.6, MeOH); UV (MeOH) $\lambda_{\max}$ ($\log \epsilon$) = 204 (4.18) nm; ECD (MeOH) $\lambda_{\max}$ ($\Delta\epsilon$) 223 ($+2.60$), 303 ($+2.57$) nm; IR (KBr) $\nu_{\max}$ 3492, 2975, 2929, 1778, 1695, 1677, 1469, 1378, 1077 cm⁻¹; ¹H and ¹³C NMR data, see Tables S2 and S4; HRESIMS: m/z 489.3190 $[M + H]^+$ (calcd for C₂₉H₄₅O₆, 489.3211).

Compound 10: Colorless crystals; mp 101–102 °C; $[\alpha]_D^{27}$ -110.0 (c 0.3, MeOH); UV (MeOH) $\lambda_{\max}$ ($\log \epsilon$) = 202 (3.95) nm; ECD (MeOH) $\lambda_{\max}$ ($\Delta\epsilon$) 203 ($+8.04$), 318 (-7.23) nm; IR (KBr) $\nu_{\max}$ 3434, 2973, 2928, 1695, 1457, 1380, 1144 cm⁻¹; ¹H and ¹³C NMR data, see Tables S2 and S4; HRESIMS: m/z 467.3142 $[M + Na]^+$ (calcd for C₂₈H₄₄O₄Na, 467.3132).

X-ray Crystallographic Analysis. Colorless crystal of **1**, **6**, **9**, **10** were obtained from MeOH–H₂O. The intensity data were collected at 100 K on a Bruker APEX DUO diffractometer equipped with an APEX II CCD using Cu K α radiation. Cell refinement and data reduction were performed with Bruker SAINT. The structures were solved by direct methods using SHELXS-97^[1], expanded using difference Fourier techniques, and refined by the program and full-matrix least-squares calculations. The non-hydrogen atoms were refined anisotropically, and hydrogen atoms were fixed at the calculated positions. Crystallographic data (excluding structure factor tables) for the reported structures have been deposited with the Cambridge Crystallographic Data Center (CCDC) as supplementary publications no. CCDC 1936567 for **1**, CCDC 1812029 for **6**, CCDC 1936569 for **9**, and CCDC 1936570 for **10**. Copies of the data can be obtained free of charge from the CCDC, 12 Union Road, Cambridge CB 1EZ, UK [fax: Int. +44(0) (1223) 336 033]; e-mail: deposit@ccdc.cam.ac.uk].

Crystal data of compound 1: C₂₇H₄₂O₇, $M = 478.60$, $a = 10.13810(10)$ Å, $b = 12.15220(10)$ Å, $c = 10.78530(10)$ Å, $\alpha = 90^\circ$, $\beta = 104.64^\circ$, $\gamma = 90^\circ$, $V = 1285.59(2)$ Å³, $T = 100(2)$ K, space group $P2_1$, $Z = 2$, $\mu(\text{Cu K}\alpha) = 0.713$ mm⁻¹, 30275 reflections measured, 5065 independent reflections ($R_{\text{int}} = 0.0225$).

The final R_1 values were 0.0257 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0658 ($I > 2\sigma(I)$). The final R_1 values were 0.0258 (all data). The final $wR(F^2)$ values were 0.0658 (all data). The goodness of fit on F^2 was 1.054. Flack parameter = 0.00(3).^[2]

Crystal data of compound 6: $C_{31}H_{46}O_6$, $M = 514.68$, $a = 10.7265(2)$ Å, $b = 15.4183(3)$ Å, $c = 16.9237(3)$ Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2798.92(9)$ Å³, $T = 100(2)$ K, space group $P2_12_12_1$, $Z = 4$, $\mu(\text{Cu K}\alpha) = 0.663$ mm⁻¹, 18027 reflections measured, 4965 independent reflections ($R_{int} = 0.0333$). The final R_1 values were 0.0315 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0791 ($I > 2\sigma(I)$). The final R_1 values were 0.0316 (all data). The final $wR(F^2)$ values were 0.0792 (all data). The goodness of fit on F^2 was 1.107. Flack parameter = 0.06(4).^[2]

Crystal data of compound 9: $C_{29}H_{44}O_6$, $M = 488.64$, $a = 11.4340(3)$ Å, $b = 11.8435(4)$ Å, $c = 20.1913(6)$ Å, $\alpha = 90^\circ$, $\beta = 95.0100(10)^\circ$, $\gamma = 90^\circ$, $V = 2723.83(14)$ Å³, $T = 100(2)$ K, space group $P2_1$, $Z = 4$, $\mu(\text{Cu K}\alpha) = 0.655$ mm⁻¹, 26357 reflections measured, 8708 independent reflections ($R_{int} = 0.0494$). The final R_1 values were 0.0563 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1465 ($I > 2\sigma(I)$). The final R_1 values were 0.0566 (all data). The final $wR(F^2)$ values were 0.1470 (all data). The goodness of fit on F^2 was 1.034. Flack parameter = 0.09(6).^[2]

Crystal data of compound 10: $C_{28}H_{44}O_4$, $M = 444.63$, $a = 6.98470(10)$ Å, $b = 43.8208(7)$ Å, $c = 8.69360(10)$ Å, $\alpha = 90^\circ$, $\beta = 90.0470(10)^\circ$, $\gamma = 90^\circ$, $V = 2660.89(6)$ Å³, $T = 296(2)$ K, space group $P2_1$, $Z = 4$, $\mu(\text{Cu K}\alpha) = 0.566$ mm⁻¹, 57480 reflections measured, 10576 independent reflections ($R_{int} = 0.0496$). The final R_1 values were 0.0688 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1955 ($I > 2\sigma(I)$). The final R_1 values were 0.0732 (all data). The final $wR(F^2)$ values were 0.1978 (all data). The goodness of fit on F^2 was 1.059. Flack parameter = 0.12(8).^[2]

Reference

- [1] Sheldrick, G. M.; Schneider, T. R. *Method. Enzymol.* **1997**, 277, 319–343.
- [2] H. Flack, G. Bernardinelli, *Chirality* **2008**, 20, 681-690.

Preparation of (S)- and (R)-MTPA Esters of 8. Hyperforone H (**8**) (0.5 mg) was dissolved in 2 mL of anhydrous CH_2Cl_2 . Dimethylaminopyridine (30 mg), triethylamine, and (R)-MTPA chloride (20 μL) were then added in sequence. The reaction mixture was stirred at room temperature for 2 h, and then

quenched by the addition of 1 mL of aqueous MeOH. The solvents were concentrated under reduced pressure, yielding a residue which was subjected to a small silica gel column eluted with petroleum ether–acetone (25:1) to provide the (S)-MTPA ester of **8** (1.2 mg). The (R)-MTPA derivative (1.0 mg) was prepared with (S)-MTPA chloride and purified in the same manner.

(S)-MTPA derivative of 8 (8a). ^1H NMR (CD_3OD , 600 MHz) δ_{H} 7.662–7.264 (10H, overlap, aromatic protons), 5.225 (1H, t, J = 7.7 Hz, H-19), 5.104 (1H, m, H-24), 4.283 (1H, dd, J = 11.9, 7.7 Hz, H-9), 2.655 (1H, dd, J = 13.8, 8.4 Hz, H-18a), 2.243 (1H, m, H-18b), 2.092 (1H, dd, J = 14.0, 2.0 Hz, H-4a), 1.935 (1H, t, J = 13.4 Hz, H-4b), 1.719 (3H, s, H-26), 1.488 (3H, s, H-31), 1.406 (3H, s, H-30), 1.237 (3H, d, J = 6.4 Hz, H-16), 1.127 (3H, d, J = 6.4 Hz, H-17), 0.957 (3H, s, H-28); HRESIMS m/z 753.3590 $[\text{M} + \text{Na}]^+$ (calcd for $\text{C}_{41}\text{H}_{53}\text{F}_3\text{NaO}_8$, 753.3590).

(R)-MTPA derivative of 8 (8b). ^1H NMR (CD_3OD , 600 MHz) δ_{H} 7.662–7.264 (10H, overlap, aromatic protons), 5.234 (1H, t, J = 7.7 Hz, H-19), 5.104 (1H, m, H-24), 4.263 (1H, dd, J = 11.9, 7.7 Hz, H-9), 2.669 (1H, dd, J = 14.1, 8.5 Hz, H-18a), 2.261 (1H, dd, J = 14.1, 7.2 Hz, H-18b), 2.099 (1H, dd, J = 14.0, 2.0 Hz, H-4a), 1.940 (1H, t, J = 13.4 Hz, H-4b), 1.722 (3H, s, H-26), 1.554 (3H, s, H-31), 1.469 (3H, s, H-30), 1.235 (3H, d, J = 6.4 Hz, H-16), 1.126 (3H, d, J = 6.4 Hz, H-17), 0.953 (3H, s, H-28); HRESIMS m/z 753.3592 $[\text{M} + \text{Na}]^+$ (calcd for $\text{C}_{41}\text{H}_{53}\text{F}_3\text{NaO}_8$, 753.3590).

HRESIMS of compound **8a**

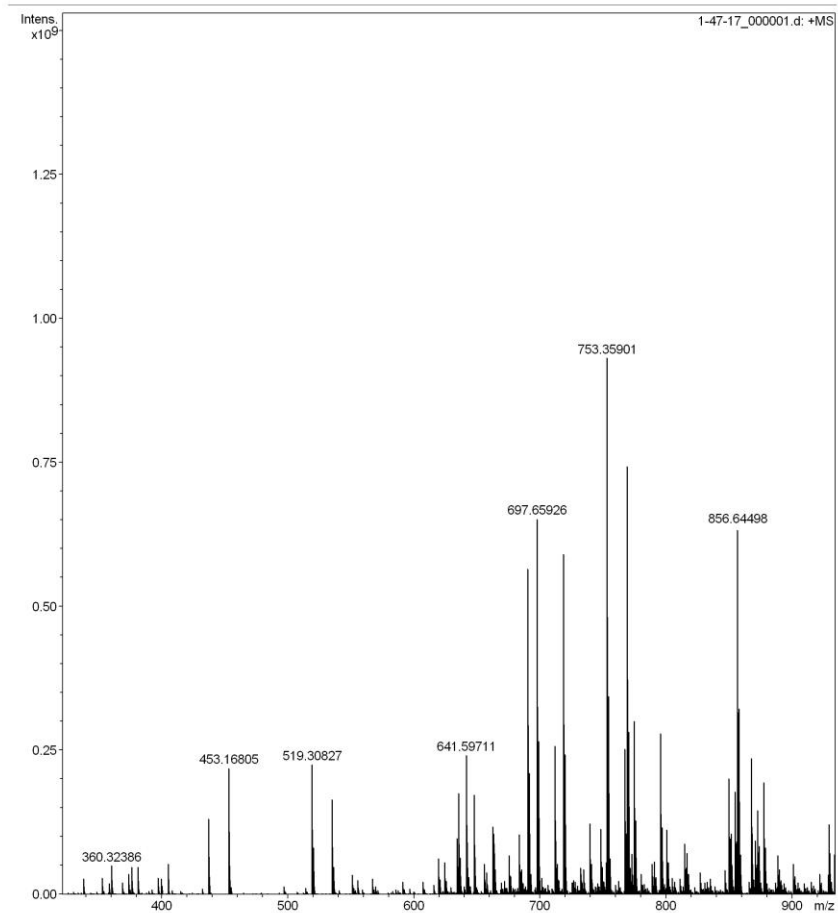
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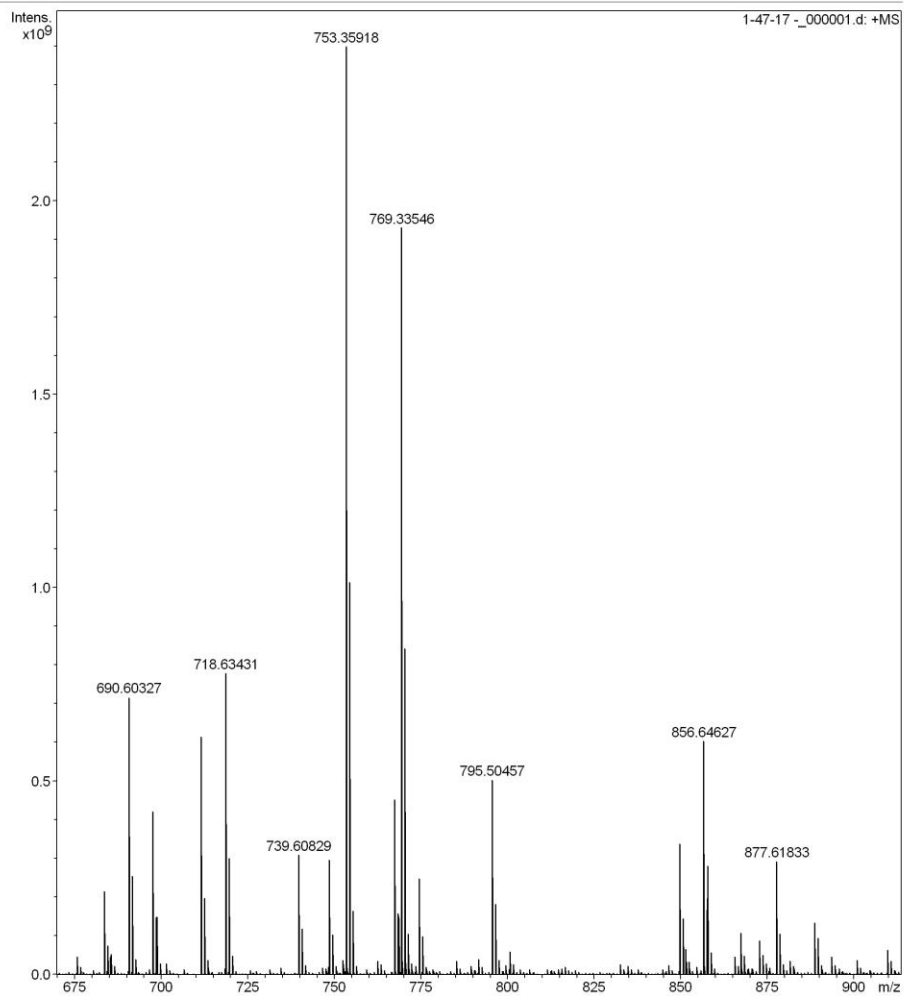
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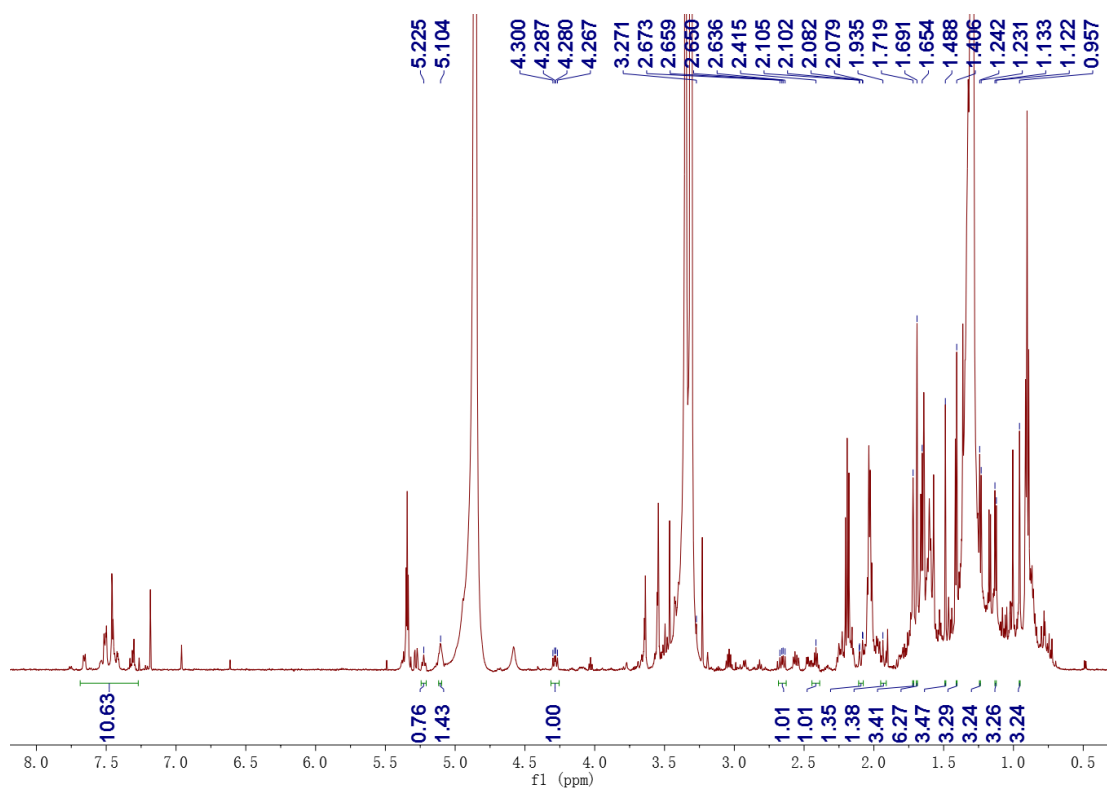
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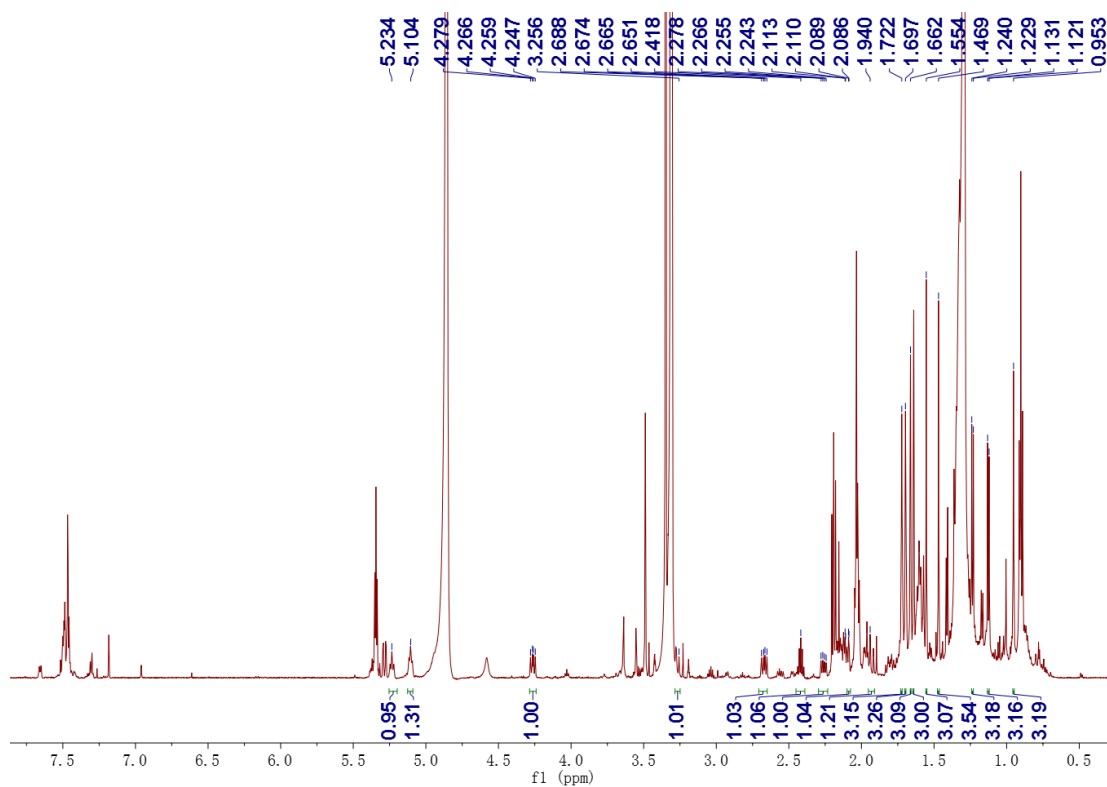
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^1H NMR of compound **8a** (600MHz, in CD_3OD)



^1H NMR of compound **8b** (600MHz, in CD_3OD)



Chemicals and Antibodies. LY2811376 and OA were purchased from Millipore (Temecula, CA, USA). SCR1693 was from Simovay (Nanjing, JS, China). Bicinchoninic acid (BCA) protein detection kit was from Pierce (Rockford, IL, USA). Reagents for cell culture were from Gibco BRL (Gaithersburg, MD, USA). Primary antibodies employed in this study are listed in Table S9. Secondary antibodies for western blotting were from Amersham Pharmacia Biotech (Little Chalfort, Buckinghamshire, UK).

Animal Experiments. Male 3 × Tg AD mice (APP^{swe}/PS1/TauP301L) were purchased from the Jackson Laboratory. The generation and characterization of the 3 × Tg AD mouse model, as well as the timing of disease progression, were previously described.^[3] All of the animal experiments were performed according to the ‘Policies on the Use of Animals and Humans in Neuroscience Research’. The animals were fed in a room under standard housing conditions (room temperature 24 to 27 °C, humidity 60–65% and 12 h light–dark cycle) with free access to food and water. The mice were aged 4 months and weighed 20 to 25 g. The mice were divided randomly into five groups (n = 10 in each). The mice were anesthetized with 6% chloral hydrate (6 mL/kg, i.p.) and different solutions (compound **6**-low (0.725 µg/µL × 5 µL), compound **6**-middle (2.9 µg/µL × 5 µL), compound **6**-high (11.6 µg/µL × 5 µL), LY2811376 (2 µg/µL × 5 µL), or DMSO 5 µL as vehicle) were infused very slowly into the cerebral ventricles of the mice every day at the same time for one month with cannulas implanted in the following coordinates: 0.2 mm anterior to posterior (AP) bregma, 0.9 mm midline to lateral (ML), and 2.3 mm dorsal to the ventral (DV) dura. 48 hours after the last administration, the behavioral tests were conducted. And then the pathological tests were also performed.

Open Field (OF) Tests. The animals were individually placed at the center of a 45 × 45 × 45 cm³ white acrylic box and left to freely move within it for 10 min. For all behavioral tests, data were gathered and analyzed with a video tracking system (HVS Imagen, UK). Room temperature was maintained at 20 °C.

Novel Object Recognition (NOR) Tests. NOR tests were performed a day after the OF test in a 45 × 45 × 45 cm³ white acrylic box. Animals were pre-trained to habituate to the box for two consecutive days, without objects present. For training, animals were placed individually at the center of the box in

the presence of two identical objects (old objects) for 10 min. After that period, the box and objects were cleaned with 50% methanol solution. For the testing at the same time of the second day, the animal was exposed to one of the old objects and a new object of a different shape and color than the old object, and the box and objects were cleaned again to continue with the next animal. The recognition index was calculated as the time spent exploring the new object divided by the time exploring both objects.

Morris Water Maze (MWM) Tests. The Morris water maze tests were performed a day after the NOR tests. The standard Morris water maze procedure was used with minor modifications as described previously. The water maze test contains acquisition training and probe trial. During the acquisition training, the mice were trained to find a submerged platform hidden 1 cm under water by using constant cues outside the pool. During each trial, mice have up to 60 s to find the hidden platform; otherwise, it would be guided to the platform and forced to stay on it for 20 s. Acquisition training contained four trials a day for six consecutive days. The probe trial was used to test the memory of animals. In the seventh day, the hidden platform was removed and each mouse was allowed to swim freely for 60 s. The swimming pathway, escape latency of mice to find the hidden platform, and the times in the target quadrant were recorded by a digital device connected to a computer.

Golgi Staining. The Golgi staining protocol was performed as previously described.^[4] The mice were anesthetized by isoflurane and perfused intracardially with 400 mL of normal saline containing 0.5% sodium nitrite, followed with 400 mL 4% formaldehyde and the Golgi dye solution containing 5% chloral hydrate, 4% formaldehyde, and 5% potassium dichromate. After being perfused, the brains were dissected into 5 mm x 5 mm sections and transferred to a vial containing Golgi dye solution for 3 days in the dark, then immersed in solution containing 1% silver nitrate for another 3 days. The brains were serially sectioned into 100- μ m-thick slices using a vibrating microtome (Leica, VT1000S, Germany). Images were observed under the microscope (Nikon, Tokyo, Japan).

Mice Brain Tissue Preparation and Protein Extraction. Mice were deeply anaesthetized with chloral hydrate and immediately perfused with saline, and the hippocampus of mice were rapidly

removed and snap frozen for biochemical analysis. For hippocampus protein extraction, hemispheres were first extracted in RIPA buffer (50 mM Tris pH 7.4, 150 mM NaCl, 1% NP-40, 0.25% sodium deoxycholate), centrifuged at 14000 g for 20 min.

PP2A and GSK-3 β Activity Assay. PP2A activity in the cell extracts and brain lysates were measured using the phosphatase kit V2460 according to the manufacturer's procedure (Promega). GSK-3 β activity in the cell extracts and brain lysates were measured using the GENMED GSK-3 β Activity Assay Kit (GENMED Scientifics INC., Arlington, MA, USA), based on its ability to phosphorylate its targeting sequence GPHRSTPESRAAV in the presence of ATP and GSK-3 α inhibitor Aloisine A, and then through a series of reactions involving pyruvate kinase and lactate dehydrogenase, the phosphorylated products in the system transform NADH (reduced nicotinamide adenine dinucleotide) to NAD (nicotinamide adenine dinucleotide), accordingly, detect the absorbance at 340 nm to evaluate the specific activity of GSK-3 β .

BACE1 Enzymatic Assay. The enzyme inhibition assay was carried out using β -Secretase Activity Assay Kit from Abnova according to the manufacturer's instructions and using a multiwall fluorescence plate reader that allowed absorption at 335–355 nm and recorded emission at 495–510 nm.^[5] The assay procedure was conducted as follows: Collect cells (5×10^6 cells/assay) by centrifugation for 5 min at $700 \times g$. Add 0.1 ml of ice-cold Extraction Buffer. For tissue sample, add 2–3 $\times$ volume of ice-cold Extraction Buffer to tissue sample and homogenize it on ice. Incubate cell lysate on ice for 10 minutes and centrifuge at $10,000 \times g$ for 5 minutes. Transfer the supernatant to a new tube and keep on ice. This should yield a lysate with a protein concentration of ~ 2 –4 mg/ml. Add 50 μ l cell lysate (~ 2 – 5×10^6 cells or 25–200 μ g of total protein) to each well in a 96-well plate. For positive control assay, add 2 μ l of Active β -secretase to 50 μ l of Extraction Buffer. For negative control assay, add 2 μ l of the β -secretase inhibitor to the 50 μ l of Sample or Positive Control well. Add 50 μ l of $2 \times$ Reaction Buffer, gently mix then pre-incubate 20 minutes at 37 °C before adding substrate. Add 2 μ l of the β -secretase substrate, pipet up and down to mix well, incubate 10 minutes at 37 °C. Cover the plate, tap gently to mix, and incubate in the dark at 37 °C for 1 hour. Read sample in a fluorescence plate reader with Ex/Em=345/500 nm.

ELISA Quantification of $A\beta_{42}$. For measurement of $A\beta_{42}$ species in cell medium, conditioned media of cells were recovered and debris was removed by centrifugation and applied to ELISA plates after 48 h of treatment. To detect the concentration of $A\beta_{42}$ in total brain lysates, the mouse brains were homogenized in buffer (2% SDS in H_2O containing 0.7 mg/ml Pepstatin A supplemented with complete Mini protease inhibitor tablet and phosphatase inhibitors 1:100), and centrifuged at 4 °C, 100,000g for 1 h. The supernatant was stored as soluble fraction. The pellet was rehomogenized in 70% formic acid (FA) and centrifuged as above. The supernatant was stored as the insoluble fraction. $A\beta_{42}$ was quantified using the Human/Mouse $A\beta_{1-42}$ ELISA Kit (Elabscience, Wuhan, China) in accordance with the manufacturer's instructions. The $A\beta_{42}$ concentrations were determined by comparison with the standard curve.

Cell Culture. The human embryonic kidney 293 (HEK293) cells stably transfected with the longest human tau (tau441) (HEK293/tau) and mouse neuroblastoma N2a cells with stable expression of APP (N2a/APP) were cultured in Dulbecco's modified Eagle's medium (Gibco, Invitrogen; Bleiswijk, Netherlands) in the presence of 200 mg/mL G418 containing 10% fetal bovine serum. The cells were maintained at 37 °C in a humidified atmosphere containing 5% CO_2 . Cells were seeded into 6-well or 12-well culture plates for 1 day. After adherence and confluence were reached, the medium in each well was replaced with 1000 mL of the appropriate fresh medium, containing the test compound in DMSO or the vehicle alone in control wells. After 24 h of treatment, further analysis was continued.

CCK8 Assay. The cell counting kit-8 (CCK-8) assay was performed following the manufacturer's protocol (Solarbio, Beijing, China). HEK293 cells were cultured in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% fetal bovine serum (FBS, Gibco BRL, Gaithersburg, MD, USA) and grown at 37 °C in a humid atmosphere containing 5% CO_2 . Cells were seeded in 96-well culture plates (1×10^4 cells per well). After 24 h of incubation, the cells were treated with compounds at different concentrations. After 24 h of treatment, the medium in each well was replaced with 110 mL of the appropriate fresh medium, containing 10% CCK8. After 30 min, the optical density at 450 nm was measured using a microplate reader.

Western Blot Analysis. Hippocampi were rapidly removed from the brains and homogenized in a

buffer containing 50 mM Tris, pH 7.4, 40 mM NaCl, 1 mM EDTA, 0.5% Triton X-100, 1.5 mM Na₃VO₄, 50 mM NaF, 10 mM sodium pyrophosphate, 10 mM sodium β -glycerophosphate, supplemented with protease inhibitors cocktail.^[6] The homogenates were mixed with one-third of sample buffer (200 mM Tris-HCl, 8% sodium dodecyl sulfate and 40% glycerol), boiled for 10 min, and centrifuged at 14000 g for 10 min. For cell samples, cells were washed with PBS and lysed with 1 $\times$ RIPA buffer. The protein concentrations of the supernatants were measured using the BCA method. The same amount of proteins was separated by 10% SDS-polyacrylamide gel electrophoresis gel, and then transferred to nitrocellulose membrane. After blocking in 3% non-fat milk for 1 h at 25 °C, the membranes were then incubated with primary antibodies at 4 °C overnight. Finally, the membranes were incubated with anti-rabbit or anti-mouse IgG conjugated to IRDyeTM (800CW) for 1 h at 25 °C and visualized using the Odyssey Infrared Imaging System (Licor biosciences, Lincoln, NE, USA).

Statistical Analyses. Data were expressed as mean $\pm$ S.E.M. and analyzed using commercial software (GraphPad Prism; GraphPad Software, Inc, La Jolla, CA). The two-way analysis of variance or one-way analysis of variance (ANOVA), or a Student's t-test was used to determine the different means among the groups. The level of significance was set at $p < 0.05$.

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Molecular Docking. The investigated compounds were subjected to molecular docking experiments using 'SYBYL-X2.0' software (TRIPOS of Chemical Computing Group Inc., on a Core i7 workstation). Molecules were built with Chemdraw and optimized at molecular mechanical and semiempirical level by using Open Babel GUI. The Molecular Mechanics calculations in vacuo, dipole bond option for electrostatics and Root Mean Square Deviation gradient of 0.01 kcal/mol

conformational searching in torsional space was performed using the multi-conformer method. Lowest energy conformer of each new analogue ‘global-minima’ was used for docking. The X-ray crystallographic structure of the PP2Ac and BACE1 was selected from the Protein Data Bank (PDB code: 2IE4 and 4YBI) for the docking study.^[7,8] All the hydrogens were added, and enzyme structure was subjected to a refinement protocol in which the constraints on the enzyme were gradually removed and minimized. Energy of binding was calculated as the difference between the energy of the complex and individual energies of the enzyme and ligands. In the docking calculation, the default Flex X scoring function was used for exhaustive searching, solid body optimizing and interaction scoring. Finally, the ligands with the lowest-energy and the most favorable orientation were selected.^[9,10]

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Cellular Thermal Shift Assay (CETSA). For all of the cell lysate CETSA experiments, cultured cells (N2a/APP cells for BACE1 and HEK293/tau cells for PP2A) from abovementioned cell lines were harvested and washed with PBS. The cells were diluted in PBS supplemented with Completed protease inhibitor cocktail. The cell suspensions were freeze-thawed three times using liquid nitrogen. The soluble fraction (lysate) was separated from the cell debris by centrifugation at $20000 \times g$ for 20 minutes at 4°C. The cell lysates were divided into two aliquots, with one aliquot being treated with compounds and the other aliquot with the diluent of the compounds (an equal amount of DMSO).

After 30 min incubation at room temperature the respective lysates were divided into smaller (50 μ L) aliquots and heated individually at different temperatures for 3 minutes (Veriti thermal cycler, Applied Biosystems/Life Technologies) followed by cooling for 3 minutes at room temperature. The appropriate temperatures were determined in preliminary CETSA experiments (data not shown). The heated lysates were centrifuged at $20000 \times g$ for 20 minutes at 4°C in order to separate the soluble fractions from precipitates. The supernatants were transferred to new microtubes and analyzed by sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE) followed by western blot analysis.

LC-MS Analyses. Chromatography was performed on an Agilent 1290II UPLC system using an Eclipse Plus C₁₈ column (3.5 μ m, 2.1 $\times$ 100 mm, Agilent). The mobile phase with a flow rate of 0.4 mL/min consisted of H₂O (solvent A) and methanol (solvent B). The flow was 0.4 mL/min, and the injection volume was 5 μ L. A linear gradient with the following proportion of phase B (t_{min} , B%) was used: (0, 60), (5, 70), (25, 90), (28,100). The UPLC was coupled with an electrospray ionization, a hybrid quadrupole time-of-flight (UPLC-ESI-Q-TOF) mass spectrometer (model 6545, Agilent). The mass acquisition was performed in negative ionization and full scan (50–1700 Da) modes. Spray parameters were as follows: gas temp. 320°C, gas flow 10 L/min, nebulizer 35 psi, sheath gas temp. 340°C, sheath gas flow 10 L/min, Vcap 3,500 V, nozzle voltage 1000 V, fragment voltage 175 V.

Stability analyses of compounds 1–10 in aqueous solution. In order to investigate whether these compounds are hydrolyzed or metabolized in aqueous solution, the following stability experiments have been designed: (i) Certain mass of these compounds were dissolved in distilled water to prepare a solution with a concentration of 200 μ M, respectively. (ii) Half volumes of the above solution were taken after ultrasonic treatment and diluted to 10 μ M using methanol and then immediately detected by UPLC-ESI-QTOF-MS as the standard group. (iii) The other half volumes of the solution were incubated at 37°C for 24 hours and subsequently diluted to 10 μ M (using the same procedures as above) as the experimental group and detected by UPLC-ESI-QTOF-MS to compare the degradation of the substances in the experimental and standard groups. The UPLC-ESI-QTOF-MS method was as described in the "LC-MS Analyses" section above.

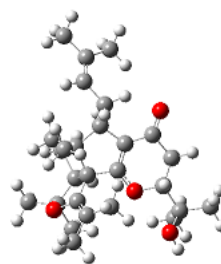
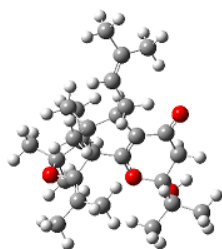
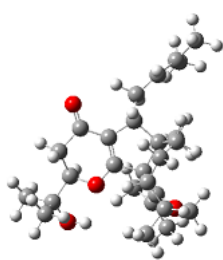
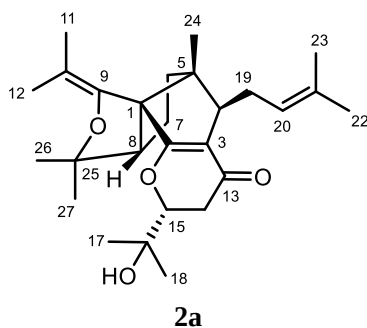
¹³C NMR calculation details of 2 and 6.

All computations were performed using Gaussian 09^[11] and figured using GaussView 5.0^[12]. Conformation search using molecular mechanics calculations was performed in Discovery Studio 3.5 Client with MMFF force field with 10 kcal mol⁻¹ upper energy limit.^[13] For the calculations of ¹³C NMR chemical shifts, mPW1PW91/6-31G(d,p) method was used to optimize the selected conformations. For all optimized structures, vibrational spectra were calculated to ensure that no imaginary frequencies for energy minimum were obtained. NMR calculations were performed at the levels of mPW1PW91/6-31G(d,p) with the gauge-independent atomic orbital (GIAO) method.^[14] The solvent effect was considered by using methanol for **2** and chloroform for **6** in the calculations to resemble the experimental condition. The polarized continuum model (PCM) of Tomasi et al. was used.^[15] The calculated ¹³C NMR chemical shifts were analyzed by subtracting the isotopic shifts for TMS calculated with the same methods.^[14] Different conformers for structure **2** and **6** were considered. The ¹³C NMR chemical shifts in each compound were considered as the average values of the same atoms in the different conformers. The average values were obtained by the Boltzmann distributions, using the relative Gibbs free energies as weighting factors.^[16] The differences $\Delta\delta$ were determined by subtracting the experimental chemical shifts δ_{exptl} from the calculated chemical shifts δ_{calcd} .

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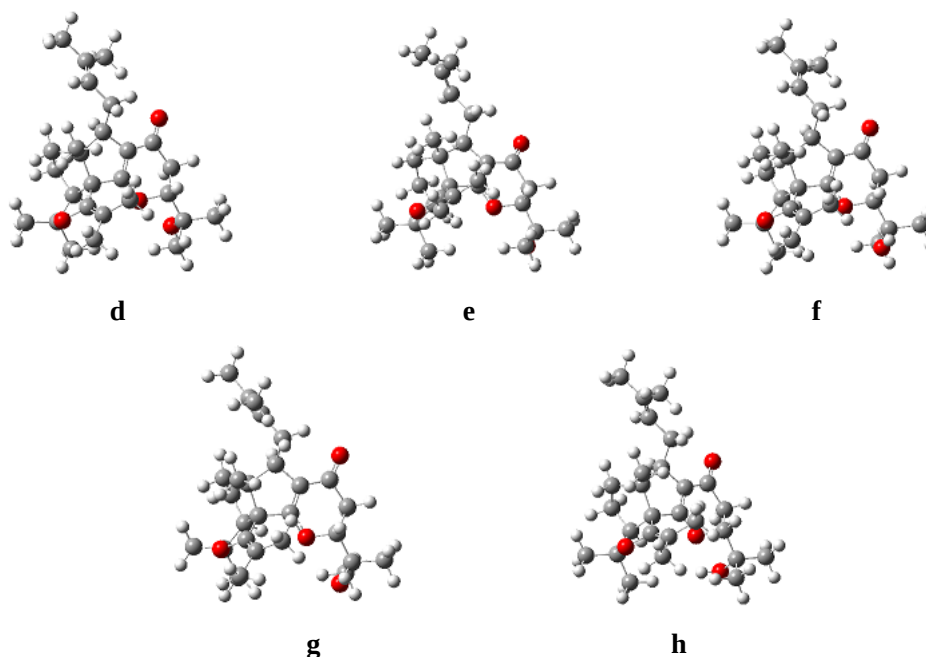


Figure S26. Optimized geometries of predominant conformers for compound **2a** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S10. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2a** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
2a-a	-1353.271583	-1353.333191	57.9
2a-b	-1353.266534	-1353.328922	0.6
2a-c	-1353.266174	-1353.328526	0.4
2a-d	-1353.267261	-1353.329507	1.2
2a-e	-1353.267465	-1353.329978	1.9
2a-f	-1353.265956	-1353.328574	0.4
2a-g	-1353.266170	-1353.328723	0.5
2a-h	-1353.270878	-1353.332771	37.1

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S11. Optimized Z-matrixes of compound **2a** in the gas phase (Å) at B3LYP/6-31G(d,p) level

2a-a				2a-b			
C	1.537616	0.690429	-0.14778	C	1.371413	1.119753	0.295863
C	-0.04546	0.96512	-0.17343	C	-0.20203	1.053977	-0.02777
C	0.293872	-1.37672	-0.5837	C	0.618419	-1.19887	0.03758
C	1.691298	-0.80109	-0.67634	C	1.883283	-0.3722	0.103088
C	2.104928	1.70422	-1.16495	C	1.938826	2.045959	-0.80308
C	1.028311	1.8322	-2.24596	C	1.069115	1.787007	-2.03644

C	-0.31345	1.812689	-1.48634	C	-0.36593	1.625766	-1.49635
C	2.773427	-1.68929	-0.01315	C	2.92693	-0.91946	1.116978
C	4.182073	-1.29215	-0.36883	C	4.323639	-0.37739	0.930278
C	5.26138	-1.19973	0.424375	C	5.28094	-0.88834	0.138475
C	6.61063	-0.83089	-0.14541	C	6.642287	-0.24156	0.049624
C	5.262202	-1.46242	1.9104	C	5.111631	-2.12338	-0.71372
C	2.158263	0.901416	1.237237	C	1.670643	1.689522	1.687589
C	-0.87955	3.171461	-0.95623	C	-1.23811	2.911568	-1.31321
O	-0.59886	3.158742	0.466472	O	-1.24046	3.157371	0.11686
C	-0.60882	1.853471	0.924181	C	-1.10253	1.960543	0.794334
C	-2.40298	3.216965	-1.14237	C	-2.68302	2.63639	-1.75263
C	-0.23395	4.439122	-1.50872	C	-0.71258	4.187777	-1.96464
C	-0.61463	-0.41478	-0.2854	C	-0.49098	-0.41605	0.001403
C	-1.0629	1.574026	2.158544	C	-1.6986	1.785676	1.986151
C	-1.02554	0.203519	2.787024	C	-1.51152	0.567822	2.853186
C	-1.63654	2.660554	3.035341	C	-2.59408	2.851323	2.568467
O	-1.94108	-0.59438	-0.16132	O	-1.75951	-0.83352	-0.10496
C	-2.34537	-1.98412	0.037534	C	-1.9718	-2.24984	0.145013
C	-1.67799	-2.87836	-1.00048	C	-0.91276	-3.08203	-0.57429
C	-0.15028	-2.70196	-0.99787	C	0.516362	-2.61489	-0.26605
O	0.589289	-3.59741	-1.39223	O	1.465912	-3.38699	-0.37515
C	-3.88728	-1.95797	0.109396	C	-3.4395	-2.56862	-0.24301
C	-4.42338	-3.31844	0.558401	C	-4.39693	-1.56299	0.40407
C	-4.52968	-1.51565	-1.214	C	-3.80075	-3.99802	0.191045
O	-4.24643	-1.04276	1.151974	O	-3.6222	-2.41882	-1.65507
H	1.960598	-0.75914	-1.74263	H	2.373494	-0.44001	-0.87811
H	3.076426	1.388323	-1.55875	H	3.003223	1.859716	-0.9802
H	2.255238	2.670298	-0.66768	H	1.838768	3.090781	-0.48444
H	1.064006	0.967176	-2.91795	H	1.370186	0.84818	-2.51532
H	1.151923	2.717471	-2.87555	H	1.156621	2.566142	-2.7986
H	-1.08438	1.338014	-2.09975	H	-0.9255	0.923242	-2.11977
H	2.6213	-1.73306	1.068822	H	2.588056	-0.72749	2.140614
H	2.59065	-2.70317	-0.39128	H	2.929059	-2.00461	0.994963
H	4.334588	-1.09773	-1.43257	H	4.574362	0.52176	1.493067
H	6.564712	-0.654	-1.22355	H	6.718047	0.644529	0.686234
H	7.008695	0.074601	0.332013	H	7.432156	-0.94364	0.348764
H	7.347249	-1.6249	0.036612	H	6.872427	0.05897	-0.98138
H	4.269859	-1.67613	2.310731	H	4.114899	-2.56398	-0.65382
H	5.909306	-2.31673	2.149625	H	5.313458	-1.88982	-1.76778
H	5.671061	-0.60292	2.457645	H	5.842507	-2.89163	-0.42719
H	1.765005	0.206869	1.984158	H	1.277785	1.066804	2.495131
H	1.956806	1.915639	1.591295	H	1.229377	2.684009	1.79242
H	3.241211	0.764722	1.187199	H	2.749877	1.786635	1.834699
H	-2.81999	4.105919	-0.66037	H	-3.32575	3.485076	-1.50072
H	-2.66496	3.242489	-2.20554	H	-2.73538	2.469418	-2.83375
H	-2.86961	2.332387	-0.69764	H	-3.07308	1.744765	-1.25285
H	-0.41714	4.536339	-2.58299	H	-0.70551	4.096796	-3.05487
H	-0.66532	5.312313	-1.01087	H	-1.36469	5.024807	-1.69892
H	0.843898	4.451127	-1.33323	H	0.297461	4.427831	-1.62563
H	-0.46138	-0.52768	2.206507	H	-0.80775	-0.15889	2.445269
H	-0.5667	0.253658	3.782965	H	-1.14289	0.857122	3.846711
H	-2.04126	-0.19001	2.926952	H	-2.47082	0.057984	3.016939
H	-1.78921	3.587989	2.482951	H	-2.79817	3.644404	1.848845
H	-2.59419	2.341679	3.467139	H	-3.54765	2.416456	2.896207
H	-0.97025	2.875386	3.881974	H	-2.13853	3.308282	3.457875
H	-1.9774	-2.25804	1.035826	H	-1.85848	-2.38627	1.230764
H	-2.03662	-2.64262	-2.0109	H	-1.05204	-2.99926	-1.66096
H	-1.90315	-3.93059	-0.81035	H	-0.99161	-4.13809	-0.30606
H	-5.49931	-3.23672	0.733118	H	-5.42414	-1.81205	0.125688

H	-3.95239	-3.62956	1.495445	H	-4.17686	-0.55082	0.064023
H	-4.25394	-4.08926	-0.19803	H	-4.3127	-1.59024	1.494895
H	-5.60787	-1.41032	-1.06881	H	-4.84806	-4.19438	-0.05329
H	-4.12933	-0.55066	-1.53857	H	-3.18883	-4.7484	-0.3217
H	-4.36081	-2.2419	-2.01538	H	-3.66805	-4.13947	1.268285
H	-3.78796	-0.21065	0.963357	H	-3.26936	-3.20566	-2.09112
2a-c				2a-d			
C	1.377378	1.096825	0.33832	C	1.368558	1.122854	0.296939
C	-0.18677	1.058056	-0.02885	C	-0.20494	1.052497	-0.02472
C	0.614576	-1.20313	-0.02482	C	0.620416	-1.19833	0.04503
C	1.883776	-0.38926	0.092556	C	1.883179	-0.36833	0.105607
C	1.981776	2.066791	-0.70104	C	1.932339	2.048797	-0.80405
C	1.146561	1.866268	-1.96866	C	1.062467	1.784732	-2.03624
C	-0.30418	1.692416	-1.47681	C	-0.37161	1.619491	-1.49468
C	2.906276	-0.98262	1.101707	C	2.930867	-0.9111	1.117774
C	4.307053	-0.43604	0.965322	C	4.326062	-0.36705	0.925697
C	5.279566	-0.9162	0.17286	C	5.280743	-0.87698	0.130078
C	6.643022	-0.2687	0.137155	C	6.640916	-0.22855	0.035382
C	5.125741	-2.11588	-0.73124	C	5.109164	-2.11257	-0.72092
C	1.637331	1.598648	1.763577	C	1.66842	1.695218	1.687435
C	-1.16963	2.977761	-1.25903	C	-1.24842	2.902284	-1.31506
O	-1.17725	3.176927	0.176749	O	-1.25247	3.152448	0.114242
C	-1.10082	1.942627	0.801687	C	-1.10745	1.958479	0.795549
C	-2.61463	2.722349	-1.71294	C	-2.69239	2.619822	-1.75344
C	-0.63373	4.269234	-1.8698	C	-0.72857	4.17896	-1.97013
C	-0.48739	-0.40929	-0.0562	C	-0.48987	-0.4184	0.009078
C	-1.76884	1.715822	1.944224	C	-1.70136	1.7856	1.98888
C	-1.68244	0.434888	2.734301	C	-1.50871	0.571297	2.859745
C	-2.68338	2.764193	2.527832	C	-2.59898	2.850573	2.569319
O	-1.75651	-0.81871	-0.19022	O	-1.75825	-0.83778	-0.09551
C	-1.9642	-2.2334	0.076498	C	-1.96709	-2.25572	0.153376
C	-0.92771	-3.07605	-0.66297	C	-0.90383	-3.09473	-0.55296
C	0.506608	-2.60972	-0.36882	C	0.520907	-2.61699	-0.2548
O	1.455809	-3.37652	-0.51424	O	1.477354	-3.38112	-0.36513
C	-3.44555	-2.54012	-0.21786	C	-3.42241	-2.57492	-0.24767
C	-3.74114	-4.02852	0.029111	C	-4.39778	-1.59298	0.419239
C	-3.86015	-2.11963	-1.63398	C	-3.7752	-4.02073	0.141163
O	-4.15145	-1.7559	0.754861	O	-3.46725	-2.42566	-1.67187
H	2.39042	-0.42088	-0.88211	H	2.371062	-0.43697	-0.87666
H	3.049665	1.881409	-0.85627	H	2.997115	1.865253	-0.98171
H	1.877162	3.09728	-0.34006	H	1.829556	3.094043	-0.48733
H	1.455882	0.946553	-2.47851	H	1.365991	0.845969	-2.51346
H	1.260242	2.676092	-2.69461	H	1.146895	2.562727	-2.79996
H	-0.84993	1.023387	-2.14794	H	-0.9283	0.912417	-2.11548
H	2.547506	-0.83305	2.125605	H	2.594771	-0.71764	2.142071
H	2.909092	-2.06167	0.93365	H	2.934213	-1.99641	0.997575
H	4.547098	0.439345	1.568835	H	4.577829	0.532695	1.487171
H	6.70748	0.589647	0.811891	H	6.718313	0.657737	0.67157
H	7.426482	-0.98409	0.421323	H	7.432956	-0.92961	0.33126
H	6.89308	0.074802	-0.87567	H	6.866371	0.072093	-0.99664
H	4.126079	-2.55338	-0.71147	H	4.112666	-2.5533	-0.658
H	5.352886	-1.84199	-1.77032	H	5.307971	-1.87955	-1.77568
H	5.846704	-2.8984	-0.45841	H	5.841037	-2.88054	-0.43607
H	1.208358	0.945595	2.527989	H	1.278642	1.072263	2.496291
H	1.204015	2.592941	1.898966	H	1.224798	2.688748	1.791988
H	2.711907	1.674504	1.951462	H	2.747646	1.795254	1.832787
H	-3.25115	3.573309	-1.45277	H	-3.33917	3.465833	-1.50268
H	-2.66217	2.572129	-2.79699	H	-2.74402	2.450538	-2.83428
H	-3.01544	1.829658	-1.22279	H	-3.07691	1.726933	-1.25146

H	-0.61657	4.208932	-2.96217	H	-0.72098	4.084954	-3.0601
H	-1.28464	5.101383	-1.58638	H	-1.38393	5.014183	-1.70656
H	0.37405	4.495079	-1.51462	H	0.280543	4.423784	-1.63186
H	-0.87683	-0.22481	2.407893	H	-0.80488	-0.15524	2.451796
H	-1.51484	0.652955	3.797018	H	-1.13755	0.864798	3.851113
H	-2.62454	-0.12374	2.662727	H	-2.46634	0.059816	3.028568
H	-2.82001	3.605947	1.848514	H	-2.808	3.639884	1.846928
H	-3.6653	2.329436	2.756689	H	-3.55005	2.413967	2.902227
H	-2.28566	3.151848	3.475807	H	-2.14241	3.313171	3.455306
H	-1.82049	-2.3593	1.158509	H	-1.87307	-2.38802	1.241146
H	-1.07528	-3.0178	-1.74985	H	-1.06223	-3.04656	-1.63698
H	-1.00674	-4.12782	-0.37985	H	-0.98026	-4.14352	-0.25766
H	-4.82187	-4.19709	-0.03055	H	-5.42406	-1.82157	0.109147
H	-3.4114	-4.32921	1.028162	H	-4.16526	-0.56598	0.136506
H	-3.26599	-4.67868	-0.71083	H	-4.35831	-1.67256	1.51071
H	-4.92646	-2.324	-1.78545	H	-4.8265	-4.21851	-0.09538
H	-3.68524	-1.05227	-1.77927	H	-3.16671	-4.73952	-0.41185
H	-3.31132	-2.6749	-2.40083	H	-3.64216	-4.19735	1.21357
H	-5.09572	-1.82945	0.562646	H	-4.37499	-2.59656	-1.9557
2a-e				2a-f			
C	1.536908	0.689182	-0.20526	C	1.375092	1.103911	0.330598
C	-0.04721	0.954268	-0.16064	C	-0.191	1.056986	-0.02744
C	0.28314	-1.40166	-0.46835	C	0.617655	-1.20129	-0.01322
C	1.674809	-0.83245	-0.6419	C	1.884773	-0.38244	0.09382
C	2.037747	1.636497	-1.31823	C	1.969709	2.067739	-0.72015
C	0.898742	1.695391	-2.33943	C	1.128299	1.853759	-1.98141
C	-0.39588	1.721591	-1.50259	C	-0.3191	1.677881	-1.4804
C	2.777512	-1.68215	0.037961	C	2.913377	-0.96586	1.102697
C	4.175099	-1.31905	-0.38981	C	4.312639	-0.41856	0.954724
C	5.284083	-1.19746	0.357173	C	5.283563	-0.90711	0.16542
C	6.614574	-0.87329	-0.27997	C	6.645759	-0.25776	0.117606
C	5.337713	-1.38269	1.853969	C	5.129553	-2.11825	-0.72322
C	2.238232	0.998916	1.12172	C	1.642815	1.618046	1.75008
C	-0.93949	3.107181	-1.02276	C	-1.19001	2.960444	-1.26985
O	-0.58438	3.178184	0.382272	O	-1.18756	3.173676	0.165183
C	-0.54742	1.903317	0.915606	C	-1.10101	1.947875	0.801159
C	-2.4706	3.137739	-1.12933	C	-2.63686	2.692575	-1.7093
C	-0.32936	4.341693	-1.68049	C	-0.66496	4.24861	-1.89639
C	-0.61971	-0.43052	-0.17941	C	-0.48723	-0.41144	-0.04308
C	-0.89775	1.69863	2.196927	C	-1.7565	1.733234	1.953467
C	-0.78023	0.37299	2.903354	C	-1.65693	0.461767	2.755796
C	-1.41025	2.831882	3.051573	C	-2.66734	2.785014	2.536236
O	-1.94019	-0.58764	-0.01172	O	-1.757	-0.82391	-0.1672
C	-2.38999	-1.9596	0.16491	C	-1.96136	-2.24076	0.079273
C	-1.69847	-2.89263	-0.82747	C	-0.91681	-3.07404	-0.66166
C	-0.17388	-2.73616	-0.82316	C	0.514399	-2.60982	-0.35346
O	0.555669	-3.65697	-1.18024	O	1.465269	-3.37655	-0.48615
C	-3.93057	-1.94462	0.080253	C	-3.44821	-2.54702	-0.22292
C	-4.51744	-0.88138	1.021252	C	-3.75741	-4.0226	0.075219
C	-4.49448	-3.33236	0.429952	C	-3.83753	-2.17958	-1.65634
O	-4.23636	-1.62159	-1.28161	O	-4.26422	-1.71284	0.608295
H	1.90851	-0.85756	-1.71732	H	2.387264	-0.41966	-0.88274
H	2.985726	1.296567	-1.74827	H	3.037474	1.885256	-0.87961
H	2.213608	2.632465	-0.89337	H	1.86301	3.100704	-0.36699
H	0.898793	0.788774	-2.95529	H	1.438689	0.931509	-2.48595
H	0.980877	2.538537	-3.03085	H	1.234437	2.658449	-2.71408
H	-1.19949	1.208338	-2.03735	H	-0.8654	1.00033	-2.14233
H	2.663334	-1.65712	1.125172	H	2.559704	-0.80837	2.127263
H	2.576171	-2.71625	-0.26968	H	2.916854	-2.04618	0.943559

H	4.289398	-1.18093	-1.46713	H	4.553046	0.464914	1.546188
H	6.530079	-0.7519	-1.36346	H	6.710683	0.609358	0.780975
H	7.038549	0.051408	0.134412	H	7.431122	-0.96818	0.408803
H	7.350511	-1.66479	-0.08426	H	6.892365	0.072909	-0.90029
H	4.35986	-1.57144	2.300023	H	4.130549	-2.55683	-0.69651
H	5.991014	-2.2262	2.114049	H	5.354648	-1.857	-1.76596
H	5.767859	-0.49771	2.341181	H	5.852005	-2.89633	-0.44187
H	1.8977	0.358199	1.93907	H	1.22151	0.969708	2.522847
H	2.052848	2.035324	1.415433	H	1.207877	2.612245	1.880721
H	3.316941	0.86126	1.01368	H	2.718377	1.698327	1.930076
H	-2.86611	4.049645	-0.67229	H	-3.27642	3.54161	-1.45056
H	-2.78778	3.106928	-2.1772	H	-2.69177	2.534579	-2.79184
H	-2.90544	2.274178	-0.61709	H	-3.02953	1.801078	-1.21059
H	-0.5678	4.374649	-2.74772	H	-0.65422	4.177125	-2.98813
H	-0.73905	5.242089	-1.21355	H	-1.31893	5.079921	-1.61774
H	0.756121	4.365897	-1.56194	H	0.343761	4.483691	-1.54989
H	-0.3619	-0.42026	2.282666	H	-0.87111	-0.21278	2.412562
H	-0.14002	0.466454	3.791146	H	-1.45767	0.687269	3.81144
H	-1.76237	0.039425	3.265662	H	-2.61046	-0.08302	2.72208
H	-1.59646	3.730206	2.462608	H	-2.80787	3.621458	1.851426
H	-2.34009	2.542086	3.558981	H	-3.64884	2.353307	2.77296
H	-0.69136	3.086939	3.842478	H	-2.26391	3.179632	3.478924
H	-2.10599	-2.24149	1.189455	H	-1.80544	-2.38166	1.161383
H	-2.064	-2.68265	-1.83982	H	-1.05926	-3.00003	-1.74793
H	-1.93242	-3.93583	-0.60436	H	-0.99911	-4.12964	-0.39374
H	-5.61098	-0.88147	0.944444	H	-4.83681	-4.17717	-0.00092
H	-4.14684	0.110453	0.76148	H	-3.44621	-4.29697	1.09109
H	-4.26026	-1.08804	2.065502	H	-3.26302	-4.70395	-0.62257
H	-5.58955	-3.29713	0.418154	H	-4.90557	-2.36391	-1.79698
H	-4.17609	-4.08403	-0.29561	H	-3.64149	-1.12205	-1.84201
H	-4.18843	-3.65634	1.430211	H	-3.28483	-2.77729	-2.38638
H	-5.19841	-1.58422	-1.36408	H	-4.11975	-1.9734	1.528682
2a-g				2a-h			
C	1.545355	0.683008	-0.16708	C	1.530441	0.690853	-0.20616
C	-0.03668	0.962219	-0.16479	C	-0.0556	0.947811	-0.16385
C	0.285023	-1.38785	-0.52722	C	0.288352	-1.40604	-0.47427
C	1.683426	-0.82246	-0.65594	C	1.677099	-0.82908	-0.64649
C	2.09181	1.666904	-1.22513	C	2.028891	1.644362	-1.31473
C	0.990587	1.769	-2.28377	C	0.892598	1.700114	-2.33894
C	-0.33299	1.776082	-1.49298	C	-0.40427	1.716776	-1.50525
C	2.771022	-1.69991	0.012882	C	2.784261	-1.67362	0.032479
C	4.176365	-1.32374	-0.37683	C	4.180207	-1.29779	-0.38988
C	5.270571	-1.22225	0.394526	C	5.285384	-1.17019	0.36177
C	6.61229	-0.87805	-0.20758	C	6.61577	-0.83428	-0.26935
C	5.295984	-1.45024	1.886082	C	5.334899	-1.35988	1.858143
C	2.19926	0.931087	1.196382	C	2.22639	1.000016	1.123723
C	-0.88034	3.149504	-0.98226	C	-0.95797	3.097687	-1.02344
O	-0.53312	3.180159	0.426125	O	-0.60079	3.169347	0.379998
C	-0.55803	1.888505	0.921535	C	-0.56153	1.893668	0.912971
C	-2.41112	3.181695	-1.09782	C	-2.4899	3.117151	-1.12536
C	-0.26453	4.399387	-1.60368	C	-0.35931	4.336816	-1.68271
C	-0.61858	-0.41645	-0.23577	C	-0.61785	-0.44089	-0.18394
C	-0.98593	1.65147	2.172236	C	-0.91308	1.687663	2.193774
C	-0.97721	0.293126	2.823597	C	-0.7881	0.363603	2.90212
C	-1.52197	2.767454	3.03427	C	-1.42908	2.819788	3.048008
O	-1.94292	-0.57496	-0.09373	O	-1.94122	-0.61355	-0.01372
C	-2.37685	-1.94947	0.082058	C	-2.37693	-1.99471	0.187423
C	-1.69907	-2.8655	-0.93568	C	-1.68263	-2.92495	-0.80204
C	-0.17035	-2.71108	-0.9221	C	-0.16053	-2.74776	-0.82159

O	0.556763	-3.62459	-1.3006	O	0.576829	-3.6589	-1.1846
C	-3.92473	-1.94077	0.098941	C	-3.92113	-1.95003	0.081718
C	-4.46006	-3.35663	0.363324	C	-4.50276	-1.02279	1.16184
C	-4.51703	-1.35581	-1.18494	C	-4.52278	-3.35179	0.20397
O	-4.36507	-1.06283	1.141948	O	-4.28372	-1.47992	-1.21971
H	1.936056	-0.81099	-1.72719	H	1.910605	-0.85093	-1.72194
H	3.053182	1.337213	-1.63262	H	2.979662	1.310944	-1.7434
H	2.255492	2.645771	-0.7581	H	2.198148	2.639868	-0.88629
H	1.007817	0.884858	-2.93134	H	0.899235	0.79533	-2.95741
H	1.102569	2.635381	-2.94135	H	0.97144	2.54572	-3.02759
H	-1.12099	1.289568	-2.07435	H	-1.20203	1.200918	-2.04719
H	2.637334	-1.71347	1.098095	H	2.667009	-1.65372	1.119428
H	2.57448	-2.72211	-0.33492	H	2.591864	-2.708	-0.27956
H	4.31126	-1.15485	-1.44737	H	4.297281	-1.15597	-1.46637
H	6.548352	-0.72628	-1.28863	H	6.534577	-0.70972	-1.35271
H	7.025959	0.035306	0.240837	H	7.031535	0.091844	0.150019
H	7.346024	-1.67349	-0.01992	H	7.356381	-1.62128	-0.07349
H	4.309571	-1.64895	2.308277	H	4.356881	-1.55612	2.300607
H	5.942714	-2.30239	2.134081	H	5.992472	-2.20019	2.117551
H	5.718691	-0.58053	2.406082	H	5.758121	-0.47391	2.349499
H	1.8189	0.2622	1.973125	H	1.887306	0.354661	1.937953
H	2.013156	1.956757	1.524577	H	2.034727	2.034443	1.42023
H	3.27982	0.7847	1.125258	H	3.305973	0.868482	1.017826
H	-2.80866	4.087735	-0.63107	H	-2.89077	4.031299	-0.67808
H	-2.7216	3.167586	-2.14822	H	-2.81242	3.071365	-2.17112
H	-2.85106	2.313977	-0.59656	H	-2.91622	2.259952	-0.59458
H	-0.48945	4.456249	-2.67292	H	-0.60031	4.368063	-2.74941
H	-0.68199	5.288168	-1.12173	H	-0.77458	5.233934	-1.21459
H	0.819328	4.422882	-1.47065	H	0.726136	4.368954	-1.56644
H	-0.44914	-0.46651	2.245613	H	-0.37202	-0.43005	2.280483
H	-0.5034	0.341953	3.812688	H	-0.14153	0.461268	3.784725
H	-2.00668	-0.05648	2.982816	H	-1.76649	0.028896	3.272383
H	-1.63542	3.693695	2.470864	H	-1.62059	3.716827	2.45885
H	-2.4961	2.490442	3.458667	H	-2.35603	2.526052	3.557991
H	-0.8551	2.964537	3.884882	H	-0.70916	3.078607	3.836611
H	-2.03478	-2.24495	1.087728	H	-2.08577	-2.2599	1.213694
H	-2.04346	-2.63819	-1.9532	H	-2.06789	-2.731	-1.81151
H	-1.93731	-3.91268	-0.73703	H	-1.89917	-3.96895	-0.5654
H	-5.54056	-3.30045	0.518778	H	-5.5843	-0.94293	1.024211
H	-4.00988	-3.79044	1.265162	H	-4.06625	-0.02244	1.101845
H	-4.2677	-4.03904	-0.46905	H	-4.30943	-1.41475	2.166276
H	-5.60467	-1.30811	-1.08861	H	-5.61338	-3.27786	0.203255
H	-4.13892	-0.34511	-1.34857	H	-4.22944	-3.98069	-0.63918
H	-4.27453	-1.97161	-2.05534	H	-4.21133	-3.83674	1.134391
H	-4.072	-1.42996	1.987596	H	-3.88425	-0.60334	-1.31704

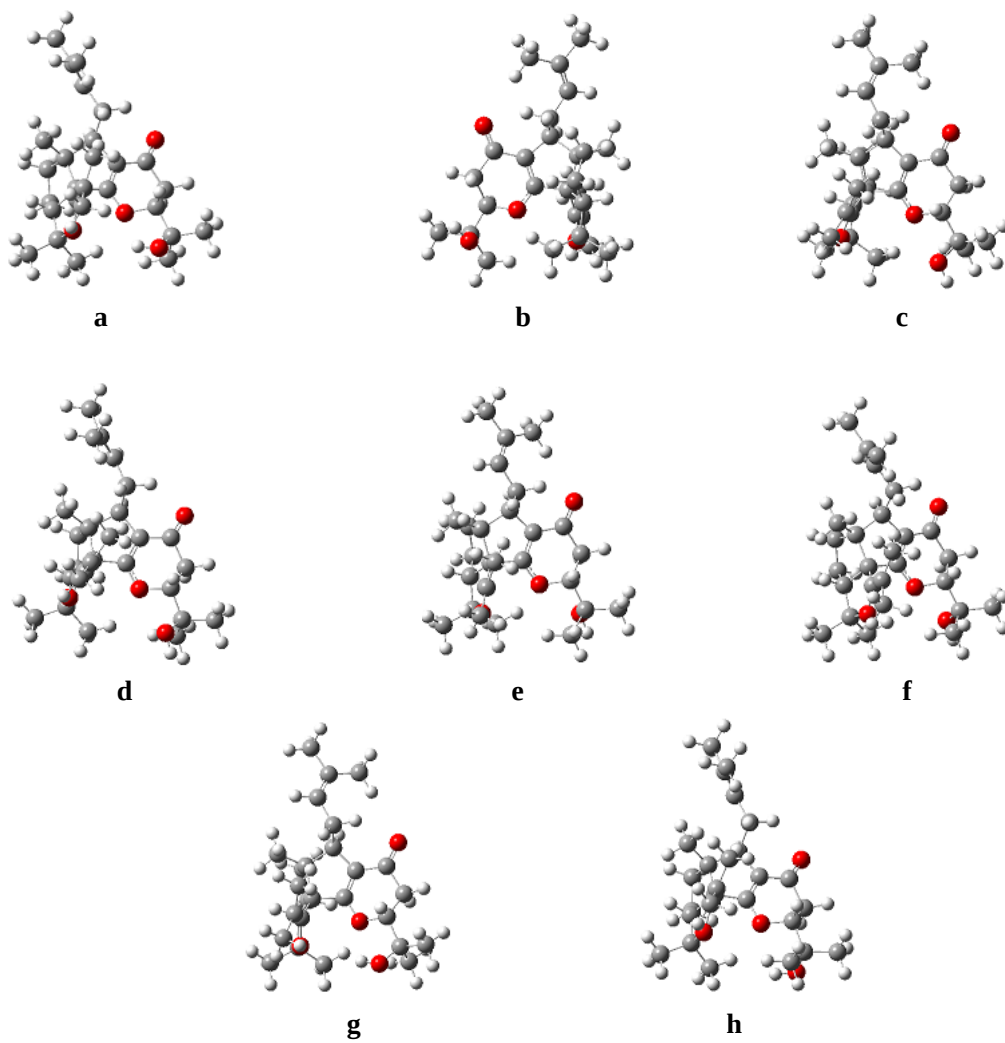
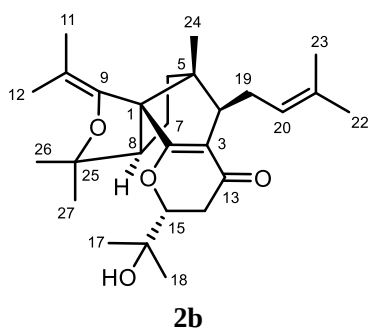


Figure S27. Optimized geometries of predominant conformers for compound **2b** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S12. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2b** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
2b-a	-1353.242939	-1353.305476	31
2b-b	-1353.240328	-1353.302755	1.7
2b-c	-1353.236644	-1353.299259	0
2b-d	-1353.236394	-1353.299814	0.1
2b-e	-1353.241340	-1353.303718	4.8
2b-f	-1353.240398	-1353.302709	1.7
2b-g	-1353.243447	-1353.305711	39.7
2b-h	-1353.242471	-1353.305111	21

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S13. Optimized Z-matrixes of compound **2b** in the gas phase (Å) at B3LYP/6-31G(d,p) level

2b-a				2b-b			
C	1.500453	0.838582	-0.88168	C	-1.39007	-1.2732	-0.50703
C	0.009799	1.066056	-0.31921	C	0.191143	-1.19605	-0.1972
C	0.37982	-1.29086	-0.73233	C	-0.75563	1.032719	-0.2585
C	1.764487	-0.72107	-0.90126	C	-1.98842	0.169791	-0.27394
C	1.362433	1.335126	-2.39156	C	-1.40845	-1.55735	-2.07673
C	-0.10519	1.755393	-2.65214	C	0.046241	-1.5536	-2.60585
C	-0.47979	2.207606	-1.25486	C	0.751545	-2.05985	-1.36463
C	2.804951	-1.3489	0.066547	C	-2.9223	0.448074	0.943048
C	4.234561	-1.13244	-0.35793	C	-4.33569	-0.06401	0.792553
C	5.298607	-0.80322	0.390531	C	-5.35582	0.570465	0.192205
C	6.672447	-0.69119	-0.22691	C	-6.72704	-0.05772	0.125416
C	5.257034	-0.52882	1.873729	C	-5.25123	1.93238	-0.45127
C	2.570848	1.672794	-0.17321	C	-2.1188	-2.40712	0.218545
C	-1.82818	2.684651	-0.71659	C	2.24306	-2.26255	-1.10429
O	-1.73288	2.283566	0.689546	O	2.293773	-2.11241	0.35249
C	-0.53333	1.636937	0.999994	C	1.063372	-1.7865	0.922746
C	-3.06476	2.044869	-1.34745	C	3.195029	-1.26453	-1.76546
C	-1.95868	4.211491	-0.7376	C	2.693722	-3.69484	-1.41514
C	-0.54793	-0.33716	-0.46329	C	0.393152	0.306761	-0.2154
C	-0.17322	1.552786	2.291388	C	0.914129	-1.9526	2.247983
C	0.962695	0.708586	2.796679	C	-0.2653	-1.45494	3.035151
C	-0.95636	2.27601	3.360538	C	1.994003	-2.61766	3.067351
O	-1.84372	-0.59261	-0.19425	O	1.624018	0.822489	-0.08561
C	-2.11449	-1.95761	0.25054	C	1.687501	2.206433	0.346628
C	-1.51219	-2.94774	-0.739	C	0.708951	3.052343	-0.46486
C	-0.01116	-2.68365	-0.92255	C	-0.7121	2.478525	-0.38813
O	0.763217	-3.57657	-1.24911	O	-1.69899	3.20214	-0.4938
C	-3.63192	-2.01676	0.528359	C	3.177756	2.625184	0.278023
C	-3.98124	-3.31493	1.261447	C	4.038542	1.644543	1.082021
C	-4.47889	-1.86564	-0.74516	C	3.357219	4.053479	0.81478
O	-3.93879	-0.96508	1.446988	O	3.652669	2.542101	-1.07059
H	2.128236	-0.98979	-1.90088	H	-2.59758	0.430024	-1.14603
H	1.705552	0.573455	-3.0957	H	-2.04638	-0.84407	-2.60368
H	2.009912	2.207247	-2.53454	H	-1.84043	-2.54942	-2.24951
H	-0.71618	0.909203	-2.98449	H	0.378451	-0.54765	-2.88351
H	-0.18127	2.542981	-3.40819	H	0.169166	-2.20162	-3.47925
H	0.214938	3.026432	-1.01644	H	0.306712	-3.0457	-1.16141
H	2.638274	-1.03236	1.097905	H	-2.48884	0.046612	1.86334
H	2.606465	-2.42843	0.040522	H	-2.93581	1.534527	1.06632
H	4.41436	-1.31765	-1.41889	H	-4.53976	-1.04598	1.217171
H	6.655792	-0.90019	-1.30006	H	-6.75378	-1.03677	0.612138

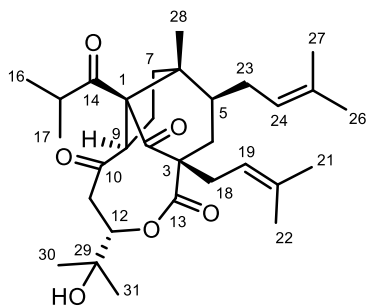
H	7.092286	0.313299	-0.08134	H	-7.47739	0.58268	0.608299
H	7.376128	-1.39092	0.243588	H	-7.05485	-0.18468	-0.91508
H	4.249858	-0.56639	2.292473	H	-4.24358	2.351753	-0.43323
H	5.87119	-1.25758	2.419161	H	-5.57498	1.884185	-1.49958
H	5.679941	0.459565	2.096998	H	-5.92738	2.643453	0.042696
H	2.743931	1.354872	0.855052	H	-2.20234	-2.23814	1.292873
H	2.282491	2.72946	-0.14955	H	-1.59436	-3.3579	0.074576
H	3.523467	1.598424	-0.70472	H	-3.13008	-2.5234	-0.18304
H	-3.94624	2.266498	-0.73775	H	4.204307	-1.40524	-1.36611
H	-3.23202	2.46097	-2.34631	H	3.234337	-1.45391	-2.84378
H	-2.96536	0.964206	-1.43219	H	2.908371	-0.22761	-1.6009
H	-1.95738	4.586673	-1.76681	H	2.613573	-3.90317	-2.48768
H	-2.89352	4.522443	-0.26213	H	3.736503	-3.83912	-1.1179
H	-1.12877	4.675772	-0.19712	H	2.079394	-4.41981	-0.8731
H	1.376834	0.058202	2.029409	H	-0.926	-0.82053	2.448416
H	1.775851	1.322461	3.207987	H	-0.85822	-2.28088	3.452039
H	0.615521	0.066446	3.617089	H	0.079586	-0.86102	3.892358
H	-1.64882	3.003685	2.937493	H	2.736371	-3.11018	2.439286
H	-1.53787	1.568598	3.967606	H	2.5175	-1.88665	3.699394
H	-0.27515	2.793114	4.048722	H	1.55564	-3.36013	3.746993
H	-1.60232	-2.05691	1.217853	H	1.369737	2.214084	1.400335
H	-1.99551	-2.85979	-1.72073	H	1.009898	3.066339	-1.52179
H	-1.64203	-3.97777	-0.39817	H	0.679086	4.084039	-0.10794
H	-5.02592	-3.27012	1.580186	H	5.090398	1.924791	0.982934
H	-3.36182	-3.43378	2.155162	H	3.907876	0.623696	0.722142
H	-3.85424	-4.19154	0.620363	H	3.767486	1.674436	2.141996
H	-5.53496	-1.83446	-0.46472	H	4.421017	4.304893	0.820626
H	-4.24069	-0.93773	-1.27189	H	2.841077	4.792046	0.191515
H	-4.33294	-2.7003	-1.43836	H	2.97566	4.15346	1.836081
H	-3.51543	-0.15817	1.115861	H	3.290743	3.288934	-1.56615
2b-c				2b-d			
C	-1.34456	-1.27534	-0.53852	C	1.472866	0.719919	-0.92301
C	0.225339	-1.20508	-0.18145	C	0.019031	1.043362	-0.30807
C	-0.74203	1.016276	-0.20312	C	0.326034	-1.34885	-0.53447
C	-1.96827	0.142684	-0.25529	C	1.71767	-0.83127	-0.789
C	-1.30463	-1.48547	-2.12166	C	1.250075	1.051639	-2.46936
C	0.17634	-1.55151	-2.58956	C	-0.21629	1.521116	-2.68142
C	0.793214	-2.09448	-1.31771	C	-0.46069	2.122195	-1.31287
C	-2.94689	0.341487	0.943311	C	2.792773	-1.3703	0.195538
C	-4.35917	-0.13236	0.685124	C	4.196566	-1.28329	-0.34621
C	-5.34536	0.563864	0.096601	C	5.318835	-0.88712	0.273976
C	-6.71742	-0.04013	-0.08347	C	6.650095	-0.92466	-0.43884
C	-5.20019	1.973986	-0.42266	C	5.388628	-0.3908	1.697355
C	-2.06685	-2.44091	0.138731	C	2.581993	1.597008	-0.34044
C	2.224421	-2.4739	-0.9399	C	-1.66162	2.83505	-0.69181
O	2.068653	-2.5708	0.507544	O	-1.26642	2.786772	0.712386
C	0.98857	-1.83366	0.998857	C	-0.34844	1.773044	0.996067
C	3.347623	-1.48903	-1.27643	C	-3.04643	2.204421	-0.86256
C	2.596497	-3.87605	-1.4306	C	-1.71331	4.316451	-1.07721
C	0.418405	0.304052	-0.21669	C	-0.58187	-0.35487	-0.33649
C	0.840453	-1.75082	2.333023	C	-0.00935	1.575297	2.282195
C	-0.20671	-0.91631	3.016545	C	0.877087	0.458644	2.75859
C	1.770896	-2.49148	3.262884	C	-0.54794	2.47049	3.371869
O	1.647894	0.841663	-0.18139	O	-1.8897	-0.54677	-0.10072
C	1.723266	2.21553	0.286933	C	-2.26481	-1.87892	0.343878
C	0.670025	3.080002	-0.40208	C	-1.60758	-2.9477	-0.52701
C	-0.72884	2.466291	-0.29125	C	-0.09463	-2.73616	-0.64374
O	-1.73396	3.170349	-0.34576	O	0.662428	-3.67252	-0.8797
C	3.185539	2.67842	0.12277	C	-3.80552	-1.92382	0.413455

C	3.362456	4.086003	0.716744	C	-4.2652	-3.27002	0.997927
C	3.659187	2.634093	-1.33716	C	-4.46728	-1.65993	-0.94652
O	3.930166	1.740527	0.90965	O	-4.13664	-0.87587	1.333017
H	-2.5591	0.433486	-1.13081	H	2.03903	-1.20812	-1.76827
H	-1.86278	-0.70253	-2.63995	H	1.503145	0.197395	-3.1018
H	-1.79649	-2.43379	-2.36513	H	1.926321	1.864193	-2.75742
H	0.566156	-0.56201	-2.852	H	-0.88732	0.681334	-2.8927
H	0.304117	-2.20526	-3.45783	H	-0.30357	2.238342	-3.50339
H	0.264816	-3.04324	-1.14472	H	0.321666	2.888126	-1.21039
H	-2.56753	-0.15257	1.840236	H	2.716379	-0.89678	1.174223
H	-2.9511	1.413266	1.159622	H	2.552697	-2.432	0.339289
H	-4.59329	-1.14342	1.016456	H	4.297958	-1.63373	-1.37534
H	-6.77332	-1.05679	0.315828	H	6.554327	-1.29251	-1.46416
H	-7.48379	0.565458	0.418841	H	7.10873	0.072764	-0.47568
H	-6.99933	-0.07444	-1.14444	H	7.363294	-1.57274	0.08813
H	-4.18871	2.373598	-0.33157	H	4.413129	-0.33285	2.183301
H	-5.48443	2.020508	-1.48256	H	6.024024	-1.04861	2.305233
H	-5.88671	2.649994	0.10532	H	5.847781	0.605705	1.73842
H	-2.11768	-2.31796	1.22307	H	2.752522	1.39304	0.718849
H	-1.55582	-3.38924	-0.05873	H	2.329773	2.658817	-0.4331
H	-3.08791	-2.53199	-0.24357	H	3.523991	1.429445	-0.86999
H	4.312179	-1.92707	-1.001	H	-3.80482	2.862208	-0.42643
H	3.36718	-1.28578	-2.35354	H	-3.28104	2.081254	-1.92636
H	3.233949	-0.55275	-0.73497	H	-3.10869	1.23966	-0.36488
H	2.729584	-3.8802	-2.51767	H	-2.00531	4.4311	-2.12664
H	3.53587	-4.1978	-0.9722	H	-2.44987	4.839857	-0.46105
H	1.822342	-4.60323	-1.16964	H	-0.74182	4.796908	-0.93005
H	-0.66518	-0.18557	2.353512	H	1.029187	-0.31226	2.005724
H	-1.00453	-1.53026	3.458737	H	1.861678	0.822855	3.086058
H	0.247642	-0.36127	3.847597	H	0.424332	-0.02655	3.633345
H	2.464021	-3.13629	2.723854	H	-1.08067	3.332014	2.970437
H	2.356429	-1.78573	3.867922	H	-1.23615	1.916765	4.025352
H	1.198393	-3.10744	3.969693	H	0.269066	2.830091	4.011581
H	1.512636	2.173413	1.364555	H	-1.88889	-1.96551	1.372762
H	0.895177	3.191155	-1.47104	H	-2.01981	-2.92948	-1.54444
H	0.639432	4.081594	0.031906	H	-1.78267	-3.94623	-0.12084
H	4.426891	4.344915	0.721986	H	-5.34668	-3.23993	1.170223
H	3.006045	4.117215	1.750579	H	-3.77877	-3.46086	1.959212
H	2.841859	4.854988	0.139153	H	-4.06365	-4.10939	0.326622
H	4.724217	2.889188	-1.3867	H	-5.55592	-1.61908	-0.82444
H	3.523825	1.636096	-1.75784	H	-4.13081	-0.70853	-1.36218
H	3.126175	3.355983	-1.96309	H	-4.25374	-2.45496	-1.66712
H	4.868853	1.93485	0.786026	H	-5.10034	-0.81027	1.367095
2b-e				2b-f			
C	-1.38885	-1.27079	-0.51268	C	1.493354	0.755549	-0.95682
C	0.191253	-1.19443	-0.19691	C	0.031256	1.040024	-0.34133
C	-0.75605	1.034467	-0.25075	C	0.360975	-1.34265	-0.62954
C	-1.98809	0.170827	-0.27359	C	1.745214	-0.80282	-0.8747
C	-1.40141	-1.54567	-2.08402	C	1.285295	1.132359	-2.49296
C	0.054954	-1.53576	-2.60843	C	-0.19708	1.516407	-2.72146
C	0.756816	-2.04948	-1.36828	C	-0.50591	2.092237	-1.35484
C	-2.92424	0.442252	0.943195	C	2.796266	-1.38048	0.11251
C	-4.33739	-0.06905	0.787763	C	4.222573	-1.19028	-0.33395
C	-5.35542	0.567482	0.186018	C	5.296134	-0.83838	0.390099
C	-6.72676	-0.05988	0.11358	C	6.663933	-0.75723	-0.24526
C	-5.24791	1.930927	-0.45374	C	5.272107	-0.5076	1.862108
C	-2.12043	-2.40924	0.20291	C	2.602832	1.630527	-0.36839
C	2.24798	-2.25055	-1.10465	C	-1.82213	2.630261	-0.79686
O	2.295873	-2.10634	0.35255	O	-1.63636	2.391572	0.636576

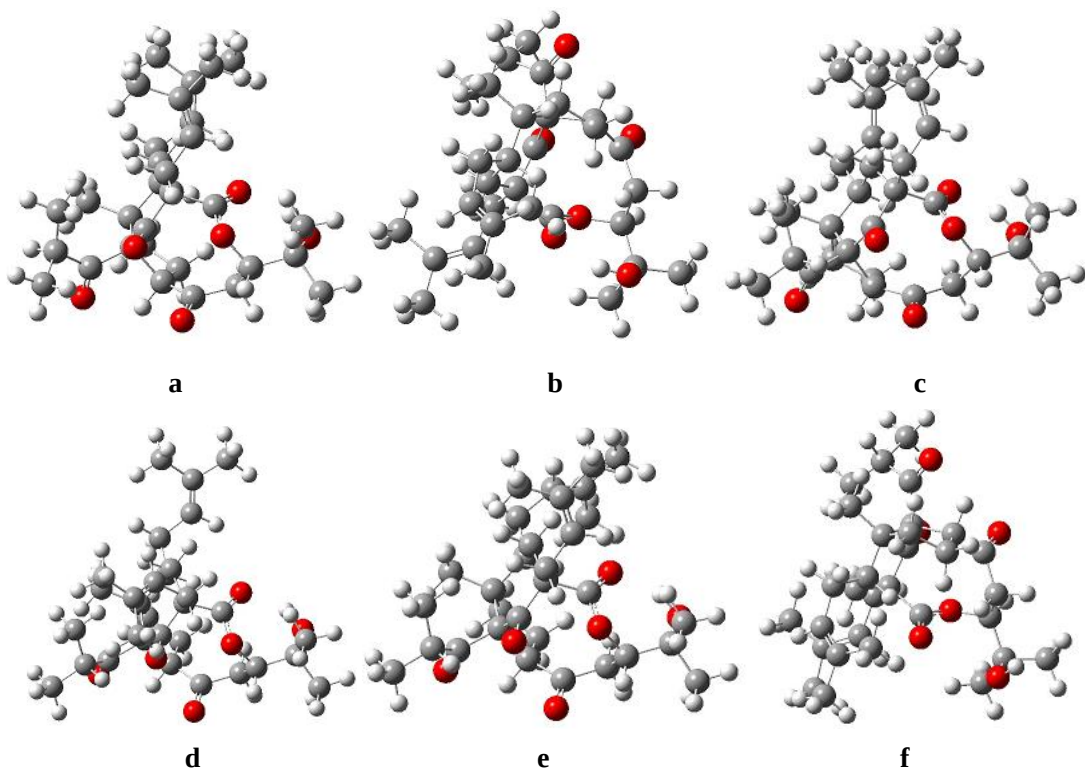
C	1.06143	-1.78995	0.921686	C	-0.44114	1.739966	0.943139
C	3.199972	-1.248	-1.75983	C	-3.1017	1.944019	-1.27891
C	2.702321	-3.68056	-1.42091	C	-1.94888	4.147851	-0.97812
C	0.39165	0.308749	-0.20672	C	-0.53974	-0.36503	-0.35128
C	0.909735	-1.96679	2.245152	C	-0.01485	1.764922	2.217348
C	-0.27463	-1.48131	3.032576	C	1.131684	0.94637	2.739707
C	1.990321	-2.63271	3.062943	C	-0.72936	2.598191	3.25401
O	1.62268	0.822397	-0.07058	O	-1.81743	-0.57117	0.000558
C	1.685773	2.207439	0.361426	C	-2.156	-1.92667	0.39675
C	0.704595	3.060802	-0.43899	C	-1.57531	-2.9329	-0.594
C	-0.71208	2.48267	-0.37247	C	-0.06816	-2.72565	-0.77441
O	-1.70365	3.200721	-0.47826	O	0.677897	-3.65237	-1.07615
C	3.167038	2.625752	0.276678	C	-3.68715	-1.96184	0.572371
C	4.045605	1.646851	1.071583	C	-4.13923	-0.86396	1.548267
C	3.352477	4.057719	0.805365	C	-4.13844	-3.34216	1.078345
O	3.49437	2.575279	-1.11842	O	-4.22335	-1.72396	-0.73596
H	-2.59581	0.435127	-1.14544	H	2.084926	-1.14285	-1.86088
H	-2.0387	-0.83025	-2.60869	H	1.610883	0.322954	-3.15061
H	-1.83092	-2.53755	-2.26419	H	1.912474	1.999184	-2.72977
H	0.385976	-0.5273	-2.87767	H	-0.81689	0.64168	-2.94543
H	0.181633	-2.17771	-3.48583	H	-0.31582	2.232624	-3.54055
H	0.313673	-3.03779	-1.17344	H	0.200938	2.925627	-1.22577
H	-2.49219	0.036259	1.862283	H	2.637621	-1.01321	1.128433
H	-2.93787	1.528081	1.071617	H	2.59288	-2.45944	0.142298
H	-4.54319	-1.05207	1.20925	H	4.390625	-1.41727	-1.38872
H	-6.75536	-1.04018	0.59773	H	6.634903	-1.00706	-1.3094
H	-7.47828	0.579627	0.595865	H	7.090083	0.25004	-0.14287
H	-7.05162	-0.18403	-0.9282	H	7.369509	-1.44195	0.244285
H	-4.24011	2.349802	-0.43127	H	4.269891	-0.52756	2.293771
H	-5.56801	1.885391	-1.50332	H	5.891714	-1.21616	2.427814
H	-5.92556	2.641088	0.039532	H	5.698836	0.487817	2.043391
H	-2.20835	-2.24708	1.277927	H	2.836958	1.379438	0.666344
H	-1.59589	-3.35942	0.054833	H	2.314339	2.687095	-0.39686
H	-3.13025	-2.52248	-0.20325	H	3.52289	1.519628	-0.94909
H	4.208674	-1.39207	-1.35912	H	-3.94886	2.298592	-0.68276
H	3.241267	-1.43257	-2.83889	H	-3.29305	2.21601	-2.3228
H	2.910636	-0.21214	-1.59167	H	-3.05923	0.859206	-1.20085
H	2.624232	-3.88473	-2.49441	H	-2.02043	4.407472	-2.04002
H	3.744849	-3.82459	-1.12231	H	-2.84755	4.518245	-0.47616
H	2.088341	-4.40881	-0.88297	H	-1.08248	4.662312	-0.55231
H	-0.93748	-0.84699	2.448263	H	1.511365	0.239379	2.005518
H	-0.86374	-2.31361	3.442173	H	1.965789	1.578573	3.074587
H	0.064328	-0.89116	3.894773	H	0.812559	0.36743	3.617206
H	2.739622	-3.11297	2.4336	H	-1.43675	3.292433	2.800601
H	2.504704	-1.90491	3.706183	H	-1.28343	1.961993	3.958517
H	1.554091	-3.38594	3.732091	H	-0.00639	3.168499	3.851962
H	1.386218	2.210914	1.420141	H	-1.69259	-2.08203	1.382529
H	1.025145	3.103354	-1.48705	H	-2.07108	-2.81834	-1.56562
H	0.672719	4.084253	-0.05953	H	-1.73906	-3.95809	-0.25551
H	5.101871	1.914938	0.950284	H	-5.2338	-0.8531	1.612396
H	3.898061	0.620945	0.733014	H	-3.7924	0.118124	1.225686
H	3.817039	1.694439	2.141503	H	-3.75468	-1.0532	2.555982
H	4.41764	4.313725	0.807717	H	-5.21716	-3.32922	1.269152
H	2.835317	4.782543	0.172892	H	-3.93824	-4.11862	0.336871
H	2.987806	4.162094	1.832737	H	-3.64247	-3.61314	2.016305
H	4.443271	2.736687	-1.20293	H	-5.18217	-1.64191	-0.649
2b-g				2b-h			
C	-1.38389	-1.30554	-0.45187	C	1.501006	0.800811	-0.91034
C	0.201413	-1.20068	-0.18528	C	0.019498	1.057284	-0.3288

C	-0.76116	1.016479	-0.33737	C	0.369236	-1.3131	-0.67872
C	-1.98803	0.144897	-0.28728	C	1.754496	-0.75935	-0.88277
C	-1.43321	-1.68615	-2.00047	C	1.343513	1.243562	-2.43441
C	0.011946	-1.73948	-2.55406	C	-0.1295	1.643047	-2.69233
C	0.740718	-2.15231	-1.29128	C	-0.48235	2.155934	-1.31102
C	-2.90909	0.478663	0.925176	C	2.79609	-1.36534	0.097753
C	-4.31929	-0.05331	0.818458	C	4.225302	-1.16805	-0.33674
C	-5.35242	0.540496	0.198975	C	5.294692	-0.82857	0.399339
C	-6.71817	-0.10269	0.180705	C	6.666363	-0.73928	-0.22653
C	-5.26892	1.868704	-0.51418	C	5.261714	-0.52069	1.876107
C	-2.08591	-2.39934	0.357486	C	2.588289	1.652072	-0.2497
C	2.240235	-2.32162	-1.04856	C	-1.8181	2.662679	-0.77389
O	2.335884	-2.0128	0.380439	O	-1.68436	2.358005	0.650694
C	1.104489	-1.68931	0.958104	C	-0.49329	1.70036	0.96893
C	3.154899	-1.38306	-1.83478	C	-3.06464	1.978033	-1.33803
C	2.699793	-3.77308	-1.22474	C	-1.96114	4.18413	-0.89162
C	0.391833	0.299502	-0.30872	C	-0.54572	-0.35029	-0.40131
C	0.992318	-1.76702	2.2945	C	-0.1085	1.672077	2.255707
C	-0.18129	-1.2479	3.076435	C	1.024919	0.834843	2.778091
C	2.111543	-2.34133	3.129646	C	-0.85802	2.458292	3.304241
O	1.622736	0.844806	-0.25174	O	-1.83176	-0.58722	-0.07725
C	1.655411	2.220441	0.239187	C	-2.12884	-1.95147	0.349865
C	0.671053	3.070512	-0.55506	C	-1.53778	-2.94574	-0.64343
C	-0.73782	2.466095	-0.49006	C	-0.04011	-2.70249	-0.84708
O	-1.74034	3.164408	-0.60947	O	0.722612	-3.60666	-1.17236
C	3.14443	2.627833	0.252638	C	-3.66376	-2.00994	0.536189
C	3.319798	3.947148	1.010054	C	-4.1102	-0.9766	1.583736
C	3.750926	2.722528	-1.15624	C	-4.1064	-3.41577	0.950381
O	3.847505	1.649642	1.022383	O	-4.30537	-1.7576	-0.71786
H	-2.60989	0.355365	-1.16393	H	2.10835	-1.06306	-1.87572
H	-2.06625	-0.99444	-2.56098	H	1.686169	0.460995	-3.1153
H	-1.88664	-2.67815	-2.10371	H	1.981089	2.116277	-2.61432
H	0.345649	-0.76079	-2.91595	H	-0.74016	0.779303	-2.97667
H	0.11284	-2.45411	-3.3768	H	-0.22152	2.395681	-3.48156
H	0.305775	-3.12154	-1.00533	H	0.217482	2.982948	-1.1197
H	-2.46117	0.129357	1.859531	H	2.633067	-1.02038	1.120836
H	-2.93245	1.569504	0.992287	H	2.591215	-2.44413	0.101098
H	-4.50938	-1.01342	1.296203	H	4.399465	-1.37873	-1.39387
H	-6.73072	-1.05545	0.717667	H	6.643259	-0.97168	-1.29473
H	-7.46912	0.555374	0.638086	H	7.093567	0.265364	-0.10508
H	-7.05593	-0.28656	-0.84801	H	7.367689	-1.43322	0.255961
H	-4.26606	2.299393	-0.52725	H	4.256555	-0.5451	2.300697
H	-5.60263	1.763714	-1.55522	H	5.87596	-1.23936	2.434721
H	-5.94819	2.59659	-0.05003	H	5.689376	0.470839	2.075344
H	-2.14331	-2.16873	1.42206	H	2.785	1.362491	0.7826
H	-1.55984	-3.35461	0.255437	H	2.3017	2.709549	-0.24902
H	-3.10611	-2.54457	-0.01037	H	3.528504	1.561168	-0.80056
H	4.167932	-1.42439	-1.42261	H	-3.92964	2.211639	-0.70989
H	3.203251	-1.69918	-2.88197	H	-3.26832	2.346303	-2.34864
H	2.807328	-0.3522	-1.79722	H	-2.94188	0.89682	-1.38134
H	2.579158	-4.09477	-2.26497	H	-1.98751	4.492223	-1.94246
H	3.755264	-3.87601	-0.95614	H	-2.88668	4.519458	-0.41429
H	2.116748	-4.44138	-0.58446	H	-1.12238	4.687421	-0.40231
H	-0.87205	-0.66949	2.467131	H	1.42094	0.150051	2.031311
H	-0.74107	-2.06025	3.559898	H	1.85128	1.454353	3.153162
H	0.169034	-0.59137	3.883866	H	0.683571	0.229391	3.628643
H	2.841026	-2.87672	2.521831	H	-1.55565	3.16828	2.860285
H	2.642812	-1.54831	3.673753	H	-1.42858	1.790298	3.964513
H	1.709498	-3.02613	3.887307	H	-0.15578	3.005791	3.946402

H	1.322808	2.165021	1.285165	H	-1.64076	-2.07634	1.327657
H	0.968313	3.126527	-1.61028	H	-2.05658	-2.84893	-1.6058
H	0.627493	4.091911	-0.16949	H	-1.6706	-3.9736	-0.29916
H	4.387938	4.144162	1.133725	H	-5.20205	-0.97371	1.643982
H	2.872146	3.884581	2.006268	H	-3.76415	0.027727	1.325934
H	2.874561	4.788404	0.471752	H	-3.71114	-1.22178	2.573689
H	4.820705	2.92804	-1.06618	H	-5.17736	-3.40712	1.168599
H	3.630805	1.783208	-1.70234	H	-3.93417	-4.13362	0.145482
H	3.296698	3.523615	-1.74823	H	-3.57409	-3.75192	1.845593
H	3.566976	0.776423	0.708079	H	-4.13483	-0.83267	-0.94367



6a



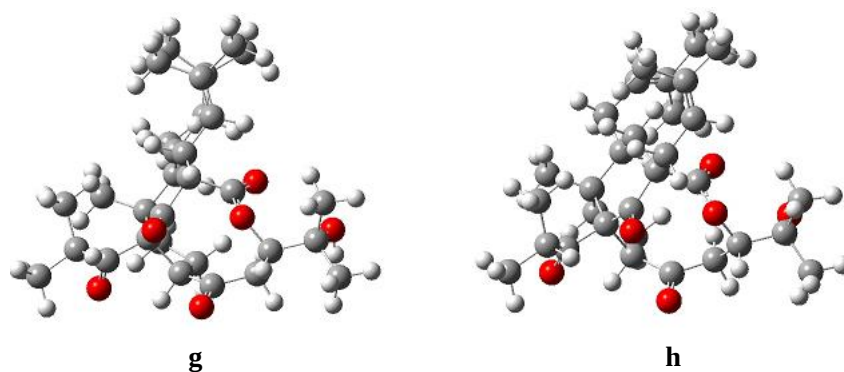


Figure S28. Optimized geometries of predominant conformers for compound **6a** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S14. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **6a** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
6a-a	-1659.274254	-1659.345283	5.9
6a-b	-1659.271846	-1659.342635	0.4
6a-c	-1659.276400	-1659.347700	76.9
6a-d	-1659.275262	-1659.345356	6.4
6a-e	-1659.274313	-1659.345810	10.4
6a-f	-1659.259380	-1659.331170	0.0
6a-g	-1659.263535	-1659.335458	0.0
6a-h	-1659.261582	-1659.334197	0.0

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S15. Optimized Z-matrixes of compound **6a** in the gas phase (Å) at B3LYP/6-31G(d,p) level

6a-a				6a-b			
C	0.346507	-2.02948	-1.36954	C	1.671349	1.122888	1.407943
C	1.464912	-1.5286	-0.34302	C	2.038716	-0.14362	0.505409
C	1.020553	-0.74237	0.883872	C	1.333825	-0.30406	-0.83353
C	-0.30324	0.043802	0.869411	C	-0.04947	0.327589	-1.06419
C	-1.35173	-0.70818	0.054324	C	-0.14965	1.668053	-0.33826
C	-0.88616	-1.07902	-1.35051	C	0.209429	1.596074	1.143734
C	-2.08141	-1.61288	-2.16871	C	-0.12601	2.937846	1.836018
C	-3.09406	-0.54479	-2.45527	C	-1.59205	3.272264	1.813472
C	-4.40254	-0.53748	-2.1675	C	-2.51038	2.954058	2.735065
C	-5.26421	0.632927	-2.55198	C	-3.94827	3.353393	2.562384
C	-5.13799	-1.64479	-1.46777	C	-2.22072	2.18123	3.989364
C	-0.08822	-3.48694	-1.16958	C	2.653557	2.2946	1.276014
C	1.071796	-1.90281	-2.72428	C	1.772146	0.541007	2.832019
C	1.835983	-0.59326	-2.64397	C	1.135697	-0.83502	2.744147
C	2.450162	-0.63999	-1.24539	C	1.727849	-1.40032	1.453706
C	2.293415	-2.76407	0.150748	C	3.583342	-0.15145	0.237289
C	1.96974	-3.62836	1.385277	C	4.293806	0.530998	-0.94792

C	3.215644	-3.65058	2.282288	C	5.14233	-0.5309	-1.66191
C	0.717325	-3.39033	2.228146	C	3.526748	1.369058	-1.97057
O	3.229812	-3.13885	-0.52423	O	4.310436	-0.66685	1.061141
O	1.746201	-0.72029	1.854546	O	1.866205	-0.96931	-1.69587
C	-0.76159	0.27393	2.336735	C	-0.27954	0.476075	-2.5943
C	-2.01029	1.091181	2.446328	C	-1.63533	1.002852	-2.94621
C	-3.19905	0.724214	2.944471	C	-1.94213	2.151086	-3.56557
C	-3.52096	-0.63493	3.496063	C	-0.9458	3.175245	-4.02788
C	-4.34106	1.700156	2.994549	C	-3.37351	2.49925	-3.86456
C	0.002925	1.405226	0.243499	C	-1.07702	-0.66406	-0.5176
O	1.058878	1.963521	0.830139	O	-0.85485	-1.88312	-1.00233
O	-0.62911	1.903319	-0.66757	O	-1.96897	-0.37539	0.255752
C	1.975627	2.822832	0.085074	C	-1.15908	-3.07897	-0.22047
C	1.424967	4.229691	-0.24472	C	-2.66543	-3.40421	-0.0888
C	0.611145	4.766202	0.9351	C	-3.38483	-3.10959	-1.40716
C	2.606334	5.157038	-0.52524	C	-2.81119	-4.88371	0.262973
O	0.650923	4.232853	-1.42494	O	-3.26818	-2.69895	0.974864
C	2.466462	2.025342	-1.11726	C	-0.40766	-2.96045	1.100605
C	2.992166	0.663368	-0.65844	C	1.062112	-2.62873	0.833283
O	3.886466	0.626509	0.159284	O	1.717012	-3.38141	0.144607
H	-1.63801	-1.60957	0.611329	H	0.498109	2.388344	-0.85441
H	-2.25111	-0.09194	-0.01719	H	-1.17222	2.036282	-0.44644
H	-0.58583	-0.14325	-1.83018	H	-0.46647	0.859343	1.58477
H	-1.71595	-2.00766	-3.12569	H	0.235972	2.913735	2.868206
H	-2.54217	-2.45637	-1.64767	H	0.421293	3.747983	1.341456
H	-2.69381	0.331805	-2.96428	H	-1.93846	3.826931	0.943259
H	-4.69067	1.413468	-3.05527	H	-4.10762	3.910841	1.637277
H	-6.0758	0.321313	-3.21979	H	-4.59981	2.472302	2.544807
H	-5.74059	1.076155	-1.6698	H	-4.28736	3.975445	3.39894
H	-5.92806	-2.04828	-2.1114	H	-2.78005	1.238814	3.993684
H	-5.63636	-1.26515	-0.56841	H	-2.54631	2.739933	4.87407
H	-4.49557	-2.4735	-1.17023	H	-1.16438	1.94046	4.112782
H	0.769543	-4.16091	-1.13104	H	3.687727	1.969285	1.404476
H	-0.6926	-3.80529	-2.02131	H	2.459094	3.02293	2.065879
H	-0.68788	-3.64191	-0.27069	H	2.573746	2.822823	0.323743
H	0.376629	-1.94913	-3.56699	H	1.303685	1.191673	3.575464
H	1.776671	-2.73342	-2.83332	H	2.827856	0.439718	3.10404
H	2.610065	-0.50717	-3.41148	H	1.37933	-1.46979	3.600561
H	1.159841	0.25461	-2.77848	H	0.046643	-0.75326	2.70779
H	3.338088	-1.27635	-1.30406	H	2.735027	-1.75532	1.691531
H	1.881925	-4.62525	0.934891	H	4.991222	1.199201	-0.42708
H	3.07629	-4.3707	3.092933	H	5.775628	-0.05474	-2.41507
H	4.098451	-3.93452	1.709233	H	5.778781	-1.0578	-0.95084
H	3.38006	-2.66302	2.718328	H	4.493703	-1.25483	-2.15963
H	-0.16271	-3.12219	1.639162	H	2.720536	1.962835	-1.53348
H	0.876637	-2.60835	2.970306	H	3.09797	0.747192	-2.75646
H	0.473175	-4.31368	2.760746	H	4.220707	2.072171	-2.43933
H	-0.88259	-0.71026	2.793713	H	0.51455	1.119676	-2.97825
H	0.063475	0.759392	2.86447	H	-0.12221	-0.50784	-3.04388
H	-1.92629	2.115623	2.084334	H	-2.46869	0.355682	-2.67359
H	-2.6889	-1.3366	3.440669	H	0.085838	2.920412	-3.78598
H	-4.36827	-1.07478	2.957925	H	-1.16525	4.151068	-3.58024
H	-3.82651	-0.56007	4.54578	H	-1.01169	3.311361	-5.11325
H	-4.68624	1.848226	4.02427	H	-3.52885	2.627606	-4.94197
H	-5.20205	1.324526	2.429523	H	-3.65178	3.449987	-3.39552
H	-4.06516	2.673658	2.585076	H	-4.06349	1.730864	-3.51093
H	2.793945	2.920618	0.800065	H	-0.68142	-3.8491	-0.82813
H	0.305577	5.791861	0.719043	H	-4.42561	-3.42846	-1.32316
H	-0.29042	4.170201	1.090494	H	-3.37563	-2.03997	-1.62596

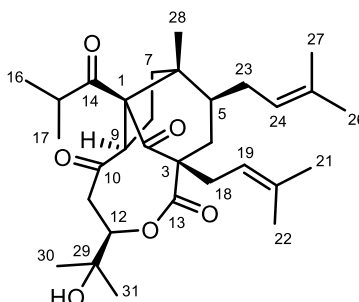
H	1.187595	4.759307	1.864187	H	-2.92355	-3.63322	-2.24892
H	2.220466	6.142951	-0.79067	H	-3.87136	-5.10879	0.392195
H	3.200822	4.798959	-1.36809	H	-2.30839	-5.11953	1.20289
H	3.254032	5.258578	0.348438	H	-2.41076	-5.52582	-0.52477
H	-0.04187	3.564141	-1.30284	H	-3.08284	-1.75841	0.821064
H	1.680847	1.968334	-1.86809	H	-0.91141	-2.24825	1.751066
H	3.306944	2.556743	-1.57193	H	-0.43213	-3.93028	1.604976
6a-c				6a-d			
C	-1.13384	-1.70056	1.291729	C	-1.19906	0.628891	-1.83768
C	-1.95489	-0.79909	0.251733	C	-0.94486	-0.84749	-1.26489
C	-1.19444	-0.24377	-0.95734	C	-0.62935	-0.97348	0.231384
C	0.336637	-0.05587	-0.89968	C	-0.00076	0.211261	0.994664
C	0.979835	-1.16179	-0.0726	C	-0.56214	1.532838	0.485421
C	0.371293	-1.3029	1.317021	C	-0.41978	1.702392	-1.02186
C	1.24136	-2.25281	2.168079	C	-0.7824	3.151059	-1.41357
C	2.580073	-1.65635	2.485635	C	0.220932	4.141327	-0.90199
C	3.797155	-2.15749	2.235343	C	0.007544	5.239818	-0.16508
C	5.033605	-1.40495	2.641552	C	1.153763	6.126139	0.236221
C	4.066239	-3.47073	1.557373	C	-1.33618	5.708749	0.31571
C	-1.27112	-3.21032	1.05891	C	-2.68104	1.013456	-1.92558
C	-1.78448	-1.31822	2.635398	C	-0.59044	0.540265	-3.25161
C	-1.97035	0.188169	2.567155	C	0.701235	-0.24044	-3.07219
C	-2.52098	0.408641	1.157416	C	0.29024	-1.38896	-2.15079
C	-3.22074	-1.61354	-0.20996	C	-2.17091	-1.74868	-1.67305
C	-3.38145	-2.21353	-1.6071	C	-3.20127	-2.29199	-0.68551
C	-2.22221	-3.08274	-2.10324	C	-3.88877	-1.2462	0.197368
C	-4.70235	-2.96989	-1.70474	C	-4.23348	-3.13951	-1.42265
O	-4.11888	-1.75086	0.595838	O	-2.27812	-2.03375	-2.84923
O	-1.80021	0.09824	-1.94903	O	-0.80412	-2.02759	0.80215
C	0.883539	-0.02616	-2.35569	C	-0.1851	0.024876	2.5314
C	2.354269	0.23861	-2.43046	C	-1.56518	0.286761	3.053296
C	3.318357	-0.56272	-2.90381	C	-2.39078	-0.5852	3.650857
C	3.099706	-1.94029	-3.46003	C	-2.09967	-2.04376	3.85323
C	4.750707	-0.10733	-2.91893	C	-3.7105	-0.12455	4.203714
C	0.587237	1.314534	-0.26882	C	1.50838	0.133931	0.754899
O	-0.15149	2.248971	-0.86237	O	1.957207	-1.09344	1.002074
O	1.355145	1.518515	0.651154	O	2.200563	1.070334	0.405602
C	-0.66322	3.397916	-0.12008	C	3.102764	-1.64956	0.288497
C	0.394021	4.469117	0.235907	C	4.473403	-1.05316	0.686529
C	1.370696	4.652437	-0.92808	C	4.520684	-0.80294	2.19561
C	-0.32841	5.785228	0.519223	C	5.564864	-2.04489	0.287621
O	1.088643	4.152767	1.422809	O	4.760333	0.132721	-0.02291
C	-1.45111	2.852805	1.06469	C	2.77716	-1.58225	-1.19852
C	-2.47461	1.824328	0.580648	C	1.392622	-2.18233	-1.449
O	-3.2941	2.155817	-0.24935	O	1.181057	-3.32985	-1.11883
H	0.885598	-2.10462	-0.62682	H	-1.61872	1.59425	0.768962
H	2.049918	-0.96106	0.018778	H	-0.05047	2.35924	0.987939
H	0.447233	-0.31937	1.788501	H	0.642668	1.586532	-1.25035
H	0.72547	-2.46855	3.112509	H	-0.82032	3.231305	-2.50775
H	1.353482	-3.21193	1.655988	H	-1.78632	3.393025	-1.05542
H	2.536107	-0.68681	2.981355	H	1.252184	3.923773	-1.17952
H	4.793344	-0.45898	3.130384	H	2.109434	5.748169	-0.1317
H	5.647851	-1.99834	3.328908	H	1.017779	7.143272	-0.14953
H	5.663697	-1.18712	1.771345	H	1.219441	6.214474	1.326846
H	4.626013	-4.13894	2.221771	H	-1.56927	6.695513	-0.10056
H	4.692389	-3.32221	0.670091	H	-1.33482	5.825942	1.405303
H	3.161479	-3.9928	1.246248	H	-2.15198	5.035933	0.051259
H	-2.31378	-3.51322	0.953798	H	-3.26705	0.251917	-2.44127
H	-0.87736	-3.74835	1.923782	H	-2.78546	1.932399	-2.50586

H	-0.72064	-3.55535	0.18139	H	-3.12987	1.18978	-0.94577
H	-1.18143	-1.64018	3.488704	H	-0.43748	1.528503	-3.69348
H	-2.76007	-1.80604	2.71292	H	-1.26972	-0.0161	-3.90282
H	-2.66643	0.563389	3.322327	H	1.100745	-0.6204	-4.01654
H	-1.01873	0.700167	2.730125	H	1.475931	0.391862	-2.6319
H	-3.59062	0.195618	1.201333	H	-0.18266	-2.14065	-2.78512
H	-3.42628	-1.33463	-2.25894	H	-2.61547	-2.93806	-0.02362
H	-2.36218	-3.29319	-3.16617	H	-4.50892	-1.76165	0.935141
H	-1.24655	-2.60476	-1.99719	H	-3.18997	-0.62013	0.755227
H	-2.19275	-4.04035	-1.57824	H	-4.54789	-0.60276	-0.39042
H	-5.545	-2.33617	-1.42757	H	-3.7592	-3.93218	-2.00205
H	-4.71335	-3.83834	-1.04098	H	-4.82234	-2.53435	-2.11655
H	-4.85192	-3.32028	-2.72926	H	-4.91668	-3.59635	-0.70187
H	0.621005	-0.98015	-2.81859	H	0.156251	-0.97695	2.786704
H	0.326962	0.741784	-2.89878	H	0.500198	0.733565	3.015012
H	2.666813	1.21528	-2.06181	H	-1.89777	1.321855	2.997988
H	2.058358	-2.26072	-3.43329	H	-1.24089	-2.39104	3.281695
H	3.692528	-2.67546	-2.90415	H	-2.96272	-2.64556	3.549392
H	3.439268	-1.99195	-4.50065	H	-1.93199	-2.25685	4.915489
H	5.150922	-0.10263	-3.93938	H	-3.77693	-0.33405	5.277508
H	5.384315	-0.78927	-2.34004	H	-4.54156	-0.66116	3.732075
H	4.864765	0.89603	-2.50446	H	-3.86765	0.945958	4.056757
H	-1.36303	3.817589	-0.84451	H	3.060951	-2.69102	0.611121
H	2.055912	5.46858	-0.69074	H	5.521286	-0.4609	2.467335
H	1.962548	3.748849	-1.08686	H	3.807821	-0.02841	2.485437
H	0.852717	4.888419	-1.86168	H	4.291684	-1.70727	2.766054
H	0.412197	6.535479	0.801977	H	6.536246	-1.61168	0.532667
H	-1.02754	5.684099	1.351687	H	5.552541	-2.23763	-0.78701
H	-0.87095	6.143261	-0.35861	H	5.460677	-2.99324	0.819565
H	1.460526	3.265033	1.295876	H	4.023313	0.740741	0.147968
H	-0.76732	2.473155	1.821483	H	2.889624	-0.56008	-1.55425
H	-2.01149	3.672978	1.521496	H	3.49839	-2.19527	-1.74564
6a-e				6a-f			
C	1.795886	0.761302	1.393009	C	1.751025	1.226719	1.271477
C	1.999252	-0.44602	0.359437	C	2.059385	-0.09182	0.418886
C	1.22393	-0.38072	-0.96065	C	1.280618	-0.3174	-0.86941
C	-0.07384	0.446957	-1.06719	C	-0.11897	0.289714	-1.03981
C	0.002689	1.695416	-0.19624	C	-0.16428	1.683437	-0.41437
C	0.381056	1.396388	1.2506	C	0.292764	1.732702	1.04124
C	0.19396	2.663252	2.11893	C	0.042224	3.14138	1.627206
C	-1.23953	3.105706	2.225024	C	-1.40822	3.543483	1.617
C	-2.12944	2.748471	3.160182	C	-2.33313	3.24964	2.539834
C	-3.53858	3.267897	3.125315	C	-3.756	3.704217	2.382827
C	-1.83484	1.814277	4.298258	C	-2.06206	2.44403	3.777293
C	2.870899	1.851038	1.303019	C	2.766381	2.356753	1.053253
C	1.89945	0.037965	2.750683	C	1.876989	0.712507	2.719932
C	1.112137	-1.24864	2.5736	C	1.216148	-0.65543	2.71187
C	1.564958	-1.75057	1.200881	C	1.788246	-1.29022	1.446559
C	3.542533	-0.60677	0.093546	C	3.585673	-0.13425	0.065713
C	4.221729	-0.2256	-1.2226	C	4.23262	0.492389	-1.18465
C	3.926379	1.181756	-1.74834	C	5.033342	-0.60408	-1.90108
C	5.725752	-0.45956	-1.12417	C	3.413951	1.294874	-2.19604
O	4.216058	-1.07672	0.988125	O	4.353307	-0.62756	0.866192
O	1.602191	-1.02272	-1.91596	O	1.768689	-1.02079	-1.72862
C	-0.312	0.793369	-2.56524	C	-0.4699	0.324854	-2.55077
C	-1.57396	1.56068	-2.80511	C	-1.87024	0.77697	-2.82438
C	-1.71022	2.783577	-3.33631	C	-2.27562	1.884709	-3.46027
C	-0.57791	3.657292	-3.7945	C	-1.36414	2.933442	-4.03053
C	-3.07404	3.385025	-3.53062	C	-3.73965	2.158583	-3.66329

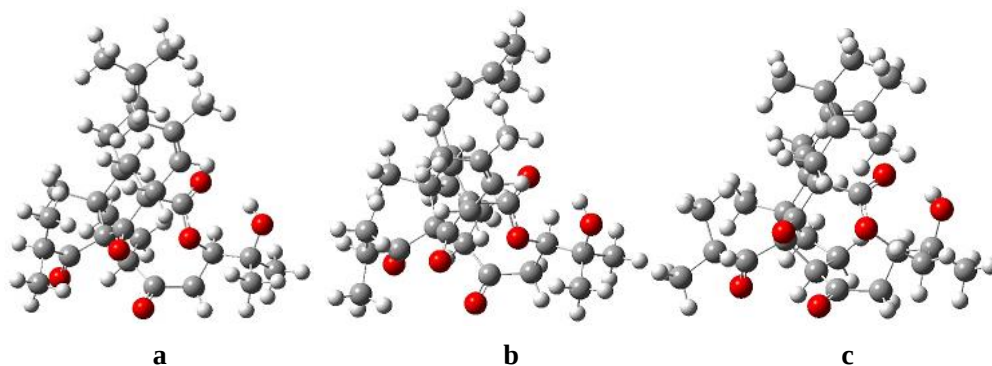
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O	-1.14555	-1.65022	-1.19703	O	-0.94562	-1.90353	-0.84019
O	-2.0688	-0.13226	0.195882	O	-1.81889	-0.37995	0.583154
C	-1.57678	-2.86534	-0.51147	C	-1.12355	-3.08675	-0.02386
C	-3.10752	-3.02563	-0.364	C	-2.59163	-3.54597	0.183647
C	-3.81038	-2.54941	-1.63759	C	-3.45908	-3.11612	-0.99089
C	-3.41728	-4.50198	-0.12121	C	-2.5946	-5.07291	0.318491
O	-3.60594	-2.34184	0.765246	O	-3.1937	-2.9686	1.330015
C	-0.79006	-2.94218	0.791056	C	-0.31848	-2.91872	1.260794
C	0.705599	-2.80544	0.502493	C	1.131396	-2.56185	0.91423
O	1.228277	-3.58307	-0.2672	O	1.772963	-3.33281	0.23369
H	0.72351	2.390047	-0.64623	H	0.445474	2.356583	-1.03162
H	-0.96894	2.19269	-0.22629	H	-1.19158	2.050528	-0.4777
H	-0.35341	0.675474	1.618542	H	-0.37998	1.06565	1.583319
H	0.604298	2.486925	3.117236	H	0.432587	3.18226	2.649505
H	0.779824	3.484488	1.691736	H	0.609256	3.883587	1.05553
H	-1.58634	3.783532	1.4472	H	-1.735	4.122997	0.755484
H	-3.70346	3.942593	2.283079	H	-3.90038	4.279922	1.466386
H	-4.25721	2.444118	3.046503	H	-4.43878	2.84733	2.356985
H	-3.78242	3.807177	4.048102	H	-4.06696	4.32651	3.230133
H	-2.4726	0.925096	4.236613	H	-2.61482	1.498399	3.74257
H	-2.05861	2.290189	5.259711	H	-2.40481	2.976297	4.671661
H	-0.79794	1.477571	4.322269	H	-1.00596	2.206041	3.909943
H	3.877733	1.431441	1.319668	H	3.792276	2.001888	1.169163
H	2.795519	2.510183	2.170246	H	2.620312	3.129626	1.810383
H	2.770698	2.472525	0.41116	H	2.675779	2.838867	0.077856
H	1.535555	0.657272	3.57487	H	1.433727	1.407231	3.438754
H	2.947927	-0.19848	2.951677	H	2.936525	0.606377	2.97569
H	1.32882	-1.98703	3.350429	H	1.459407	-1.24868	3.59806
H	0.038203	-1.05105	2.614195	H	0.128283	-0.55627	2.676491
H	2.513541	-2.26871	1.351778	H	2.807381	-1.61566	1.680599
H	3.797476	-0.93355	-1.94252	H	4.962192	1.175905	-0.73188
H	4.300312	1.268475	-2.77133	H	5.624529	-0.16406	-2.70856
H	2.860861	1.416467	-1.77545	H	5.706987	-1.10603	-1.20638
H	4.429443	1.942733	-1.14724	H	4.353152	-1.34282	-2.33005
H	5.950746	-1.48324	-0.8244	H	2.634107	1.909396	-1.74022
H	6.182886	0.206071	-0.38738	H	2.940835	0.645459	-2.93244
H	6.193032	-0.26919	-2.09376	H	4.083878	1.975189	-2.7291
H	0.565084	1.342639	-2.91439	H	0.264858	0.968027	-3.04038
H	-0.32219	-0.14871	-3.11956	H	-0.31222	-0.68146	-2.94597
H	-2.49145	1.044266	-2.52384	H	-2.64817	0.102493	-2.46732
H	0.406287	3.219057	-3.6301	H	-0.30634	2.722593	-3.87417
H	-0.60751	4.623462	-3.27838	H	-1.58131	3.911287	-3.58587
H	-0.67176	3.875394	-4.86431	H	-1.52913	3.04061	-5.10861
H	-3.25705	3.6084	-4.58799	H	-3.98063	2.234842	-4.72996
H	-3.16307	4.335879	-2.99276	H	-4.02605	3.115233	-3.21127
H	-3.86732	2.721381	-3.18164	H	-4.36551	1.377079	-3.22847
H	-1.20486	-3.63178	-1.1932	H	-0.62074	-3.83752	-0.63719
H	-4.88079	-2.74455	-1.54668	H	-4.4495	-3.56499	-0.89297
H	-3.67291	-1.47593	-1.78219	H	-3.57308	-2.03182	-0.9862
H	-3.43402	-3.06265	-2.52673	H	-3.02157	-3.42379	-1.94283
H	-4.49466	-4.61465	0.012399	H	-3.61005	-5.41037	0.535677
H	-2.93383	-4.86477	0.788021	H	-1.94475	-5.41044	1.133485
H	-3.1025	-5.12319	-0.96279	H	-2.25499	-5.56087	-0.59816
H	-3.32094	-1.41804	0.67514	H	-2.80725	-3.3765	2.110721
H	-1.17293	-2.209	1.498506	H	-0.8023	-2.18942	1.907905
H	-0.94104	-3.92812	1.238966	H	-0.28322	-3.87964	1.78469
6a-g				6a-h			
C	-0.65317	-1.99366	1.22015	C	1.876351	0.906933	1.267098

C	-1.68	-1.2672	0.222985	C	2.032004	-0.3691	0.304213
C	-1.08482	-0.49885	-0.96346	C	1.183601	-0.39873	-0.97128
C	0.349238	0.059819	-0.88724	C	-0.13663	0.390679	-1.0436
C	1.254317	-0.90323	-0.12843	C	-0.01029	1.713474	-0.29588
C	0.725624	-1.27063	1.252029	C	0.46597	1.558076	1.142606
C	1.80858	-2.04668	2.031406	C	0.353994	2.911311	1.884582
C	2.986207	-1.17885	2.36254	C	-1.05502	3.436823	1.95301
C	4.282834	-1.39818	2.10673	C	-1.99608	3.106245	2.846512
C	5.325607	-0.40146	2.530406	C	-3.37573	3.695188	2.772926
C	4.830913	-2.609	1.406782	C	-1.78757	2.125834	3.9642
C	-0.45304	-3.48577	0.928118	C	2.964935	1.96911	1.069169
C	-1.34349	-1.80778	2.586103	C	2.010464	0.271603	2.665579
C	-1.86239	-0.3788	2.56852	C	1.206563	-1.01602	2.589058
C	-2.49439	-0.26298	1.181786	C	1.648044	-1.61098	1.252571
C	-2.72945	-2.33445	-0.26283	C	3.558771	-0.54828	-0.03385
C	-2.76973	-2.902	-1.68136	C	4.165177	-0.24217	-1.40339
C	-1.44892	-3.45872	-2.2208	C	3.83135	1.12815	-1.99977
C	-3.88078	-3.94025	-1.80055	C	5.673954	-0.46383	-1.37227
O	-3.55922	-2.70642	0.542699	O	4.280381	-0.97162	0.846806
O	-1.76415	-0.27969	-1.94303	O	1.522284	-1.09292	-1.90551
C	0.856926	0.314651	-2.33257	C	-0.50153	0.602902	-2.53784
C	2.194054	0.984952	-2.3823	C	-1.83345	1.254423	-2.73853
C	3.352287	0.494281	-2.84416	C	-2.10076	2.439448	-3.30423
C	3.539206	-0.8851	-3.40782	C	-1.07087	3.385704	-3.85166
C	4.597691	1.335745	-2.83466	C	-3.51936	2.9152	-3.44847
C	0.245949	1.405423	-0.15564	C	-1.20303	-0.50597	-0.39759
O	-0.65452	2.188865	-0.77258	O	-1.20593	-1.70853	-0.99729
O	0.858103	1.712682	0.836681	O	-1.91705	-0.19628	0.52314
C	-1.47313	3.121079	-0.02638	C	-1.50756	-2.91584	-0.25792
C	-0.80127	4.472406	0.33877	C	-3.01535	-3.21317	-0.02969
C	0.290911	4.816822	-0.66351	C	-3.86318	-2.55905	-1.11083
C	-1.88735	5.553932	0.339442	C	-3.20313	-4.73388	-0.04684
O	-0.16207	4.444935	1.604065	O	-3.49658	-2.6924	1.198968
C	-2.0953	2.378995	1.15231	C	-0.66074	-2.93164	1.010829
C	-2.8241	1.129838	0.64721	C	0.816105	-2.74289	0.65168
O	-3.71357	1.262133	-0.16594	O	1.342118	-3.54062	-0.09453
H	1.387796	-1.80558	-0.73999	H	0.671496	2.364475	-0.85926
H	2.243861	-0.45093	-0.02605	H	-0.98613	2.204569	-0.30039
H	0.592234	-0.32688	1.784467	H	-0.25485	0.896764	1.626017
H	1.380335	-2.42292	2.96984	H	0.764028	2.808234	2.894628
H	2.12029	-2.92744	1.463768	H	0.975923	3.658117	1.380332
H	2.732323	-0.2506	2.874048	H	-1.33569	4.148702	1.178931
H	4.884197	0.461795	3.031811	H	-3.47542	4.395281	1.941045
H	6.053389	-0.85775	3.211784	H	-4.12873	2.908814	2.647644
H	5.894669	-0.03812	1.666627	H	-3.62822	4.225687	3.698519
H	5.516721	-3.15606	2.063964	H	-2.40208	1.232719	3.803624
H	5.415743	-2.31239	0.528514	H	-2.09945	2.555357	4.922707
H	4.060437	-3.30591	1.076915	H	-0.75025	1.802474	4.061056
H	-1.40143	-4.01428	0.822825	H	3.964954	1.533648	1.064469
H	0.072268	-3.9526	1.763828	H	2.938234	2.676441	1.900353
H	0.142031	-3.66058	0.029455	H	2.831434	2.541578	0.148999
H	-0.66257	-2.00894	3.417697	H	1.670892	0.947999	3.454737
H	-2.18385	-2.50318	2.665153	H	3.06174	0.037593	2.857176
H	-2.59915	-0.18602	3.353518	H	1.423593	-1.70001	3.414506
H	-1.04287	0.329196	2.714996	H	0.135117	-0.80302	2.619934
H	-3.47532	-0.73838	1.247216	H	2.616705	-2.08414	1.427682
H	-3.02647	-2.03234	-2.29539	H	3.707829	-0.99522	-2.05404
H	-1.55482	-3.65777	-3.28985	H	4.143185	1.148845	-3.04675
H	-0.61066	-2.76962	-2.10455	H	2.765133	1.36038	-1.97797

H	-1.18868	-4.40121	-1.73341	H	4.366372	1.926578	-1.48018
H	-4.84334	-3.53051	-1.49371	H	5.921856	-1.46654	-1.02368
H	-3.67966	-4.81112	-1.17125	H	6.165358	0.247104	-0.70283
H	-3.96006	-4.27815	-2.8371	H	6.087208	-0.3305	-2.37536
H	0.867764	-0.64882	-2.84812	H	0.304086	1.185453	-2.99127
H	0.106796	0.926311	-2.83915	H	-0.48127	-0.37699	-3.02066
H	2.208998	2.006543	-2.00323	H	-2.68692	0.671864	-2.39231
H	2.628475	-1.4835	-3.40027	H	-0.04644	3.038123	-3.719
H	4.303073	-1.42914	-2.84069	H	-1.15836	4.366534	-3.37087
H	3.899189	-0.83312	-4.44164	H	-1.23268	3.550965	-4.92293
H	4.994053	1.463042	-3.84875	H	-3.77273	3.080408	-4.50217
H	5.390478	0.855738	-2.24922	H	-3.66512	3.875349	-2.94019
H	4.417332	2.326368	-2.41315	H	-4.2334	2.20039	-3.03515
H	-2.26583	3.323879	-0.74964	H	-1.11134	-3.67562	-0.93491
H	0.656653	5.826769	-0.46776	H	-4.89843	-2.89085	-1.0091
H	1.124177	4.122748	-0.55066	H	-3.83651	-1.4757	-0.99055
H	-0.07999	4.765202	-1.68922	H	-3.50331	-2.81625	-2.10915
H	-1.45007	6.499599	0.666186	H	-4.24244	-4.96987	0.190742
H	-2.7072	5.305749	1.022949	H	-2.56477	-5.229	0.693569
H	-2.31839	5.695665	-0.65446	H	-2.96482	-5.15921	-1.02449
H	-0.84178	4.456047	2.284537	H	-3.16275	-3.24708	1.910428
H	-1.33356	2.165353	1.900294	H	-1.0359	-2.18966	1.713407
H	-2.85833	3.017424	1.610169	H	-0.74114	-3.91933	1.477432



6b



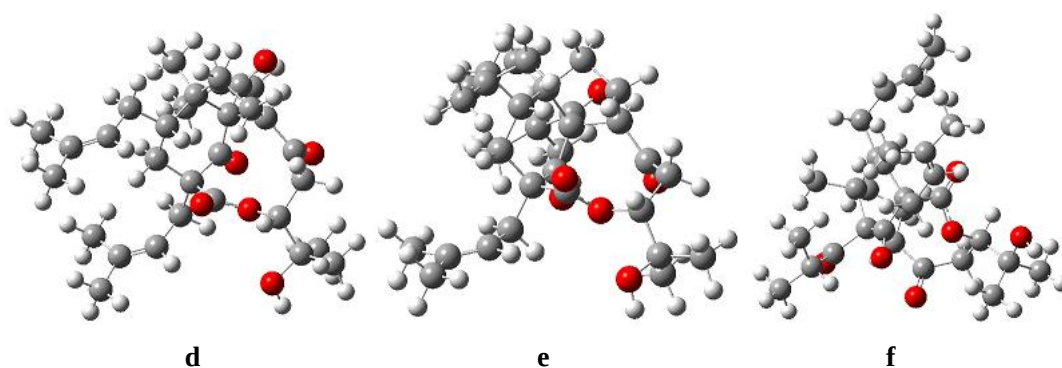


Figure S29. Optimized geometries of predominant conformers for compound **6b** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S16. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **6b** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
6b-a	-1659.269902	-1659.341102	5.9
6b-b	-1659.267847	-1659.339544	0.4
6b-c	-1659.270206	-1659.342030	76.9
6b-d	-1659.266869	-1659.338664	6.4
6b-e	-1659.265188	-1659.338097	0.0
6b-f	-1659.267047	-1659.339636	10.4

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S17. Optimized Z-matrixes of compound **6b** in the gas phase (Å) at B3LYP/6-31G(d,p) level

6b-a				6b-b			
C	-0.09913	-1.99236	-1.34038	C	-0.82441	-1.78029	1.394849
C	1.06771	-1.73525	-0.26037	C	-1.77302	-0.92093	0.41561
C	0.740687	-0.8357	0.929817	C	-1.16733	-0.42654	-0.89587
C	-0.36226	0.225658	0.812736	C	0.347622	-0.20786	-1.00811
C	-1.56269	-0.38549	0.091738	C	1.069253	-1.38547	-0.35397
C	-1.20749	-0.88879	-1.30252	C	0.700211	-1.55331	1.115961
C	-2.49003	-1.28356	-2.06492	C	1.601608	-2.6202	1.780119
C	-3.37116	-0.09993	-2.33264	C	3.068451	-2.29461	1.69828
C	-4.65299	0.082514	-1.9885	C	3.778657	-1.54202	2.548523
C	-5.37154	1.350158	-2.35799	C	5.241341	-1.28769	2.320553
C	-5.49152	-0.90695	-1.23096	C	3.207897	-0.88079	3.769634
C	-0.71566	-3.39416	-1.24031	C	-1.16919	-3.27587	1.405056
C	0.644619	-1.85747	-2.68781	C	-1.13531	-1.17943	2.78364
C	1.652447	-0.73887	-2.47576	C	-1.32038	0.31011	2.54115
C	2.252427	-1.12072	-1.12831	C	-2.23387	0.303483	1.321627
C	1.582763	-3.10866	0.295801	C	-3.06584	-1.74103	0.075248
C	1.016052	-3.86145	1.513903	C	-3.23185	-2.72251	-1.09958
C	2.172416	-4.11018	2.492957	C	-4.43514	-2.25862	-1.93308
C	-0.21743	-3.36327	2.265469	C	-2.06224	-3.08796	-2.01235

O	2.453371	-3.68796	-0.32084	O	-4.00803	-1.67044	0.837752
O	1.36689	-0.97287	1.958463	O	-1.8986	-0.20821	-1.83749
C	-0.72388	0.74891	2.229555	C	0.73249	-0.03611	-2.50311
C	-1.72448	1.862193	2.231773	C	2.182795	0.258249	-2.72747
C	-2.96615	1.851539	2.735828	C	3.080706	-0.48651	-3.38719
C	-3.62036	0.672678	3.397433	C	2.798276	-1.81386	-4.03071
C	-3.8234	3.084918	2.677579	C	4.497272	-0.00941	-3.54628
C	0.195915	1.384865	-0.00256	C	0.68525	1.083782	-0.27431
O	1.509737	1.505551	0.213547	O	-0.32897	1.948753	-0.38108
O	-0.43108	2.093341	-0.7602	O	1.705256	1.313257	0.338688
C	2.315642	2.154936	-0.79353	C	-0.46249	2.980251	0.621149
C	2.617296	3.60433	-0.37868	C	0.077898	4.315255	0.084753
C	3.382032	3.693053	0.936261	C	-0.65925	4.791948	-1.16106
C	3.376249	4.295731	-1.5129	C	0.016912	5.359136	1.20145
O	1.38383	4.270243	-0.15368	O	1.427267	4.123063	-0.31336
C	3.514283	1.219929	-0.99716	C	-1.93921	2.934376	1.032196
C	3.2456	-0.18643	-0.4441	C	-2.6046	1.611372	0.6301
O	3.892802	-0.58478	0.497396	O	-3.49249	1.622414	-0.1919
H	-1.96545	-1.19623	0.711345	H	0.844867	-2.29438	-0.92593
H	-2.34816	0.370355	0.014123	H	2.145246	-1.21592	-0.43839
H	-0.80787	-0.02152	-1.83834	H	0.9775	-0.61077	1.597195
H	-2.21155	-1.72953	-3.02901	H	1.302985	-2.7423	2.826421
H	-3.02967	-2.0583	-1.51433	H	1.43547	-3.59072	1.30132
H	-2.88463	0.709775	-2.87665	H	3.598932	-2.70878	0.842869
H	-6.25031	1.138771	-2.97843	H	5.438986	-0.215	2.213639
H	-5.73958	1.866368	-1.46369	H	5.838959	-1.63223	3.172491
H	-4.72639	2.039947	-2.90523	H	5.60658	-1.78996	1.422706
H	-6.3613	-1.20923	-1.82537	H	3.266839	0.209487	3.675243
H	-5.88621	-0.45217	-0.31519	H	3.784044	-1.14892	4.662253
H	-4.9505	-1.81034	-0.94967	H	2.164599	-1.14223	3.950638
H	0.054155	-4.1676	-1.24569	H	-2.23569	-3.43558	1.572163
H	-1.35025	-3.58152	-2.10849	H	-0.64919	-3.76986	2.227913
H	-1.3344	-3.53059	-0.35091	H	-0.88292	-3.7908	0.485724
H	-0.04888	-1.67263	-3.51304	H	-0.35049	-1.41385	3.508481
H	1.178862	-2.78756	-2.90951	H	-2.0711	-1.60097	3.166454
H	2.412294	-0.7056	-3.26182	H	-1.78374	0.819012	3.391298
H	1.154158	0.235695	-2.4666	H	-0.35669	0.795578	2.358281
H	2.866279	-2.01296	-1.31106	H	-3.21054	-0.05239	1.677127
H	0.761404	-4.83089	1.06688	H	-3.53909	-3.63589	-0.57443
H	1.840434	-4.76988	3.29906	H	-4.67317	-3.01024	-2.69043
H	3.015001	-4.57689	1.982476	H	-5.30896	-2.11192	-1.298
H	2.503802	-3.16511	2.927521	H	-4.20181	-1.31707	-2.43382
H	-0.99174	-2.95595	1.611374	H	-1.11825	-3.21978	-1.47872
H	0.039945	-2.60002	2.999326	H	-1.90948	-2.34087	-2.79063
H	-0.66446	-4.20594	2.800257	H	-2.28562	-4.04045	-2.501
H	-1.07049	-0.11141	2.806072	H	0.416779	-0.94543	-3.01855
H	0.205944	1.073943	2.705785	H	0.113737	0.769057	-2.91074
H	-1.38229	2.792553	1.781698	H	2.532212	1.203386	-2.31529
H	-3.89652	0.915924	4.429698	H	2.984411	-1.764	-5.10955
H	-2.99233	-0.21768	3.421121	H	1.775479	-2.16093	-3.88466
H	-4.55158	0.412965	2.881155	H	3.47352	-2.58145	-3.63603
H	-3.30992	3.915838	2.190611	H	4.658981	0.956264	-3.06401
H	-4.11621	3.406811	3.6837	H	4.760508	0.090083	-4.60574
H	-4.75341	2.890609	2.130696	H	5.204361	-0.72872	-3.11706
H	1.705651	2.203346	-1.70144	H	0.179721	2.690681	1.459154
H	3.411741	4.739041	1.24771	H	-0.12388	5.650498	-1.57129
H	2.873792	3.118958	1.712336	H	-0.67576	4.006353	-1.91783
H	4.409434	3.335232	0.845564	H	-1.68451	5.100015	-0.94652
H	3.522642	5.34582	-1.25314	H	0.481415	6.281878	0.848762

H	2.802406	4.258647	-2.4438	H	0.572594	5.020333	2.080992
H	4.356605	3.845005	-1.6905	H	-1.00963	5.584105	1.503697
H	0.693257	3.848613	-0.68278	H	1.803405	3.382457	0.181406
H	3.763404	1.167502	-2.06144	H	-2.02595	3.089584	2.112108
H	4.392596	1.576517	-0.45867	H	-2.51625	3.710333	0.528592
6b-c				6b-d			
C	-1.28895	-1.43139	1.326705	C	0.586139	2.174795	-1.02031
C	-1.94733	-0.35103	0.318621	C	-0.73136	1.870684	-0.1462
C	-1.17889	-0.06583	-0.98171	C	-0.65104	0.752043	0.887451
C	0.340163	-0.29999	-1.04543	C	0.318811	-0.41506	0.666903
C	0.681714	-1.61439	-0.35068	C	1.658584	0.134366	0.184632
C	0.249953	-1.6165	1.109195	C	1.543825	0.942007	-1.10228
C	0.823391	-2.8552	1.838653	C	2.949795	1.294563	-1.63188
C	2.327224	-2.89466	1.845615	C	3.714797	0.072242	-2.04436
C	3.148155	-2.36224	2.760178	C	4.93285	-0.32275	-1.65059
C	4.639434	-2.47455	2.618547	C	5.537688	-1.58916	-2.1896
C	2.688519	-1.61237	3.97697	C	5.805243	0.415251	-0.67555
C	-1.98692	-2.79716	1.292947	C	1.342152	3.431466	-0.56786
C	-1.48361	-0.76528	2.705581	C	0.007071	2.411538	-2.43058
C	-1.22363	0.715343	2.468399	C	-1.11223	1.393965	-2.57336
C	-2.05576	0.965354	1.21592	C	-1.84274	1.543631	-1.24301
C	-3.43637	-0.77319	0.017808	C	-1.18624	3.178644	0.586686
C	-3.90792	-1.3341	-1.32039	C	-0.70945	3.649135	1.973727
C	-3.10897	-2.52462	-1.85915	C	-1.95187	3.866438	2.84908
C	-5.39566	-1.66457	-1.2599	C	0.363489	2.892823	2.756727
O	-4.24574	-0.62365	0.911503	O	-1.92048	3.945024	-0.00353
O	-1.75697	0.360015	-1.95736	O	-1.37914	0.792629	1.856331
C	0.794289	-0.28368	-2.53187	C	0.456839	-1.22402	1.983222
C	2.265008	-0.4878	-2.72017	C	1.24851	-2.48577	1.831464
C	2.877322	-1.47621	-3.38698	C	2.438594	-2.78488	2.369698
C	2.182139	-2.61542	-4.07595	C	3.242165	-1.87039	3.249327
C	4.37542	-1.50017	-3.5086	C	3.074113	-4.12434	2.121672
C	1.017471	0.860689	-0.32756	C	-0.31524	-1.31693	-0.39287
O	0.275763	1.967658	-0.44399	O	-1.61942	-1.44869	-0.11547
O	2.064099	0.811884	0.28159	O	0.239895	-1.81575	-1.34121
C	0.428078	3.011054	0.543141	C	-2.50759	-1.93496	-1.13415
C	1.328718	4.133646	0.002153	C	-3.44613	-2.9568	-0.47633
C	0.768299	4.778639	-1.26003	C	-4.18668	-2.37876	0.725135
C	1.546707	5.169115	1.107299	C	-4.41488	-3.52532	-1.51486
O	2.576117	3.569592	-0.37167	O	-2.55599	-3.98996	-0.06234
C	-1.00771	3.394999	0.923837	C	-3.18084	-0.69224	-1.75919
C	-2.01618	2.316315	0.511501	C	-2.96042	0.560573	-0.89934
O	-2.84883	2.570139	-0.32992	O	-3.72741	0.811587	0.00408
H	0.209696	-2.43695	-0.90393	H	2.093675	0.741269	0.989289
H	1.761359	-1.76747	-0.41624	H	2.342462	-0.70241	0.020985
H	0.751654	-0.76166	1.571617	H	1.117428	0.258322	-1.84064
H	0.444407	-2.88094	2.864758	H	2.847877	1.949351	-2.50771
H	0.455604	-3.76648	1.355965	H	3.502576	1.868245	-0.88336
H	2.791682	-3.40551	1.004179	H	3.191885	-0.56723	-2.75552
H	5.102522	-1.48282	2.561534	H	6.484995	-1.38663	-2.70301
H	5.081157	-2.97611	3.48749	H	5.768055	-2.2902	-1.37877
H	4.922477	-3.03163	1.723371	H	4.870287	-2.09204	-2.89187
H	3.048707	-0.57779	3.945439	H	6.750935	0.704465	-1.14822
H	3.103275	-2.05853	4.887886	H	6.06773	-0.23113	0.169867
H	1.603293	-1.58331	4.079997	H	5.34344	1.318246	-0.27636
H	-3.0694	-2.70448	1.379611	H	0.673957	4.29039	-0.48204
H	-1.65691	-3.40036	2.140751	H	2.092316	3.696099	-1.31557
H	-1.75969	-3.36004	0.384958	H	1.864075	3.303949	0.382721
H	-0.83198	-1.20797	3.463809	H	0.778224	2.32629	-3.20143

H	-2.51788	-0.90251	3.036366	H	-0.41043	3.422376	-2.49158
H	-1.55843	1.338867	3.302436	H	-1.77117	1.612783	-3.41881
H	-0.1554	0.908089	2.328697	H	-0.7136	0.385912	-2.72478
H	-3.09596	0.914239	1.557767	H	-2.38045	2.499792	-1.28862
H	-3.7546	-0.5006	-2.01346	H	-0.30746	4.642709	1.73765
H	-3.4039	-2.71706	-2.89338	H	-1.66354	4.338584	3.792076
H	-2.03086	-2.35485	-1.85939	H	-2.67292	4.507678	2.341779
H	-3.31462	-3.43063	-1.28376	H	-2.42562	2.907626	3.068605
H	-5.98217	-0.79999	-0.94824	H	1.171213	2.507396	2.130676
H	-5.59549	-2.47063	-0.5491	H	-0.05846	2.055586	3.312011
H	-5.74283	-1.9839	-2.24602	H	0.818568	3.578997	3.476521
H	0.208488	-1.04434	-3.05208	H	0.891916	-0.55506	2.729445
H	0.484472	0.673557	-2.96197	H	-0.55302	-1.45468	2.332423
H	2.900778	0.275108	-2.27417	H	0.777745	-3.24967	1.213718
H	2.395953	-2.60112	-5.15071	H	3.417278	-2.33307	4.2273
H	1.099305	-2.60465	-3.95249	H	2.769353	-0.90291	3.417134
H	2.554528	-3.57496	-3.69984	H	4.230411	-1.68927	2.81127
H	4.839947	-0.65716	-2.99401	H	2.458376	-4.75435	1.477236
H	4.683652	-1.4699	-4.56015	H	3.24357	-4.65975	3.063267
H	4.788525	-2.4257	-3.091	H	4.056295	-4.01038	1.648222
H	0.948557	2.563599	1.39644	H	-1.90584	-2.46925	-1.87187
H	1.531887	5.43806	-1.67716	H	-4.84986	-3.13907	1.151837
H	0.530962	4.016557	-2.00375	H	-3.47513	-2.06203	1.488165
H	-0.12601	5.37357	-1.06428	H	-4.79161	-1.5107	0.457434
H	2.25222	5.92202	0.750986	H	-4.97911	-4.34745	-1.06577
H	1.978103	4.702256	1.997835	H	-3.86847	-3.92393	-2.37319
H	0.619703	5.674015	1.392764	H	-5.14017	-2.78835	-1.86675
H	2.717532	2.749861	0.121509	H	-3.04	-4.56272	0.539867
H	-1.06799	3.575149	2.001631	H	-2.8003	-0.54067	-2.77042
H	-1.32655	4.301096	0.408211	H	-4.26083	-0.82859	-1.82663
6b-e				6b-f			
C	0.444826	-2.27153	0.87948	C	0.348939	-2.20425	-0.90624
C	-0.91892	-1.75672	0.193647	C	1.467758	-1.3026	-0.16119
C	-0.80246	-0.70703	-0.90631	C	0.968424	-0.3875	0.967055
C	0.383514	0.263559	-0.90612	C	-0.47828	0.129373	0.938307
C	1.664732	-0.50737	-0.59619	C	-1.41835	-1.01544	0.577723
C	1.613115	-1.24075	0.738897	C	-1.09824	-1.62245	-0.78019
C	2.99793	-1.84262	1.074523	C	-2.19888	-2.62889	-1.19255
C	4.0903	-0.80976	1.153864	C	-3.56443	-2.0027	-1.28905
C	4.407054	-0.04895	2.209459	C	-4.07677	-1.34172	-2.33505
C	5.511943	0.965317	2.129128	C	-5.45318	-0.7435	-2.27447
C	3.703063	-0.1103	3.533959	C	-3.34708	-1.11524	-3.62748
C	0.874377	-3.66586	0.404457	C	0.364086	-3.67304	-0.46441
C	0.062976	-2.34266	2.372866	C	0.760836	-2.08978	-2.38825
C	-0.81875	-1.1298	2.613045	C	1.190163	-0.64164	-2.5649
C	-1.76847	-1.19745	1.422104	C	2.095893	-0.44329	-1.35439
C	-1.71014	-2.9787	-0.38717	C	2.628311	-2.24387	0.33665
C	-1.54071	-3.57541	-1.79741	C	2.861377	-2.61364	1.799911
C	-2.92029	-3.59006	-2.47077	C	1.643471	-3.13737	2.566358
C	-0.48269	-3.05523	-2.76997	C	4.030612	-3.58614	1.918089
O	-2.4739	-3.57344	0.346023	O	3.388459	-2.68126	-0.50484
O	-1.66821	-0.64421	-1.75328	O	1.710661	-0.04997	1.863636
C	0.454554	0.988214	-2.27554	C	-0.82325	0.753427	2.316834
C	1.520412	2.036877	-2.34349	C	-2.19186	1.356655	2.375038
C	2.576999	2.087372	-3.16632	C	-3.2081	1.020519	3.181401
C	2.915831	1.053894	-4.20231	C	-3.17282	-0.07725	4.205973
C	3.53153	3.247375	-3.11167	C	-4.51122	1.767516	3.117744
C	0.096339	1.304825	0.177219	C	-0.53714	1.238147	-0.11331
O	-1.199	1.641431	0.109188	O	0.595505	1.953018	-0.03697

O	0.881393	1.746173	0.979975	O	-1.42934	1.443761	-0.89803
C	-1.81231	2.322314	1.215355	C	0.958348	2.836751	-1.10852
C	-2.62962	3.489379	0.64222	C	1.247907	4.21649	-0.49914
C	-3.64242	3.03052	-0.40187	C	2.31215	4.149278	0.592352
C	-3.30097	4.267387	1.775335	C	1.628058	5.207243	-1.60071
O	-1.63523	4.314738	0.04227	O	-0.00725	4.597619	0.054653
C	-2.61025	1.253939	1.995753	C	2.146875	2.163936	-1.83099
C	-2.7441	-0.04626	1.189419	C	2.647251	0.944411	-1.04673
O	-3.67516	-0.18665	0.427334	O	3.541226	1.072591	-0.23881
H	1.85874	-1.20384	-1.42231	H	-1.36649	-1.77274	1.371686
H	2.495172	0.202621	-0.58144	H	-2.44177	-0.63268	0.571863
H	1.451917	-0.46375	1.49002	H	-1.18707	-0.80163	-1.49547
H	2.932635	-2.39112	2.020246	H	-1.93068	-3.08752	-2.15021
H	3.274304	-2.58004	0.313889	H	-2.24494	-3.4462	-0.46596
H	4.667813	-0.65892	0.243622	H	-4.18943	-2.08587	-0.40176
H	5.130928	1.973506	2.32813	H	-5.41474	0.340155	-2.43397
H	6.284125	0.768634	2.882062	H	-6.09655	-1.15302	-3.06204
H	5.987904	0.971474	1.146569	H	-5.9343	-0.92659	-1.31163
H	3.176105	0.830793	3.727592	H	-3.12231	-0.0502	-3.75486
H	4.421048	-0.24313	4.350926	H	-3.96633	-1.41104	-4.48153
H	2.971976	-0.91751	3.592505	H	-2.40547	-1.66245	-3.68763
H	0.052554	-4.38095	0.473551	H	1.3705	-4.09201	-0.47517
H	1.66901	-4.04399	1.050434	H	-0.22921	-4.27116	-1.15859
H	1.256337	-3.67756	-0.61831	H	-0.06018	-3.81475	0.531766
H	0.948667	-2.37767	3.013659	H	-0.05204	-2.38999	-3.05525
H	-0.51488	-3.25395	2.561682	H	1.612823	-2.74797	-2.58617
H	-1.36057	-1.18733	3.561728	H	1.734051	-0.47879	-3.50016
H	-0.22897	-0.20785	2.630007	H	0.328663	0.033918	-2.56883
H	-2.44522	-2.04152	1.610238	H	3.005856	-1.01138	-1.57962
H	-1.28935	-4.61752	-1.56188	H	3.142739	-1.65917	2.256969
H	-2.86715	-4.13917	-3.4147	H	1.880273	-3.17481	3.63237
H	-3.65782	-4.06966	-1.827	H	0.761072	-2.50543	2.456285
H	-3.24446	-2.56841	-2.67824	H	1.384423	-4.15111	2.251323
H	0.467587	-2.80957	-2.29083	H	4.929068	-3.18844	1.445847
H	-0.82823	-2.17044	-3.30371	H	3.802531	-4.54126	1.437643
H	-0.27441	-3.83449	-3.50849	H	4.245999	-3.77696	2.972731
H	0.588123	0.221172	-3.04155	H	-0.68829	-0.02714	3.068774
H	-0.52651	1.434757	-2.4604	H	-0.06648	1.512839	2.532628
H	1.398297	2.862401	-1.64346	H	-2.36181	2.179653	1.682251
H	2.915347	1.499604	-5.20362	H	-3.35305	0.327454	5.208465
H	2.22934	0.207334	-4.21461	H	-2.22771	-0.61954	4.231647
H	3.927079	0.664491	-4.03849	H	-3.9723	-0.80288	4.017776
H	3.249283	3.970184	-2.34407	H	-4.4947	2.550048	2.357002
H	3.571142	3.769325	-4.07497	H	-4.74492	2.23282	4.082542
H	4.55205	2.906804	-2.90133	H	-5.34207	1.089136	2.891364
H	-1.01417	2.747044	1.827342	H	0.090201	2.936686	-1.7631
H	-4.2153	3.890428	-0.76532	H	2.498663	5.151941	0.991586
H	-3.12929	2.566765	-1.24487	H	1.976955	3.503167	1.404252
H	-4.34544	2.298305	-0.00055	H	3.259251	3.75227	0.222255
H	-3.76736	5.16745	1.364894	H	1.716662	6.208602	-1.16988
H	-2.56163	4.581312	2.51625	H	0.852353	5.24055	-2.36957
H	-4.08525	3.695817	2.276704	H	2.584704	4.970783	-2.0721
H	-2.08818	4.95255	-0.51718	H	0.14571	5.360192	0.620454
H	-2.12971	1.068502	2.957794	H	1.854958	1.881865	-2.84437
H	-3.6272	1.595502	2.191771	H	2.996048	2.843923	-1.90394

ECD calculation details of 2–5.

The theoretical calculations of compounds 2–5 were performed using Gaussian 09^[17] and figured using GaussView 5.0.^[18] Conformation search using molecular mechanics calculations was performed in Discovery Studio 3.5 Client with MMFF force field with 20 kcal mol⁻¹ upper energy limit.^[19]

The optimized conformation geometries and thermodynamic parameters of all selected conformations were provided. The predominant conformers were optimized at B3LYP/6-31G(d,p) level. The theoretical calculation of ECD was performed using time dependent Density Functional Theory (TDDFT) at B3LYP/6-31G(d,p) level in MeOH with PCM model.^[20] The ECD spectra of compound 2–5 were obtained by weighing the Boltzmann distribution rate of each geometric conformation.^[21]

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

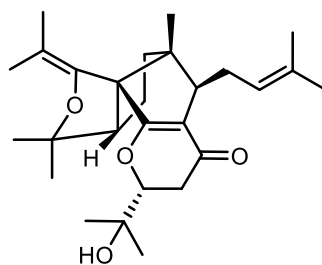
$$\Delta\epsilon(E) = \frac{1}{2.297 \times 10^{-39}} \times \frac{1}{\sqrt{2\pi}\sigma} \sum_i^A \Delta E_i R_i e^{-[(E-E_i)/(2\sigma)]^2}$$

The σ represented the width of the band at 1/e height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i , respectively. R_{vel} had been used in this work.

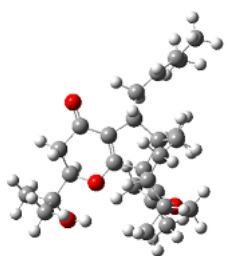
Reference

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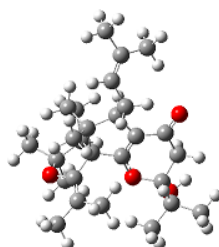
- [20] (a) Miertus, S.; Scrocc, E.; Tomasi, J. *J. Chem. Phys.* **1981**, 55, 117. (b) Miertus, S.; Tomasi, J. *J. Chem. Phys.* **1982**, 65, 239. (c) Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J. *Chem. Phys. Lett.* **1996**, 255, 327.
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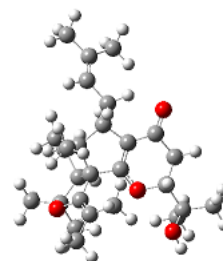
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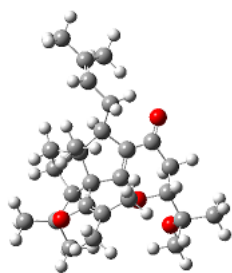
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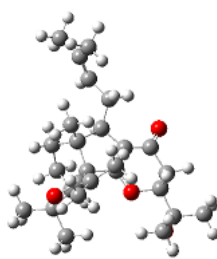
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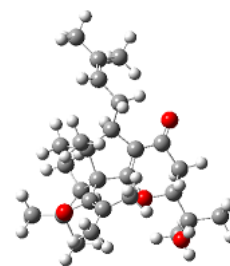
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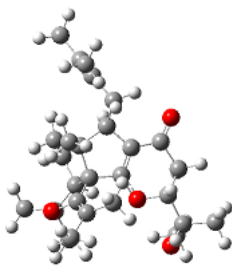
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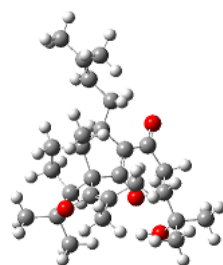
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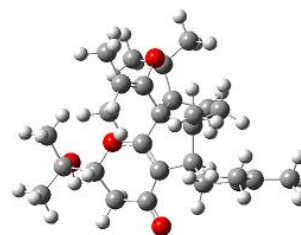
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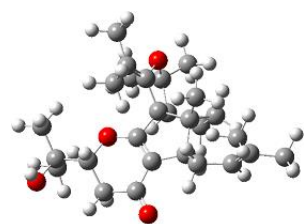
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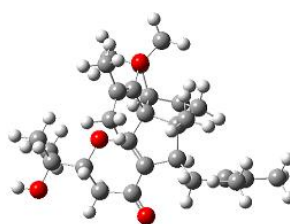
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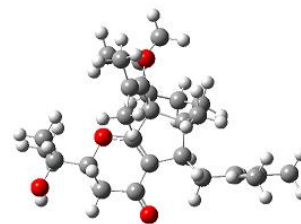
i



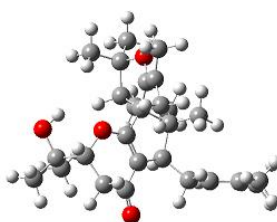
j



k



l



m

Figure S30. Optimized geometries of predominant conformers for compound **2** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S18. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
2-a	-1353.271583	-1353.333191	50.9
2-b	-1353.266534	-1353.328922	0.6
2-c	-1353.266174	-1353.328526	0.4
2-d	-1353.267261	-1353.329507	1
2-e	-1353.267465	-1353.329978	1.7
2-f	-1353.265956	-1353.328574	0.4
2-g	-1353.266170	-1353.328723	0.4
2-h	-1353.270878	-1353.332771	32.6
2-i	-1353.266726	-1353.329374	0.9
2-j	-1353.268571	-1353.330738	3.8
2-k	-1353.268614	-1353.330910	4.5
2-l	-1353.268199	-1353.330407	2.7
2-m	-1353.265325	-1353.327093	0.1

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S19. Optimized Z-matrixes of compound **2** in the gas phase (Å) at B3LYP/6-31G(d,p) level

2-a				2-b			
C	1.537616	0.690429	-0.14778	C	1.371413	1.119753	0.295863
C	-0.04546	0.96512	-0.17343	C	-0.20203	1.053977	-0.02777
C	0.293872	-1.37672	-0.5837	C	0.618419	-1.19887	0.03758
C	1.691298	-0.80109	-0.67634	C	1.883283	-0.3722	0.103088
C	2.104928	1.70422	-1.16495	C	1.938826	2.045959	-0.80308
C	1.028311	1.8322	-2.24596	C	1.069115	1.787007	-2.03644
C	-0.31345	1.812689	-1.48634	C	-0.36593	1.625766	-1.49635
C	2.773427	-1.68929	-0.01315	C	2.92693	-0.91946	1.116978
C	4.182073	-1.29215	-0.36883	C	4.323639	-0.37739	0.930278
C	5.26138	-1.19973	0.424375	C	5.28094	-0.88834	0.138475
C	6.61063	-0.83089	-0.14541	C	6.642287	-0.24156	0.049624
C	5.262202	-1.46242	1.9104	C	5.111631	-2.12338	-0.71372
C	2.158263	0.901416	1.237237	C	1.670643	1.689522	1.687589
C	-0.87955	3.171461	-0.95623	C	-1.23811	2.911568	-1.31321
O	-0.59886	3.158742	0.466472	O	-1.24046	3.157371	0.11686
C	-0.60882	1.853471	0.924181	C	-1.10253	1.960543	0.794334
C	-2.40298	3.216965	-1.14237	C	-2.68302	2.63639	-1.75263

C	-0.23395	4.439122	-1.50872	C	-0.71258	4.187777	-1.96464
C	-0.61463	-0.41478	-0.2854	C	-0.49098	-0.41605	0.001403
C	-1.0629	1.574026	2.158544	C	-1.6986	1.785676	1.986151
C	-1.02554	0.203519	2.787024	C	-1.51152	0.567822	2.853186
C	-1.63654	2.660554	3.035341	C	-2.59408	2.851323	2.568467
O	-1.94108	-0.59438	-0.16132	O	-1.75951	-0.83352	-0.10496
C	-2.34537	-1.98412	0.037534	C	-1.9718	-2.24984	0.145013
C	-1.67799	-2.87836	-1.00048	C	-0.91276	-3.08203	-0.57429
C	-0.15028	-2.70196	-0.99787	C	0.516362	-2.61489	-0.26605
O	0.589289	-3.59741	-1.39223	O	1.465912	-3.38699	-0.37515
C	-3.88728	-1.95797	0.109396	C	-3.4395	-2.56862	-0.24301
C	-4.42338	-3.31844	0.558401	C	-4.39693	-1.56299	0.40407
C	-4.52968	-1.51565	-1.214	C	-3.80075	-3.99802	0.191045
O	-4.24643	-1.04276	1.151974	O	-3.6222	-2.41882	-1.65507
H	1.960598	-0.75914	-1.74263	H	2.373494	-0.44001	-0.87811
H	3.076426	1.388323	-1.55875	H	3.003223	1.859716	-0.9802
H	2.255238	2.670298	-0.66768	H	1.838768	3.090781	-0.48444
H	1.064006	0.967176	-2.91795	H	1.370186	0.84818	-2.51532
H	1.151923	2.717471	-2.87555	H	1.156621	2.566142	-2.7986
H	-1.08438	1.338014	-2.09975	H	-0.9255	0.923242	-2.11977
H	2.6213	-1.73306	1.068822	H	2.588056	-0.72749	2.140614
H	2.59065	-2.70317	-0.39128	H	2.929059	-2.00461	0.994963
H	4.334588	-1.09773	-1.43257	H	4.574362	0.52176	1.493067
H	6.564712	-0.654	-1.22355	H	6.718047	0.644529	0.686234
H	7.008695	0.074601	0.332013	H	7.432156	-0.94364	0.348764
H	7.347249	-1.6249	0.036612	H	6.872427	0.05897	-0.98138
H	4.269859	-1.67613	2.310731	H	4.114899	-2.56398	-0.65382
H	5.909306	-2.31673	2.149625	H	5.313458	-1.88982	-1.76778
H	5.671061	-0.60292	2.457645	H	5.842507	-2.89163	-0.42719
H	1.765005	0.206869	1.984158	H	1.277785	1.066804	2.495131
H	1.956806	1.915639	1.591295	H	1.229377	2.684009	1.79242
H	3.241211	0.764722	1.187199	H	2.749877	1.786635	1.834699
H	-2.81999	4.105919	-0.66037	H	-3.32575	3.485076	-1.50072
H	-2.66496	3.242489	-2.20554	H	-2.73538	2.469418	-2.83375
H	-2.86961	2.332387	-0.69764	H	-3.07308	1.744765	-1.25285
H	-0.41714	4.536339	-2.58299	H	-0.70551	4.096796	-3.05487
H	-0.66532	5.312313	-1.01087	H	-1.36469	5.024807	-1.69892
H	0.843898	4.451127	-1.33323	H	0.297461	4.427831	-1.62563
H	-0.46138	-0.52768	2.206507	H	-0.80775	-0.15889	2.445269
H	-0.5667	0.253658	3.782965	H	-1.14289	0.857122	3.846711
H	-2.04126	-0.19001	2.926952	H	-2.47082	0.057984	3.016939
H	-1.78921	3.587989	2.482951	H	-2.79817	3.644404	1.848845
H	-2.59419	2.341679	3.467139	H	-3.54765	2.416456	2.896207
H	-0.97025	2.875386	3.881974	H	-2.13853	3.308282	3.457875
H	-1.9774	-2.25804	1.035826	H	-1.85848	-2.38627	1.230764
H	-2.03662	-2.64262	-2.0109	H	-1.05204	-2.99926	-1.66096
H	-1.90315	-3.93059	-0.81035	H	-0.99161	-4.13809	-0.30606
H	-5.49931	-3.23672	0.733118	H	-5.42414	-1.81205	0.125688
H	-3.95239	-3.62956	1.495445	H	-4.17686	-0.55082	0.064023
H	-4.25394	-4.08926	-0.19803	H	-4.3127	-1.59024	1.494895
H	-5.60787	-1.41032	-1.06881	H	-4.84806	-4.19438	-0.05329
H	-4.12933	-0.55066	-1.53857	H	-3.18883	-4.7484	-0.3217
H	-4.36081	-2.2419	-2.01538	H	-3.66805	-4.13947	1.268285
H	-3.78796	-0.21065	0.963357	H	-3.26936	-3.20566	-2.09112
2-c				2-d			
C	1.377378	1.096825	0.33832	C	1.368558	1.122854	0.296939
C	-0.18677	1.058056	-0.02885	C	-0.20494	1.052497	-0.02472
C	0.614576	-1.20313	-0.02482	C	0.620416	-1.19833	0.04503
C	1.883776	-0.38926	0.092556	C	1.883179	-0.36833	0.105607
C	1.981776	2.066791	-0.70104	C	1.932339	2.048797	-0.80405
C	1.146561	1.866268	-1.96866	C	1.062467	1.784732	-2.03624
C	-0.30418	1.692416	-1.47681	C	-0.37161	1.619491	-1.49468
C	2.906276	-0.98262	1.101707	C	2.930867	-0.9111	1.117774

C	4.307053	-0.43604	0.965322	C	4.326062	-0.36705	0.925697
C	5.279566	-0.9162	0.17286	C	5.280743	-0.87698	0.130078
C	6.643022	-0.2687	0.137155	C	6.640916	-0.22855	0.035382
C	5.125741	-2.11588	-0.73124	C	5.109164	-2.11257	-0.72092
C	1.637331	1.598648	1.763577	C	1.66842	1.695218	1.687435
C	-1.16963	2.977761	-1.25903	C	-1.24842	2.902284	-1.31506
O	-1.17725	3.176927	0.176749	O	-1.25247	3.152448	0.114242
C	-1.10082	1.942627	0.801687	C	-1.10745	1.958479	0.795549
C	-2.61463	2.722349	-1.71294	C	-2.69239	2.619822	-1.75344
C	-0.63373	4.269234	-1.8698	C	-0.72857	4.17896	-1.97013
C	-0.48739	-0.40929	-0.0562	C	-0.48987	-0.4184	0.009078
C	-1.76884	1.715822	1.944224	C	-1.70136	1.7856	1.98888
C	-1.68244	0.434888	2.734301	C	-1.50871	0.571297	2.859745
C	-2.68338	2.764193	2.527832	C	-2.59898	2.850573	2.569319
O	-1.75651	-0.81871	-0.19022	O	-1.75825	-0.83778	-0.09551
C	-1.9642	-2.2334	0.076498	C	-1.96709	-2.25572	0.153376
C	-0.92771	-3.07605	-0.66297	C	-0.90383	-3.09473	-0.55296
C	0.506608	-2.60972	-0.36882	C	0.520907	-2.61699	-0.2548
O	1.455809	-3.37652	-0.51424	O	1.477354	-3.38112	-0.36513
C	-3.44555	-2.54012	-0.21786	C	-3.42241	-2.57492	-0.24767
C	-3.74114	-4.02852	0.029111	C	-4.39778	-1.59298	0.419239
C	-3.86015	-2.11963	-1.63398	C	-3.7752	-4.02073	0.141163
O	-4.15145	-1.7559	0.754861	O	-3.46725	-2.42566	-1.67187
H	2.39042	-0.42088	-0.88211	H	2.371062	-0.43697	-0.87666
H	3.049665	1.881409	-0.85627	H	2.997115	1.865253	-0.98171
H	1.877162	3.09728	-0.34006	H	1.829556	3.094043	-0.48733
H	1.455882	0.946553	-2.47851	H	1.365991	0.845969	-2.51346
H	1.260242	2.676092	-2.69461	H	1.146895	2.562727	-2.79996
H	-0.84993	1.023387	-2.14794	H	-0.9283	0.912417	-2.11548
H	2.547506	-0.83305	2.125605	H	2.594771	-0.71764	2.142071
H	2.909092	-2.06167	0.93365	H	2.934213	-1.99641	0.997575
H	4.547098	0.439345	1.568835	H	4.577829	0.532695	1.487171
H	6.70748	0.589647	0.811891	H	6.718313	0.657737	0.67157
H	7.426482	-0.98409	0.421323	H	7.432956	-0.92961	0.33126
H	6.89308	0.074802	-0.87567	H	6.866371	0.072093	-0.99664
H	4.126079	-2.55338	-0.71147	H	4.112666	-2.5533	-0.658
H	5.352886	-1.84199	-1.77032	H	5.307971	-1.87955	-1.77568
H	5.846704	-2.8984	-0.45841	H	5.841037	-2.88054	-0.43607
H	1.208358	0.945595	2.527989	H	1.278642	1.072263	2.496291
H	1.204015	2.592941	1.898966	H	1.224798	2.688748	1.791988
H	2.711907	1.674504	1.951462	H	2.747646	1.795254	1.832787
H	-3.25115	3.573309	-1.45277	H	-3.33917	3.465833	-1.50268
H	-2.66217	2.572129	-2.79699	H	-2.74402	2.450538	-2.83428
H	-3.01544	1.829658	-1.22279	H	-3.07691	1.726933	-1.25146
H	-0.61657	4.208932	-2.96217	H	-0.72098	4.084954	-3.0601
H	-1.28464	5.101383	-1.58638	H	-1.38393	5.014183	-1.70656
H	0.37405	4.495079	-1.51462	H	0.280543	4.423784	-1.63186
H	-0.87683	-0.22481	2.407893	H	-0.80488	-0.15524	2.451796
H	-1.51484	0.652955	3.797018	H	-1.13755	0.864798	3.851113
H	-2.62454	-0.12374	2.662727	H	-2.46634	0.059816	3.028568
H	-2.82001	3.605947	1.848514	H	-2.808	3.639884	1.846928
H	-3.6653	2.329436	2.756689	H	-3.55005	2.413967	2.902227
H	-2.28566	3.151848	3.475807	H	-2.14241	3.313171	3.455306
H	-1.82049	-2.3593	1.158509	H	-1.87307	-2.38802	1.241146
H	-1.07528	-3.0178	-1.74985	H	-1.06223	-3.04656	-1.63698
H	-1.00674	-4.12782	-0.37985	H	-0.98026	-4.14352	-0.25766
H	-4.82187	-4.19709	-0.03055	H	-5.42406	-1.82157	0.109147
H	-3.4114	-4.32921	1.028162	H	-4.16526	-0.56598	0.136506
H	-3.26599	-4.67868	-0.71083	H	-4.35831	-1.67256	1.51071
H	-4.92646	-2.324	-1.78545	H	-4.8265	-4.21851	-0.09538
H	-3.68524	-1.05227	-1.77927	H	-3.16671	-4.73952	-0.41185
H	-3.31132	-2.6749	-2.40083	H	-3.64216	-4.19735	1.21357
H	-5.09572	-1.82945	0.562646	H	-4.37499	-2.59656	-1.9557

2-e				2-f			
C	1.536908	0.689182	-0.20526	C	1.375092	1.103911	0.330598
C	-0.04721	0.954268	-0.16064	C	-0.191	1.056986	-0.02744
C	0.28314	-1.40166	-0.46835	C	0.617655	-1.20129	-0.01322
C	1.674809	-0.83245	-0.6419	C	1.884773	-0.38244	0.09382
C	2.037747	1.636497	-1.31823	C	1.969709	2.067739	-0.72015
C	0.898742	1.695391	-2.33943	C	1.128299	1.853759	-1.98141
C	-0.39588	1.721591	-1.50259	C	-0.3191	1.677881	-1.4804
C	2.777512	-1.68215	0.037961	C	2.913377	-0.96586	1.102697
C	4.175099	-1.31905	-0.38981	C	4.312639	-0.41856	0.954724
C	5.284083	-1.19746	0.357173	C	5.283563	-0.90711	0.16542
C	6.614574	-0.87329	-0.27997	C	6.645759	-0.25776	0.117606
C	5.337713	-1.38269	1.853969	C	5.129553	-2.11825	-0.72322
C	2.238232	0.998916	1.12172	C	1.642815	1.618046	1.75008
C	-0.93949	3.107181	-1.02276	C	-1.19001	2.960444	-1.26985
O	-0.58438	3.178184	0.382272	O	-1.18756	3.173676	0.165183
C	-0.54742	1.903317	0.915606	C	-1.10101	1.947875	0.801159
C	-2.4706	3.137739	-1.12933	C	-2.63686	2.692575	-1.7093
C	-0.32936	4.341693	-1.68049	C	-0.66496	4.24861	-1.89639
C	-0.61971	-0.43052	-0.17941	C	-0.48723	-0.41144	-0.04308
C	-0.89775	1.69863	2.196927	C	-1.7565	1.733234	1.953467
C	-0.78023	0.37299	2.903354	C	-1.65693	0.461767	2.755796
C	-1.41025	2.831882	3.051573	C	-2.66734	2.785014	2.536236
O	-1.94019	-0.58764	-0.01172	O	-1.757	-0.82391	-0.1672
C	-2.38999	-1.9596	0.16491	C	-1.96136	-2.24076	0.079273
C	-1.69847	-2.89263	-0.82747	C	-0.91681	-3.07404	-0.66166
C	-0.17388	-2.73616	-0.82316	C	0.514399	-2.60982	-0.35346
O	0.555669	-3.65697	-1.18024	O	1.465269	-3.37655	-0.48615
C	-3.93057	-1.94462	0.080253	C	-3.44821	-2.54702	-0.22292
C	-4.51744	-0.88138	1.021252	C	-3.75741	-4.0226	0.075219
C	-4.49448	-3.33236	0.429952	C	-3.83753	-2.17958	-1.65634
O	-4.23636	-1.62159	-1.28161	O	-4.26422	-1.71284	0.608295
H	1.90851	-0.85756	-1.71732	H	2.387264	-0.41966	-0.88274
H	2.985726	1.296567	-1.74827	H	3.037474	1.885256	-0.87961
H	2.213608	2.632465	-0.89337	H	1.86301	3.100704	-0.36699
H	0.898793	0.788774	-2.95529	H	1.438689	0.931509	-2.48595
H	0.980877	2.538537	-3.03085	H	1.234437	2.658449	-2.71408
H	-1.19949	1.208338	-2.03735	H	-0.8654	1.00033	-2.14233
H	2.663334	-1.65712	1.125172	H	2.559704	-0.80837	2.127263
H	2.576171	-2.71625	-0.26968	H	2.916854	-2.04618	0.943559
H	4.289398	-1.18093	-1.46713	H	4.553046	0.464914	1.546188
H	6.530079	-0.7519	-1.36346	H	6.710683	0.609358	0.780975
H	7.038549	0.051408	0.134412	H	7.431122	-0.96818	0.408803
H	7.350511	-1.66479	-0.08426	H	6.892365	0.072909	-0.90029
H	4.35986	-1.57144	2.300023	H	4.130549	-2.55683	-0.69651
H	5.991014	-2.2262	2.114049	H	5.354648	-1.857	-1.76596
H	5.767859	-0.49771	2.341181	H	5.852005	-2.89633	-0.44187
H	1.8977	0.358199	1.93907	H	1.22151	0.969708	2.522847
H	2.052848	2.035324	1.415433	H	1.207877	2.612245	1.880721
H	3.316941	0.86126	1.01368	H	2.718377	1.698327	1.930076
H	-2.86611	4.049645	-0.67229	H	-3.27642	3.54161	-1.45056
H	-2.78778	3.106928	-2.1772	H	-2.69177	2.534579	-2.79184
H	-2.90544	2.274178	-0.61709	H	-3.02953	1.801078	-1.21059
H	-0.5678	4.374649	-2.74772	H	-0.65422	4.177125	-2.98813
H	-0.73905	5.242089	-1.21355	H	-1.31893	5.079921	-1.61774
H	0.756121	4.365897	-1.56194	H	0.343761	4.483691	-1.54989
H	-0.3619	-0.42026	2.282666	H	-0.87111	-0.21278	2.412562
H	-0.14002	0.466454	3.791146	H	-1.45767	0.687269	3.81144
H	-1.76237	0.039425	3.265662	H	-2.61046	-0.08302	2.72208
H	-1.59646	3.730206	2.462608	H	-2.80787	3.621458	1.851426
H	-2.34009	2.542086	3.558981	H	-3.64884	2.353307	2.77296
H	-0.69136	3.086939	3.842478	H	-2.26391	3.179632	3.478924
H	-2.10599	-2.24149	1.189455	H	-1.80544	-2.38166	1.161383

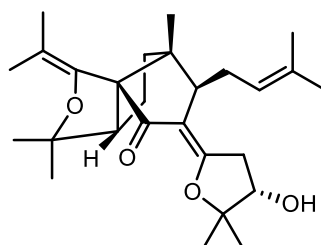
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H	-1.93242	-3.93583	-0.60436	H	-0.99911	-4.12964	-0.39374
H	-5.61098	-0.88147	0.944444	H	-4.83681	-4.17717	-0.00092
H	-4.14684	0.110453	0.76148	H	-3.44621	-4.29697	1.09109
H	-4.26026	-1.08804	2.065502	H	-3.26302	-4.70395	-0.62257
H	-5.58955	-3.29713	0.418154	H	-4.90557	-2.36391	-1.79698
H	-4.17609	-4.08403	-0.29561	H	-3.64149	-1.12205	-1.84201
H	-4.18843	-3.65634	1.430211	H	-3.28483	-2.77729	-2.38638
H	-5.19841	-1.58422	-1.36408	H	-4.11975	-1.9734	1.528682
2-g				2-h			
C	1.545355	0.683008	-0.16708	C	1.530441	0.690853	-0.20616
C	-0.03668	0.962219	-0.16479	C	-0.0556	0.947811	-0.16385
C	0.285023	-1.38785	-0.52722	C	0.288352	-1.40604	-0.47427
C	1.683426	-0.82246	-0.65594	C	1.677099	-0.82908	-0.64649
C	2.09181	1.666904	-1.22513	C	2.028891	1.644362	-1.31473
C	0.990587	1.769	-2.28377	C	0.892598	1.700114	-2.33894
C	-0.33299	1.776082	-1.49298	C	-0.40427	1.716776	-1.50525
C	2.771022	-1.69991	0.012882	C	2.784261	-1.67362	0.032479
C	4.176365	-1.32374	-0.37683	C	4.180207	-1.29779	-0.38988
C	5.270571	-1.22225	0.394526	C	5.285384	-1.17019	0.36177
C	6.61229	-0.87805	-0.20758	C	6.61577	-0.83428	-0.26935
C	5.295984	-1.45024	1.886082	C	5.334899	-1.35988	1.858143
C	2.19926	0.931087	1.196382	C	2.22639	1.000016	1.123723
C	-0.88034	3.149504	-0.98226	C	-0.95797	3.097687	-1.02344
O	-0.53312	3.180159	0.426125	O	-0.60079	3.169347	0.379998
C	-0.55803	1.888505	0.921535	C	-0.56153	1.893668	0.912971
C	-2.41112	3.181695	-1.09782	C	-2.4899	3.117151	-1.12536
C	-0.26453	4.399387	-1.60368	C	-0.35931	4.336816	-1.68271
C	-0.61858	-0.41645	-0.23577	C	-0.61785	-0.44089	-0.18394
C	-0.98593	1.65147	2.172236	C	-0.91308	1.687663	2.193774
C	-0.97721	0.293126	2.823597	C	-0.7881	0.363603	2.90212
C	-1.52197	2.767454	3.03427	C	-1.42908	2.819788	3.048008
O	-1.94292	-0.57496	-0.09373	O	-1.94122	-0.61355	-0.01372
C	-2.37685	-1.94947	0.082058	C	-2.37693	-1.99471	0.187423
C	-1.69907	-2.8655	-0.93568	C	-1.68263	-2.92495	-0.80204
C	-0.17035	-2.71108	-0.9221	C	-0.16053	-2.74776	-0.82159
O	0.556763	-3.62459	-1.3006	O	0.576829	-3.6589	-1.1846
C	-3.92473	-1.94077	0.098941	C	-3.92113	-1.95003	0.081718
C	-4.46006	-3.35663	0.363324	C	-4.50276	-1.02279	1.16184
C	-4.51703	-1.35581	-1.18494	C	-4.52278	-3.35179	0.20397
O	-4.36507	-1.06283	1.141948	O	-4.28372	-1.47992	-1.21971
H	1.936056	-0.81099	-1.72719	H	1.910605	-0.85093	-1.72194
H	3.053182	1.337213	-1.63262	H	2.979662	1.310944	-1.7434
H	2.255492	2.645771	-0.7581	H	2.198148	2.639868	-0.88629
H	1.007817	0.884858	-2.93134	H	0.899235	0.79533	-2.95741
H	1.102569	2.635381	-2.94135	H	0.97144	2.54572	-3.02759
H	-1.12099	1.289568	-2.07435	H	-1.20203	1.200918	-2.04719
H	2.637334	-1.71347	1.098095	H	2.667009	-1.65372	1.119428
H	2.57448	-2.72211	-0.33492	H	2.591864	-2.708	-0.27956
H	4.31126	-1.15485	-1.44737	H	4.297281	-1.15597	-1.46637
H	6.548352	-0.72628	-1.28863	H	6.534577	-0.70972	-1.35271
H	7.025959	0.035306	0.240837	H	7.031535	0.091844	0.150019
H	7.346024	-1.67349	-0.01992	H	7.356381	-1.62128	-0.07349
H	4.309571	-1.64895	2.308277	H	4.356881	-1.55612	2.300607
H	5.942714	-2.30239	2.134081	H	5.992472	-2.20019	2.117551
H	5.718691	-0.58053	2.406082	H	5.758121	-0.47391	2.349499
H	1.8189	0.2622	1.973125	H	1.887306	0.354661	1.937953
H	2.013156	1.956757	1.524577	H	2.034727	2.034443	1.42023
H	3.27982	0.7847	1.125258	H	3.305973	0.868482	1.017826
H	-2.80866	4.087735	-0.63107	H	-2.89077	4.031299	-0.67808
H	-2.7216	3.167586	-2.14822	H	-2.81242	3.071365	-2.17112
H	-2.85106	2.313977	-0.59656	H	-2.91622	2.259952	-0.59458
H	-0.48945	4.456249	-2.67292	H	-0.60031	4.368063	-2.74941

H	-0.68199	5.288168	-1.12173	H	-0.77458	5.233934	-1.21459
H	0.819328	4.422882	-1.47065	H	0.726136	4.368954	-1.56644
H	-0.44914	-0.46651	2.245613	H	-0.37202	-0.43005	2.280483
H	-0.5034	0.341953	3.812688	H	-0.14153	0.461268	3.784725
H	-2.00668	-0.05648	2.982816	H	-1.76649	0.028896	3.272383
H	-1.63542	3.693695	2.470864	H	-1.62059	3.716827	2.45885
H	-2.4961	2.490442	3.458667	H	-2.35603	2.526052	3.557991
H	-0.8551	2.964537	3.884882	H	-0.70916	3.078607	3.836611
H	-2.03478	-2.24495	1.087728	H	-2.08577	-2.2599	1.213694
H	-2.04346	-2.63819	-1.9532	H	-2.06789	-2.731	-1.81151
H	-1.93731	-3.91268	-0.73703	H	-1.89917	-3.96895	-0.5654
H	-5.54056	-3.30045	0.518778	H	-5.5843	-0.94293	1.024211
H	-4.00988	-3.79044	1.265162	H	-4.06625	-0.02244	1.101845
H	-4.2677	-4.03904	-0.46905	H	-4.30943	-1.41475	2.166276
H	-5.60467	-1.30811	-1.08861	H	-5.61338	-3.27786	0.203255
H	-4.13892	-0.34511	-1.34857	H	-4.22944	-3.98069	-0.63918
H	-4.27453	-1.97161	-2.05534	H	-4.21133	-3.83674	1.134391
H	-4.072	-1.42996	1.987596	H	-3.88425	-0.60334	-1.31704
2-i				2-j			
C	1.539588	0.686759	-0.20663	C	1.532609	0.695054	-0.20427
C	-0.04393	0.955997	-0.16392	C	-0.05191	0.961746	-0.16935
C	0.280985	-1.40003	-0.47674	C	0.278223	-1.39208	-0.50164
C	1.675029	-0.83474	-0.64475	C	1.672416	-0.82222	-0.65567
C	2.044345	1.634229	-1.31783	C	2.043689	1.655014	-1.30196
C	0.906536	1.698831	-2.33994	C	0.912172	1.731747	-2.33001
C	-0.38871	1.728228	-1.50427	C	-0.3882	1.75004	-1.50204
C	2.772883	-1.68848	0.03793	C	2.768843	-1.67969	0.024647
C	4.172912	-1.32895	-0.38516	C	4.17008	-1.31222	-0.3874
C	5.279583	-1.21076	0.365758	C	5.272747	-1.20012	0.370343
C	6.61301	-0.88935	-0.26659	C	6.608956	-0.87074	-0.25189
C	5.327576	-1.39687	1.862622	C	5.313372	-1.40216	1.865342
C	2.23946	0.993468	1.121788	C	2.223677	0.98926	1.1316
C	-0.92744	3.114783	-1.02078	C	-0.93341	3.129073	-1.0055
O	-0.57161	3.18015	0.38438	O	-0.58668	3.178818	0.401942
C	-0.54245	1.903836	0.914247	C	-0.55752	1.896247	0.91737
C	-2.45821	3.151722	-1.12763	C	-2.46414	3.162443	-1.11891
C	-0.31181	4.348305	-1.67529	C	-0.31853	4.371906	-1.64262
C	-0.62077	-0.42665	-0.18771	C	-0.62502	-0.42186	-0.2123
C	-0.89598	1.6964	2.194125	C	-0.91448	1.675216	2.194193
C	-0.78565	0.368004	2.896328	C	-0.79838	0.341275	2.884923
C	-1.40648	2.828763	3.051053	C	-1.42658	2.79889	3.061757
O	-1.94153	-0.58212	-0.02278	O	-1.95122	-0.5853	-0.0592
C	-2.39323	-1.95215	0.155778	C	-2.37613	-1.96637	0.113304
C	-1.70727	-2.87497	-0.84884	C	-1.69689	-2.88067	-0.90068
C	-0.17864	-2.73062	-0.83659	C	-0.17211	-2.72832	-0.87392
O	0.542872	-3.65739	-1.19294	O	0.566483	-3.64053	-1.23141
C	-3.94298	-1.93659	0.088276	C	-3.926	-1.98395	0.110891
C	-4.5107	-0.84948	1.006326	C	-4.51186	-1.56956	-1.23951
C	-4.50176	-3.31128	0.487918	C	-4.46671	-1.09576	1.238361
O	-4.37852	-1.59053	-1.23116	O	-4.33811	-3.34308	0.312207
H	1.91224	-0.85896	-1.71941	H	1.914987	-0.83654	-1.72935
H	2.991748	1.292266	-1.74753	H	2.993267	1.317565	-1.73024
H	2.222745	2.628844	-0.89104	H	2.220145	2.644731	-0.86307
H	0.904281	0.793453	-2.95778	H	0.913938	0.833815	-2.95853
H	0.992244	2.543038	-3.02958	H	1.001619	2.584265	-3.0089
H	-1.19432	1.220186	-2.04104	H	-1.18854	1.247244	-2.05184
H	2.655293	-1.66368	1.124748	H	2.645356	-1.66608	1.111038
H	2.570191	-2.72207	-0.27062	H	2.570375	-2.71042	-0.2955
H	4.291168	-1.19037	-1.462	H	4.293673	-1.16274	-1.46217
H	6.532599	-0.76696	-1.35026	H	6.53384	-0.73699	-1.33459
H	7.037618	0.034018	0.150007	H	7.030724	0.048467	0.176627
H	7.346264	-1.68276	-0.06875	H	7.341872	-1.66564	-0.05888
H	4.348077	-1.58521	2.305206	H	4.331407	-1.59318	2.301289

H	5.979435	-2.2409	2.124484	H	5.962163	-2.25036	2.121261
H	5.756569	-0.51243	2.351761	H	5.741942	-0.52391	2.365857
H	1.896151	0.352788	1.938006	H	1.877535	0.338676	1.938642
H	2.055664	2.029917	1.41615	H	2.0359	2.022061	1.436126
H	3.318047	0.853767	1.01533	H	3.303144	0.853126	1.029744
H	-2.84983	4.065006	-0.67013	H	-2.86086	4.071506	-0.65751
H	-2.77563	3.123175	-2.17544	H	-2.77759	3.139501	-2.16818
H	-2.89788	2.290202	-0.61621	H	-2.9017	2.297251	-0.61119
H	-0.55006	4.384991	-2.74243	H	-0.5514	4.420408	-2.7105
H	-0.71816	5.249069	-1.20623	H	-0.72922	5.266151	-1.16499
H	0.773752	4.368094	-1.55641	H	0.766335	4.392698	-1.51814
H	-0.36737	-0.42458	2.274635	H	-0.39004	-0.44708	2.251442
H	-0.14853	0.456293	3.786836	H	-0.14933	0.421729	3.767547
H	-1.77033	0.036606	3.253461	H	-1.77871	0.009485	3.253057
H	-1.58698	3.729842	2.464596	H	-1.61144	3.704366	2.48347
H	-2.33933	2.540983	3.553881	H	-2.35681	2.504044	3.565267
H	-0.68912	3.077799	3.845228	H	-0.70764	3.043786	3.855763
H	-2.09079	-2.24165	1.173286	H	-2.03906	-2.25963	1.121162
H	-2.04808	-2.63319	-1.86489	H	-2.0265	-2.64283	-1.92039
H	-1.95025	-3.92184	-0.65327	H	-1.96984	-3.91932	-0.70769
H	-5.60264	-0.87465	0.964044	H	-5.60257	-1.54358	-1.17278
H	-4.17055	0.136236	0.688405	H	-4.24302	-2.28801	-2.01765
H	-4.1957	-1.00931	2.04219	H	-4.15152	-0.57991	-1.53057
H	-5.5942	-3.27569	0.46561	H	-5.55835	-1.15499	1.264399
H	-4.17617	-4.1005	-0.19873	H	-4.08132	-1.42578	2.211658
H	-4.18916	-3.59805	1.496989	H	-4.16922	-0.0536	1.102489
H	-4.30401	-2.37524	-1.79018	H	-4.17094	-3.57284	1.236986
2-k				2-l			
C	1.529557	0.697078	-0.20438	C	1.532745	0.694174	-0.20438
C	-0.0559	0.958345	-0.16956	C	-0.0521	0.957556	-0.16863
C	0.282726	-1.39465	-0.49845	C	0.28306	-1.39608	-0.49389
C	1.674486	-0.81993	-0.65471	C	1.675585	-0.82355	-0.65312
C	2.037347	1.657999	-1.30269	C	2.040807	1.652985	-1.30438
C	0.905716	1.729532	-2.33103	C	0.908887	1.723516	-2.33247
C	-0.3948	1.743976	-1.50318	C	-0.39141	1.740051	-1.50426
C	2.774282	-1.67312	0.025471	C	2.775527	-1.67667	0.026844
C	4.174147	-1.30073	-0.38668	C	4.175025	-1.30556	-0.38801
C	5.276528	-1.18531	0.37099	C	5.278156	-1.18822	0.368257
C	6.611645	-0.85141	-0.25121	C	6.612492	-0.85555	-0.25624
C	5.317885	-1.38787	1.865906	C	5.321216	-1.38694	1.863626
C	2.219589	0.994321	1.131353	C	2.223812	0.992306	1.130611
C	-0.94461	3.121686	-1.00821	C	-0.94064	3.119139	-1.01183
O	-0.59744	3.174796	0.398623	O	-0.58954	3.176062	0.39378
C	-0.56433	1.892648	0.916071	C	-0.55895	1.895224	0.91485
C	-2.47563	3.149447	-1.12087	C	-2.47191	3.146055	-1.12084
C	-0.33475	4.365902	-1.64756	C	-0.33249	4.361393	-1.65651
C	-0.62393	-0.42759	-0.21012	C	-0.62289	-0.42722	-0.2055
C	-0.92023	1.672322	2.193248	C	-0.91598	1.678089	2.192158
C	-0.79993	0.339899	2.886249	C	-0.79865	0.346803	2.887978
C	-1.43524	2.795951	3.059275	C	-1.43039	2.804173	3.0553
O	-1.94932	-0.59554	-0.05821	O	-1.94695	-0.59263	-0.05204
C	-2.36641	-1.97655	0.124391	C	-2.37676	-1.97127	0.136277
C	-1.68637	-2.89848	-0.88275	C	-1.69039	-2.89935	-0.86312
C	-0.16263	-2.73245	-0.87015	C	-0.16374	-2.73197	-0.85944
O	0.579471	-3.63706	-1.23966	O	0.570511	-3.64268	-1.22916
C	-3.91174	-1.98434	0.115246	C	-3.9278	-1.97681	0.119452
C	-4.49546	-1.53123	-1.22935	C	-4.50215	-1.46399	-1.20638
C	-4.44759	-1.11747	1.263028	C	-4.46131	-1.15914	1.297689
O	-4.22536	-3.36338	0.35706	O	-4.35185	-3.32427	0.367213
H	1.916196	-0.83447	-1.72862	H	1.915678	-0.83949	-1.72732
H	2.98825	1.323685	-1.7305	H	2.991459	1.317582	-1.73188
H	2.210016	2.64877	-0.86463	H	2.213935	2.644287	-0.86783
H	0.910843	0.830781	-2.95836	H	0.913461	0.823949	-2.95871

H	0.992131	2.581567	-3.01097	H	0.995512	2.574539	-3.01358
H	-1.19328	1.237704	-2.05253	H	-1.19034	1.233081	-2.05236
H	2.650775	-1.6601	1.111832	H	2.653629	-1.66148	1.113314
H	2.579454	-2.70451	-0.29479	H	2.580238	-2.70877	-0.2909
H	4.297168	-1.15048	-1.46145	H	4.29679	-1.15792	-1.46326
H	6.53598	-0.71736	-1.33386	H	6.535733	-0.72436	-1.33915
H	7.030646	0.068888	0.177708	H	7.031507	0.066004	0.169884
H	7.347097	-1.64411	-0.05871	H	7.348356	-1.64748	-0.06229
H	4.336507	-1.58193	2.301792	H	4.340548	-1.58058	2.301283
H	5.969119	-2.23432	2.121446	H	5.973395	-2.23223	2.120505
H	5.743948	-0.50859	2.366783	H	5.747243	-0.50609	2.361699
H	1.875424	0.342981	1.938596	H	1.878898	0.342901	1.9391
H	2.02842	2.02667	1.435362	H	2.034087	2.025368	1.432951
H	3.299505	0.861602	1.029627	H	3.30349	0.858047	1.02869
H	-2.87528	4.058102	-0.66115	H	-2.87057	4.056447	-0.66379
H	-2.78977	3.123047	-2.16989	H	-2.78862	3.115647	-2.16899
H	-2.90941	2.28389	-0.6105	H	-2.90451	2.282789	-0.60567
H	-0.56822	4.412016	-2.71543	H	-0.56799	4.403818	-2.72409
H	-0.74845	5.259335	-1.17096	H	-0.74578	5.256186	-1.18219
H	0.75007	4.390811	-1.52358	H	0.752553	4.387291	-1.53457
H	-0.39114	-0.44897	2.253837	H	-0.38519	-0.4428	2.259413
H	-0.14943	0.423752	3.767471	H	-0.15316	0.432913	3.772595
H	-1.77856	0.00607	3.25645	H	-1.779	0.01255	3.252827
H	-1.62211	3.700464	2.48008	H	-1.6165	3.707389	2.473871
H	-2.36472	2.499245	3.563057	H	-2.36009	2.509161	3.559438
H	-0.71703	3.043227	3.853198	H	-0.71206	3.052746	3.848666
H	-2.04138	-2.26769	1.133278	H	-2.05715	-2.25981	1.147341
H	-2.02401	-2.68245	-1.90477	H	-2.02974	-2.70206	-1.88905
H	-1.94586	-3.93594	-0.6668	H	-1.92339	-3.94045	-0.62878
H	-5.59013	-1.52655	-1.17786	H	-5.5945	-1.4827	-1.16219
H	-4.20175	-2.20963	-2.03408	H	-4.18866	-2.08692	-2.05223
H	-4.16693	-0.51962	-1.48236	H	-4.17596	-0.44048	-1.4068
H	-5.54324	-1.15128	1.282653	H	-5.55449	-1.16688	1.290739
H	-4.07742	-1.49087	2.222526	H	-4.1247	-1.60035	2.240615
H	-4.14161	-0.0746	1.151894	H	-4.10874	-0.12673	1.247392
H	-5.18687	-3.43755	0.419719	H	-4.27127	-3.82179	-0.45742
2-m							
C	1.354888	0.705479	-0.26992				
C	-0.21279	0.943606	-0.02734				
C	0.202409	-1.41514	0.13264				
C	1.495241	-0.86701	-0.43695				
C	1.642541	1.443166	-1.59594				
C	0.361191	1.303801	-2.42275				
C	-0.79316	1.451102	-1.41054				
C	2.767214	-1.53931	0.133805				
C	4.020064	-1.21249	-0.63543				
C	5.244734	-0.91874	-0.17005				
C	6.393507	-0.67052	-1.11858				
C	5.6108	-0.82805	1.291224				
C	2.231237	1.259593	0.859149				
C	-1.32435	2.889075	-1.09964				
O	-0.74212	3.224226	0.184547				
C	-0.58428	2.068246	0.928853				
C	-2.85122	2.865506	-0.93664				
C	-0.90207	3.992064	-2.06515				
C	-0.71235	-0.4299	0.313805				
C	-0.73865	2.098674	2.263267				
C	-0.47826	0.92794	3.175462				
C	-1.16357	3.366294	2.96338				
O	-2.00247	-0.56544	0.667678				
C	-2.55917	-1.91825	0.795538				
C	-1.48206	-2.95019	1.148594				
C	-0.166	-2.79836	0.377138				

O	0.504994	-3.77956	0.070865				
C	-3.42846	-2.20562	-0.46012				
C	-4.32875	-3.41861	-0.20344				
C	-2.61434	-2.40372	-1.74816				
O	-4.32684	-1.10305	-0.61685				
H	1.503704	-1.09242	-1.51448				
H	2.527656	1.043441	-2.10124				
H	1.840648	2.501235	-1.3852				
H	0.309219	0.305117	-2.87163				
H	0.300266	2.016796	-3.2493				
H	-1.64328	0.838649	-1.72444				
H	2.873378	-1.31495	1.198685				
H	2.585462	-2.61944	0.065554				
H	3.905893	-1.26967	-1.72004				
H	6.084372	-0.74929	-2.16453				
H	6.826344	0.327201	-0.9652				
H	7.207219	-1.38882	-0.9508				
H	4.757838	-0.96234	1.958562				
H	6.357818	-1.59076	1.548291				
H	6.070197	0.142826	1.518482				
H	2.050155	0.761754	1.815437				
H	2.039133	2.326284	0.999819				
H	3.287	1.132245	0.607499				
H	-3.21569	3.844313	-0.61181				
H	-3.34341	2.608089	-1.88064				
H	-3.14004	2.129004	-0.17964				
H	-1.31561	3.81859	-3.0631				
H	-1.27761	4.954016	-1.70466				
H	0.185033	4.063004	-2.14202				
H	-0.1019	0.044193	2.659856				
H	0.258828	1.199499	3.943045				
H	-1.39413	0.644721	3.711264				
H	-1.45872	4.140597	2.255161				
H	-2.00349	3.167436	3.641947				
H	-0.34951	3.765351	3.583947				
H	-1.85876	-3.96457	1.003308				
H	-1.23211	-2.85471	2.213274				
H	-5.04991	-3.49802	-1.02107				
H	-4.88958	-3.29694	0.728061				
H	-3.75971	-4.35073	-0.15831				
H	-3.30616	-2.54897	-2.58234				
H	-1.99939	-1.52756	-1.97139				
H	-1.95391	-3.27427	-1.69125				
H	-3.79149	-0.29794	-0.56979				
H	-3.26042	-1.81414	1.627543				



3

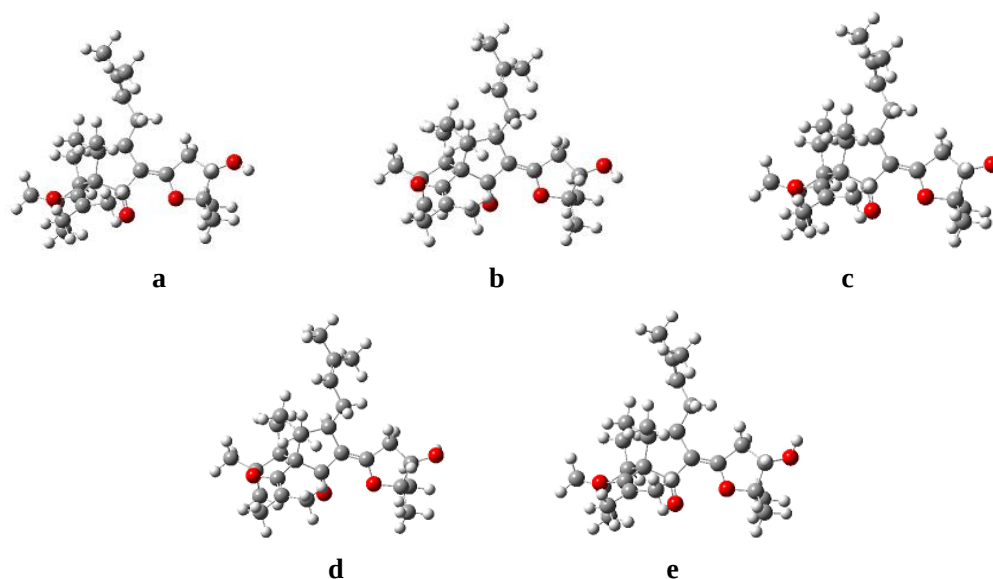


Figure S31. Optimized geometries of predominant conformers for compound **3** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S20. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **3** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
3-a	-1353.253726	-1353.316577	20.1
3-b	-1353.253226	-1353.316995	31.3
3-c	-1353.253468	-1353.316240	14.1
3-d	-1353.252947	-1353.316478	18.1
3-e	-1353.253362	-1353.316385	16.4

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S21. Optimized Z-matrixes of compound **3** in the gas phase (Å) at B3LYP/6-31G(d,p) level

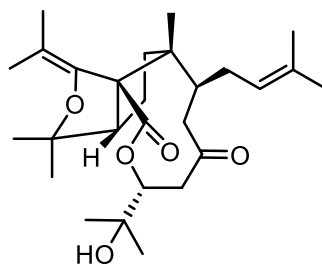
3-a				3-b			
C	-1.22357	0.957783	0.083322	C	-1.18273	0.97344	0.610697
C	-1.4713	-0.58595	-0.14349	C	-1.57199	-0.39526	-0.07926
C	-0.07839	-1.22163	-0.26534	C	-0.24291	-1.09615	-0.40044
C	0.935849	-0.14214	-0.32018	C	0.871056	-0.16402	-0.10437
C	0.21066	1.187293	-0.54122	C	0.283132	1.236344	0.080895
C	-2.3486	1.625429	-0.73607	C	-2.21036	1.97279	0.036781
C	-2.50882	0.755015	-1.98605	C	-2.42155	1.540539	-1.41786
C	-2.26612	-0.69663	-1.51174	C	-2.34429	-0.00289	-1.4071
C	-3.51538	-1.55763	-1.14241	C	-3.68628	-0.79482	-1.30134
O	-3.65916	-1.37352	0.286463	O	-3.8353	-1.04816	0.116325
C	-2.39394	-1.28992	0.84418	C	-2.57856	-1.27529	0.652337
C	0.938565	2.48034	-0.10414	C	1.12308	2.267098	0.878278
C	0.234172	3.756902	-0.48786	C	0.528095	3.650878	0.987833
C	0.016765	4.855126	0.252999	C	0.798327	4.720151	0.221152
C	-0.65981	6.066213	-0.34443	C	0.131894	6.049373	0.484113
C	0.415253	5.015953	1.699638	C	1.756924	4.724134	-0.94454
C	-1.27261	1.406016	1.549179	C	-1.22794	0.939038	2.143996
C	-3.2268	-3.04025	-1.42215	C	-3.55629	-2.14065	-2.0308
C	-4.84289	-1.13381	-1.76318	C	-4.9492	-0.0589	-1.73798
C	-2.16365	-1.8089	2.062317	C	-2.42531	-2.16961	1.643966

C	-0.84219	-1.74173	2.781851	C	-1.11771	-2.46677	2.329823
C	-3.25776	-2.52412	2.817177	C	-3.60098	-2.9668	2.154706
C	2.265934	-0.41331	-0.25	C	2.164642	-0.57968	-0.09464
O	2.691743	-1.6953	-0.08855	O	2.462596	-1.88738	-0.32469
C	4.139076	-1.80646	-0.18463	C	3.896965	-2.11178	-0.41775
C	4.613894	-0.37841	0.194273	C	4.479701	-0.92119	0.389896
C	3.469351	0.504793	-0.30726	C	3.447743	0.184387	0.157997
O	5.833572	0.035001	-0.3946	O	5.76068	-0.47741	-0.01944
C	4.503364	-2.18737	-1.62059	C	4.30142	-2.07557	-1.89251
C	4.564465	-2.87687	0.813891	C	4.170791	-3.4715	0.214785
O	0.103332	-2.42705	-0.34627	O	-0.17566	-2.22367	-0.86559
H	0.069674	1.285562	-1.62921	H	0.181211	1.668048	-0.92603
H	-2.1442	2.676049	-0.95965	H	-1.88751	3.013329	0.129569
H	-3.27095	1.594113	-0.14247	H	-3.14811	1.865127	0.596091
H	-3.47713	0.890697	-2.47357	H	-3.35516	1.920661	-1.83933
H	-1.75458	1.019588	-2.73569	H	-1.6211	1.937602	-2.05181
H	-1.68362	-1.24431	-2.25736	H	-1.80725	-0.36051	-2.28972
H	1.161805	2.449042	0.965927	H	1.31439	1.880588	1.88702
H	1.905658	2.498242	-0.62052	H	2.096533	2.350598	0.391678
H	-0.08657	3.793284	-1.53034	H	-0.19117	3.794389	1.792789
H	-0.92337	5.911815	-1.3943	H	-0.55213	6.00286	1.335802
H	-1.57767	6.316499	0.203891	H	0.876789	6.829996	0.688663
H	-0.01226	6.951059	-0.28323	H	-0.43738	6.387488	-0.39186
H	0.865626	4.11906	2.128032	H	2.233851	3.757843	-1.11866
H	1.135303	5.837566	1.810459	H	1.236898	5.008593	-1.86848
H	-0.45421	5.282949	2.314086	H	2.548176	5.470369	-0.79445
H	-2.19799	1.067375	2.020745	H	-2.19391	0.563561	2.489103
H	-0.43843	1.009574	2.134971	H	-0.45182	0.294973	2.566906
H	-1.23946	2.497126	1.611685	H	-1.09207	1.940856	2.56154
H	-4.0214	-3.66433	-1.002	H	-4.41969	-2.77439	-1.8065
H	-3.17533	-3.22445	-2.50097	H	-3.51088	-1.98781	-3.11477
H	-2.27149	-3.33418	-0.97787	H	-2.64459	-2.65884	-1.71967
H	-4.79496	-1.17207	-2.85586	H	-4.88937	0.233262	-2.79092
H	-5.63455	-1.81338	-1.43416	H	-5.81556	-0.71588	-1.6171
H	-5.12139	-0.12253	-1.4573	H	-5.11963	0.834566	-1.13266
H	-0.0595	-1.22795	2.224496	H	-0.27438	-1.89601	1.942373
H	-0.95071	-1.23595	3.751415	H	-1.18918	-2.27043	3.408738
H	-0.47812	-2.75542	2.994871	H	-0.86846	-3.53027	2.219467
H	-4.15356	-2.64721	2.208519	H	-4.49545	-2.79606	1.555666
H	-2.91375	-3.51464	3.143719	H	-3.36941	-4.04032	2.145294
H	-3.53553	-1.97569	3.728193	H	-3.83242	-2.70812	3.197461
H	4.671349	-0.31309	1.291426	H	4.486789	-1.19619	1.455531
H	3.353783	1.406025	0.291722	H	3.382757	0.869467	1.001037
H	3.683398	0.815921	-1.3377	H	3.742203	0.76843	-0.72326
H	6.557216	-0.42256	0.052882	H	6.415904	-1.11754	0.287284
H	5.584914	-2.30124	-1.73036	H	5.373775	-2.25463	-2.00525
H	4.018437	-3.13171	-1.88053	H	3.752438	-2.84568	-2.44031
H	4.174981	-1.42493	-2.33178	H	4.076146	-1.10592	-2.34421
H	5.655216	-2.98224	0.819077	H	5.24546	-3.68555	0.209565
H	4.233579	-2.61606	1.823243	H	3.814876	-3.49439	1.248764
H	4.130935	-3.8451	0.55057	H	3.663716	-4.265	-0.3402
3-c				3-d			
C	-1.2284	0.953211	0.082699	C	-1.18844	0.962476	0.61185
C	-1.46845	-0.59116	-0.14678	C	-1.56486	-0.40815	-0.08141
C	-0.07278	-1.21806	-0.27741	C	-0.22923	-1.09163	-0.41063
C	0.935779	-0.13214	-0.33278	C	0.875654	-0.1474	-0.11469
C	0.201223	1.192992	-0.54921	C	0.271263	1.245348	0.074471
C	-2.36151	1.61643	-0.72916	C	-2.23162	1.951083	0.047869
C	-2.5229	0.748357	-1.98059	C	-2.44499	1.522544	-1.40757
C	-2.27013	-0.70307	-1.51102	C	-2.34803	-0.01986	-1.40414
C	-3.51312	-1.57123	-1.13676	C	-3.67966	-0.82875	-1.29567
O	-3.64955	-1.39137	0.293245	O	-3.81932	-1.08848	0.121722
C	-2.38149	-1.30344	0.843947	C	-2.55752	-1.30329	0.651108

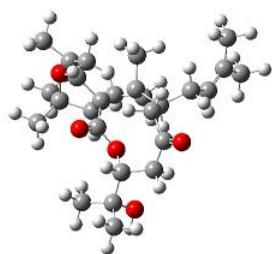
C	0.923016	2.489677	-0.11252	C	1.102052	2.284708	0.870324
C	0.207623	3.763241	-0.48573	C	0.488092	3.659193	0.993895
C	-0.01247	4.856061	0.262352	C	0.730741	4.734995	0.227228
C	-0.7011	6.065505	-0.32447	C	0.050477	6.053959	0.505631
C	0.393658	5.011912	1.707388	C	1.670387	4.755897	-0.95363
C	-1.27187	1.397295	1.549971	C	-1.22387	0.920698	2.145203
C	-3.21899	-3.05168	-1.42214	C	-3.53621	-2.17023	-2.03055
C	-4.84609	-1.15227	-1.7491	C	-4.9533	-0.10689	-1.72459
C	-2.14086	-1.82593	2.058516	C	-2.38875	-2.20071	1.637343
C	-0.81537	-1.75418	2.770151	C	-1.07452	-2.48569	2.315681
C	-3.22628	-2.55028	2.817179	C	-3.5524	-3.01464	2.149199
C	2.267245	-0.39661	-0.26556	C	2.173197	-0.54999	-0.1065
O	2.698739	-1.6765	-0.09884	O	2.48215	-1.85663	-0.33126
C	4.146922	-1.7872	-0.16477	C	3.916654	-2.08311	-0.39782
C	4.620308	-0.3509	0.179855	C	4.495566	-0.87311	0.381257
C	3.467041	0.525078	-0.34019	C	3.450903	0.228323	0.130096
O	5.908417	-0.00727	-0.28531	O	5.830743	-0.5342	0.071227
C	4.531626	-2.21174	-1.58506	C	4.334197	-2.09012	-1.87138
C	4.572434	-2.82381	0.866587	C	4.199363	-3.42107	0.272426
O	0.116103	-2.4215	-0.36778	O	-0.14953	-2.21454	-0.88438
H	0.053595	1.292475	-1.63628	H	0.158194	1.677622	-0.93109
H	-2.16463	2.668877	-0.95082	H	-1.92174	2.995235	0.143801
H	-3.28052	1.577825	-0.13093	H	-3.16485	1.828774	0.611704
H	-3.4942	0.880027	-2.46321	H	-3.38556	1.892624	-1.8224
H	-1.77368	1.01901	-2.73316	H	-1.65315	1.932766	-2.04404
H	-1.68893	-1.24624	-2.26096	H	-1.8106	-0.36686	-2.29079
H	1.154445	2.455454	0.955693	H	1.308158	1.895288	1.874954
H	1.88629	2.516351	-0.63579	H	2.069998	2.385782	0.375757
H	-0.12012	3.802673	-1.52591	H	-0.2201	3.789348	1.810737
H	-0.97033	5.914887	-1.37345	H	-0.61798	5.995363	1.368787
H	-1.61711	6.306554	0.230971	H	0.787793	6.844313	0.699924
H	-0.0593	6.954447	-0.26248	H	-0.53851	6.386536	-0.35934
H	0.853697	4.1164	2.128319	H	2.152906	3.794804	-1.14122
H	1.107744	5.838628	1.81844	H	1.132923	5.040936	-1.86731
H	-0.47417	5.268592	2.328454	H	2.456953	5.508661	-0.81149
H	-2.19257	1.051877	2.025708	H	-2.18269	0.530742	2.494101
H	-0.43218	1.004226	2.130132	H	-0.43686	0.284976	2.560519
H	-1.24496	2.48838	1.615129	H	-1.0991	1.922191	2.566861
H	-4.00804	-3.68064	-0.9989	H	-4.39104	-2.81513	-1.8054
H	-3.17319	-3.23282	-2.50173	H	-3.4968	-2.01283	-3.11411
H	-2.2597	-3.34231	-0.98433	H	-2.61724	-2.67864	-1.72478
H	-4.80383	-1.18707	-2.84213	H	-4.90124	0.18984	-2.77668
H	-5.63251	-1.83683	-1.4179	H	-5.81096	-0.77498	-1.60282
H	-5.12811	-0.14338	-1.43866	H	-5.1326	0.782136	-1.11528
H	-0.03961	-1.23157	2.211275	H	-0.23981	-1.90248	1.928057
H	-0.92129	-1.25502	3.743358	H	-1.14363	-2.29648	3.395948
H	-0.44292	-2.7665	2.974722	H	-0.81273	-3.54533	2.198027
H	-4.12528	-2.67572	2.21377	H	-4.45121	-2.85272	1.554231
H	-2.87469	-3.54019	3.137323	H	-3.30725	-4.08503	2.134501
H	-3.50105	-2.00716	3.732218	H	-3.783	-2.76306	3.193824
H	4.679614	-0.25993	1.269483	H	4.507407	-1.12299	1.447331
H	3.351951	1.437356	0.241795	H	3.385911	0.928235	0.960826
H	3.656501	0.825067	-1.38113	H	3.717739	0.809116	-0.76489
H	5.887452	0.006356	-1.25193	H	5.861365	-0.23565	-0.84792
H	5.614054	-2.34693	-1.66881	H	5.403319	-2.30091	-1.96942
H	4.043881	-3.15875	-1.82766	H	3.777756	-2.86401	-2.40531
H	4.209329	-1.47652	-2.33101	H	4.11648	-1.13387	-2.36037
H	5.66467	-2.8775	0.908206	H	5.2794	-3.59191	0.316133
H	4.198365	-2.55121	1.857356	H	3.803324	-3.42765	1.291709
H	4.181038	-3.81237	0.611958	H	3.735608	-4.24157	-0.28166
3-e							
C	-1.22759	0.956211	0.081048				
C	-1.4691	-0.58882	-0.14072				

C	-0.07316	-1.2201	-0.25124				
C	0.937154	-0.13732	-0.31302				
C	0.20734	1.188589	-0.54103				
C	-2.35298	1.616641	-0.74346				
C	-2.50482	0.74237	-1.99192				
C	-2.25489	-0.70699	-1.51374				
C	-3.50051	-1.57545	-1.15021				
O	-3.65655	-1.38513	0.276537				
C	-2.39595	-1.29223	0.843482				
C	0.928847	2.485923	-0.10534				
C	0.21989	3.759271	-0.49137				
C	-0.00529	4.856632	0.248489				
C	-0.68691	6.063844	-0.35105				
C	0.387151	5.019625	1.69656				
C	-1.28164	1.409268	1.545261				
C	-3.19905	-3.0572	-1.42084				
C	-4.82624	-1.16438	-1.78329				
C	-2.17209	-1.80511	2.065394				
C	-0.8562	-1.72908	2.794231				
C	-3.2682	-2.52292	2.814897				
C	2.268654	-0.40517	-0.24808				
O	2.699829	-1.68223	-0.07807				
C	4.148577	-1.7939	-0.17573				
C	4.620701	-0.36973	0.187899				
C	3.47104	0.515339	-0.32359				
O	5.885776	-0.10742	-0.3923				
C	4.508858	-2.19078	-1.6089				
C	4.586013	-2.85045	0.830855				
O	0.113547	-2.42536	-0.32076				
H	0.068618	1.2837	-1.62958				
H	-2.15328	2.667797	-0.96897				
H	-3.27704	1.582027	-0.15277				
H	-3.47272	0.871468	-2.48198				
H	-1.75039	1.009789	-2.74036				
H	-1.66443	-1.25183	-2.25519				
H	1.151798	2.456851	0.964937				
H	1.895931	2.507075	-0.62178				
H	-0.0985	3.793528	-1.53461				
H	-0.9461	5.908076	-1.40179				
H	-1.60809	6.308467	0.194187				
H	-0.04502	6.952662	-0.28746				
H	0.842871	4.125915	2.126008				
H	1.099908	5.84718	1.810675				
H	-0.48651	5.279042	2.308257				
H	-2.2064	1.067772	2.01594				
H	-0.44697	1.018383	2.134079				
H	-1.25379	2.500701	1.604328				
H	-3.99234	-3.68499	-1.00381				
H	-3.13823	-3.24597	-2.49837				
H	-2.24504	-3.34232	-0.96813				
H	-4.76888	-1.20565	-2.87541				
H	-5.61504	-1.84942	-1.45876				
H	-5.11571	-0.15453	-1.48291				
H	-0.07123	-1.21565	2.239803				
H	-0.9737	-1.21863	3.7603				
H	-0.49002	-2.74026	3.015107				
H	-4.15848	-2.65372	2.199779				
H	-2.92121	-3.51001	3.148507				
H	-3.55612	-1.97199	3.721234				
H	4.674804	-0.29499	1.284358				
H	3.349123	1.423746	0.265255				
H	3.675212	0.810541	-1.36067				
H	6.218064	0.72329	-0.02974				

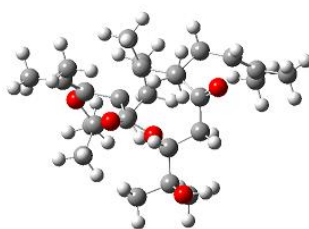
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H	4.171969	-1.44124	-2.33014				
H	5.678145	-2.91619	0.845822				
H	4.234681	-2.59465	1.834501				
H	4.179915	-3.82968	0.564326				



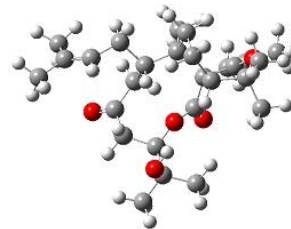
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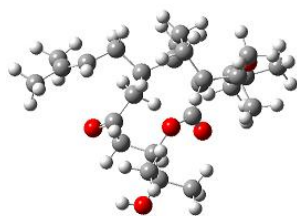
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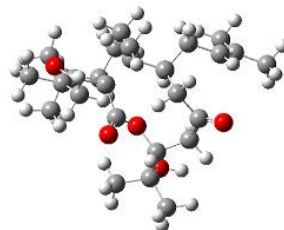
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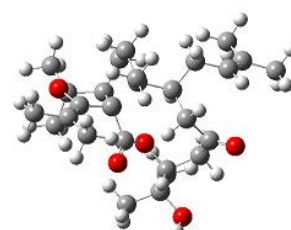
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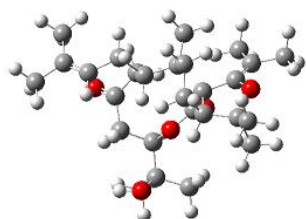
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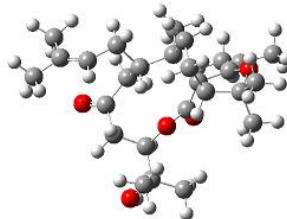
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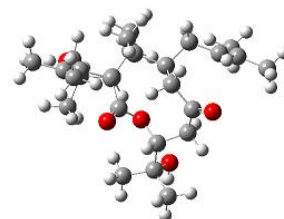
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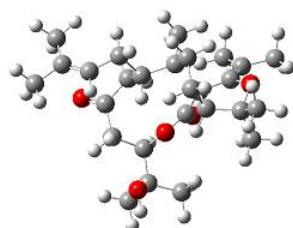
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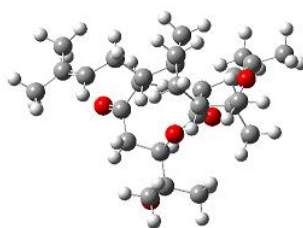
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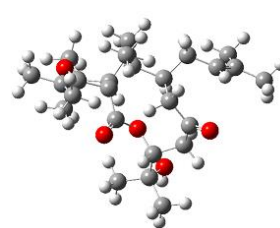
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l

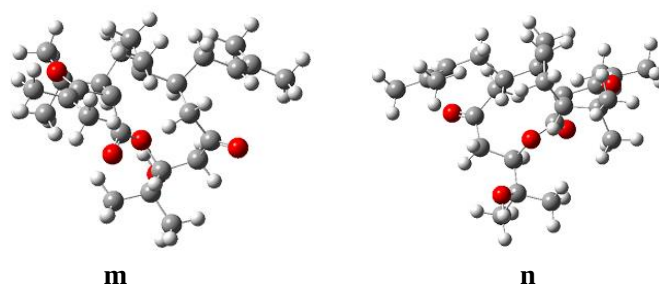


Figure S32. Optimized geometries of predominant conformers for compound **4** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S22. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **4** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
4-a	-1429.660519	-1429.724414	0.0
4-b	-1429.665914	-1429.729604	0.7
4-c	-1429.669610	-1429.733625	50.4
4-d	-1429.666836	-1429.730503	1.8
4-e	-1429.666050	-1429.729771	0.9
4-f	-1429.667626	-1429.731153	3.7
4-g	-1429.666748	-1429.729949	1.0
4-h	-1429.668364	-1429.731546	5.6
4-i	-1429.666640	-1429.730637	2.1
4-j	-1429.667396	-1429.730962	3.0
4-k	-1429.667504	-1429.730894	2.8
4-l	-1429.666640	-1429.730639	2.1
4-m	-1429.668682	-1429.732915	23.8
4-n	-1429.666640	-1429.730635	2.1

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p)

level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S23. Optimized Z-matrixes of compound **4** in the gas phase (Å) at B3LYP/6-31G(d,p) level

4-a				4-b			
C	1.077017	0.730273	-0.00978	C	-0.49208	-1.67951	-0.5329
C	1.415031	0.842576	-1.52916	C	-0.8472	-2.65901	0.612854
C	0.463051	1.873306	-2.10791	C	-0.77854	-1.82634	1.88734
C	-0.8851	1.503743	-1.47936	C	-1.44431	-0.48364	1.506489
C	-0.53946	1.09509	0.013671	C	-1.42707	-0.41192	-0.08477
C	-1.8764	2.676715	-1.33965	C	-2.94892	-0.33693	1.852793
O	-1.37809	3.336381	-0.15599	O	-3.60738	-0.9365	0.719776
C	-0.96556	2.377924	0.767945	C	-2.92081	-0.59562	-0.44161
C	1.864731	1.813621	0.753283	C	-0.8663	-2.32911	-1.87392
C	-1.42914	-0.07967	0.432019	C	-0.89132	0.94226	-0.56339
O	-1.15333	-1.19202	-0.29842	O	0.185063	1.334622	0.175634
C	0.864087	-1.29313	1.761058	C	1.459743	-0.47022	-1.77185
C	1.50489	-0.72082	0.460316	C	1.045998	-1.30537	-0.52172
C	-1.6214	-2.46871	0.218726	C	1.086374	2.328902	-0.37944
C	-0.37806	-3.30463	0.552759	C	2.453392	1.645383	-0.51493

C	0.561133	-2.78565	1.653634	C	2.569932	0.564533	-1.59792
C	3.042398	-0.93435	0.619276	C	1.984242	-2.54146	-0.38873
C	3.882974	-0.85535	-0.62613	C	3.449207	-2.18218	-0.37225
C	5.076618	-0.26331	-0.79418	C	4.282037	-2.16981	0.68227
C	5.802577	-0.35386	-2.11562	C	5.733823	-1.79129	0.508671
C	5.815755	0.512773	0.268598	C	3.896161	-2.52829	2.096779
O	1.079403	-3.58691	2.410567	O	3.539968	0.566031	-2.33425
C	-2.55332	-3.12919	-0.82478	C	1.081612	3.599168	0.519761
C	-3.21098	-4.38774	-0.23228	C	-0.31691	4.221711	0.53437
C	-3.63385	-2.13897	-1.28313	C	1.568701	3.31948	1.946574
O	-1.71286	-3.48713	-1.92955	O	1.920446	4.57412	-0.11487
O	-2.28115	-0.05996	1.296904	O	-1.31626	1.601694	-1.48636
C	-1.04151	2.690718	2.072486	C	-3.62981	-0.49177	-1.58217
C	-0.60796	1.807884	3.209535	C	-3.08989	-0.21651	-2.9611
C	-1.60764	4.020938	2.51082	C	-5.13018	-0.68631	-1.55622
C	-1.83915	3.698146	-2.47529	C	-3.34621	1.14664	1.941326
C	-3.32279	2.214183	-1.10376	C	-3.4416	-1.08407	3.089594
H	-1.32095	0.66065	-2.0229	H	-0.89101	0.346302	1.943874
H	2.46677	1.089034	-1.69023	H	-1.87491	-3.00724	0.459883
H	1.232567	-0.12252	-2.01627	H	-0.21306	-3.54818	0.625899
H	0.430112	1.858812	-3.20212	H	0.263704	-1.65041	2.175137
H	0.759791	2.881699	-1.80124	H	-1.25397	-2.31333	2.74068
H	1.568844	2.817643	0.442287	H	-0.2986	-3.25741	-1.99652
H	1.720263	1.754582	1.834172	H	-1.92624	-2.58561	-1.9
H	2.932476	1.706376	0.548581	H	-0.65138	-1.7006	-2.73898
H	-0.06998	-0.7976	2.026418	H	0.601845	0.085577	-2.16631
H	1.531435	-1.17166	2.618876	H	1.784787	-1.12746	-2.583
H	1.192447	-1.37581	-0.35436	H	1.22762	-0.69727	0.365072
H	-2.21277	-2.26291	1.114067	H	0.70654	2.632405	-1.35752
H	-0.67199	-4.30613	0.872733	H	3.21877	2.384923	-0.7617
H	0.201534	-3.43084	-0.36895	H	2.726643	1.185782	0.443361
H	3.149938	-1.95344	1.021043	H	1.732459	-3.09342	0.518408
H	3.42694	-0.27814	1.404862	H	1.802073	-3.22538	-1.22855
H	3.478529	-1.40169	-1.47951	H	3.870819	-1.89764	-1.33425
H	5.237105	-0.92811	-2.85458	H	6.003752	-0.94832	1.158593
H	5.993007	0.644366	-2.53217	H	6.394008	-2.62222	0.791514
H	6.784778	-0.82999	-1.99494	H	5.960899	-1.51083	-0.52288
H	5.263797	0.60191	1.205875	H	4.111369	-1.69495	2.778393
H	6.777426	0.033514	0.494616	H	2.841502	-2.78645	2.209042
H	6.051677	1.525397	-0.08363	H	4.49053	-3.37872	2.455931
H	-3.89195	-4.82836	-0.96915	H	-0.28643	5.163495	1.088623
H	-2.46798	-5.14478	0.027585	H	-0.65436	4.429562	-0.48397
H	-3.80028	-4.1533	0.659985	H	-1.04136	3.556975	1.01018
H	-4.32313	-2.63349	-1.97716	H	1.513082	4.236393	2.53984
H	-3.1789	-1.29079	-1.79696	H	2.608626	2.973076	1.959067
H	-4.21835	-1.76356	-0.43794	H	0.956687	2.554008	2.43144
H	-2.27324	-3.8905	-2.60571	H	2.840171	4.37295	0.101725
H	-0.06485	0.919634	2.898267	H	-2.02028	-0.03828	-2.99357
H	0.037814	2.364444	3.902078	H	-3.33392	-1.04698	-3.63792
H	-1.48044	1.475239	3.786058	H	-3.57492	0.677234	-3.37297
H	-2.07568	4.558246	1.686794	H	-5.41448	-1.59939	-2.09716
H	-2.35123	3.873254	3.304843	H	-5.52107	-0.75821	-0.54227
H	-0.82236	4.662005	2.935088	H	-5.62767	0.145629	-2.07111
H	-2.52429	4.521263	-2.25278	H	-4.43051	1.237317	2.053289
H	-2.15682	3.237278	-3.41591	H	-2.86909	1.626664	2.802262
H	-0.8414	4.117958	-2.61171	H	-3.05911	1.692408	1.037589
H	-3.40144	1.560596	-0.23303	H	-3.33266	-2.16403	2.971969
H	-3.96433	3.083219	-0.92986	H	-2.89337	-0.76814	3.982582
H	-3.70453	1.67846	-1.9798	H	-4.50273	-0.87216	3.24935
4-c				4-d			
C	0.42287	-1.72168	-0.14469	C	0.422423	-1.74227	-0.07408
C	0.95203	-2.31561	-1.47488	C	0.954398	-2.40545	-1.36912
C	1.152293	-1.12088	-2.39777	C	1.141147	-1.26338	-2.35938
C	1.81667	-0.05721	-1.49863	C	1.777032	-0.13218	-1.52117
C	1.451711	-0.45011	0.003499	C	1.451912	-0.46753	0.002653

C	3.369711	-0.01398	-1.49392	C	3.325766	-0.03599	-1.54286
O	3.730671	-0.95276	-0.4619	O	3.730726	-0.9438	-0.49906
C	2.822518	-0.8532	0.586587	C	2.840829	-0.84316	0.565528
C	0.545213	-2.79096	0.952947	C	0.53619	-2.7534	1.07742
C	0.860032	0.765419	0.727478	C	0.866085	0.763986	0.70427
O	-0.07325	1.390117	-0.04797	O	-0.05026	1.390308	-0.08931
C	-1.66155	-0.77958	1.09842	C	-1.67452	-0.75425	1.117419
C	-1.08166	-1.25182	-0.26816	C	-1.07889	-1.26885	-0.22827
C	-1.02768	2.295064	0.581294	C	-1.01654	2.28292	0.524567
C	-2.41257	1.667228	0.372168	C	-2.39975	1.656798	0.287952
C	-2.68276	0.356344	1.117237	C	-2.69525	0.380605	1.085348
C	-2.04	-2.3179	-0.87585	C	-2.0345	-2.34646	-0.81901
C	-3.37622	-1.72412	-1.24229	C	-3.36452	-1.76004	-1.21871
C	-4.56776	-1.90307	-0.65046	C	-4.56286	-1.91306	-0.63307
C	-5.78843	-1.16395	-1.1408	C	-5.77526	-1.1858	-1.16034
C	-4.80881	-2.7704	0.559111	C	-4.81975	-2.73763	0.602757
O	-3.69817	0.256492	1.785378	O	-3.71973	0.313831	1.742036
C	-0.85467	3.68405	-0.09062	C	-0.84638	3.714955	-0.06153
C	-1.87411	4.6929	0.445574	C	0.544164	4.255322	0.281894
C	0.572386	4.20861	0.135135	C	-1.09577	3.770344	-1.57329
O	-1.11984	3.568345	-1.49319	O	-1.76389	4.572491	0.630345
O	1.142599	1.160411	1.836814	O	1.134419	1.159854	1.81691
C	3.262151	-1.11469	1.831835	C	3.312784	-1.07468	1.805296
C	2.431269	-1.16178	3.087016	C	2.515305	-1.106	3.082516
C	4.72188	-1.43526	2.064886	C	4.7824	-1.37042	2.008913
C	3.869797	1.384973	-1.09554	C	3.786098	1.38626	-1.1798
C	4.067634	-0.47978	-2.76864	C	4.020775	-0.50181	-2.81937
H	1.437292	0.933005	-1.74917	H	1.354358	0.829035	-1.81003
H	1.920304	-2.78909	-1.2766	H	1.928491	-2.85501	-1.1457
H	0.301032	-3.09024	-1.8853	H	0.312232	-3.2106	-1.73265
H	0.185847	-0.74776	-2.75418	H	0.172447	-0.93202	-2.74912
H	1.738671	-1.35752	-3.28791	H	1.74096	-1.54471	-3.22709
H	-0.06146	-3.65925	0.674682	H	-0.0707	-3.63399	0.840657
H	1.577008	-3.12928	1.0592	H	1.56683	-3.08714	1.206062
H	0.200729	-2.45394	1.931277	H	0.186768	-2.36721	2.035486
H	-0.8582	-0.44308	1.764689	H	-0.87859	-0.39307	1.77948
H	-2.13842	-1.61318	1.619665	H	-2.15504	-1.57156	1.660671
H	-1.09886	-0.40654	-0.95676	H	-1.0797	-0.44248	-0.94002
H	-0.77295	2.371854	1.641386	H	-0.79882	2.348169	1.592941
H	-3.18951	2.35491	0.709944	H	-3.18153	2.364462	0.573409
H	-2.55703	1.517331	-0.70413	H	-2.51683	1.430276	-0.77876
H	-1.59991	-2.72856	-1.79055	H	-1.58421	-2.78187	-1.71697
H	-2.15457	-3.15645	-0.18217	H	-2.16007	-3.16631	-0.10484
H	-3.34343	-1.04406	-2.09582	H	-3.32029	-1.11136	-2.09607
H	-6.59569	-1.85978	-1.40349	H	-6.5847	-1.88606	-1.40352
H	-6.18071	-0.51049	-0.35069	H	-6.16994	-0.50132	-0.39805
H	-5.57059	-0.54618	-2.01646	H	-5.54723	-0.60267	-2.05709
H	-5.70762	-3.38413	0.424793	H	-5.72024	-3.35141	0.480608
H	-3.97608	-3.43995	0.784392	H	-3.99235	-3.40293	0.857922
H	-4.97509	-2.13455	1.437748	H	-4.99101	-2.07196	1.45802
H	-1.66135	5.679903	0.02682	H	0.6199	5.29385	-0.05109
H	-2.89071	4.421179	0.155009	H	0.710681	4.224906	1.361627
H	-1.82352	4.762923	1.53645	H	1.327454	3.671291	-0.20652
H	0.68323	5.178154	-0.35755	H	-0.93061	4.788815	-1.93554
H	1.317586	3.52615	-0.28304	H	-2.12424	3.485806	-1.82388
H	0.791542	4.327512	1.2005	H	-0.42311	3.0963	-2.11072
H	-0.4754	2.940045	-1.84865	H	-2.64039	4.459943	0.239932
H	1.382616	-0.92341	2.93857	H	1.463529	-0.86926	2.958231
H	2.504901	-2.15427	3.552467	H	2.603454	-2.09114	3.561102
H	2.822046	-0.4416	3.816448	H	2.925187	-0.37473	3.790195
H	4.847912	-2.48304	2.370501	H	4.929948	-2.40866	2.336726
H	5.328285	-1.26709	1.175889	H	5.364432	-1.21607	1.101393
H	5.1171	-0.82349	2.886032	H	5.189263	-0.73374	2.805051
H	4.955171	1.370536	-0.96127	H	4.873694	1.410075	-1.06604
H	3.627679	2.121138	-1.86943	H	3.505073	2.098398	-1.96287

H	3.421558	1.712996	-0.15265	H	3.345402	1.719142	-0.23524
H	3.84792	-1.52771	-2.98305	H	3.843551	-1.56306	-3.00517
H	3.764102	0.128425	-3.62629	H	3.675108	0.071741	-3.68495
H	5.150721	-0.38382	-2.65007	H	5.100677	-0.35631	-2.7242
4-e				4-f			
C	-0.49926	-1.67845	-0.53762	C	-0.49583	-1.67283	-0.55035
C	-0.86166	-2.6556	0.607829	C	-0.85741	-2.66808	0.579717
C	-0.78782	-1.82247	1.881713	C	-0.7883	-1.85481	1.866671
C	-1.44606	-0.47605	1.500685	C	-1.44844	-0.504	1.504822
C	-1.42847	-0.40579	-0.09163	C	-1.42975	-0.40944	-0.08523
C	-2.95055	-0.32424	1.845862	C	-2.95268	-0.35664	1.851993
O	-3.61131	-0.92071	0.711135	O	-3.61291	-0.93686	0.709893
C	-2.92224	-0.58322	-0.4488	C	-2.92356	-0.58419	-0.44605
C	-0.87376	-2.32582	-1.87965	C	-0.86862	-2.30067	-1.90186
C	-0.8883	0.948475	-0.56547	C	-0.89078	0.949683	-0.54338
O	0.197658	1.320692	0.162998	O	0.184594	1.330213	0.201543
C	1.46295	-0.47639	-1.76666	C	1.46632	-0.45487	-1.76644
C	1.040909	-1.31452	-0.52171	C	1.043619	-1.30357	-0.52889
C	1.08954	2.326761	-0.37955	C	1.097474	2.315941	-0.34873
C	2.454711	1.636031	-0.50165	C	2.464804	1.636677	-0.47804
C	2.574108	0.555364	-1.58278	C	2.58121	0.57508	-1.5765
C	1.971716	-2.55678	-0.39311	C	1.977134	-2.54453	-0.40694
C	3.438389	-2.20466	-0.36974	C	3.443222	-2.18981	-0.38718
C	4.2651	-2.19329	0.689568	C	4.274721	-2.18409	0.668388
C	5.719174	-1.8201	0.523834	C	5.72691	-1.80557	0.498924
C	3.869258	-2.54618	2.102651	C	3.885985	-2.54789	2.080738
O	3.547076	0.558348	-2.31614	O	3.547391	0.584018	-2.31827
C	1.099771	3.575897	0.546934	C	1.099308	3.591722	0.53951
C	1.843231	4.732901	-0.13973	C	-0.3081	4.199468	0.60139
C	-0.3313	4.000677	0.886394	C	1.643436	3.332645	1.945071
O	1.714154	3.262888	1.803482	O	2.010019	4.52445	-0.05945
O	-1.32129	1.624076	-1.47494	O	-1.31295	1.624114	-1.45804
C	-3.62814	-0.47591	-1.59097	C	-3.63063	-0.46478	-1.58634
C	-3.08169	-0.20014	-2.96718	C	-3.08783	-0.17344	-2.96084
C	-5.12916	-0.66466	-1.56978	C	-5.13143	-0.65658	-1.56531
C	-3.34375	1.15986	1.935742	C	-3.34462	1.126995	1.962101
C	-3.44701	-1.07117	3.081294	C	-3.44935	-1.11975	3.077376
H	-0.88697	0.350494	1.937489	H	-0.89218	0.31723	1.954754
H	-1.89146	-2.99743	0.454317	H	-1.88599	-3.01057	0.419405
H	-0.23308	-3.54878	0.621074	H	-0.22608	-3.55928	0.580579
H	0.255054	-1.6517	2.16975	H	0.253899	-1.68689	2.158974
H	-1.26591	-2.30621	2.735356	H	-1.26726	-2.35262	2.711729
H	-0.31309	-3.25866	-2.0001	H	-0.30285	-3.22834	-2.03743
H	-1.9356	-2.57397	-1.90938	H	-1.92906	-2.55438	-1.93446
H	-0.65083	-1.69928	-2.74429	H	-0.6495	-1.65957	-2.75659
H	0.607628	0.081453	-2.16437	H	0.611261	0.108456	-2.15706
H	1.791812	-1.13099	-2.57845	H	1.790644	-1.10344	-2.58492
H	1.224838	-0.71187	0.367999	H	1.223897	-0.70719	0.366037
H	0.701084	2.62702	-1.35671	H	0.716609	2.607971	-1.33286
H	3.241155	2.359331	-0.73025	H	3.222617	2.394494	-0.68546
H	2.688464	1.183209	0.469956	H	2.721542	1.161064	0.476689
H	1.714416	-3.11199	0.510439	H	1.723453	-3.10368	0.495333
H	1.788683	-3.23529	-1.23708	H	1.792545	-3.2201	-1.25299
H	3.866459	-1.92311	-1.32987	H	3.866323	-1.90043	-1.34704
H	5.987609	-0.97591	1.172821	H	5.9951	-0.96431	1.151581
H	6.374953	-2.65213	0.81367	H	6.386323	-2.63752	0.780689
H	5.953765	-1.54374	-0.50719	H	5.956001	-1.52165	-0.5312
H	4.077701	-1.70939	2.782046	H	4.097391	-1.71588	2.765086
H	2.814104	-2.80485	2.20809	H	2.831607	-2.80891	2.189449
H	4.462064	-3.39427	2.469893	H	4.481473	-3.39795	2.438913
H	1.846952	5.602187	0.523461	H	-0.26435	5.159793	1.122836
H	2.884266	4.479152	-0.36825	H	-0.71278	4.362051	-0.4038
H	1.357473	5.018658	-1.07768	H	-1.00525	3.547567	1.133765
H	-0.31156	4.936756	1.45053	H	1.567046	4.245337	2.541883
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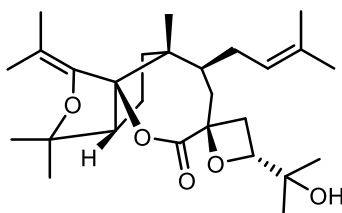
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H	-3.32223	-1.02971	-3.64643	H	-3.32993	-0.99596	-3.64796
H	-3.56397	0.694369	-3.38084	H	-3.57256	0.724759	-3.36347
H	-5.41614	-1.57395	-2.11577	H	-5.41676	-1.56119	-2.11977
H	-5.52227	-0.73991	-0.55689	H	-5.524	-0.7424	-0.55308
H	-5.62266	0.171775	-2.08146	H	-5.62686	0.183598	-2.06883
H	-4.4281	1.253284	2.045801	H	-4.42866	1.220074	2.074701
H	-2.86629	1.636886	2.798023	H	-2.86622	1.592366	2.830347
H	-3.05246	1.706215	1.033998	H	-3.05495	1.684853	1.066551
H	-3.3425	-2.15146	2.962511	H	-3.3451	-2.19825	2.943581
H	-2.89767	-0.75832	3.974621	H	-2.90001	-0.81965	3.975103
H	-4.50735	-0.85498	3.240851	H	-4.50961	-0.90558	3.239899
4-g				4-h			
C	0.416627	-1.74741	-0.04606	C	0.425512	-1.74255	-0.05581
C	0.952322	-2.4326	-1.32763	C	0.96236	-2.42488	-1.33861
C	1.136481	-1.30734	-2.33767	C	1.148878	-1.29842	-2.34664
C	1.763835	-0.15689	-1.5185	C	1.778839	-0.15167	-1.5251
C	1.448108	-0.47433	0.01197	C	1.454812	-0.46594	0.003681
C	3.311443	-0.05095	-1.54755	C	3.326926	-0.04905	-1.5476
O	3.726218	-0.94775	-0.49667	O	3.735514	-0.9411	-0.49157
C	2.840526	-0.84337	0.570274	C	2.844664	-0.83126	0.571109
C	0.522376	-2.73826	1.123468	C	0.536999	-2.73558	1.111447
C	0.868384	0.766157	0.702467	C	0.867745	0.773759	0.688015
O	-0.05359	1.375564	-0.0907	O	-0.04693	1.390093	-0.11363
C	-1.68702	-0.73435	1.114062	C	-1.67994	-0.74328	1.113425
C	-1.08266	-1.27366	-0.21788	C	-1.07593	-1.2729	-0.22233
C	-1.00215	2.291058	0.511324	C	-1.02614	2.273543	0.492032
C	-2.38592	1.673968	0.251615	C	-2.40728	1.651489	0.246943
C	-2.70037	0.40572	1.052867	C	-2.70382	0.390617	1.063424
C	-2.0362	-2.36024	-0.79553	C	-2.02716	-2.35915	-0.80482
C	-3.36498	-1.78027	-1.20842	C	-3.35843	-1.77994	-1.21106
C	-4.56524	-1.92647	-0.62513	C	-4.55577	-1.92722	-0.62193
C	-5.77635	-1.20731	-1.16631	C	-5.76915	-1.20571	-1.15461
C	-4.82603	-2.73425	0.620966	C	-4.80991	-2.73751	0.62389
O	-3.73421	0.353535	1.697128	O	-3.72425	0.330937	1.727747
C	-0.82363	3.708321	-0.10293	C	-0.86497	3.710013	-0.08048
C	-1.64718	4.733923	0.692114	C	0.541813	4.245245	0.217602
C	0.65416	4.108332	-0.10069	C	-1.17293	3.786606	-1.57626
O	-1.21893	3.709973	-1.48069	O	-1.84904	4.535676	0.557622
O	1.147636	1.180178	1.807547	O	1.133661	1.184544	1.79688
C	3.318467	-1.06331	1.809953	C	3.317197	-1.04637	1.813664
C	2.52611	-1.08256	3.090612	C	2.51942	-1.06464	3.09096
C	4.789574	-1.35371	2.010029	C	4.787617	-1.33557	2.020862
C	3.766488	1.3766	-1.20049	C	3.781324	1.379922	-1.20375
C	4.004536	-0.52443	-2.82243	C	4.024584	-0.52866	-2.81755
H	1.329031	0.795179	-1.81984	H	1.35165	0.803037	-1.82853
H	1.927461	-2.87522	-1.095	H	1.936926	-2.86882	-1.10598
H	0.312966	-3.24621	-1.6772	H	0.322567	-3.23693	-1.69068
H	0.16835	-0.98793	-2.73803	H	0.180749	-0.97642	-2.74517
H	1.741164	-1.60188	-3.19743	H	1.752542	-1.59223	-3.20748
H	-0.08294	-3.62297	0.89842	H	-0.06762	-3.62054	0.885646
H	1.552245	-3.06946	1.264426	H	1.567682	-3.06574	1.248966
H	0.166559	-2.33526	2.072427	H	0.182639	-2.3355	2.061967
H	-0.89408	-0.3688	1.777561	H	-0.88732	-0.37276	1.77466
H	-2.17833	-1.53963	1.665551	H	-2.16	-1.55537	1.664916
H	-1.07735	-0.45979	-0.94382	H	-1.07487	-0.45516	-0.94404
H	-0.78172	2.34841	1.580979	H	-0.81018	2.324394	1.564303
H	-3.1814	2.379374	0.503612	H	-3.17608	2.384247	0.498552
H	-2.45528	1.451026	-0.81981	H	-2.50573	1.407745	-0.81754
H	-1.58255	-2.80833	-1.68546	H	-1.57443	-2.80156	-1.69816
H	-2.16425	-3.1697	-0.06989	H	-2.15144	-3.17268	-0.08308
H	-3.31742	-1.14302	-2.09384	H	-3.31566	-1.14072	-2.09527
H	-6.58593	-1.91086	-1.39945	H	-6.58077	-1.90795	-1.38451

H	-6.17181	-0.51002	-0.41602	H	-6.15883	-0.50959	-0.4004
H	-5.54633	-0.63917	-2.07209	H	-5.5438	-0.63523	-2.06002
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H	-5.00675	-2.05719	1.465314	H	-4.97986	-2.06169	1.47144
H	-1.51768	5.723366	0.245236	H	0.599087	5.296599	-0.07805
H	-2.71711	4.499144	0.68708	H	0.77637	4.166311	1.28523
H	-1.32327	4.783384	1.736159	H	1.307985	3.689083	-0.3284
H	0.754501	5.141923	-0.44198	H	-0.98709	4.801476	-1.9376
H	1.218707	3.468114	-0.78034	H	-2.22137	3.549047	-1.77105
H	1.083711	4.019761	0.900923	H	-0.54209	3.092874	-2.13825
H	-2.18382	3.74954	-1.5182	H	-1.58661	4.653451	1.481577
H	1.474691	-0.84302	2.968057	H	1.467316	-0.83105	2.9634
H	2.612364	-2.06395	3.577294	H	2.608685	-2.04415	3.580733
H	2.941373	-0.34697	3.790805	H	2.92833	-0.32507	3.790671
H	4.94134	-2.38784	2.348886	H	4.938381	-2.37024	2.358351
H	5.366579	-1.20823	1.097827	H	5.36952	-1.18801	1.112116
H	5.199227	-0.70708	2.796789	H	5.192278	-0.69023	2.811171
H	4.854451	1.406037	-1.09084	H	4.868757	1.409712	-1.08972
H	3.479316	2.078721	-1.99021	H	3.497999	2.079825	-1.99698
H	3.327163	1.718655	-0.25885	H	3.33865	1.724251	-0.26419
H	3.837265	-1.58946	-2.99524	H	3.853313	-1.59337	-2.98827
H	3.648102	0.03581	-3.69229	H	3.675436	0.030581	-3.69105
H	5.083441	-0.36687	-2.73494	H	5.103672	-0.37571	-2.72473
4-i				4-j			
C	-0.49627	-1.68253	-0.52731	C	0.41266	-1.74642	-0.05698
C	-0.85766	-2.65167	0.625229	C	0.948232	-2.42388	-1.34278
C	-0.78523	-1.80893	1.892779	C	1.136409	-1.29193	-2.34442
C	-1.4457	-0.46665	1.501568	C	1.767065	-0.14975	-1.5165
C	-1.42662	-0.40744	-0.09132	C	1.446051	-0.47519	0.011303
C	-2.95069	-0.3147	1.844228	C	3.315195	-0.04971	-1.541
O	-3.61039	-0.9175	0.712723	O	3.724833	-0.9512	-0.49265
C	-2.91972	-0.58722	-0.44873	C	2.835698	-0.84923	0.572062
C	-0.87066	-2.34049	-1.86433	C	0.516897	-2.74576	1.105522
C	-0.88613	0.944392	-0.5724	C	0.86685	0.764171	0.704859
O	0.197909	1.319604	0.155915	O	-0.05361	1.375127	-0.08778
C	1.463182	-0.48502	-1.76455	C	-1.68745	-0.73672	1.110113
C	1.043437	-1.31667	-0.51481	C	-1.08571	-1.26898	-0.22553
C	1.092793	2.323897	-0.38834	C	-1.00314	2.291305	0.51475
C	2.460235	1.638611	-0.51597	C	-2.39152	1.680299	0.266493
C	2.574536	0.549057	-1.58681	C	-2.69954	0.406279	1.058369
C	1.975051	-2.55794	-0.38065	C	-2.04105	-2.35101	-0.80874
C	3.44147	-2.20453	-0.36196	C	-3.36971	-1.76608	-1.21477
C	4.267897	-2.17875	0.697122	C	-4.56897	-1.91544	-0.63049
C	5.720155	-1.80053	0.527796	C	-5.77891	-1.18641	-1.16082
C	3.872516	-2.5153	2.114254	C	-4.82886	-2.73422	0.608652
O	3.547937	0.540595	-2.32041	O	-3.73253	0.344465	1.704169
C	1.094933	3.567566	0.531365	C	-0.81868	3.700359	-0.09578
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C	-0.34105	4.035214	0.809723	C	0.657349	4.120981	-0.04414
O	1.721389	3.149699	1.751206	O	-1.25354	3.595242	-1.45773
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C	-3.62444	-0.48691	-1.59221	C	3.308924	-1.07577	1.812285
C	-3.07565	-0.21966	-2.96912	C	2.511211	-1.09864	3.089527
C	-5.1254	-0.67613	-1.57189	C	4.778401	-1.37122	2.016588
C	-3.3454	1.169771	1.92511	C	3.774547	1.374962	-1.18683
C	-3.44782	-1.05487	3.083504	C	4.010019	-0.52064	-2.8159
H	-0.88769	0.363738	1.932533	H	1.336228	0.805789	-1.81273
H	-1.88681	-2.99676	0.474131	H	1.921788	-2.87131	-1.11244
H	-0.22714	-3.5433	0.645427	H	0.306446	-3.23268	-1.69892
H	0.257375	-1.63378	2.178783	H	0.16926	-0.96612	-2.74175
H	-1.26219	-2.28705	2.750302	H	1.740242	-1.58183	-3.20647
H	-0.30914	-3.27371	-1.97723	H	-0.0902	-3.62758	0.874046
H	-1.93234	-2.5898	-1.89245	H	1.546068	-3.0802	1.244331
H	-0.64757	-1.72055	-2.73362	H	0.161425	-2.34892	2.057117

H	0.606871	0.069353	-2.16512	H	-0.89298	-0.37742	1.775381
H	1.792016	-1.14395	-2.57291	H	-2.17958	-1.54471	1.656996
H	1.228828	-0.70869	0.371006	H	-1.08076	-0.45082	-0.94655
H	0.700231	2.628452	-1.36226	H	-0.77508	2.355139	1.58214
H	3.236451	2.36697	-0.7564	H	-3.1763	2.389539	0.534631
H	2.713361	1.209343	0.459844	H	-2.48316	1.481577	-0.80656
H	1.719853	-3.10816	0.526655	H	-1.5895	-2.79366	-1.70263
H	1.790783	-3.24143	-1.22036	H	-2.16858	-3.16514	-0.08823
H	3.868089	-1.93083	-1.32491	H	-3.32219	-1.11861	-2.09257
H	5.982151	-0.94501	1.164287	H	-6.59247	-1.88423	-1.39766
H	6.380249	-2.62462	0.830471	H	-6.1679	-0.49428	-0.4025
H	5.954107	-1.5374	-0.50679	H	-5.5492	-0.61007	-2.06137
H	4.071566	-1.6665	2.781385	H	-5.72885	-3.34912	0.487487
H	2.819492	-2.78219	2.221157	H	-4.0018	-3.39786	0.869433
H	4.472308	-3.3526	2.49479	H	-5.00258	-2.06407	1.459948
H	1.874559	5.589884	0.531777	H	-1.53092	5.72103	0.231219
H	2.949369	4.428784	-0.25498	H	-2.74699	4.487844	0.581397
H	1.484098	4.996292	-1.08479	H	-1.41259	4.776477	1.718603
H	-0.32509	4.951353	1.411392	H	0.767436	5.144971	-0.41933
H	-0.88937	3.271282	1.363084	H	1.262792	3.460421	-0.66661
H	-0.88097	4.248923	-0.1173	H	1.047368	4.092117	0.977526
H	1.720776	3.905351	2.353704	H	-1.13261	4.460138	-1.87169
H	-2.00555	-0.04215	-2.99478	H	1.461214	-0.85454	2.963617
H	-3.31457	-1.05365	-3.6435	H	2.591518	-2.08292	3.571336
H	-3.55742	0.672052	-3.38941	H	2.926209	-0.3683	3.795373
H	-5.41115	-1.58985	-2.1111	H	4.925679	-2.40648	2.353965
H	-5.52002	-0.74371	-0.55902	H	5.358893	-1.2259	1.10655
H	-5.61854	0.15599	-2.09092	H	5.187676	-0.7275	2.805968
H	-4.42991	1.263328	2.033636	H	4.862362	1.400488	-1.07458
H	-2.86915	1.652079	2.785283	H	3.491683	2.081473	-1.97437
H	-3.05372	1.710477	1.019977	H	3.33427	1.713626	-0.24434
H	-3.34108	-2.1356	2.971252	H	3.837765	-1.58397	-2.99397
H	-2.9002	-0.73604	3.975811	H	3.658985	0.045062	-3.68446
H	-4.50881	-0.83965	3.240225	H	5.089465	-0.36898	-2.72438
4-k				4-l			
C	0.4177	-1.7419	-0.05779	C	-0.49608	-1.68253	-0.52721
C	0.950328	-2.42138	-1.34395	C	-0.85741	-2.65165	0.625342
C	1.137664	-1.2918	-2.34837	C	-0.78517	-1.80885	1.892885
C	1.772094	-0.14965	-1.52374	C	-1.44569	-0.46663	1.501589
C	1.450935	-0.46934	0.004391	C	-1.42662	-0.40752	-0.09134
C	3.320343	-0.05097	-1.54955	C	-2.95066	-0.31468	1.844236
O	3.729001	-0.94978	-0.49962	O	-3.61036	-0.91758	0.712786
C	2.841115	-0.84231	0.566212	C	-2.91971	-0.58745	-0.44876
C	0.527543	-2.73946	1.105725	C	-0.87035	-2.34052	-1.86424
C	0.871265	0.769915	0.696838	C	-0.8862	0.94425	-0.5726
O	-0.04495	1.393014	-0.09905	O	0.197642	1.319822	0.155842
C	-1.6814	-0.73869	1.11951	C	1.463396	-0.48497	-1.76447
C	-1.08234	-1.26627	-0.21973	C	1.043592	-1.31649	-0.51463
C	-1.01602	2.278051	0.514255	C	1.092467	2.324067	-0.38847
C	-2.40269	1.666271	0.27209	C	2.459988	1.638943	-0.51606
C	-2.70495	0.395514	1.071837	C	2.574592	0.549254	-1.58671
C	-2.0374	-2.34803	-0.80437	C	1.975269	-2.55768	-0.38024
C	-3.36581	-1.76437	-1.21328	C	3.44167	-2.20424	-0.36177
C	-4.56557	-1.91135	-0.62931	C	4.26832	-2.17862	0.697129
C	-5.77499	-1.18382	-1.16277	C	5.720517	-1.80031	0.527534
C	-4.82591	-2.72519	0.612877	C	3.873261	-2.51532	2.11431
O	-3.73562	0.325188	1.718698	O	3.548108	0.540841	-2.32017
C	-0.84057	3.703824	-0.06809	C	1.094481	3.567754	0.531205
C	0.558701	4.240544	0.263762	C	1.90187	4.706452	-0.11557
C	-1.1056	3.766735	-1.57835	C	-0.34155	4.035321	0.809375
O	-1.8316	4.461472	0.64089	O	1.72081	3.149881	1.751119
O	1.145261	1.174939	1.805029	O	-1.31982	1.616002	-1.48486
C	3.316271	-1.06541	1.806298	C	-3.62457	-0.48741	-1.5922
C	2.52213	-1.08602	3.085831	C	-3.07585	-0.22072	-2.96925
C	4.786152	-1.36115	2.008125	C	-5.12552	-0.67673	-1.5716

C	3.779614	1.374911	-1.19901	C	-3.34538	1.169794	1.924968
C	4.013689	-0.52538	-2.82388	C	-3.44782	-1.05473	3.083559
H	1.346372	0.807294	-1.82225	H	-0.88768	0.363805	1.932463
H	1.924266	-2.86845	-1.11475	H	-1.8865	-2.99688	0.474216
H	0.308038	-3.23068	-1.69777	H	-0.22678	-3.5432	0.645635
H	0.169418	-0.96601	-2.74357	H	0.257387	-1.63365	2.179009
H	1.738819	-1.58397	-3.21154	H	-1.26219	-2.287	2.750362
H	-0.08124	-3.62115	0.878242	H	-0.30831	-3.27338	-1.97743
H	1.557157	-3.0743	1.239914	H	-1.93188	-2.59044	-1.89214
H	0.17685	-2.3411	2.058282	H	-0.64784	-1.72028	-2.73348
H	-0.88655	-0.37073	1.779295	H	0.607073	0.069272	-2.16519
H	-2.16173	-1.55165	1.669492	H	1.792377	-1.144	-2.57267
H	-1.07995	-0.44594	-0.93857	H	1.228884	-0.70838	0.371113
H	-0.80126	2.340608	1.583544	H	0.699865	2.628597	-1.36238
H	-3.1664	2.398388	0.539052	H	3.236115	2.36739	-0.75652
H	-2.5116	1.433749	-0.79424	H	2.713196	1.209832	0.459817
H	-1.58475	-2.7918	-1.69711	H	1.72017	-3.10762	0.527267
H	-2.166	-3.16143	-0.08329	H	1.790938	-3.24144	-1.21972
H	-3.3182	-1.12165	-2.09476	H	3.868097	-1.93037	-1.32476
H	-6.58939	-1.88194	-1.39544	H	5.982677	-0.945	1.164231
H	-6.16251	-0.48747	-0.40764	H	6.380721	-2.62448	0.829753
H	-5.54552	-0.61244	-2.06663	H	5.954187	-1.53683	-0.50702
H	-5.7288	-3.33645	0.495649	H	4.473307	-3.35252	2.494661
H	-4.00098	-3.39157	0.873416	H	4.072282	-1.66652	2.781451
H	-4.99394	-2.05139	1.46233	H	2.820311	-2.78242	2.221409
H	0.639696	5.287524	-0.05195	H	1.483873	4.996494	-1.0849
H	0.748078	4.185926	1.338655	H	1.87388	5.590144	0.531773
H	1.339254	3.678012	-0.255	H	2.949005	4.429181	-0.2547
H	-0.93251	4.784658	-1.94584	H	-0.32574	4.951396	1.411143
H	-2.14	3.499102	-1.80688	H	-0.88999	3.271317	1.362517
H	-0.43832	3.096261	-2.12757	H	-0.8813	4.249148	-0.11772
H	-1.74057	5.385635	0.373564	H	1.719031	3.905192	2.354039
H	1.470965	-0.84606	2.962693	H	-3.31339	-1.05566	-3.64296
H	2.607821	-2.06839	3.570493	H	-3.55885	0.669875	-3.39048
H	2.936856	-0.35189	3.78778	H	-2.00601	-0.04164	-2.99472
H	4.933459	-2.39677	2.344231	H	-5.52002	-0.7433	-0.55862
H	5.365751	-1.21513	1.097659	H	-5.61874	0.154838	-2.09141
H	5.196162	-0.71835	2.797755	H	-5.41128	-1.59104	-2.10981
H	4.867471	1.401062	-1.08807	H	-4.42989	1.263365	2.033558
H	3.49589	2.080065	-1.9875	H	-2.86909	1.652226	2.785046
H	3.340776	1.714965	-0.25614	H	-3.05378	1.710371	1.019734
H	3.839274	-1.5887	-3	H	-3.34108	-2.13547	2.97145
H	3.663839	0.039476	-3.69351	H	-2.90027	-0.73579	3.97587
H	5.093412	-0.37576	-2.73288	H	-4.50883	-0.83951	3.240189
4-m				4-n			
C	0.4177	-1.7419	-0.05779	C	-0.49608	-1.68253	-0.52721
C	0.950328	-2.42138	-1.34395	C	-0.85741	-2.65165	0.625342
C	1.137664	-1.2918	-2.34837	C	-0.78517	-1.80885	1.892885
C	1.772094	-0.14965	-1.52374	C	-1.44569	-0.46663	1.501589
C	1.450935	-0.46934	0.004391	C	-1.42662	-0.40752	-0.09134
C	3.320343	-0.05097	-1.54955	C	-2.95066	-0.31468	1.844236
O	3.729001	-0.94978	-0.49962	O	-3.61036	-0.91758	0.712786
C	2.841115	-0.84231	0.566212	C	-2.91971	-0.58745	-0.44876
C	0.527543	-2.73946	1.105725	C	-0.87035	-2.34052	-1.86424
C	0.871265	0.769915	0.696838	C	-0.8862	0.94425	-0.5726
O	-0.04495	1.393014	-0.09905	O	0.197642	1.319822	0.155842
C	-1.6814	-0.73869	1.11951	C	1.463396	-0.48497	-1.76447
C	-1.08234	-1.26627	-0.21973	C	1.043592	-1.31649	-0.51463
C	-1.01602	2.278051	0.514255	C	1.092467	2.324067	-0.38847
C	-2.40269	1.666271	0.27209	C	2.459988	1.638943	-0.51606
C	-2.70495	0.395514	1.071837	C	2.574592	0.549254	-1.58671
C	-2.0374	-2.34803	-0.80437	C	1.975269	-2.55768	-0.38024
C	-3.36581	-1.76437	-1.21328	C	3.44167	-2.20424	-0.36177
C	-4.56557	-1.91135	-0.62931	C	4.26832	-2.17862	0.697129
C	-5.77499	-1.18382	-1.16277	C	5.720517	-1.80031	0.527534

C	-4.82591	-2.72519	0.612877	C	3.873261	-2.51532	2.11431
O	-3.73562	0.325188	1.718698	O	3.548108	0.540841	-2.32017
C	-0.84057	3.703824	-0.06809	C	1.094481	3.567754	0.531205
C	0.558701	4.240544	0.263762	C	1.90187	4.706452	-0.11557
C	-1.1056	3.766735	-1.57835	C	-0.34155	4.035321	0.809375
O	-1.8316	4.461472	0.64089	O	1.72081	3.149881	1.751119
O	1.145261	1.174939	1.805029	O	-1.31982	1.616002	-1.48486
C	3.316271	-1.06541	1.806298	C	-3.62457	-0.48741	-1.5922
C	2.52213	-1.08602	3.085831	C	-3.07585	-0.22072	-2.96925
C	4.786152	-1.36115	2.008125	C	-5.12552	-0.67673	-1.5716
C	3.779614	1.374911	-1.19901	C	-3.34538	1.169794	1.924968
C	4.013689	-0.52538	-2.82388	C	-3.44782	-1.05473	3.083559
H	1.346372	0.807294	-1.82225	H	-0.88768	0.363805	1.932463
H	1.924266	-2.86845	-1.11475	H	-1.8865	-2.99688	0.474216
H	0.308038	-3.23068	-1.69777	H	-0.22678	-3.5432	0.645635
H	0.169418	-0.96601	-2.74357	H	0.257387	-1.63365	2.179009
H	1.738819	-1.58397	-3.21154	H	-1.26219	-2.287	2.750362
H	-0.08124	-3.62115	0.878242	H	-0.30831	-3.27338	-1.97743
H	1.557157	-3.0743	1.239914	H	-1.93188	-2.59044	-1.89214
H	0.17685	-2.3411	2.058282	H	-0.64784	-1.72028	-2.73348
H	-0.88655	-0.37073	1.779295	H	0.607073	0.069272	-2.16519
H	-2.16173	-1.55165	1.669492	H	1.792377	-1.144	-2.57267
H	-1.07995	-0.44594	-0.93857	H	1.228884	-0.70838	0.371113
H	-0.80126	2.340608	1.583544	H	0.699865	2.628597	-1.36238
H	-3.1664	2.398388	0.539052	H	3.236115	2.36739	-0.75652
H	-2.5116	1.433749	-0.79424	H	2.713196	1.209832	0.459817
H	-1.58475	-2.7918	-1.69711	H	1.72017	-3.10762	0.527267
H	-2.166	-3.16143	-0.08329	H	1.790938	-3.24144	-1.21972
H	-3.3182	-1.12165	-2.09476	H	3.868097	-1.93037	-1.32476
H	-6.58939	-1.88194	-1.39544	H	5.982677	-0.945	1.164231
H	-6.16251	-0.48747	-0.40764	H	6.380721	-2.62448	0.829753
H	-5.54552	-0.61244	-2.06663	H	5.954187	-1.53683	-0.50702
H	-5.7288	-3.33645	0.495649	H	4.473307	-3.35252	2.494661
H	-4.00098	-3.39157	0.873416	H	4.072282	-1.66652	2.781451
H	-4.99394	-2.05139	1.46233	H	2.820311	-2.78242	2.221409
H	0.639696	5.287524	-0.05195	H	1.483873	4.996494	-1.0849
H	0.748078	4.185926	1.338655	H	1.87388	5.590144	0.531773
H	1.339254	3.678012	-0.255	H	2.949005	4.429181	-0.2547
H	-0.93251	4.784658	-1.94584	H	-0.32574	4.951396	1.411143
H	-2.14	3.499102	-1.80688	H	-0.88999	3.271317	1.362517
H	-0.43832	3.096261	-2.12757	H	-0.8813	4.249148	-0.11772
H	-1.74057	5.385635	0.373564	H	1.719031	3.905192	2.354039
H	1.470965	-0.84606	2.962693	H	-3.31339	-1.05566	-3.64296
H	2.607821	-2.06839	3.570493	H	-3.55885	0.669875	-3.39048
H	2.936856	-0.35189	3.78778	H	-2.00601	-0.04164	-2.99472
H	4.933459	-2.39677	2.344231	H	-5.52002	-0.7433	-0.55862
H	5.365751	-1.21513	1.097659	H	-5.61874	0.154838	-2.09141
H	5.196162	-0.71835	2.797755	H	-5.41128	-1.59104	-2.10981
H	4.867471	1.401062	-1.08807	H	-4.42989	1.263365	2.033558
H	3.49589	2.080065	-1.9875	H	-2.86909	1.652226	2.785046
H	3.340776	1.714965	-0.25614	H	-3.05378	1.710371	1.019734
H	3.839274	-1.5887	-3	H	-3.34108	-2.13547	2.97145
H	3.663839	0.039476	-3.69351	H	-2.90027	-0.73579	3.97587
H	5.093412	-0.37576	-2.73288	H	-4.50883	-0.83951	3.240189



5

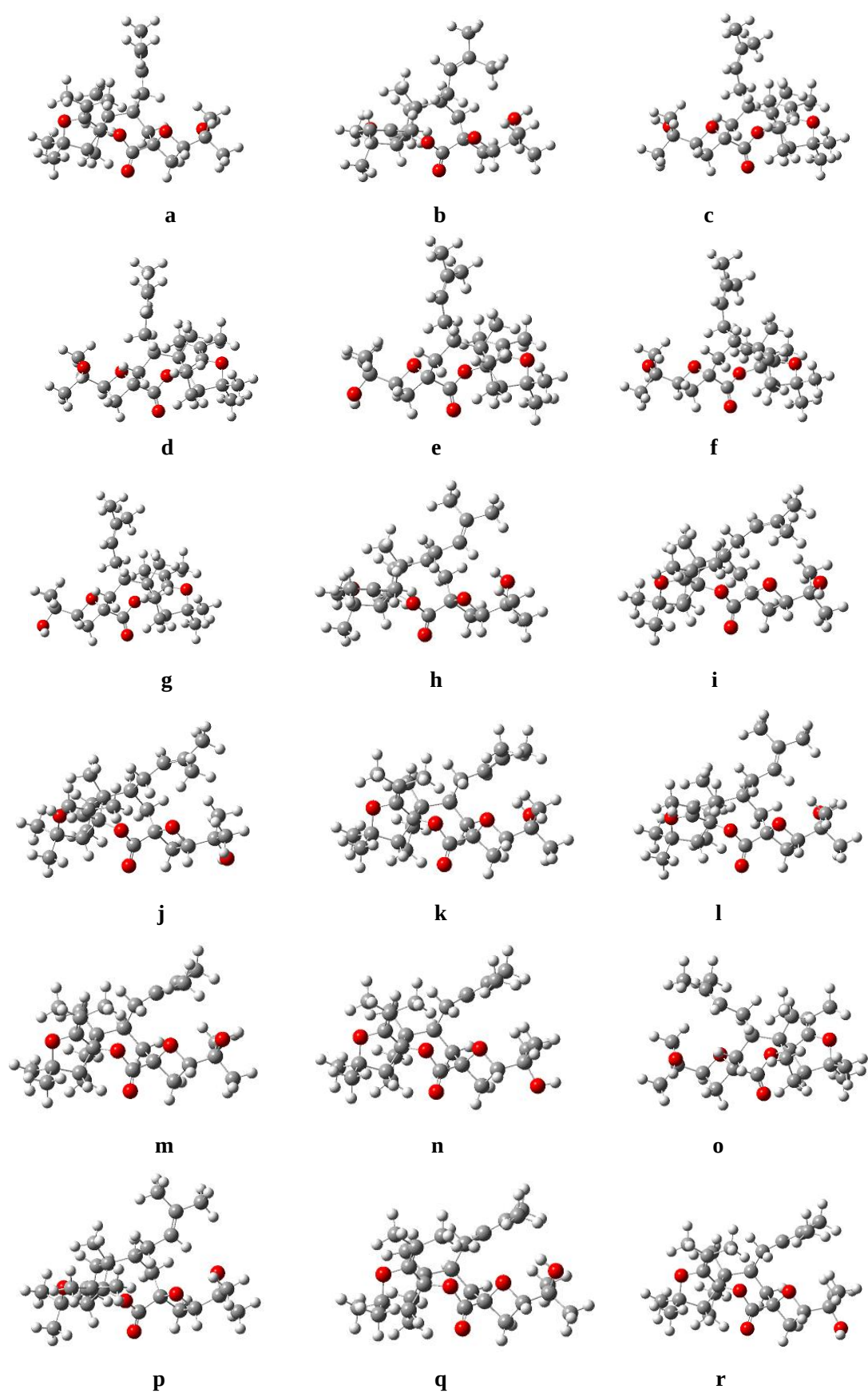


Figure S33. Optimized geometries of predominant conformers for compound 5 at the

B3LYP/6-31G(d,p) level in the gas phase.

Table S24. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound 5 at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
5-a	-1429.627366	-1429.691280	0.1
5-b	-1429.628234	-1429.691929	0.2
5-c	-1429.622453	-1429.687920	0
5-d	-1429.625721	-1429.689486	0
5-e	-1429.624612	-1429.689908	0
5-f	-1429.622837	-1429.688038	0
5-g	-1429.624246	-1429.689693	0
5-h	-1429.632894	-1429.696343	25.2
5-i	-1429.626958	-1429.689719	0
5-j	-1429.626944	-1429.691383	0.1
5-k	-1429.635329	-1429.697323	71
5-l	-1429.630536	-1429.693993	2.1
5-m	-1429.626156	-1429.688872	0
5-n	-1429.626749	-1429.691077	0.1
5-o	-1429.626547	-1429.691333	0.1
5-p	-1429.629072	-1429.692418	0.4
5-q	-1429.629832	-1429.692565	0.5
5-r	-1429.627220	-1429.691534	0.2

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S25. Optimized Z-matrixes of compound 5 in the gas phase (Å) at B3LYP/6-31G(d,p) level

5-a				5-b			
C	-1.17553	0.28062	-1.29478	C	-1.29138	0.798807	-1.07801
C	-1.61679	-0.52481	0.029505	C	-1.86285	-0.24246	0.006155
C	-1.90608	1.636982	-1.39386	C	-1.89673	2.207468	-0.88348
C	-1.67105	-0.62199	-2.47666	C	-1.80008	0.248251	-2.45448
C	-2.01863	-2.00518	-1.90947	C	-2.33508	-1.17409	-2.23269
C	-2.44073	-1.76492	-0.45404	C	-2.79633	-1.22795	-0.76921
C	-3.92781	-1.38439	-0.15034	C	-4.24287	-0.75562	-0.40759
O	-3.86145	-0.02413	0.369442	O	-4.04907	0.41339	0.441582
C	-2.61205	0.189518	0.93064	C	-2.80356	0.344252	1.046809
C	-2.48976	0.899618	2.063976	C	-2.63993	0.754146	2.315431
C	-1.18666	1.259397	2.730211	C	-1.32501	0.798643	3.051842
C	-3.71923	1.430051	2.762897	C	-3.82424	1.247047	3.11284
C	-4.48786	-2.28336	0.959961	C	-4.95692	-1.82541	0.428958
C	-4.88682	-1.34493	-1.33671	C	-5.12996	-0.30525	-1.56477
O	-0.44996	-0.88476	0.81328	O	-0.7656	-0.91122	0.681334
C	0.339949	-1.93572	0.448282	C	-0.07322	-1.91046	0.061946
C	1.630874	-1.4509	-0.1897	C	1.291644	-1.42297	-0.39662
C	1.308837	-0.69379	-1.48329	C	1.124619	-0.30556	-1.43311
C	0.374628	0.54666	-1.4428	C	0.278056	0.952302	-1.09672
C	0.975989	1.66657	-0.54128	C	0.89737	1.735625	0.11449
C	0.908415	3.051956	-1.14226	C	1.301333	3.14699	-0.22892
C	0.867948	4.235176	-0.51107	C	2.540486	3.649683	-0.35083
C	0.85283	5.5293	-1.28921	C	2.750303	5.107502	-0.68703

C	0.845051	4.402905	0.988099	C	3.816869	2.863853	-0.16931
O	0.043757	-3.09329	0.630002	O	-0.4935	-3.03561	-0.0741
O	2.383349	-0.66847	0.791816	O	2.071173	-1.04872	0.786087
C	3.470413	-1.63265	0.783687	C	3.016767	-2.12718	0.550404
C	2.753886	-2.50217	-0.26857	C	2.292876	-2.54001	-0.74605
C	4.818042	-1.00211	0.410952	C	4.465106	-1.63432	0.455922
C	5.91476	-2.07696	0.452138	C	5.396026	-2.82832	0.19595
C	5.130677	0.158861	1.363371	C	4.847939	-0.8934	1.743324
O	4.674927	-0.51088	-0.93067	O	4.50914	-0.73591	-0.66388
H	-2.9883	1.496333	-1.35363	H	-2.98739	2.169817	-0.90953
H	-1.62744	2.322542	-0.59313	H	-1.61009	2.658903	0.067723
H	-1.66013	2.119163	-2.34595	H	-1.55847	2.86526	-1.69137
H	-2.5628	-0.1686	-2.92139	H	-2.60214	0.895898	-2.82293
H	-0.93235	-0.68194	-3.2829	H	-1.01752	0.277326	-3.2197
H	-1.13717	-2.65608	-1.90827	H	-1.53549	-1.91104	-2.36556
H	-2.78072	-2.52291	-2.49958	H	-3.12203	-1.44337	-2.94332
H	-2.17811	-2.62415	0.163196	H	-2.65701	-2.23159	-0.36709
H	-1.20073	0.922584	3.775453	H	-1.41259	0.246889	3.997329
H	-0.31479	0.818634	2.252643	H	-0.49571	0.372319	2.492873
H	-1.06131	2.350391	2.763089	H	-1.07151	1.832701	3.324971
H	-3.7437	2.527838	2.728107	H	-3.71919	2.315907	3.344048
H	-4.63839	1.056514	2.311839	H	-4.76437	1.106689	2.579581
H	-3.70507	1.153048	3.825115	H	-3.88024	0.725098	4.077004
H	-5.49811	-1.96735	1.237129	H	-5.93802	-1.46656	0.754367
H	-4.52802	-3.32717	0.630498	H	-5.09692	-2.74372	-0.15139
H	-3.85198	-2.2309	1.848716	H	-4.36601	-2.07021	1.316593
H	-4.52144	-0.69826	-2.13685	H	-4.6504	0.464895	-2.17204
H	-5.04845	-2.34781	-1.743	H	-5.38843	-1.14961	-2.21067
H	-5.85364	-0.95549	-1.00474	H	-6.05921	0.111026	-1.16508
H	0.920942	-1.43613	-2.19406	H	0.741561	-0.78424	-2.34507
H	2.274747	-0.36475	-1.8801	H	2.138819	0.032863	-1.67062
H	0.441198	0.931724	-2.47036	H	0.432848	1.593007	-1.97509
H	0.524043	1.639954	0.451234	H	0.178061	1.767358	0.936985
H	2.030481	1.416471	-0.37769	H	1.748672	1.176773	0.499337
H	0.945264	3.078874	-2.2333	H	0.47461	3.837036	-0.40156
H	0.873805	5.357004	-2.369	H	1.802885	5.642259	-0.79709
H	-0.04356	6.120533	-1.05748	H	3.336039	5.612864	0.092944
H	1.713754	6.160277	-1.0294	H	3.31752	5.222174	-1.62077
H	0.846025	3.45343	1.525441	H	3.659313	1.790218	-0.05614
H	1.718649	4.977115	1.325243	H	4.47808	3.013568	-1.03366
H	-0.03831	4.973688	1.304824	H	4.373533	3.225267	0.70665
H	3.570087	-2.10392	1.770644	H	2.956369	-2.87086	1.356376
H	2.455386	-3.49798	0.05899	H	1.863496	-3.54165	-0.75947
H	3.256109	-2.54633	-1.23521	H	2.864647	-2.34928	-1.65477
H	6.87832	-1.64497	0.159305	H	6.433451	-2.48703	0.106189
H	5.68642	-2.89088	-0.24209	H	5.126471	-3.33492	-0.73517
H	6.031293	-2.49696	1.456556	H	5.356536	-3.55562	1.013372
H	6.07428	0.641329	1.081072	H	5.865731	-0.49245	1.665943
H	4.329783	0.899878	1.3242	H	4.156831	-0.06721	1.921965
H	5.234587	-0.18955	2.396042	H	4.822201	-1.56323	2.608879
H	5.464516	0.004646	-1.14034	H	5.380286	-0.3185	-0.67455
5-c				5-d			
C	1.269756	0.403178	1.232353	C	1.172288	0.272161	1.29612
C	1.595948	-0.57681	0.000343	C	1.615112	-0.52848	-0.03009
C	2.12036	1.692089	1.183113	C	1.912505	1.622372	1.408157
C	1.702556	-0.40682	2.501999	C	1.653911	-0.64105	2.475385
C	1.942937	-1.86397	2.081012	C	1.992008	-2.02399	1.90201
C	2.341576	-1.81368	0.599098	C	2.425151	-1.77865	0.450639
C	3.841658	-1.57849	0.222455	C	3.917259	-1.40861	0.158055
O	3.853278	-0.29191	-0.46358	O	3.864952	-0.04433	-0.35239
C	2.601987	-0.05196	-1.01109	C	2.621278	0.182222	-0.92165
C	2.48615	0.524488	-2.21873	C	2.512727	0.897954	-2.0528
C	1.186078	0.892318	-2.88752	C	1.217582	1.271254	-2.72695

C	3.722102	0.872773	-3.01396	C	3.751478	1.421737	-2.74025
C	4.309717	-2.64508	-0.7763	C	4.475806	-2.30463	-0.9554
C	4.833289	-1.46035	1.376458	C	4.869765	-1.38572	1.350039
O	0.366411	-0.92632	-0.68761	O	0.44781	-0.87447	-0.82165
C	-0.4791	-1.86154	-0.16891	C	-0.3486	-1.92248	-0.46886
C	-1.71381	-1.20976	0.441019	C	-1.6395	-1.43806	0.171711
C	-1.29472	-0.28431	1.589289	C	-1.32031	-0.68366	1.467783
C	-0.24252	0.834125	1.349945	C	-0.37645	0.55029	1.434509
C	-0.73044	1.860869	0.272712	C	-0.96102	1.677012	0.530592
C	-0.99056	3.228029	0.853948	C	-0.88926	3.059334	1.138408
C	-0.62403	4.432256	0.388651	C	-0.83693	4.244574	0.512143
C	-1.00987	5.694646	1.122788	C	-0.82142	5.535449	1.29556
C	0.170675	4.663639	-0.87266	C	-0.80283	4.417936	-0.9861
O	-0.27555	-3.05211	-0.21664	O	-0.06135	-3.08079	-0.66132
O	-2.4756	-0.55443	-0.62046	O	-2.3975	-0.65311	-0.79987
C	-3.50273	-1.58861	-0.56333	C	-3.48576	-1.61667	-0.79252
C	-2.87007	-2.19265	0.704874	C	-2.75693	-2.49564	0.244171
C	-4.93798	-1.05016	-0.53153	C	-4.83433	-0.98031	-0.40665
C	-5.11943	0.105483	0.458211	C	-5.94123	-2.04064	-0.47816
C	-5.89947	-2.21124	-0.22999	C	-5.13	0.200433	-1.33398
O	-5.15621	-0.58017	-1.86989	O	-4.77315	-0.42317	0.916351
H	3.184672	1.451652	1.149748	H	2.993757	1.473408	1.372875
H	1.89785	2.311784	0.313819	H	1.643173	2.315553	0.610902
H	1.92987	2.290519	2.08017	H	1.664886	2.09965	2.362245
H	2.626318	0.023195	2.90168	H	2.54768	-0.19797	2.926237
H	0.964866	-0.32786	3.307414	H	0.911216	-0.69824	3.278238
H	1.020129	-2.44818	2.167297	H	1.104556	-2.66683	1.891305
H	2.683778	-2.36653	2.709785	H	2.745482	-2.55265	2.493435
H	2.00063	-2.71244	0.085126	H	2.159486	-2.63196	-0.17349
H	1.126581	0.407134	-3.87086	H	1.237372	0.940327	-3.77392
H	0.30304	0.604382	-2.32266	H	0.338631	0.834698	-2.25869
H	1.146545	1.973475	-3.08125	H	1.100547	2.363228	-2.75436
H	3.820926	1.961568	-3.12154	H	3.784172	2.519075	-2.69985
H	4.630246	0.494684	-2.54483	H	4.664376	1.038823	-2.28441
H	3.650208	0.465377	-4.03081	H	3.742615	1.149992	-3.80383
H	5.330201	-2.43595	-1.11096	H	5.490236	-1.99531	-1.2246
H	4.290518	-3.64017	-0.31884	H	4.505277	-3.35105	-0.63316
H	3.654033	-2.66089	-1.65201	H	3.845507	-2.24032	-1.84734
H	4.536439	-0.69419	2.095277	H	4.505959	-0.74113	2.152587
H	4.935967	-2.41383	1.902932	H	5.020301	-2.39273	1.750324
H	5.815303	-1.18665	0.979792	H	5.841824	-1.00271	1.026019
H	-0.97176	-0.93429	2.414246	H	-0.94449	-1.42725	2.18372
H	-2.21292	0.204274	1.937068	H	-2.28707	-0.34161	1.852786
H	-0.24325	1.377226	2.304917	H	-0.44736	0.933503	2.462386
H	-0.02057	1.91656	-0.55158	H	-0.49694	1.651159	-0.45631
H	-1.65639	1.486465	-0.17435	H	-2.0154	1.436734	0.353255
H	-1.57961	3.217705	1.774262	H	-0.93573	3.081975	2.229108
H	-1.5863	5.481997	2.027574	H	-0.84922	5.358835	2.374477
H	-0.12111	6.270809	1.413606	H	0.078215	6.124548	1.07106
H	-1.6113	6.356524	0.485111	H	-1.67899	6.169911	1.033533
H	0.471215	3.739227	-1.3682	H	-0.80789	3.470658	-1.52728
H	-0.41309	5.251429	-1.59356	H	-1.67023	4.999583	-1.32613
H	1.076476	5.246807	-0.6603	H	0.086722	4.983457	-1.29493
H	-3.42099	-2.24172	-1.44125	H	-3.58516	-2.08472	-1.78152
H	-2.60339	-3.24858	0.66474	H	-2.45537	-3.48584	-0.0968
H	-3.41366	-1.97736	1.62797	H	-3.23803	-2.57118	1.222202
H	-6.15053	0.475983	0.41564	H	-6.896	-1.60095	-0.17567
H	-4.44202	0.922827	0.205341	H	-5.72743	-2.88651	0.187622
H	-4.93121	-0.20306	1.491618	H	-6.05191	-2.4381	-1.49165
H	-6.9369	-1.86497	-0.29804	H	-6.08174	0.660989	-1.05616
H	-5.76603	-3.0172	-0.95774	H	-4.33881	0.947598	-1.2472
H	-5.75189	-2.61808	0.775569	H	-5.18722	-0.12618	-2.37697
H	-6.02206	-0.15087	-1.89209	H	-4.91686	-1.13833	1.549667

5-e				5-f			
C	1.261689	0.404364	1.233312	C	1.267296	0.399816	1.232879
C	1.590245	-0.57259	-0.00075	C	1.584633	-0.58506	0.002343
C	2.10115	1.699901	1.179649	C	2.125597	1.683113	1.177644
C	1.70623	-0.40335	2.500185	C	1.698096	-0.41071	2.502733
C	1.945471	-1.86011	2.078151	C	1.917115	-1.87197	2.085332
C	2.340371	-1.8083	0.595444	C	2.315411	-1.82997	0.603197
C	3.839247	-1.56901	0.216326	C	3.818396	-1.61346	0.226467
O	3.846566	-0.28005	-0.46571	O	3.845711	-0.32666	-0.45851
C	2.59454	-0.043	-1.01176	C	2.598285	-0.07292	-1.00817
C	2.476761	0.5344	-2.21879	C	2.491306	0.502753	-2.21697
C	1.175267	0.898964	-2.88645	C	1.196774	0.884385	-2.8886
C	3.711071	0.887145	-3.01448	C	3.732404	0.835772	-3.01067
C	4.307026	-2.63145	-0.78698	C	4.272664	-2.68527	-0.77312
C	4.833501	-1.45263	1.368178	C	4.811939	-1.50861	1.380063
O	0.36189	-0.92535	-0.68965	O	0.35284	-0.92338	-0.68861
C	-0.47686	-1.8706	-0.17647	C	-0.50048	-1.85365	-0.17481
C	-1.71093	-1.23238	0.448168	C	-1.72542	-1.19629	0.448964
C	-1.29449	-0.30738	1.596596	C	-1.2985	-0.27404	1.59556
C	-0.25356	0.821854	1.359974	C	-0.24206	0.839644	1.354791
C	-0.75545	1.853245	0.294006	C	-0.72761	1.872369	0.282409
C	-0.98026	3.226519	0.876215	C	-0.93858	3.250054	0.859146
C	-0.61298	4.424091	0.394676	C	-0.55157	4.441231	0.377373
C	-0.96179	5.694273	1.133895	C	-0.89111	5.718031	1.10945
C	0.148566	4.640526	-0.88958	C	0.222787	4.644302	-0.90136
O	-0.2695	-3.05928	-0.24532	O	-0.31354	-3.04607	-0.24357
O	-2.48126	-0.57752	-0.61361	O	-2.48986	-0.53529	-0.60974
C	-3.5091	-1.61058	-0.54021	C	-3.52197	-1.56016	-0.54575
C	-2.86163	-2.22254	0.713888	C	-2.88505	-2.17392	0.71722
C	-4.9441	-1.05461	-0.50482	C	-4.95652	-1.00934	-0.52374
C	-5.24369	-0.34699	-1.83261	C	-5.16333	0.078991	0.529066
C	-5.20327	-0.12004	0.674857	C	-5.9348	-2.17828	-0.32591
O	-5.82333	-2.17382	-0.31291	O	-5.21679	-0.35758	-1.77425
H	3.16722	1.468031	1.141125	H	3.188317	1.435844	1.141695
H	1.868644	2.317238	0.311247	H	1.903172	2.301651	0.307599
H	1.910311	2.297381	2.077176	H	1.94158	2.285205	2.073496
H	2.632593	0.028464	2.89183	H	2.629963	0.008926	2.894522
H	0.97487	-0.32477	3.31138	H	0.966778	-0.31927	3.312621
H	1.022823	-2.44441	2.166706	H	0.985973	-2.44275	2.173983
H	2.687843	-2.36331	2.704541	H	2.651015	-2.38406	2.714538
H	2.001317	-2.70782	0.081494	H	1.964295	-2.72573	0.090671
H	1.114912	0.411679	-3.86883	H	1.132164	0.3961	-3.87019
H	0.294202	0.610239	-2.31876	H	0.309799	0.610016	-2.32308
H	1.133622	1.979649	-3.08221	H	1.171003	1.965066	-3.0866
H	3.807428	1.976348	-3.1201	H	3.844503	1.92324	-3.11841
H	4.620345	0.51032	-2.54659	H	4.635298	0.447004	-2.54017
H	3.639624	0.481341	-4.03204	H	3.657087	0.428916	-4.02751
H	5.326147	-2.41904	-1.12367	H	5.29557	-2.48874	-1.10797
H	4.291333	-3.62788	-0.33238	H	4.241221	-3.68023	-0.31607
H	3.649069	-2.64633	-1.66102	H	3.616645	-2.69253	-1.64871
H	4.537924	-0.68828	2.089388	H	4.525655	-0.73866	2.099077
H	4.938138	-2.40723	1.892211	H	4.902435	-2.46346	1.906307
H	5.814352	-1.17739	0.969738	H	5.797231	-1.24782	0.982879
H	-0.96131	-0.95957	2.415652	H	-0.97592	-0.92664	2.418572
H	-2.21529	0.169012	1.953712	H	-2.21348	0.21784	1.946751
H	-0.25526	1.357946	2.318855	H	-0.23783	1.380323	2.311058
H	-0.06962	1.894681	-0.55145	H	-0.0368	1.903053	-0.55931
H	-1.70051	1.491061	-0.12256	H	-1.67463	1.520835	-0.13889
H	-1.54254	3.227305	1.813043	H	-1.5094	3.261122	1.790732
H	-1.51548	5.492841	2.055217	H	-1.4543	5.526294	2.027088
H	-0.05769	6.259659	1.397172	H	0.017377	6.274111	1.377566
H	-1.57199	6.361445	0.510297	H	-1.48905	6.3896	0.478775
H	0.41867	3.710791	-1.39267	H	0.488272	3.709719	-1.39789

H	-0.44531	5.238526	-1.59365	H	-0.35999	5.243859	-1.61325
H	1.070215	5.207756	-0.70414	H	1.148101	5.203949	-0.71098
H	-3.42925	-2.27598	-1.41432	H	-3.43324	-2.22751	-1.4182
H	-2.58802	-3.27535	0.653469	H	-2.62329	-3.23078	0.670998
H	-3.40133	-2.02949	1.642148	H	-3.42451	-1.95902	1.642313
H	-6.27324	0.021856	-1.84229	H	-6.17603	0.480254	0.438062
H	-5.11643	-1.03489	-2.67793	H	-4.4522	0.891237	0.368748
H	-4.5631	0.495276	-1.98652	H	-5.04002	-0.31121	1.543414
H	-6.22381	0.267828	0.618182	H	-6.962	-1.80997	-0.39306
H	-5.10438	-0.65136	1.624921	H	-5.79746	-2.94201	-1.10132
H	-4.50564	0.720486	0.660358	H	-5.80297	-2.66274	0.647094
H	-5.79456	-2.71423	-1.11492	H	-5.07156	-1.0001	-2.48287
5-g				5-h			
C	1.260723	0.400021	1.233969	C	-1.31743	0.980629	-0.93919
C	1.590874	-0.57438	-0.00188	C	-1.88699	-0.18799	0.008369
C	2.09622	1.698127	1.179795	C	-1.97705	2.340319	-0.61466
C	1.710342	-0.40748	2.499393	C	-1.77187	0.567267	-2.38159
C	1.961016	-1.86175	2.074804	C	-2.2276	-0.89794	-2.33356
C	2.350964	-1.80542	0.590905	C	-2.73625	-1.13304	-0.9045
C	3.846961	-1.55583	0.206933	C	-4.21917	-0.77687	-0.55587
O	3.84309	-0.26732	-0.47599	O	-4.11942	0.330965	0.386017
C	2.587329	-0.03846	-1.01715	C	-2.90292	0.262306	1.047051
C	2.460624	0.53747	-2.22398	C	-2.81787	0.577787	2.34975
C	1.154243	0.893477	-2.88679	C	-1.53983	0.62808	3.147053
C	3.689445	0.897131	-3.02507	C	-4.05931	0.95529	3.1228
C	4.319231	-2.61566	-0.79697	C	-4.88782	-1.9504	0.172093
C	4.843682	-1.43151	1.355862	C	-5.10022	-0.28995	-1.70248
O	0.361332	-0.93365	-0.68571	O	-0.79181	-0.87505	0.670902
C	-0.47276	-1.87826	-0.16658	C	-0.0553	-1.81259	0.003812
C	-1.71151	-1.23766	0.446427	C	1.291388	-1.26071	-0.45094
C	-1.29498	-0.31723	1.599488	C	1.100166	-0.05282	-1.37211
C	-0.25546	0.814136	1.364453	C	0.252896	1.16085	-0.90558
C	-0.761	1.848608	0.303336	C	0.817814	1.816385	0.388792
C	-0.97905	3.221571	0.88903	C	2.276625	2.207649	0.310187
C	-0.61689	4.419296	0.404076	C	2.80393	3.320874	-0.22545
C	-0.95807	5.689231	1.14725	C	4.294037	3.563155	-0.20687
C	0.131156	4.636024	-0.88801	C	1.992321	4.416918	-0.87098
O	-0.25756	-3.0666	-0.21375	O	-0.42673	-2.95007	-0.16302
O	-2.4764	-0.57921	-0.61244	O	2.105051	-0.98062	0.736851
C	-3.50647	-1.61261	-0.55159	C	2.993915	-2.10349	0.428042
C	-2.86197	-2.2293	0.707359	C	2.283458	-2.34276	-0.91594
C	-4.94045	-1.05389	-0.51942	C	4.463911	-1.65948	0.411496
C	-5.25038	-0.39776	-1.86599	C	5.348819	-2.79317	-0.10893
C	-5.18848	-0.07252	0.630257	C	4.892388	-1.21893	1.820112
O	-5.82485	-2.18121	-0.41987	O	4.625647	-0.5762	-0.51027
H	3.162861	1.469408	1.139674	H	-3.06001	2.279248	-0.73758
H	1.860838	2.314855	0.311763	H	-1.79028	2.670919	0.407755
H	1.904724	2.294847	2.077664	H	-1.59987	3.107198	-1.30109
H	2.632981	0.030544	2.892872	H	-2.60677	1.205047	-2.68804
H	0.977795	-0.33624	3.31026	H	-0.9829	0.730618	-3.12284
H	1.043882	-2.45424	2.165294	H	-1.38166	-1.57153	-2.51187
H	2.709806	-2.35881	2.698419	H	-2.97118	-1.13289	-3.10072
H	2.015912	-2.70663	0.077419	H	-2.55982	-2.16624	-0.60526
H	1.092166	0.403341	-3.86758	H	-1.66191	0.057805	4.077022
H	0.276794	0.60187	-2.31502	H	-0.68332	0.22052	2.616616
H	1.106446	1.973394	-3.08523	H	-1.31002	1.659831	3.447921
H	3.778441	1.986803	-3.1321	H	-4.00931	2.002508	3.450898
H	4.60301	0.526445	-2.56066	H	-4.96524	0.828343	2.53039
H	3.616167	0.489921	-4.0419	H	-4.1417	0.34824	4.033695
H	5.335956	-2.39651	-1.13655	H	-5.89545	-1.67529	0.497805
H	4.31158	-3.61193	-0.34183	H	-4.96058	-2.82431	-0.48409
H	3.65906	-2.63551	-1.66924	H	-4.30419	-2.23341	1.053228
H	4.544483	-0.66913	2.077701	H	-4.66054	0.562483	-2.2241

H	4.957077	-2.38509	1.8799	H	-5.27717	-1.09059	-2.42671
H	5.821235	-1.14899	0.954446	H	-6.06917	0.023852	-1.30344
H	-0.959	-0.97202	2.415411	H	0.702926	-0.43918	-2.31962
H	-2.21555	0.157918	1.959264	H	2.105604	0.313436	-1.60394
H	-0.25641	1.346657	2.325326	H	0.421485	1.903798	-1.69814
H	-0.08009	1.889448	-0.54614	H	0.224548	2.705896	0.61288
H	-1.70916	1.489402	-0.10871	H	0.691209	1.133243	1.229116
H	-1.53165	3.222017	1.831641	H	2.964703	1.505515	0.776437
H	-1.50233	5.487595	2.074143	H	4.838744	2.727066	0.240574
H	-0.05127	6.254473	1.401333	H	4.683166	3.714238	-1.22236
H	-1.57454	6.356549	0.530057	H	4.539561	4.472942	0.357176
H	0.395717	3.706474	-1.39436	H	0.916124	4.242556	-0.81363
H	-0.47008	5.234323	-1.5855	H	2.204091	5.38391	-0.39623
H	1.05475	5.203072	-0.71206	H	2.259746	4.529166	-1.92998
H	-3.43237	-2.27699	-1.4219	H	2.853732	-2.91103	1.15841
H	-2.58573	-3.28163	0.645547	H	1.848979	-3.32965	-1.07101
H	-3.39209	-2.03451	1.643117	H	2.880236	-2.03623	-1.77648
H	-6.27041	-0.00373	-1.86982	H	6.390233	-2.46131	-0.13936
H	-5.1645	-1.13297	-2.67128	H	5.056769	3.08081	-1.12276
H	-4.5513	0.419694	-2.06147	H	5.28403	-3.6732	0.53822
H	-6.22098	0.284995	0.589528	H	5.913525	-0.82888	1.789331
H	-5.0392	-0.54544	1.608074	H	4.230601	-0.43333	2.198083
H	-4.51656	0.786947	0.564954	H	4.859719	-2.05384	2.528097
H	-5.73537	-2.54902	0.470148	H	4.007181	0.116651	-0.23378
5-i				5-j			
C	-1.50829	0.573061	-1.38003	C	-1.48919	0.62257	-1.34035
C	-1.956	-0.10647	0.004828	C	-1.94568	-0.11602	0.009552
C	-2.20614	1.935766	-1.59601	C	-2.17794	1.997952	-1.49848
C	-2.04215	-0.40469	-2.48369	C	-2.02346	-0.30046	-2.49075
C	-2.43447	-1.7228	-1.80135	C	-2.45137	-1.63808	-1.86981
C	-2.82704	-1.35159	-0.36404	C	-2.83988	-1.32496	-0.41749
C	-4.29498	-0.90053	-0.0685	C	-4.29923	-0.86024	-0.10168
O	-4.1769	0.493144	0.339015	O	-4.1543	0.504737	0.386742
C	-2.90972	0.720917	0.852694	C	-2.8806	0.684172	0.902433
C	-2.73763	1.552515	1.892988	C	-2.68691	1.460608	1.980874
C	-1.40386	1.952281	2.469238	C	-1.34208	1.809797	2.564386
C	-3.93106	2.198257	2.556066	C	-3.86464	2.089626	2.686583
C	-4.86171	-1.68814	1.119883	C	-4.88943	-1.70317	1.03624
C	-5.27256	-0.9255	-1.23991	C	-5.27087	-0.79633	-1.27686
O	-0.78674	-0.45462	0.794691	O	-0.7786	-0.52108	0.773721
C	-0.06176	-1.57317	0.500387	C	-0.07257	-1.63349	0.413674
C	1.220709	-1.24993	-0.2635	C	1.222505	-1.27819	-0.31187
C	0.92289	-0.50783	-1.56884	C	0.944079	-0.45473	-1.57296
C	0.04932	0.775856	-1.54852	C	0.069961	0.825487	-1.49373
C	0.691218	1.882479	-0.66981	C	0.723249	1.884084	-0.56577
C	1.996676	2.390638	-1.2328	C	1.961519	2.496705	-1.17578
C	3.09894	2.759296	-0.56029	C	3.069588	2.928066	-0.5524
C	4.30425	3.299814	-1.2933	C	4.180332	3.599879	-1.32466
C	3.256116	2.684634	0.93881	C	3.299307	2.83631	0.936235
O	-0.3849	-2.68065	0.861756	O	-0.42095	-2.75693	0.69101
O	2.122496	-0.52894	0.636655	O	2.11797	-0.63426	0.651818
C	2.973754	-1.70079	0.773931	C	2.950758	-1.83383	0.719322
C	2.196631	-2.44131	-0.3328	C	2.185335	-2.4727	-0.45669
C	4.475735	-1.41255	0.620874	C	4.461152	-1.55507	0.613578
C	4.825854	-0.7223	-0.69706	C	4.937657	-0.85897	1.889238
C	5.253257	-2.72749	0.789442	C	4.839004	-0.74139	-0.62787
O	4.87398	-0.48096	1.639952	O	5.117597	-2.83313	0.603187
H	-3.29131	1.81636	-1.59697	H	-3.26398	1.887106	-1.5037
H	-1.96713	2.666785	-0.82293	H	-1.93457	2.694167	-0.69508
H	-1.9076	2.35127	-2.56506	H	-1.87672	2.451844	-2.44926
H	-2.92008	0.042007	-2.96091	H	-2.88479	0.181718	-2.96346
H	-1.31308	-0.55735	-3.28624	H	-1.28517	-0.43492	-3.28795
H	-1.57791	-2.40553	-1.75891	H	-1.61334	-2.34429	-1.85779

H	-3.22301	-2.25703	-2.3395	H	-3.25203	-2.12513	-2.43407
H	-2.58302	-2.16657	0.317811	H	-2.61192	-2.1749	0.225975
H	-1.39936	1.775483	3.552775	H	-1.32621	1.565295	3.634598
H	-0.56597	1.410226	2.039073	H	-0.51456	1.288174	2.09096
H	-1.23264	3.029238	2.333347	H	-1.16208	2.891697	2.494352
H	-3.9186	3.2862	2.404218	H	-3.84127	3.183235	2.584596
H	-4.87372	1.813007	2.167698	H	-4.81617	1.733234	2.292215
H	-3.90018	2.035897	3.641335	H	-3.8234	1.87718	3.762769
H	-5.85495	-1.31578	1.387915	H	-5.87745	-1.32782	1.319027
H	-4.9427	-2.75327	0.877682	H	-4.98881	-2.75087	0.732655
H	-4.20651	-1.58498	1.989972	H	-4.23892	-1.66307	1.915041
H	-4.90234	-0.35546	-2.09452	H	-4.88206	-0.18989	-2.09753
H	-5.47014	-1.95197	-1.56275	H	-5.49195	-1.79824	-1.65657
H	-6.22195	-0.48202	-0.92605	H	-6.21066	-0.34713	-0.94293
H	0.493418	-1.24314	-2.2619	H	0.525695	-1.14953	-2.31327
H	1.897355	-0.2328	-1.98647	H	1.924031	-0.15551	-1.96128
H	0.117766	1.148087	-2.58208	H	0.139391	1.245419	-2.50852
H	-0.00097	2.730388	-0.61621	H	0.006233	2.692846	-0.38712
H	0.82428	1.521351	0.348103	H	0.943386	1.446519	0.407229
H	2.00992	2.51456	-2.31862	H	1.906618	2.658427	-2.25497
H	4.15848	3.304208	-2.37746	H	3.957753	3.660402	-2.3937
H	4.530227	4.326893	-0.97672	H	4.35558	4.619944	-0.95704
H	5.199623	2.704713	-1.07077	H	5.129502	3.061252	-1.20317
H	2.3262	2.436711	1.451231	H	2.594438	2.168859	1.433566
H	3.995842	1.922999	1.213967	H	4.313975	2.47822	1.149869
H	3.613871	3.645438	1.331253	H	3.217609	3.827749	1.402465
H	2.817015	-2.15549	1.765878	H	2.77575	-2.36689	1.662402
H	1.769205	-3.40787	-0.0683	H	1.741613	-3.45089	-0.27425
H	2.72589	-2.50811	-1.28537	H	2.720162	-2.47178	-1.40973
H	5.874276	-0.41335	-0.66913	H	6.013649	-0.67027	1.837697
H	4.202102	0.16243	-0.83804	H	4.743507	-1.49421	2.758373
H	4.694321	-1.39404	-1.55005	H	4.415515	0.09141	2.025927
H	6.326883	-2.52712	0.740449	H	5.915044	-0.54633	-0.6269
H	5.038758	-3.18975	1.760373	H	4.603046	-1.28269	-1.55193
H	5.00009	-3.4529	0.009156	H	4.30173	0.210058	-0.65162
H	4.5663	-0.81602	2.493923	H	4.934508	-3.25087	-0.24968
5-k				5-l			
C	-1.4453	0.439131	-1.39859	C	-1.29805	0.847067	-1.04802
C	-1.95535	-0.12111	0.020647	C	-1.88661	-0.21214	0.008673
C	-2.05467	1.82651	-1.7036	C	-1.91211	2.250563	-0.83784
C	-2.02913	-0.57024	-2.449	C	-1.79173	0.320795	-2.44072
C	-2.55779	-1.79815	-1.69203	C	-2.31214	-1.1114	-2.25224
C	-2.93047	-1.30319	-0.28714	C	-2.79605	-1.1961	-0.79764
C	-4.35489	-0.7069	-0.0411	C	-4.25416	-0.74894	-0.45241
O	-4.11678	0.689327	0.30443	O	-4.08963	0.418377	0.403838
C	-2.83604	0.832796	0.812867	C	-2.85462	0.364223	1.030629
C	-2.59255	1.703117	1.806441	C	-2.71587	0.791409	2.296306
C	-1.22864	2.016034	2.366429	C	-1.40924	0.873946	3.042581
C	-3.72561	2.487144	2.424687	C	-3.91828	1.274245	3.072266
C	-5.01062	-1.38077	1.171177	C	-4.96148	-1.83418	0.370028
C	-5.31248	-0.6991	-1.22922	C	-5.13325	-0.30714	-1.61891
O	-0.82676	-0.51898	0.840699	O	-0.8043	-0.88741	0.703225
C	-0.16362	-1.68778	0.594203	C	-0.09928	-1.88269	0.088515
C	1.170131	-1.42253	-0.08496	C	1.262725	-1.39262	-0.38192
C	0.92925	-0.78751	-1.45945	C	1.094475	-0.28012	-1.42208
C	0.123594	0.534448	-1.57124	C	0.277301	0.990077	-1.06129
C	0.829801	1.685248	-0.81029	C	0.902257	1.746759	0.148986
C	2.192226	1.999898	-1.38749	C	2.327601	2.1729	-0.10064
C	3.22628	2.602935	-0.776	C	2.783716	3.408531	-0.3642
C	4.513858	2.881846	-1.51481	C	4.25884	3.649372	-0.58562
C	3.194546	3.08309	0.654467	C	1.931117	4.650256	-0.46187
O	-0.58528	-2.77716	0.902206	O	-0.50912	-3.01352	-0.03086
O	2.003076	-0.62606	0.819393	O	2.049498	-1.00483	0.790285

C	2.934044	-1.74231	0.995341	C	2.98259	-2.09794	0.572896
C	2.171513	-2.58966	-0.03906	C	2.261711	-2.51498	-0.72408
C	4.372945	-1.29928	0.68212	C	4.439707	-1.62999	0.487117
C	5.292346	-2.51537	0.561528	C	5.353649	-2.84534	0.269023
C	4.864626	-0.3447	1.782558	C	4.817145	-0.86229	1.760457
O	4.400141	-0.64397	-0.58712	O	4.516494	-0.76096	-0.6543
H	-3.14466	1.770878	-1.71796	H	-2.99753	2.217537	-0.9499
H	-1.78566	2.582341	-0.96477	H	-1.70652	2.659331	0.152001
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H	-3.70313	2.394803	3.518269	H	-3.97569	0.766439	4.043856
H	-5.96858	-0.90556	1.402653	H	-5.95151	-1.49173	0.685914
H	-5.18743	-2.44404	0.976712	H	-5.08096	-2.75139	-0.21659
H	-4.36188	-1.29786	2.048292	H	-4.37725	-2.07479	1.263235
H	-4.87673	-0.21199	-2.10402	H	-4.65913	0.475469	-2.21454
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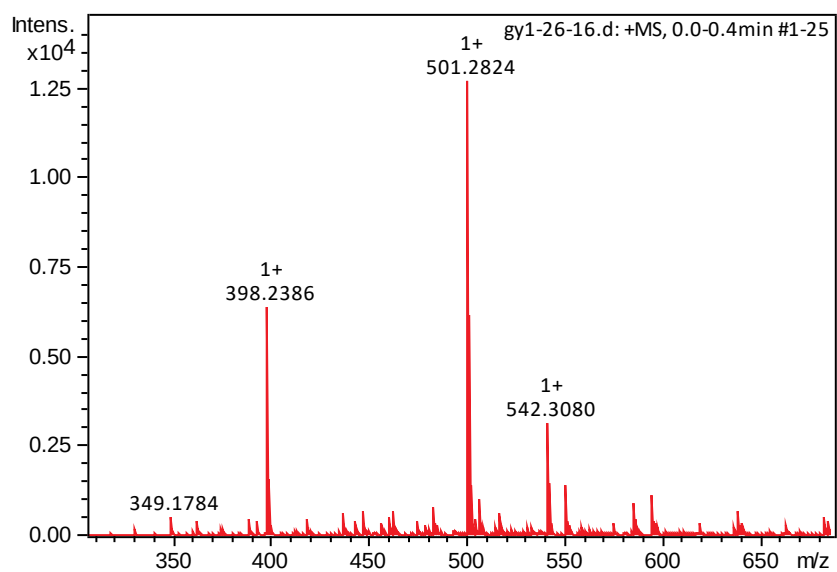
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C	0.928548	-0.54546	-1.55181	C	0.945587	-0.47324	-1.57113
C	0.054691	0.73906	-1.55582	C	0.076417	0.810655	-1.49494
C	0.689732	1.858975	-0.6889	C	0.732533	1.867711	-0.56723
C	1.993667	2.370218	-1.25214	C	1.967796	2.483519	-1.18052
C	3.086604	2.760685	-0.57669	C	3.069168	2.932218	-0.55759
C	4.291846	3.30342	-1.30835	C	4.178861	3.60251	-1.33257
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C	2.981029	-1.68317	0.816492	C	2.945124	-1.85391	0.720819
C	2.202778	-2.45242	-0.26857	C	2.181483	-2.49299	-0.45052
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H	-3.89999	2.102458	3.602264	H	-3.80832	1.896092	3.75911
H	-5.86806	-1.26988	1.399138	H	-5.88358	-1.303	1.32132
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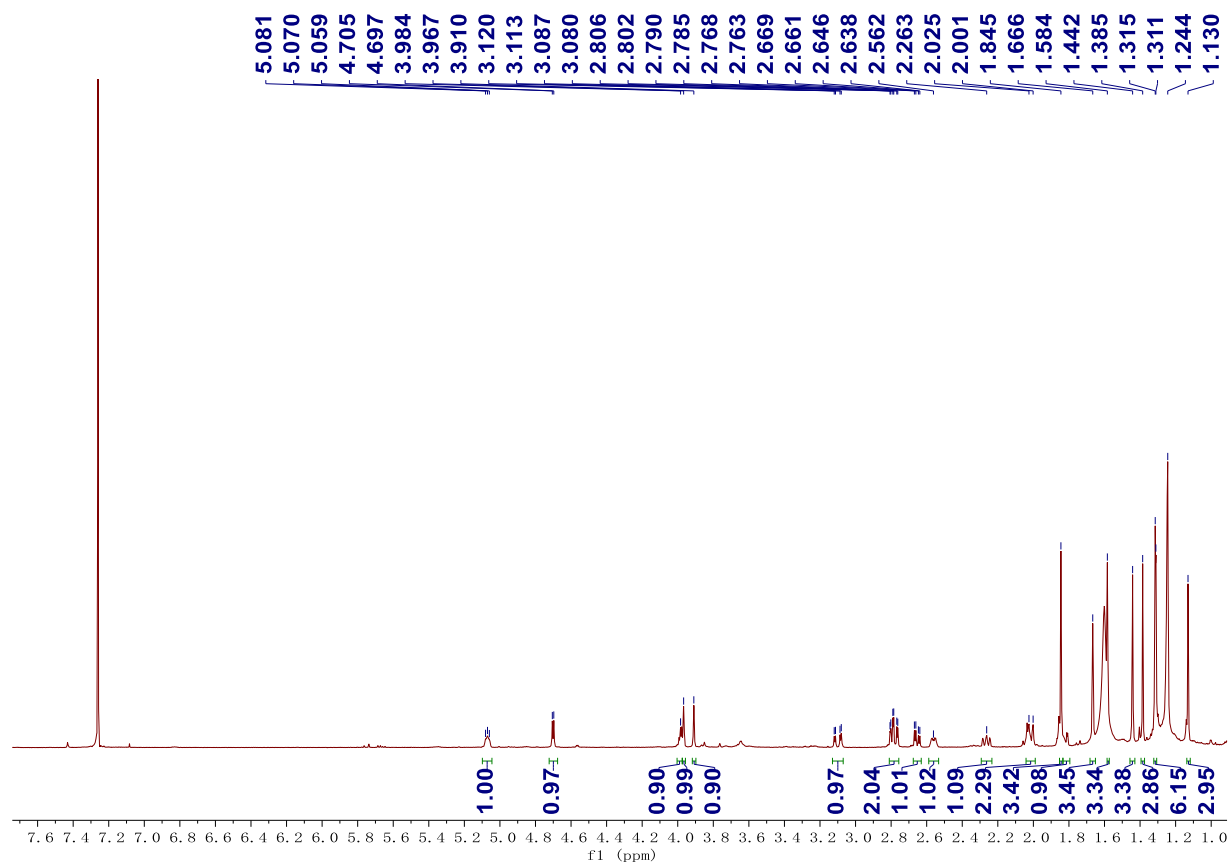
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C	-2.87691	-1.2969	-0.42922	C	-2.83126	-1.32556	-0.4281
C	-4.32294	-0.80039	-0.10089	C	-4.29371	-0.87162	-0.1109
O	-4.14205	0.552188	0.409744	O	-4.15755	0.491328	0.385945
C	-2.86085	0.693947	0.917917	C	-2.88566	0.675059	0.904333
C	-2.64095	1.44843	2.007027	C	-2.69796	1.446726	1.987229
C	-1.28414	1.756812	2.586151	C	-1.35568	1.800729	2.57361
C	-3.79843	2.093138	2.731843	C	-3.88012	2.064916	2.695046
C	-4.93174	-1.64672	1.024584	C	-4.87985	-1.7249	1.02142
C	-5.29601	-0.69221	-1.27186	C	-5.26474	-0.80651	-1.28651
O	-0.7886	-0.55567	0.757269	O	-0.77812	-0.51937	0.773136
C	-0.10192	-1.67071	0.372056	C	-0.06765	-1.62923	0.410072
C	1.206056	-1.31133	-0.32547	C	1.221552	-1.27183	-0.3244
C	0.935002	-0.4814	-1.58428	C	0.943959	-0.43491	-1.57574
C	0.076341	0.810132	-1.49816	C	0.068355	0.843077	-1.48643
C	0.747679	1.864711	-0.57729	C	0.720107	1.894378	-0.54913
C	2.010115	2.430733	-1.18316	C	1.954655	2.516533	-1.15689
C	3.139152	2.812405	-0.56482	C	3.065924	2.940369	-0.53426
C	4.279055	3.425582	-1.34332	C	4.172866	3.621064	-1.30407
C	3.380828	2.706498	0.920727	C	3.302834	2.831165	0.952079
O	-0.47724	-2.79678	0.598394	O	-0.40661	-2.75211	0.701218
O	2.080857	-0.66499	0.656146	O	2.120528	-0.63917	0.648927
C	2.935108	-1.85359	0.718407	C	2.950068	-1.84043	0.696176
C	2.179689	-2.49831	-0.45932	C	2.185697	-2.46357	-0.48278
C	4.420801	-1.47409	0.638415	C	4.461309	-1.56538	0.592406
C	4.803095	-0.77451	-0.67312	C	4.939821	-0.84886	1.861148
C	5.287509	-2.71029	0.881003	C	4.840355	-0.773	-0.65699
O	4.671054	-0.58875	1.740557	O	5.108896	-2.84122	0.460485
H	-3.2412	1.922644	-1.48849	H	-3.26817	1.89711	-1.48872
H	-1.90461	2.695017	-0.65963	H	-1.93944	2.702278	-0.67664
H	-1.84152	2.482509	-2.41816	H	-1.88332	2.471024	-2.43226
H	-2.88426	0.233537	-2.97036	H	-2.88715	0.200159	-2.95888
H	-1.29991	-0.42245	-3.29031	H	-1.28411	-0.40287	-3.29284
H	-1.68658	-2.3353	-1.8855	H	-1.59495	-2.32507	-1.87421
H	-3.32033	-2.06092	-2.45262	H	-3.23487	-2.11558	-2.4505
H	-2.66597	-2.15888	0.203733	H	-2.59934	-2.17869	0.209874
H	-1.26801	1.498657	3.653127	H	-1.3383	1.548972	3.642181
H	-0.473	1.219963	2.10133	H	-0.52481	1.287894	2.096415
H	-1.07746	2.834664	2.528404	H	-1.18267	2.884248	2.511068
H	-3.75092	3.187397	2.646693	H	-3.86414	3.159114	2.597877
H	-4.76086	1.764641	2.339737	H	-4.82899	1.703852	2.298479
H	-3.75368	1.862905	3.80421	H	-3.83819	1.848042	3.770357
H	-5.90971	-1.25182	1.315537	H	-5.87026	-1.35704	1.305758
H	-5.05749	-2.68663	0.704408	H	-4.97295	-2.77125	0.711263
H	-4.27898	-1.63706	1.902615	H	-4.23021	-1.68649	1.900943
H	-4.89387	-0.08349	-2.08438	H	-4.87879	-0.19279	-2.10305
H	-5.54458	-1.68185	-1.66637	H	-5.47928	-1.80743	-1.67254
H	-6.22252	-0.22363	-0.92765	H	-6.20756	-0.36508	-0.95077
H	0.503827	-1.16934	-2.3237	H	0.528059	-1.12336	-2.32325

H	1.916078	-0.19436	-1.97828	H	1.924216	-0.13221	-1.96029
H	0.14562	1.228611	-2.51356	H	0.137503	1.272046	-2.49743
H	0.051149	2.696439	-0.42563	H	0.001172	2.699053	-0.35964
H	0.941114	1.437923	0.405826	H	0.944433	1.44714	0.418588
H	1.960478	2.595814	-2.2621	H	1.894478	2.691088	-2.23374
H	4.057769	3.487701	-2.41247	H	3.94375	3.696143	-2.37078
H	4.502859	4.438882	-0.98387	H	4.352143	4.635865	-0.92393
H	5.20114	2.84274	-1.21862	H	5.121718	3.079046	-1.19603
H	2.570096	2.202577	1.44947	H	2.606262	2.150339	1.443138
H	4.317165	2.169465	1.12209	H	4.322065	2.480603	1.156492
H	3.500572	3.703774	1.364427	H	3.213508	3.815354	1.432182
H	2.770975	-2.37091	1.672158	H	2.76704	-2.38083	1.63823
H	1.739398	-3.4777	-0.27446	H	1.744517	-3.44469	-0.31167
H	2.727186	-2.50244	-1.4036	H	2.732595	-2.45672	-1.42649
H	5.838245	-0.42999	-0.60009	H	6.020854	-0.68721	1.820049
H	4.161103	0.093012	-0.85046	H	4.71525	-1.44675	2.753534
H	4.730733	-1.44378	-1.53673	H	4.441396	0.117482	1.976904
H	6.342168	-2.4223	0.90703	H	5.911625	-0.55409	-0.64419
H	5.038673	-3.17194	1.840822	H	4.634236	-1.35148	-1.56142
H	5.151734	-3.45104	0.086529	H	4.28239	0.16515	-0.70002
H	3.992607	0.101222	1.697247	H	5.007992	-3.31223	1.299631

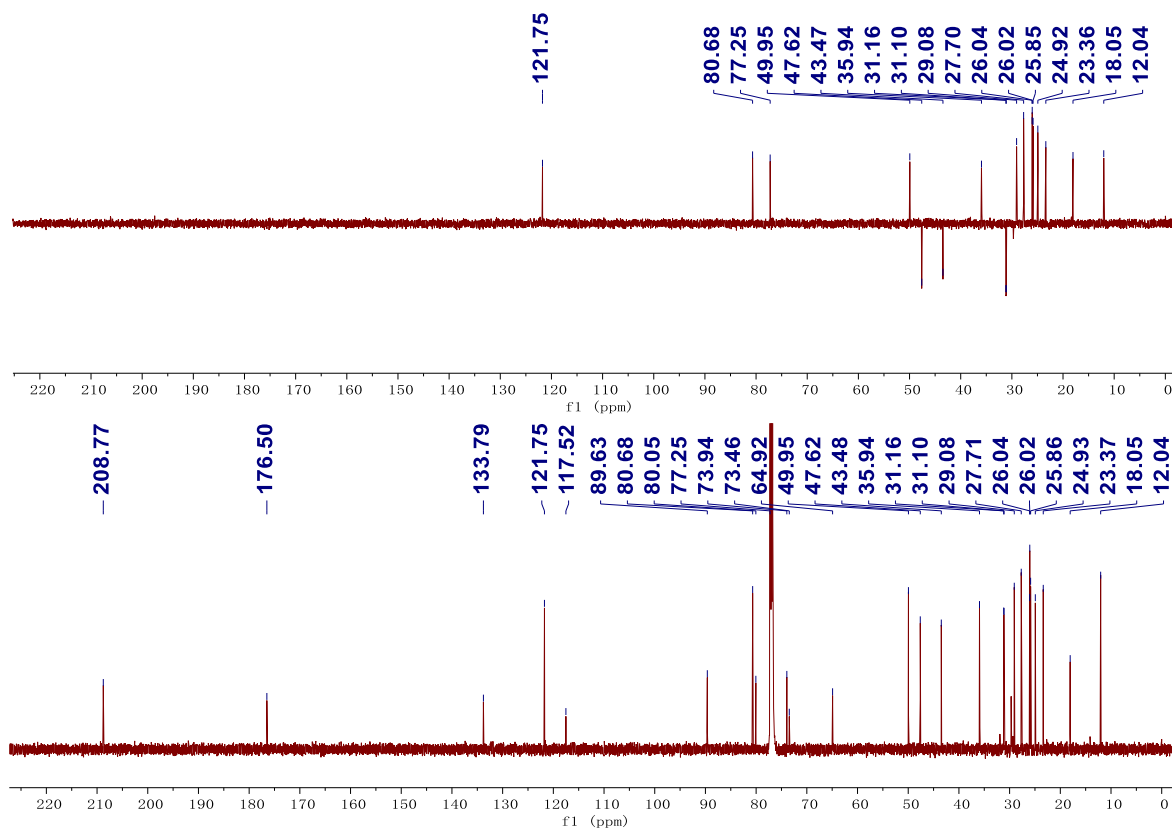
HRESIMS of compound **1**



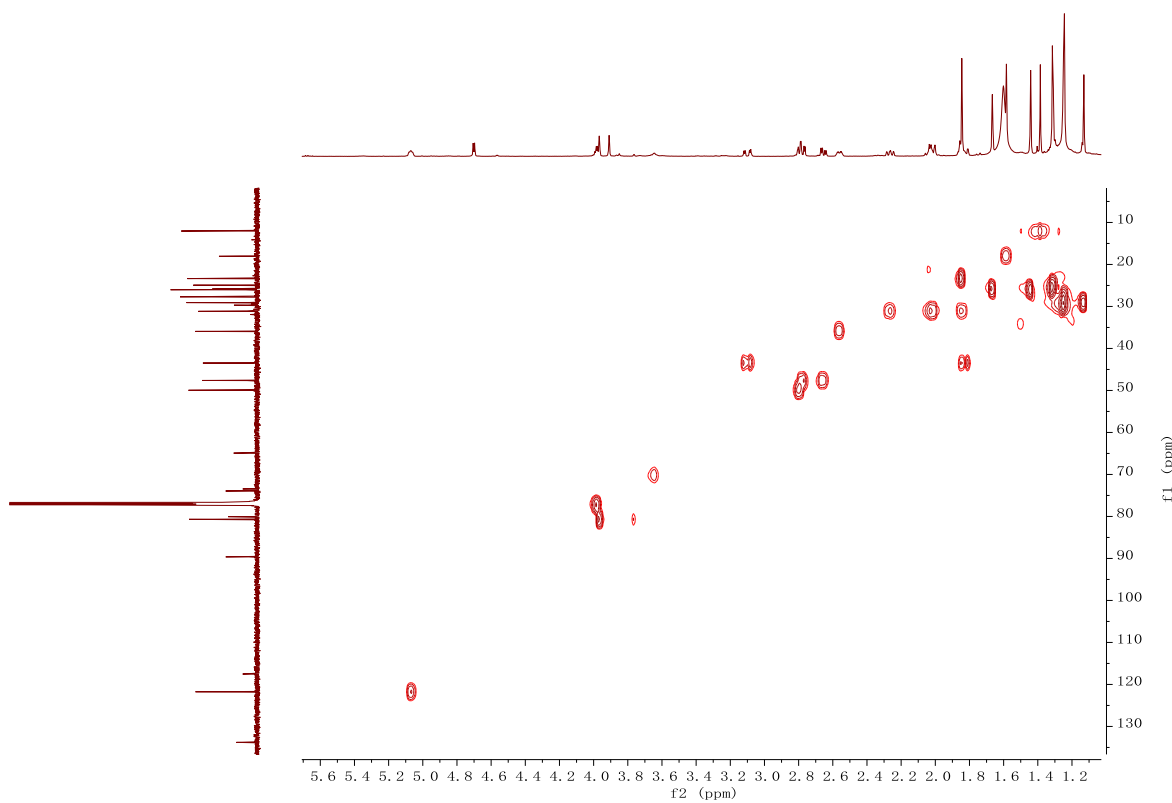
¹H NMR of compound **1** (600MHz, in CDCl₃)



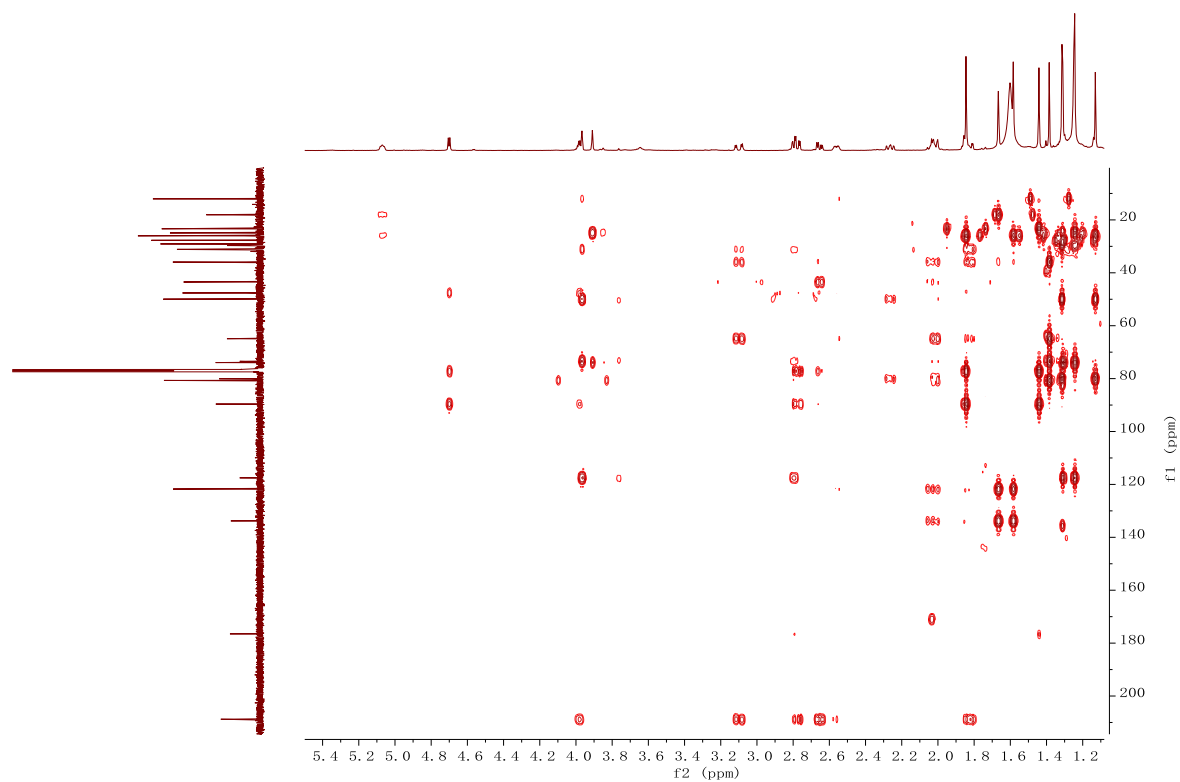
^{13}C NMR of compound **1** (150MHz, in CDCl_3)



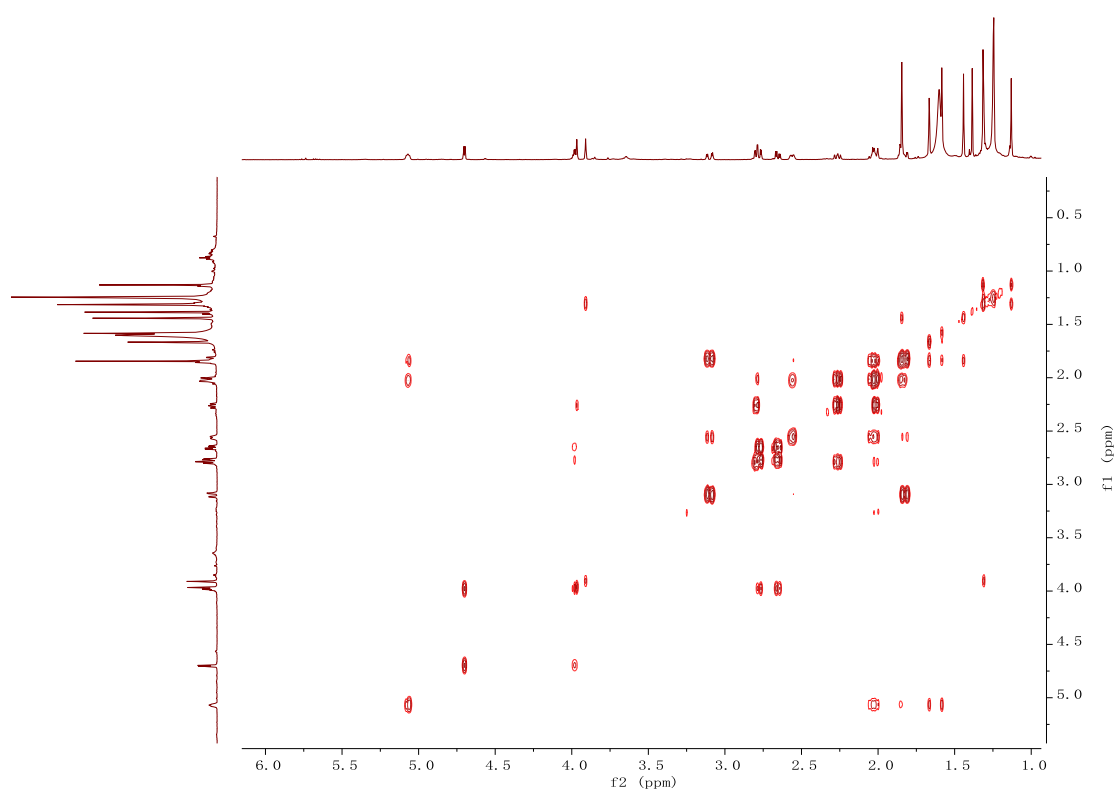
HSQC of compound **1** (600MHz, in CDCl_3)



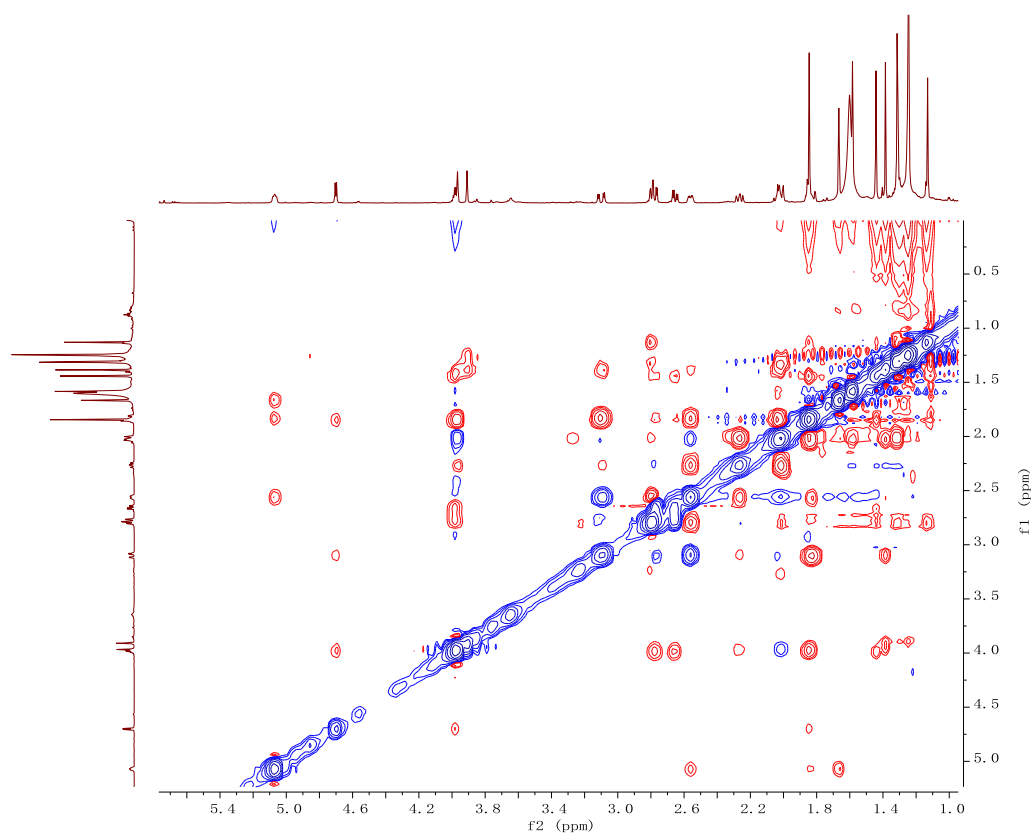
HMBC of compound **1** (600MHz, in CDCl₃)



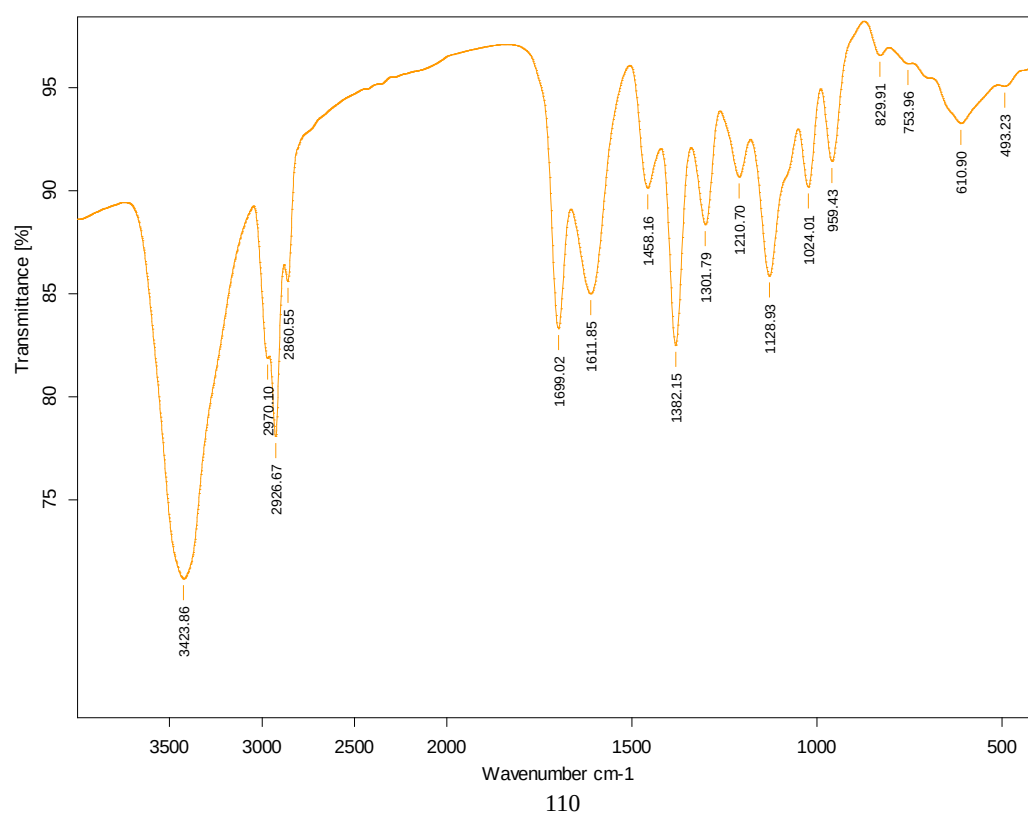
¹H-¹H COSY of compound **1** (600MHz, in CDCl₃)



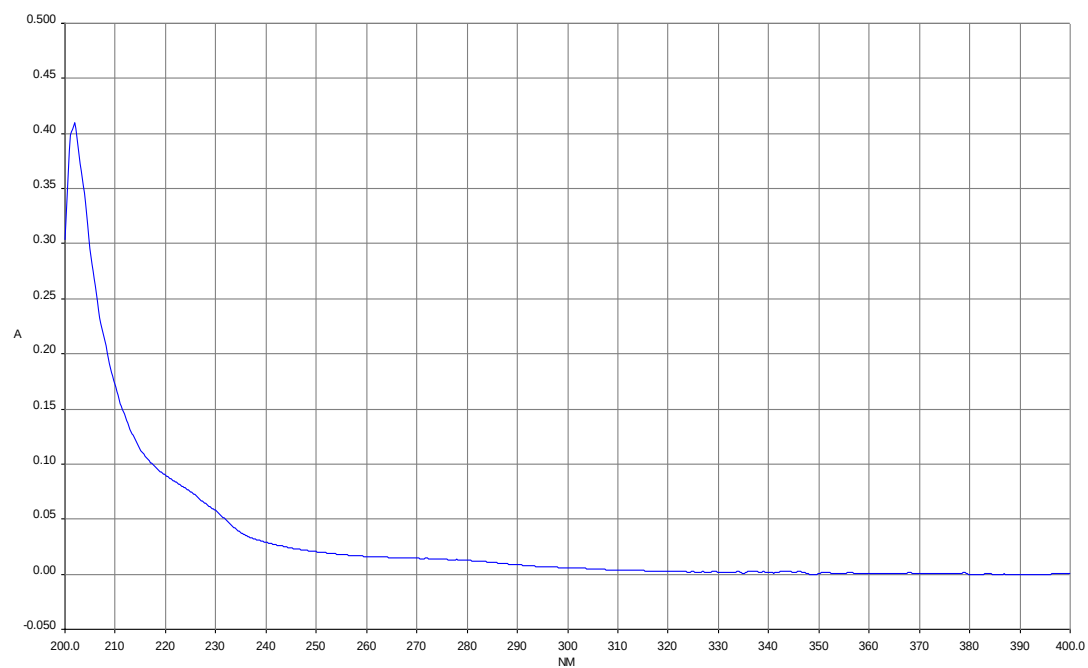
ROESY of compound **1** (600MHz, in CDCl₃)



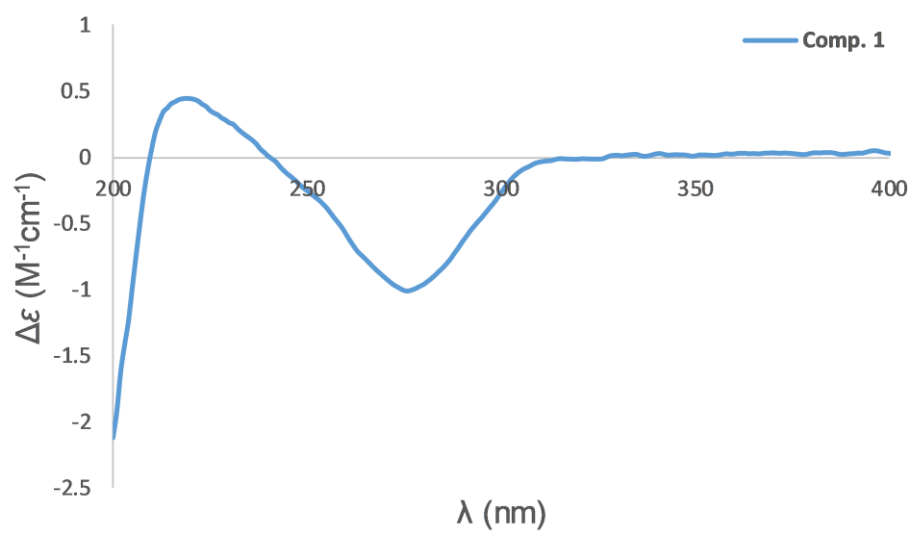
IR of compound **1**



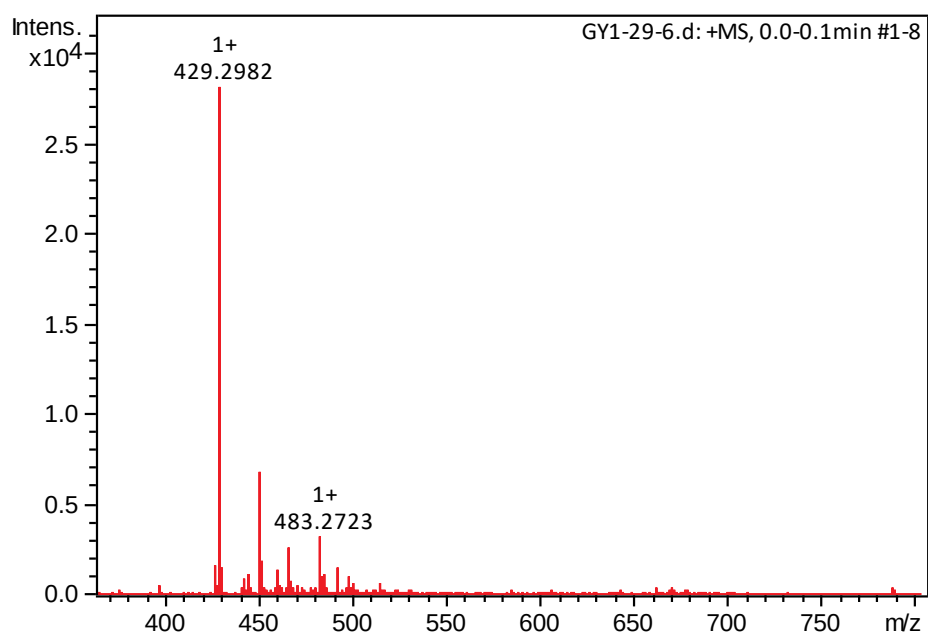
UV of compound 1



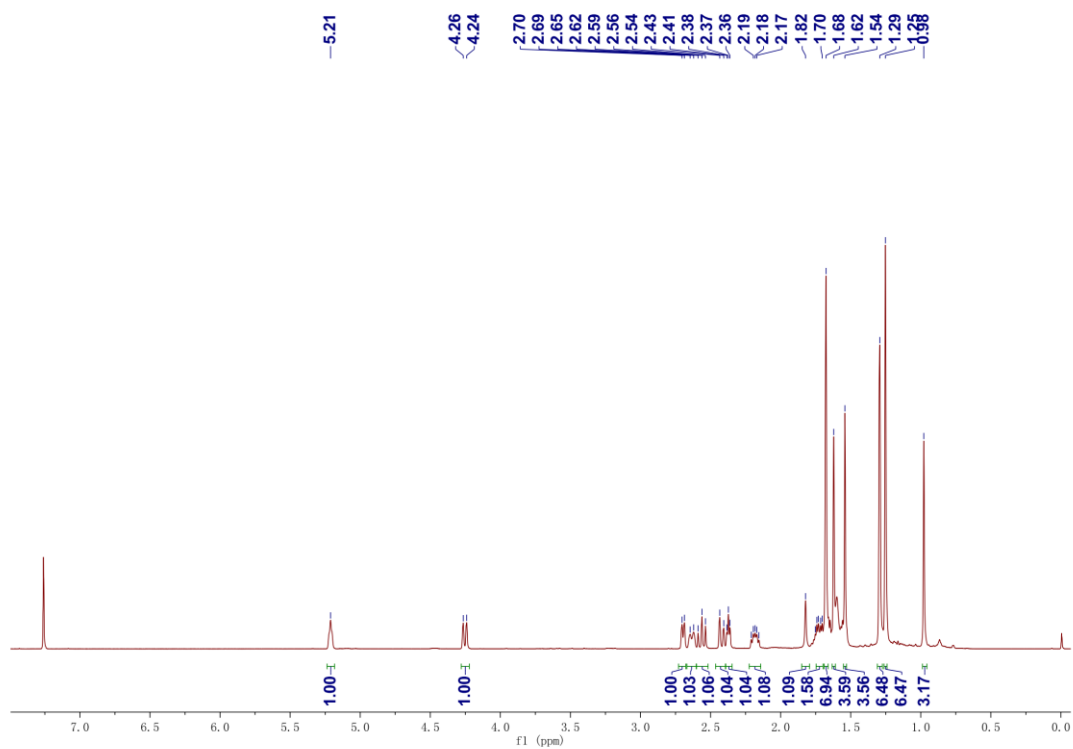
CD of compound 1



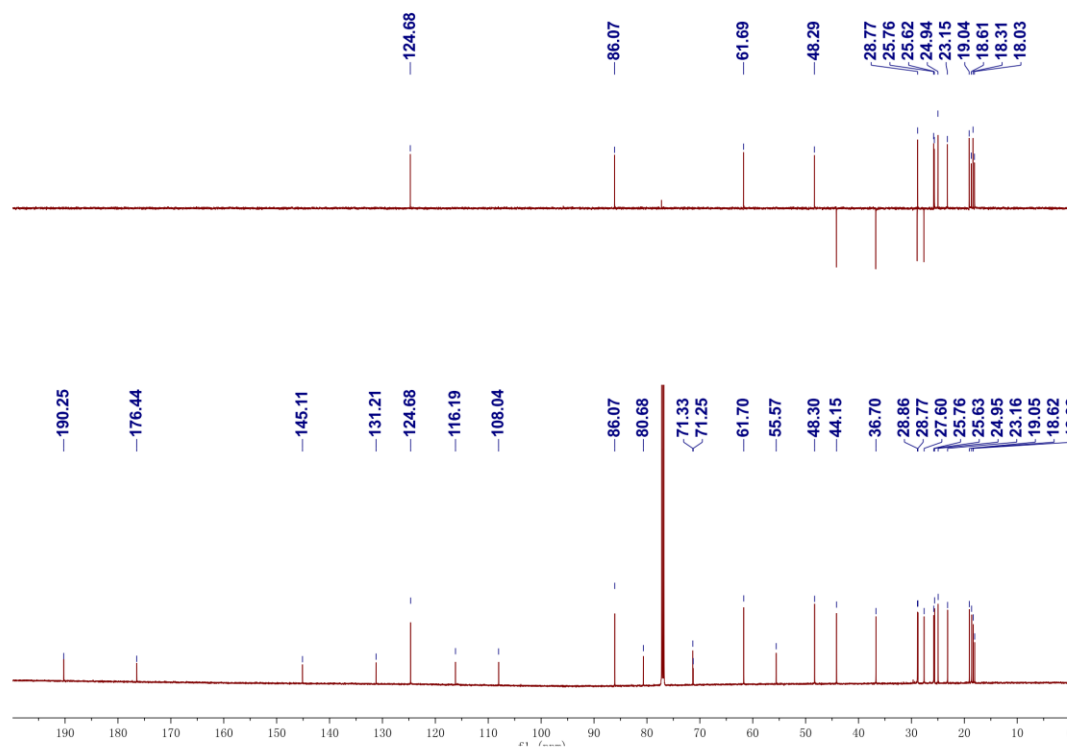
HRESIMS of compound 2



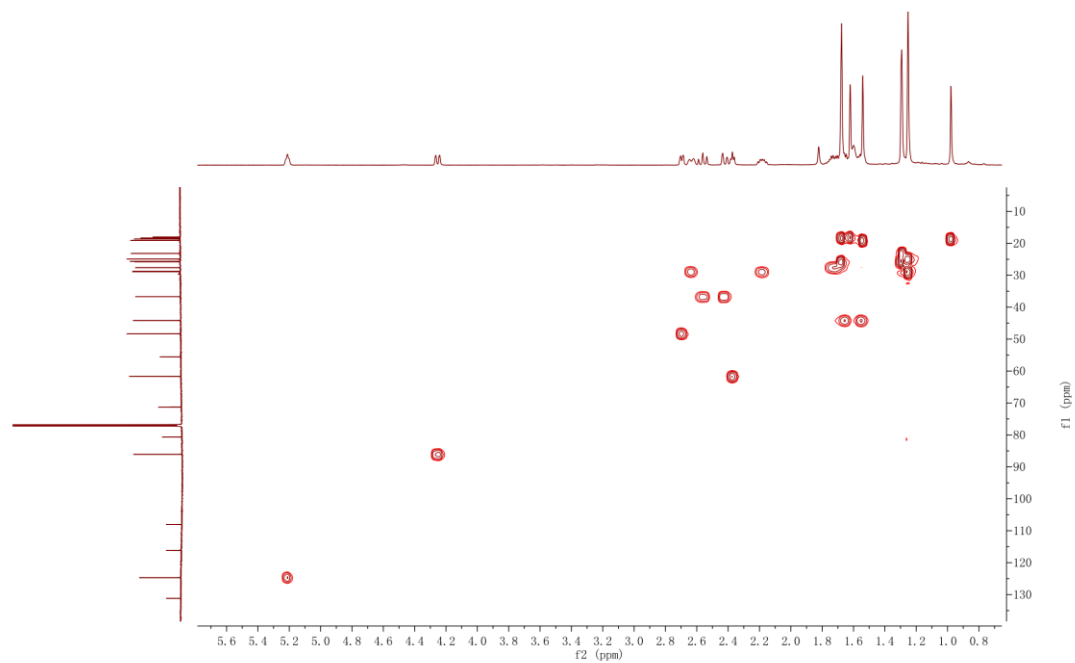
¹H NMR of compound 2 (600MHz, in CDCl₃)



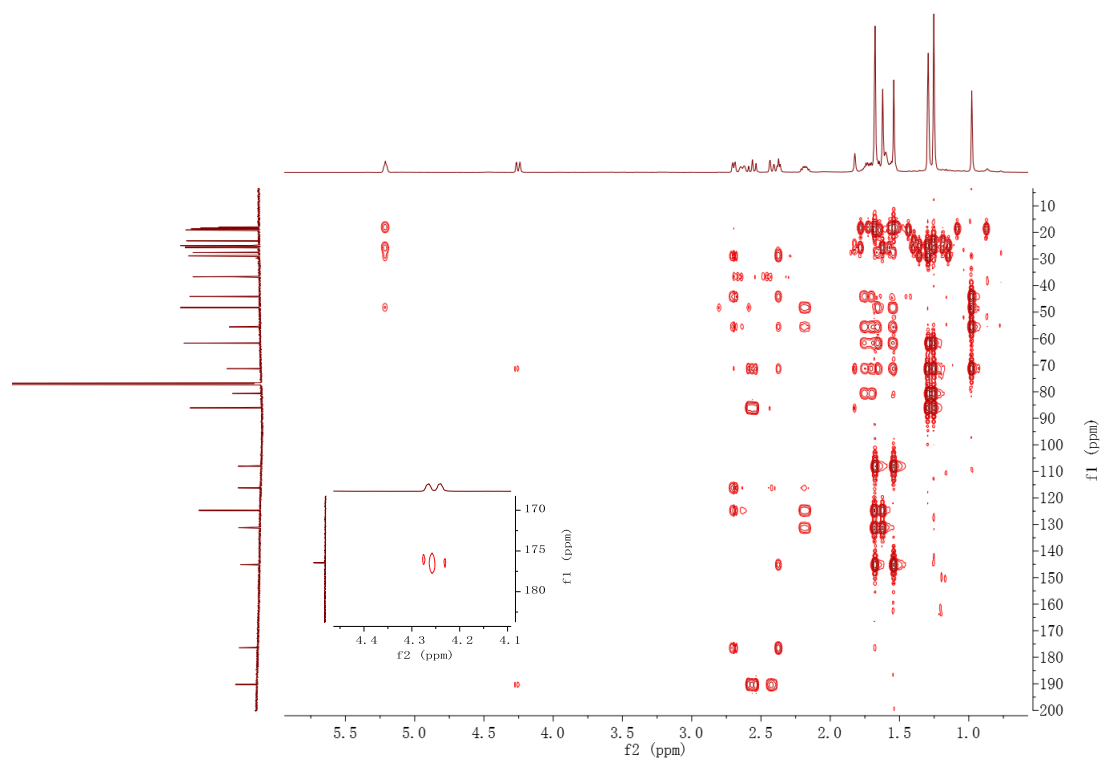
^{13}C NMR of compound 2 (150MHz, in CDCl_3)



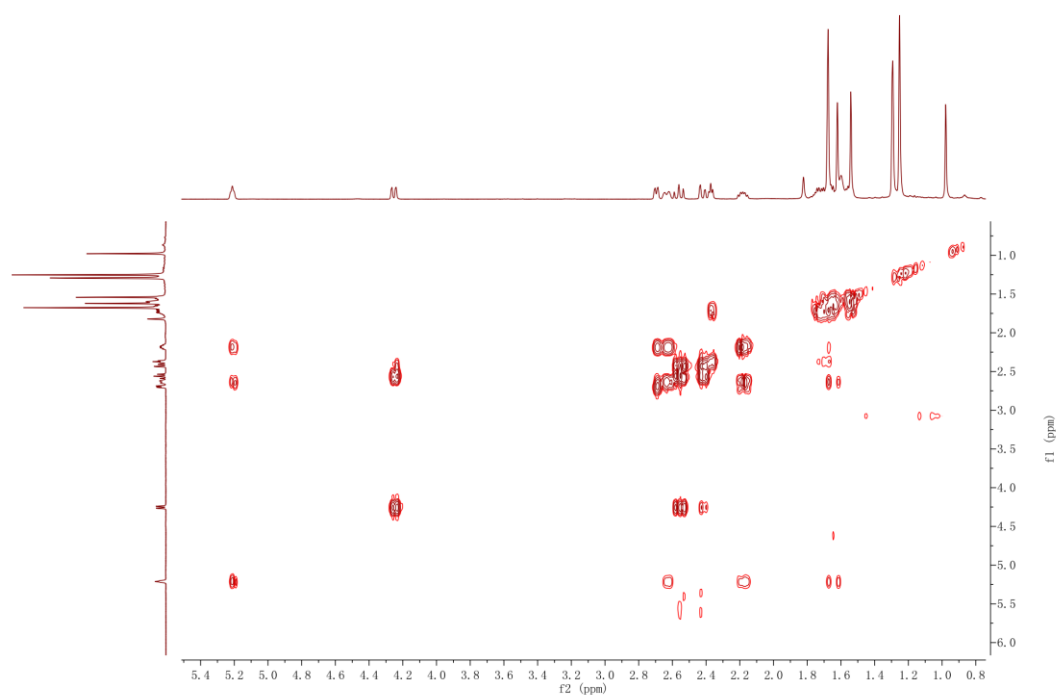
HSQC of compound 2 (600MHz, in CDCl_3)



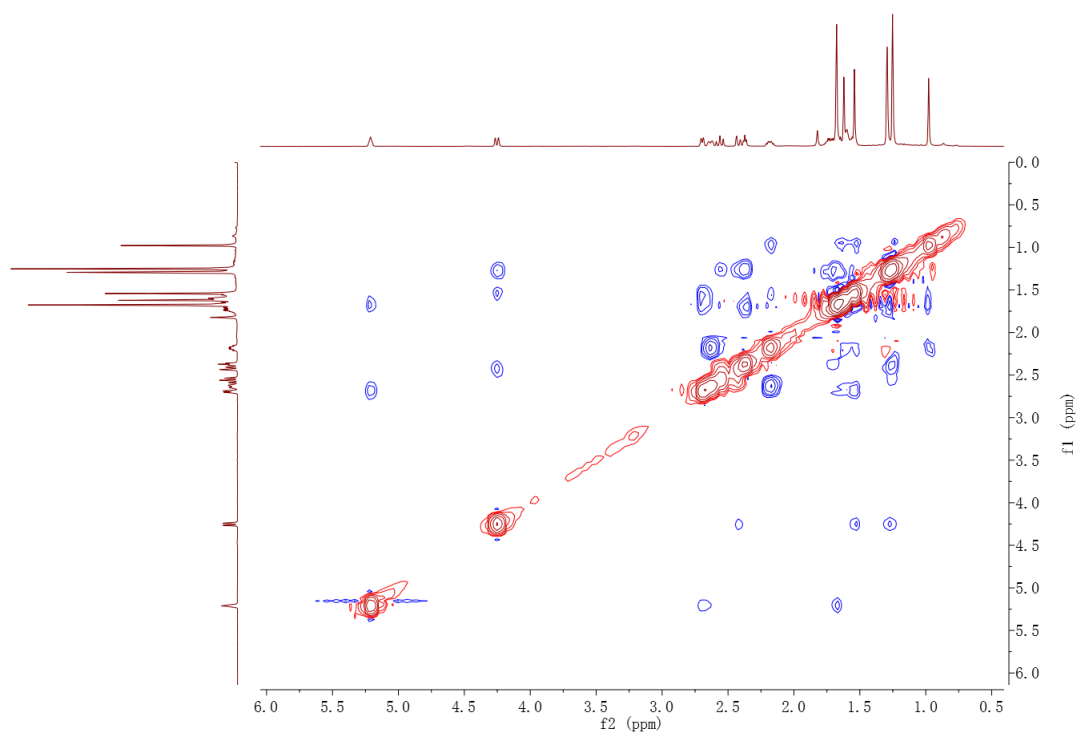
HMBC of compound 2 (600MHz, in CDCl₃)



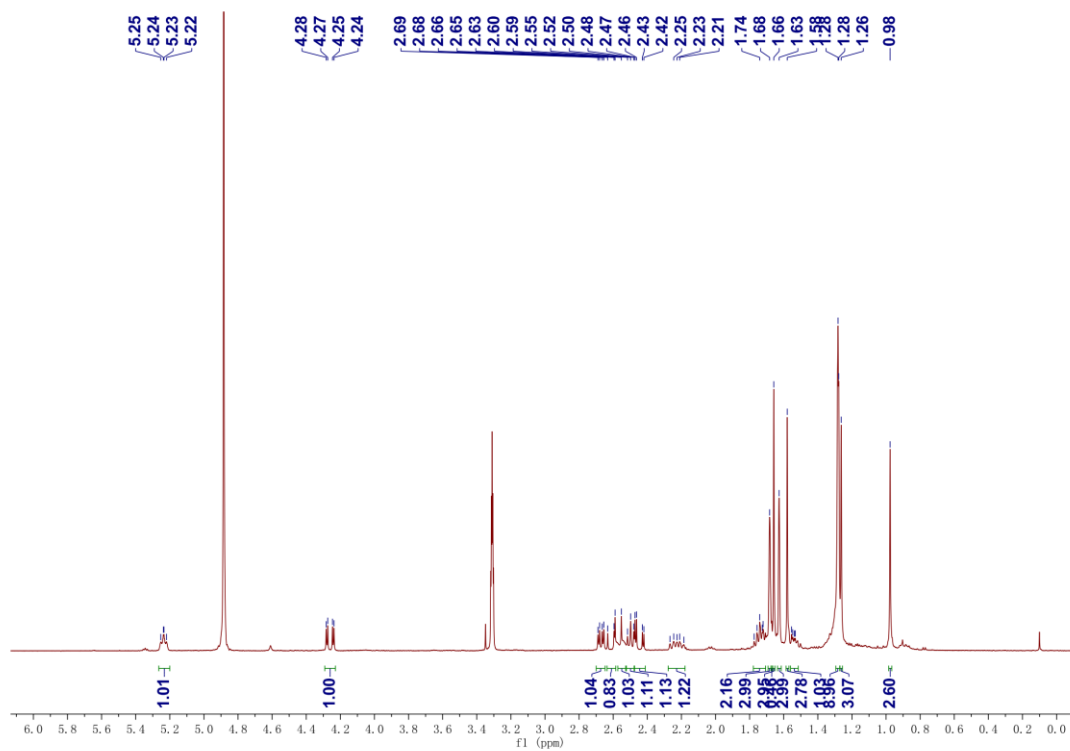
¹H-¹H COSY of compound 2 (600MHz, in CDCl₃)



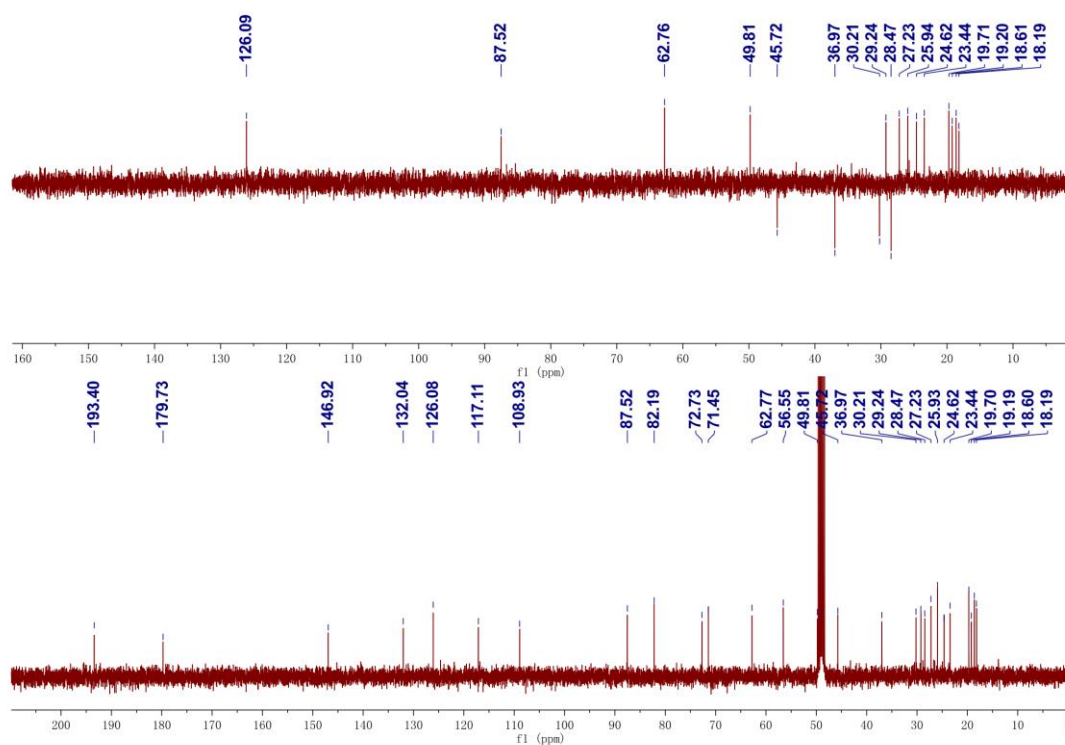
ROESY of compound 2 (600MHz, in CDCl₃)



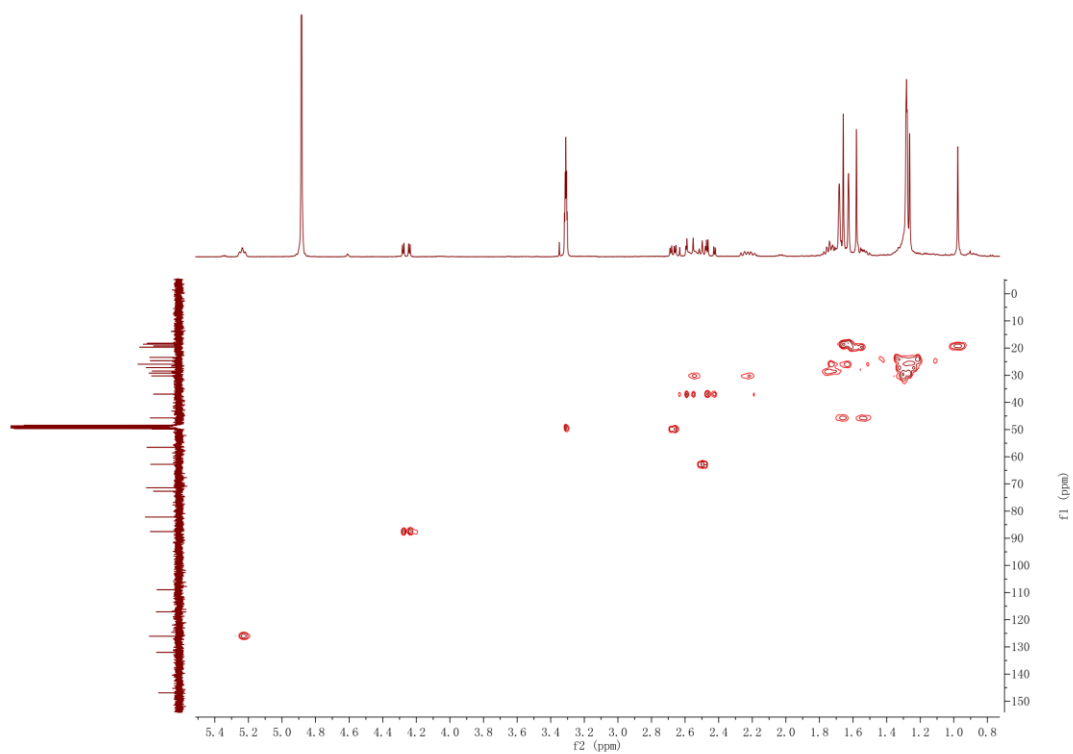
¹H NMR of compound 2 (400MHz, in CD₃OD)



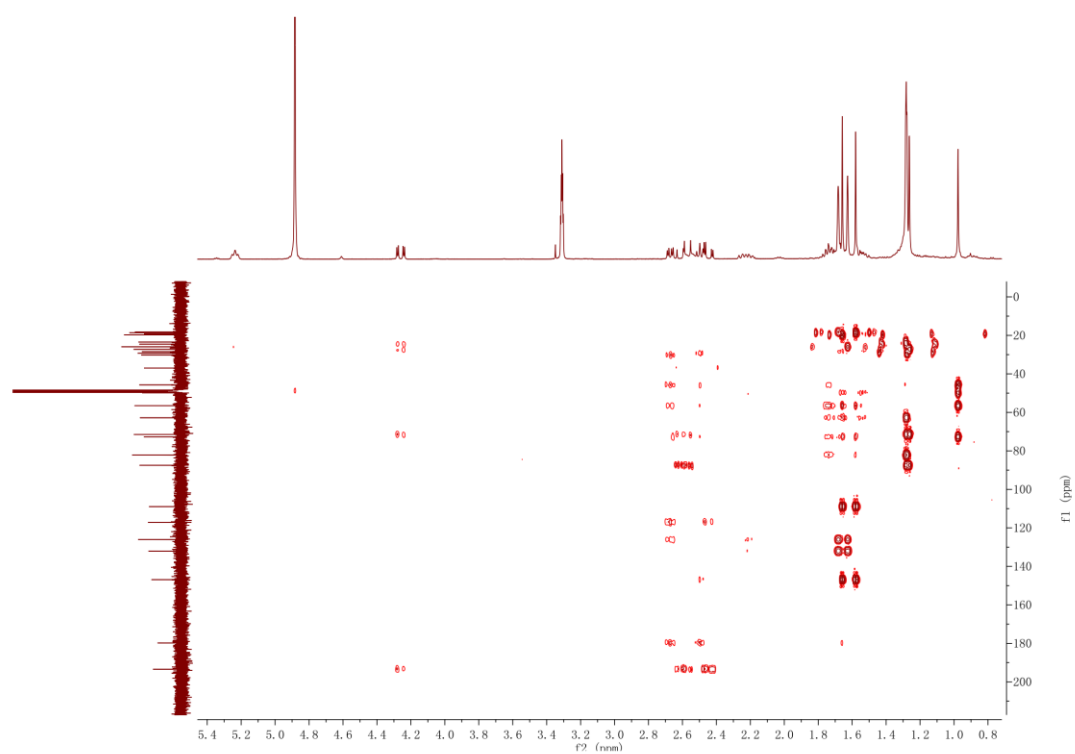
^{13}C NMR of compound 2 (100MHz, in CD_3OD)



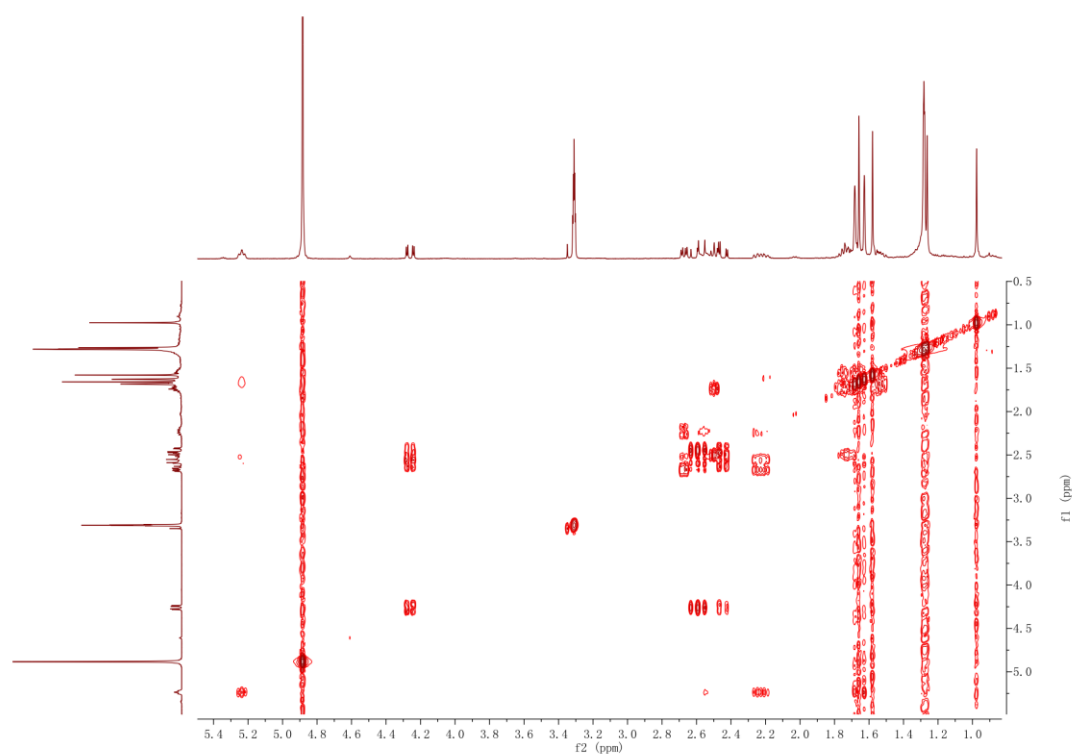
HSQC of compound 2 (400MHz, in CD_3OD)



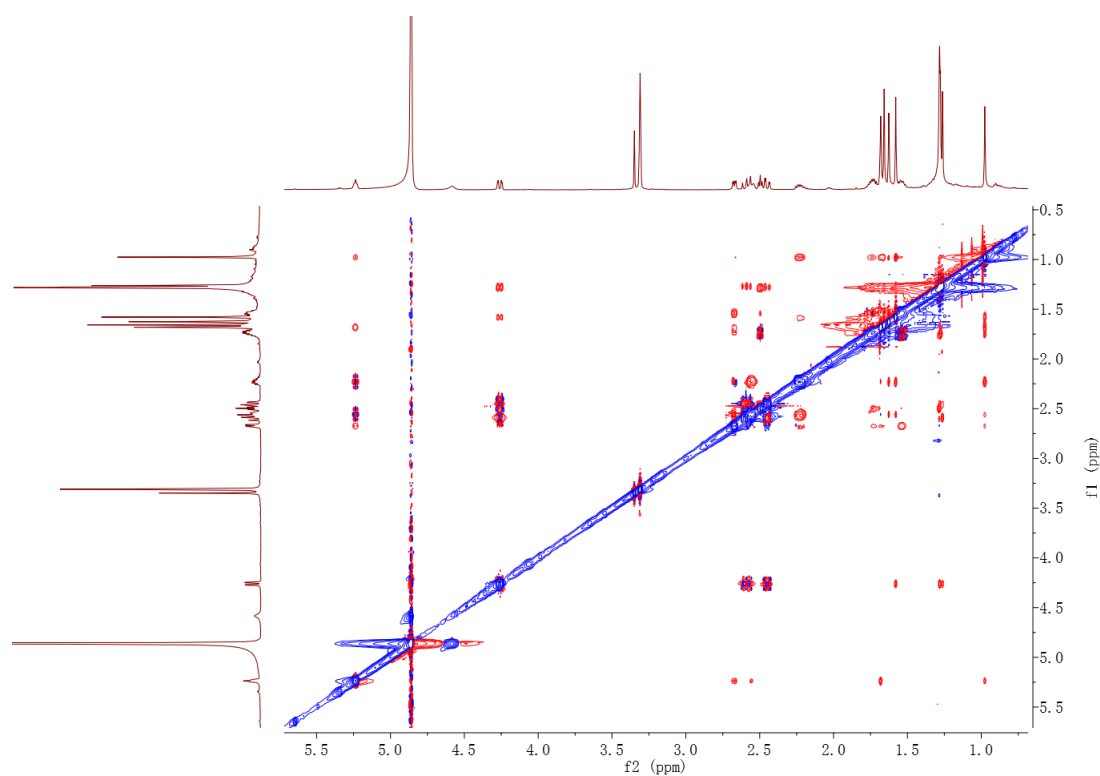
HMBC of compound 2 (400MHz, in CD₃OD)



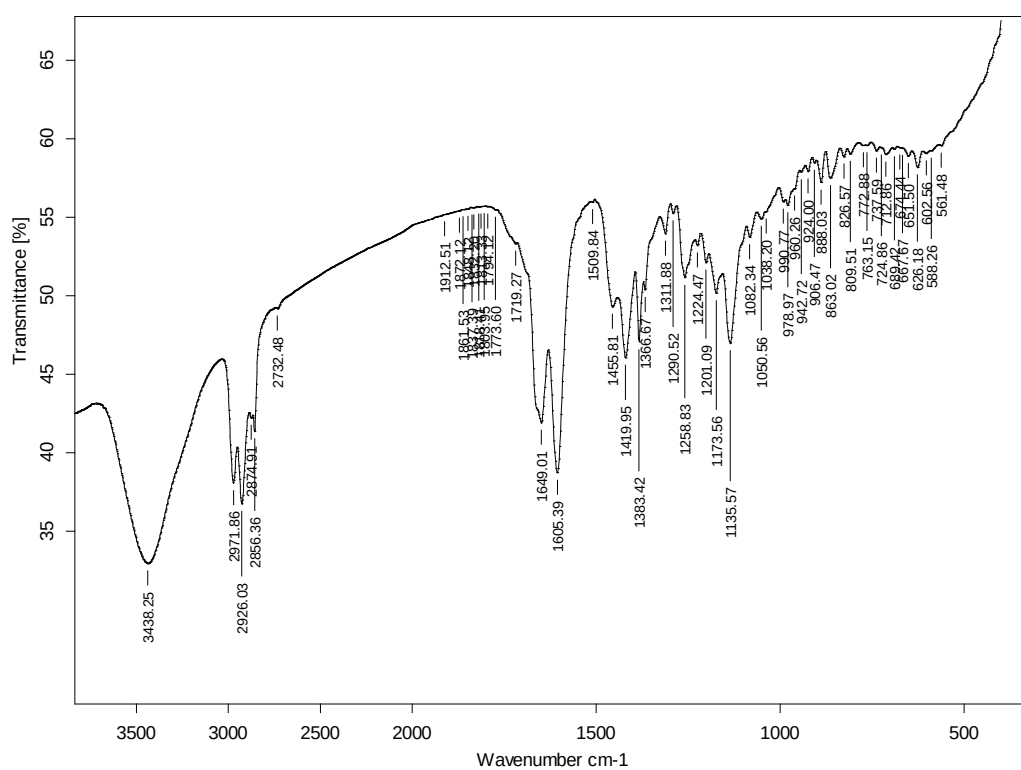
¹H-¹H COSY of compound 2 (400MHz, in CD₃OD)



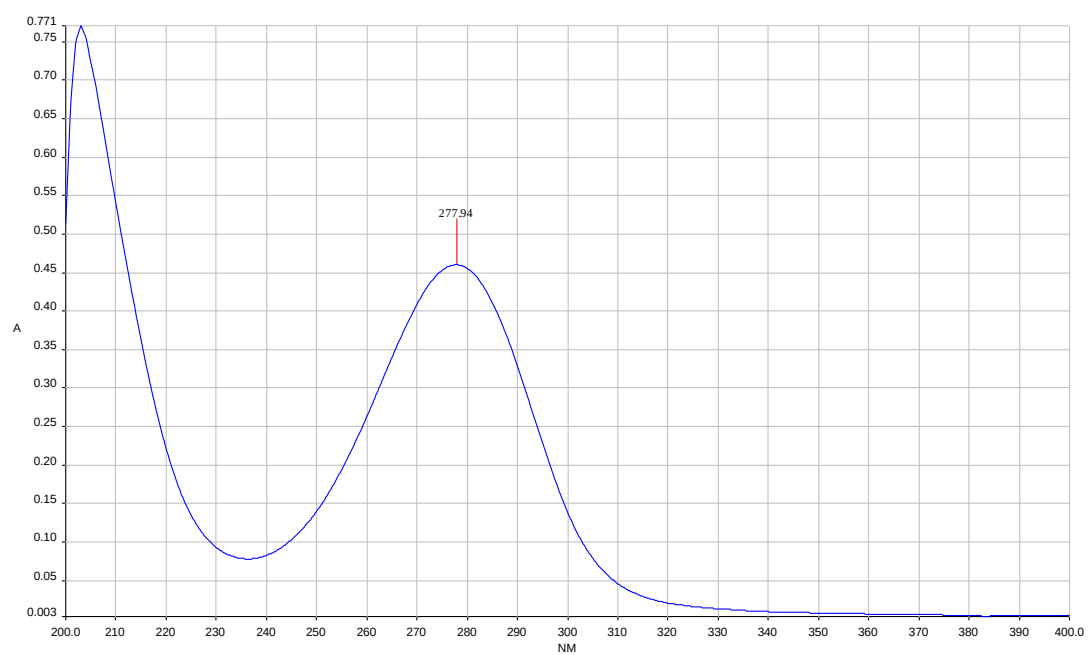
NOESY of compound 2 (600MHz, in CD₃OD)



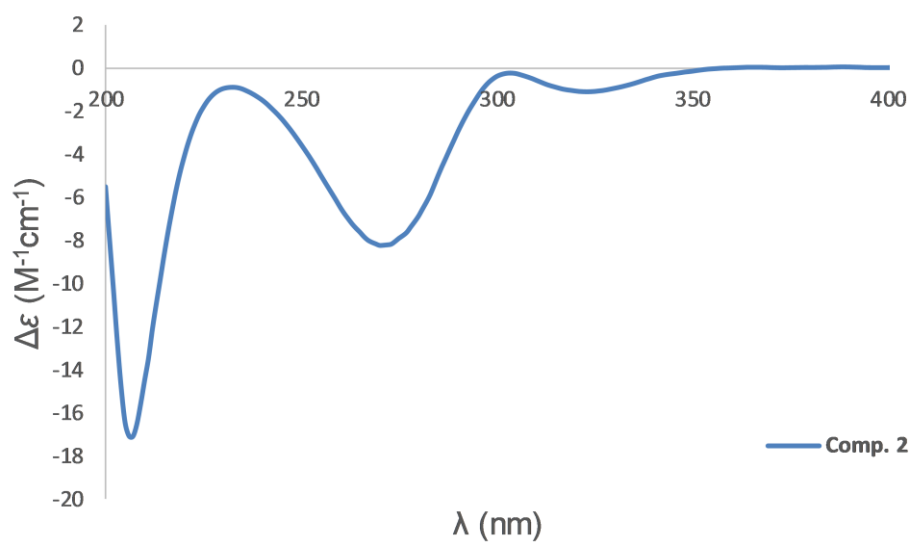
IR of compound 2



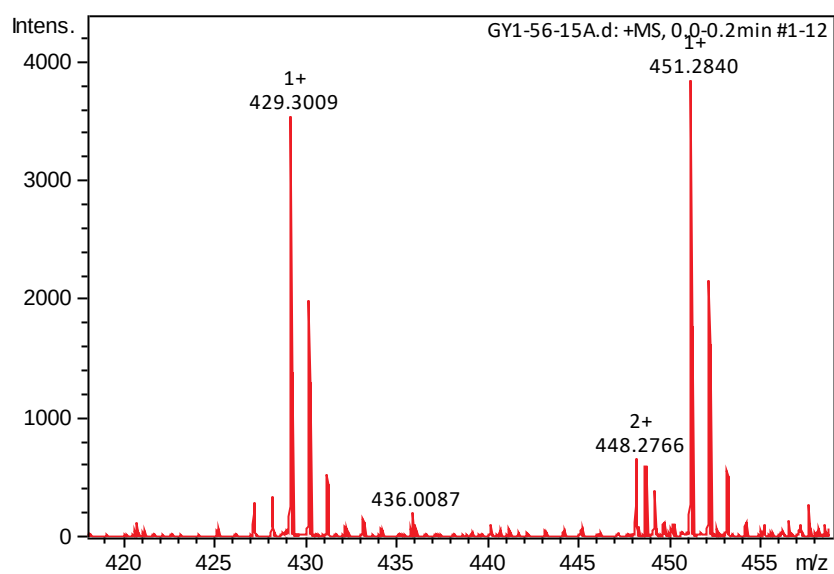
UV of compound 2



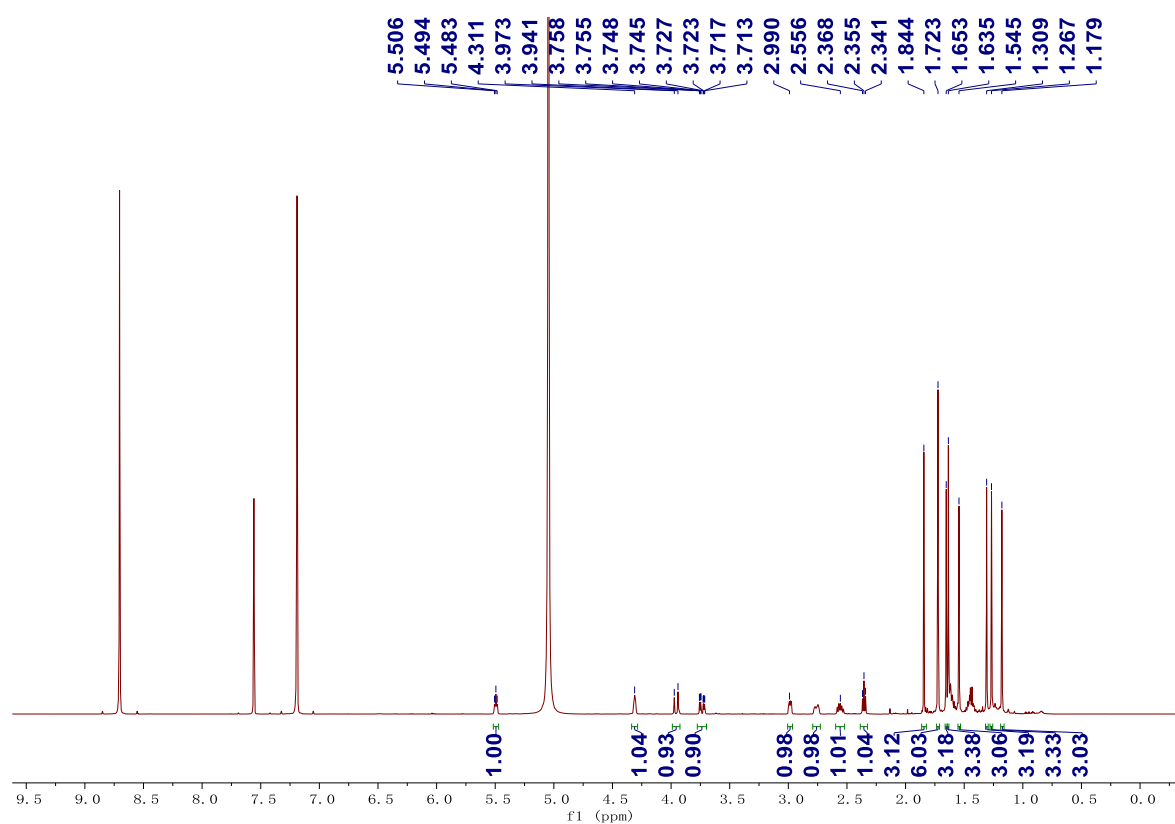
CD of compound 2



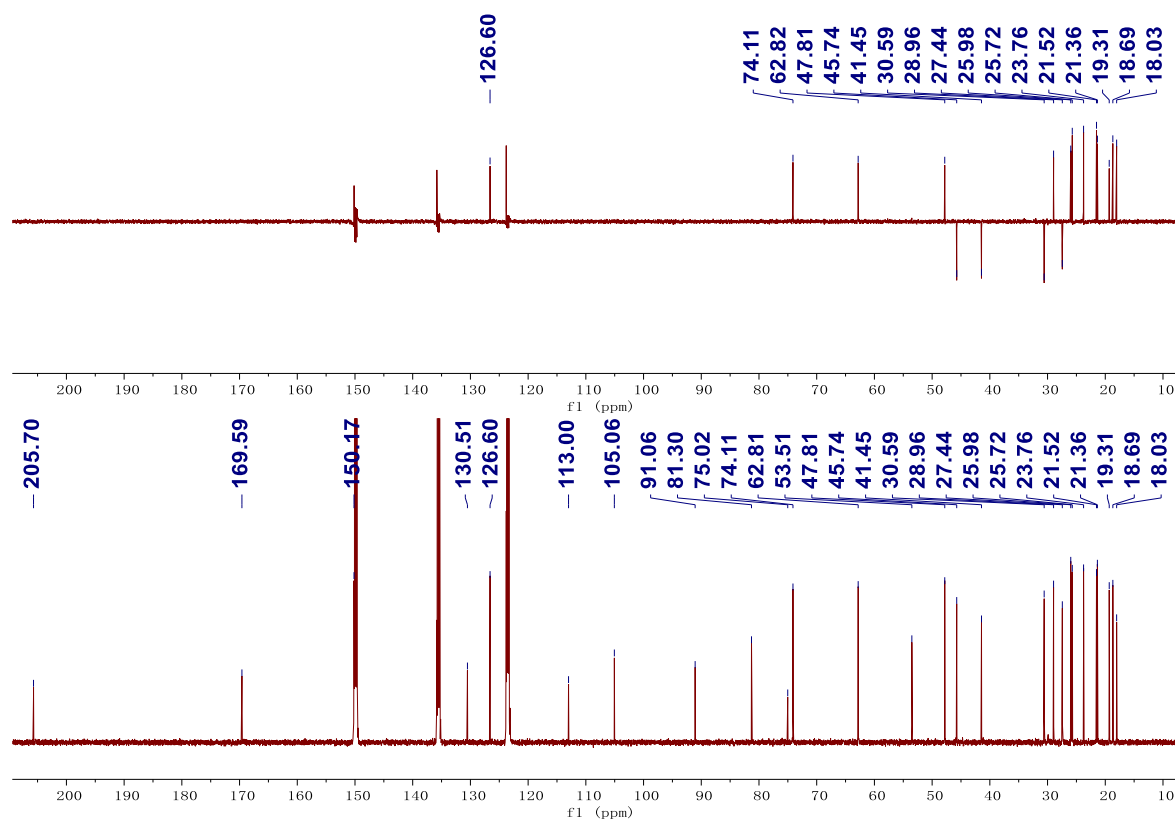
HRESIMS of compound **3**



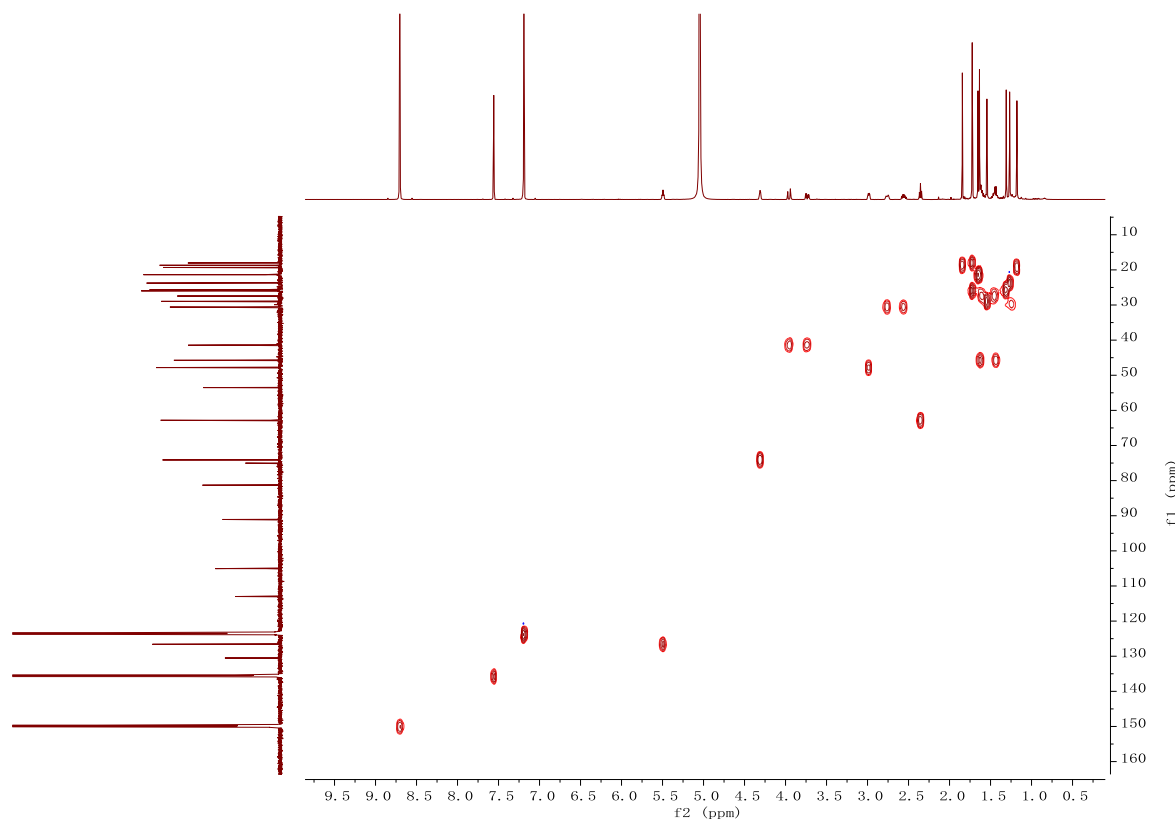
^1H NMR of compound **3** (600MHz, in $\text{C}_5\text{D}_5\text{N}$)



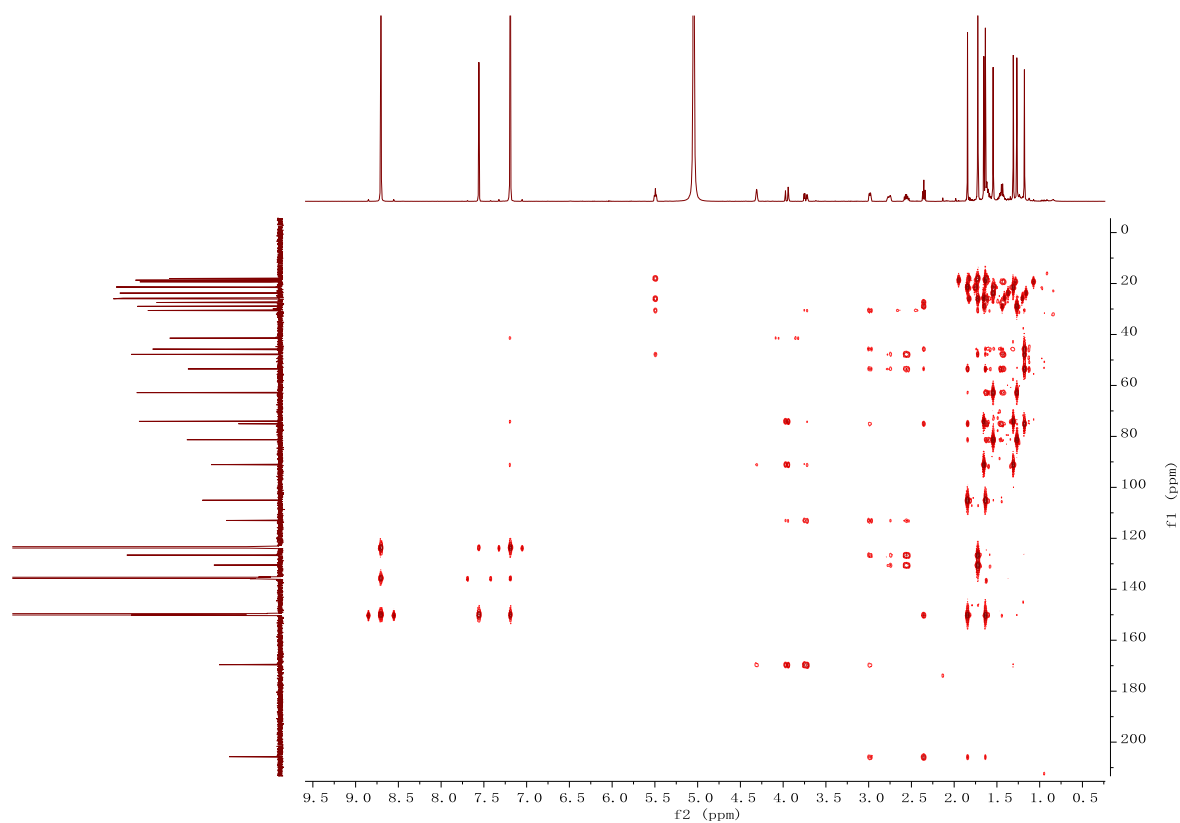
^{13}C NMR of compound **3** (150MHz, in $\text{C}_5\text{D}_5\text{N}$)



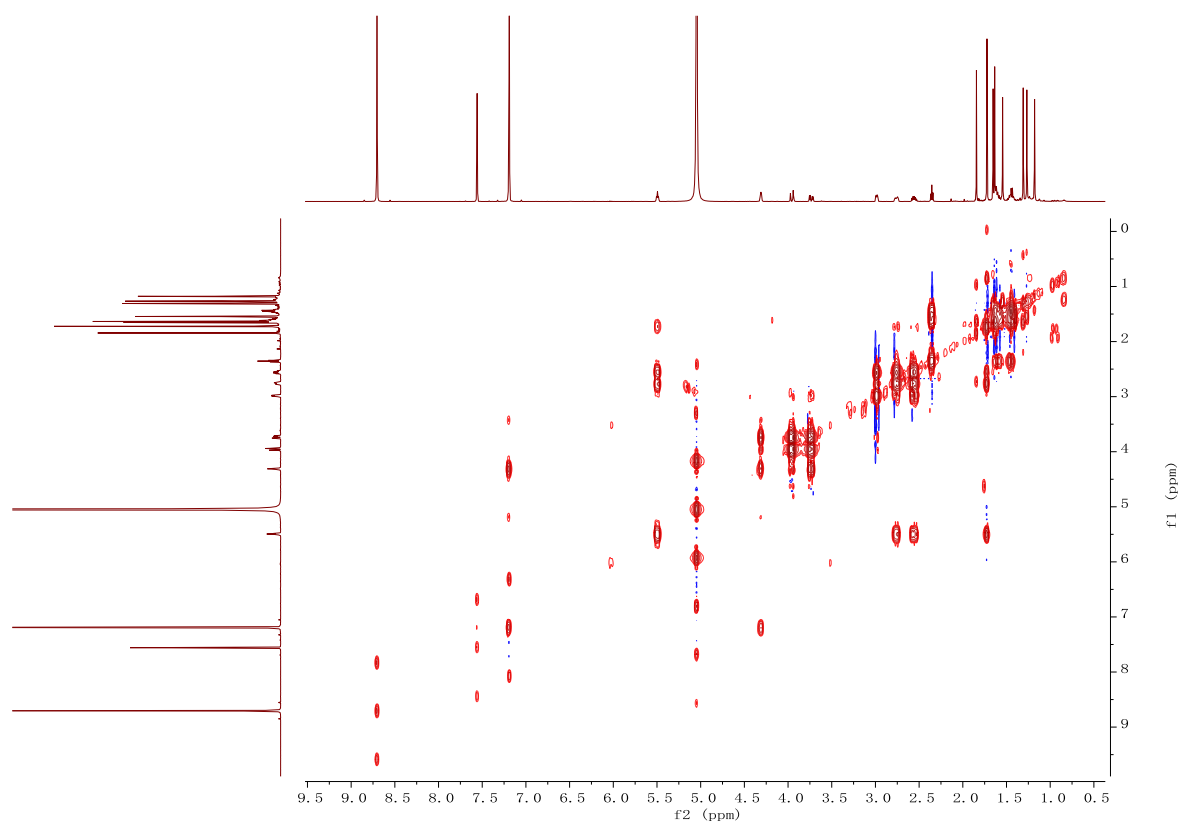
HSQC of compound **3** (600MHz, in $\text{C}_5\text{D}_5\text{N}$)



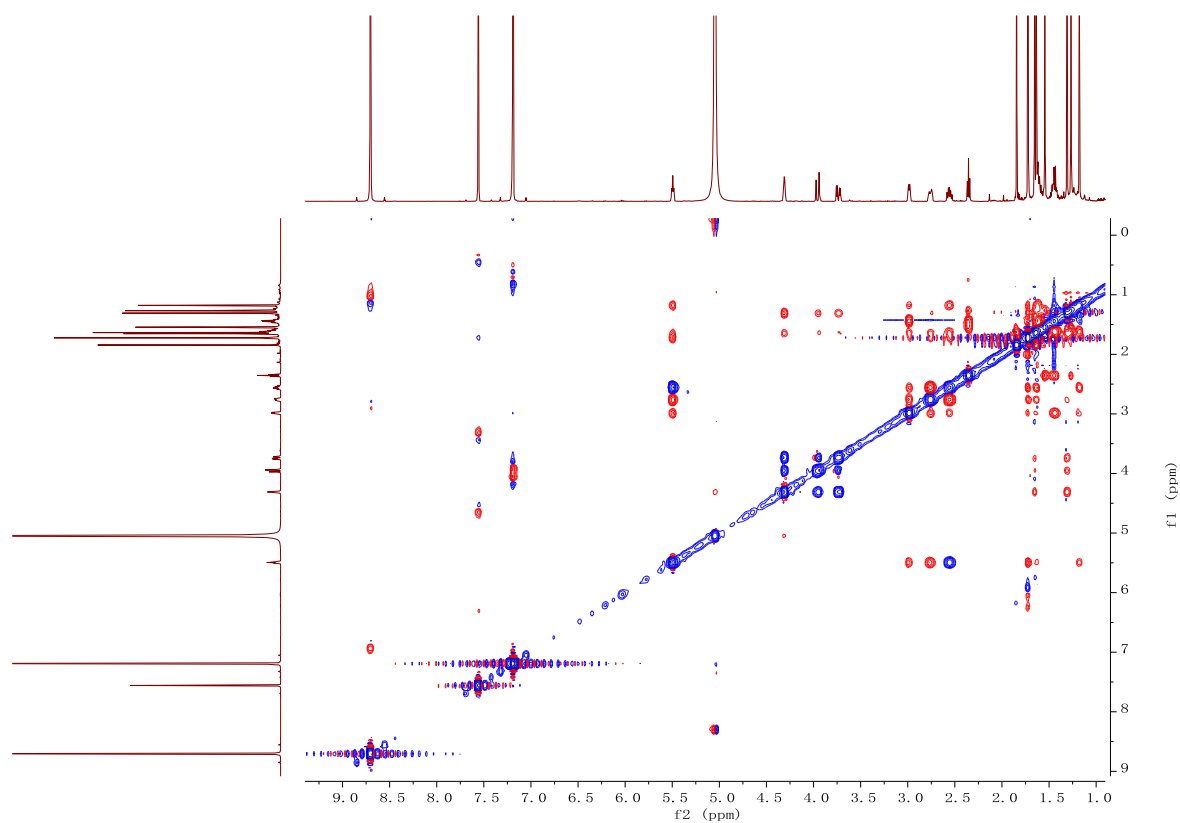
HMBC of compound **3** (600MHz, in C₅D₅N)



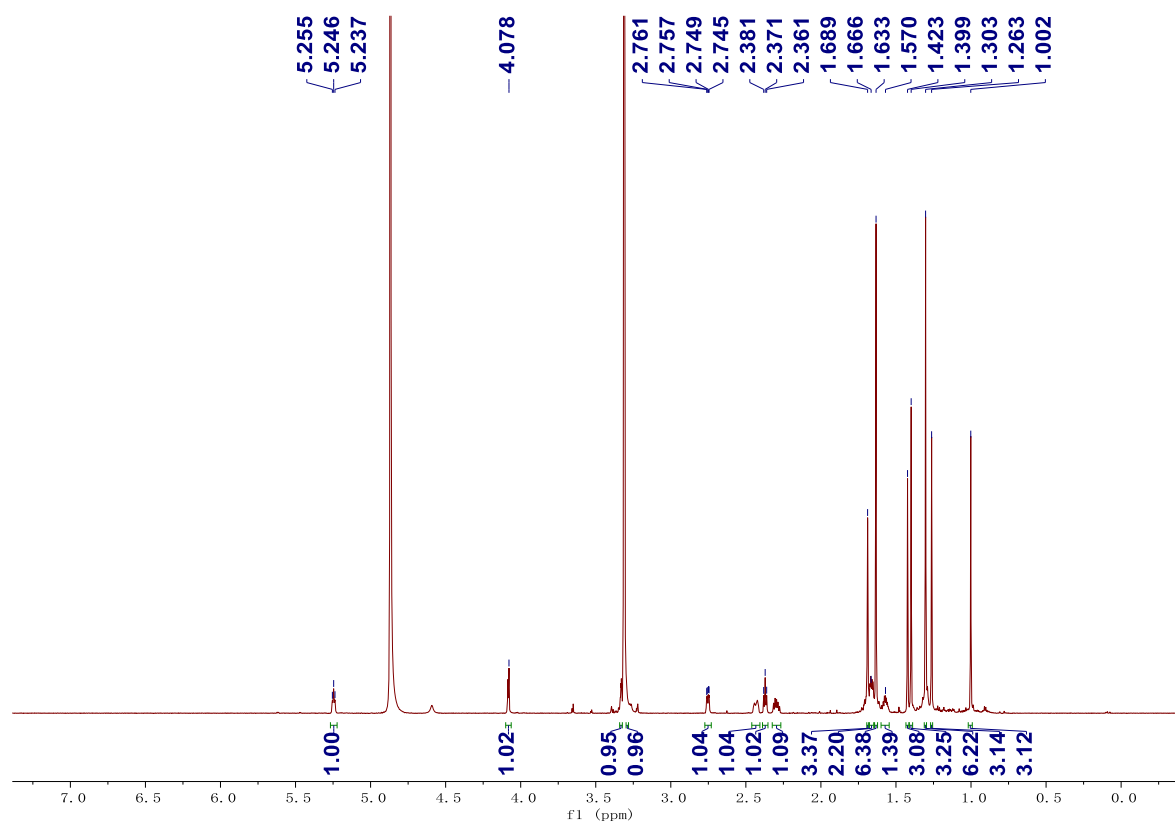
¹H-¹H COSY of compound **3** (600MHz, in C₅D₅N)



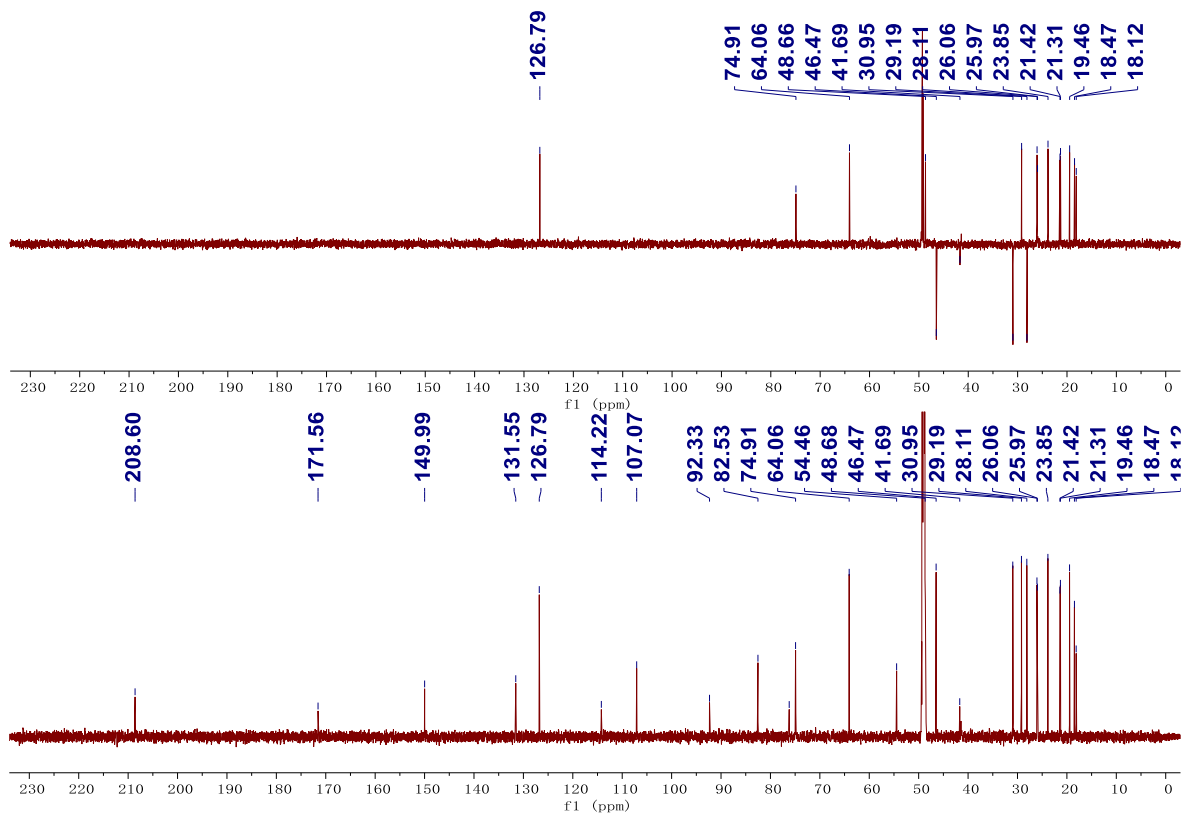
ROESY of compound **3** (600MHz, in C₅D₅N)



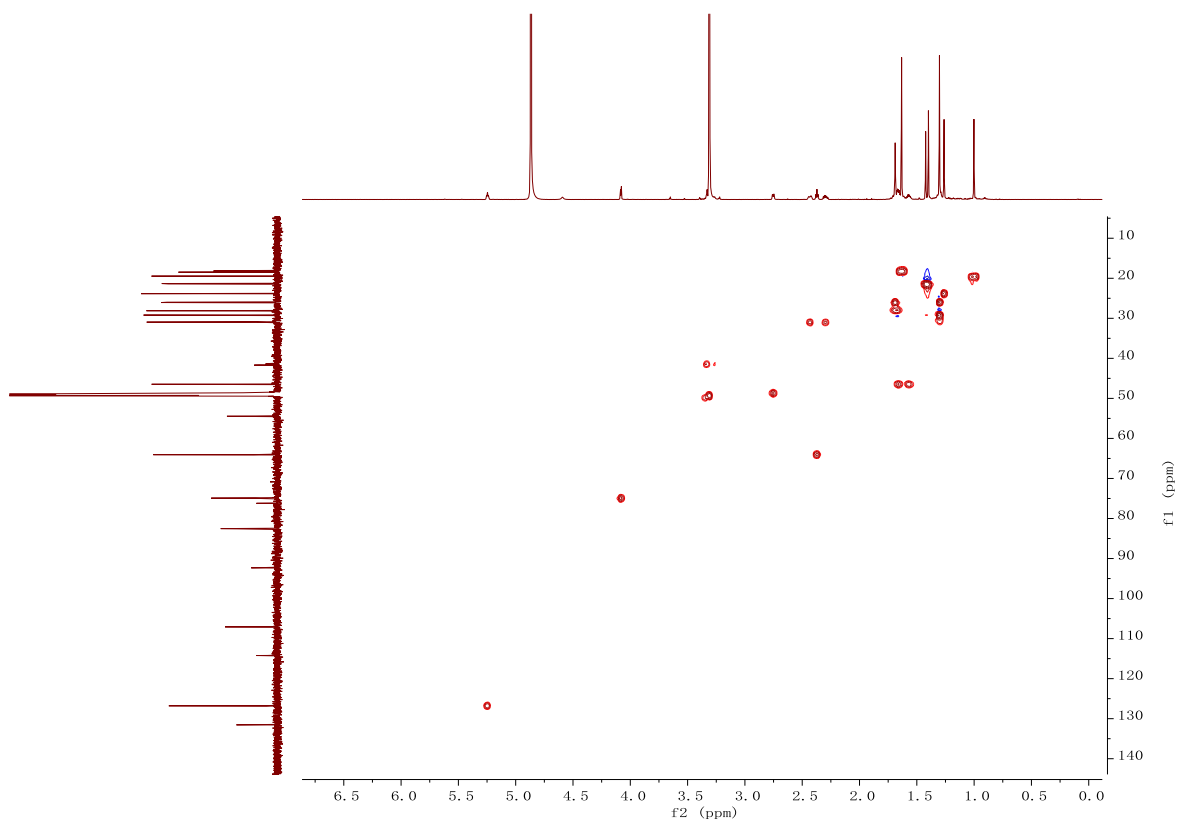
¹H NMR of compound **3** (800MHz, in CD₃OD)



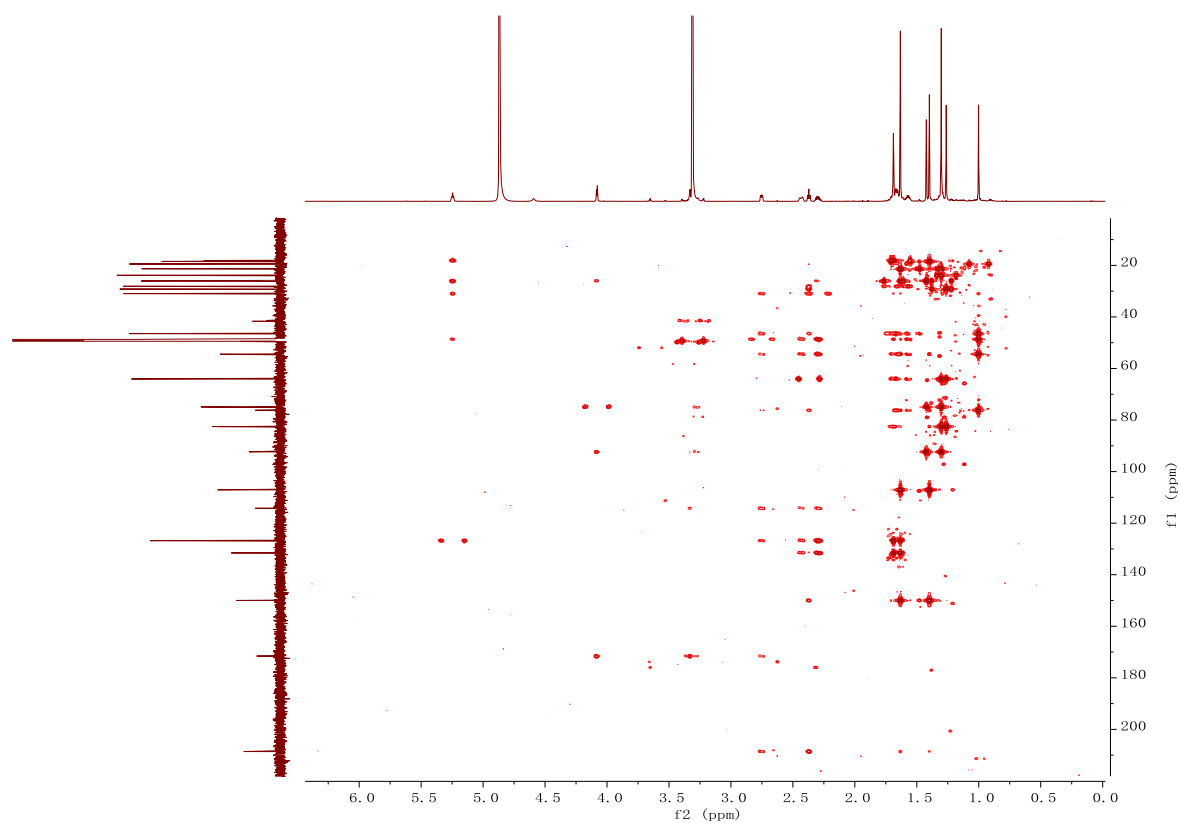
^{13}C NMR of compound **3** (200MHz, in CD_3OD)



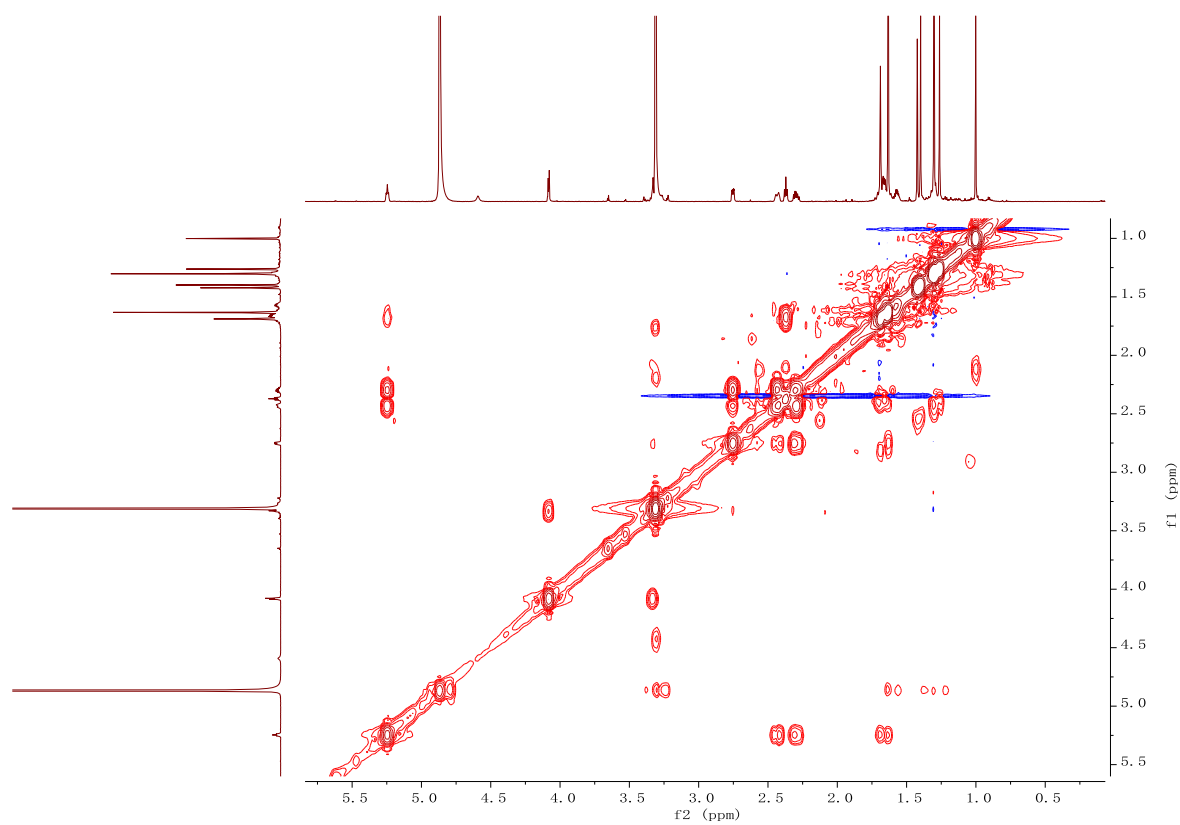
HSQC of compound **3** (800MHz, in CD_3OD)



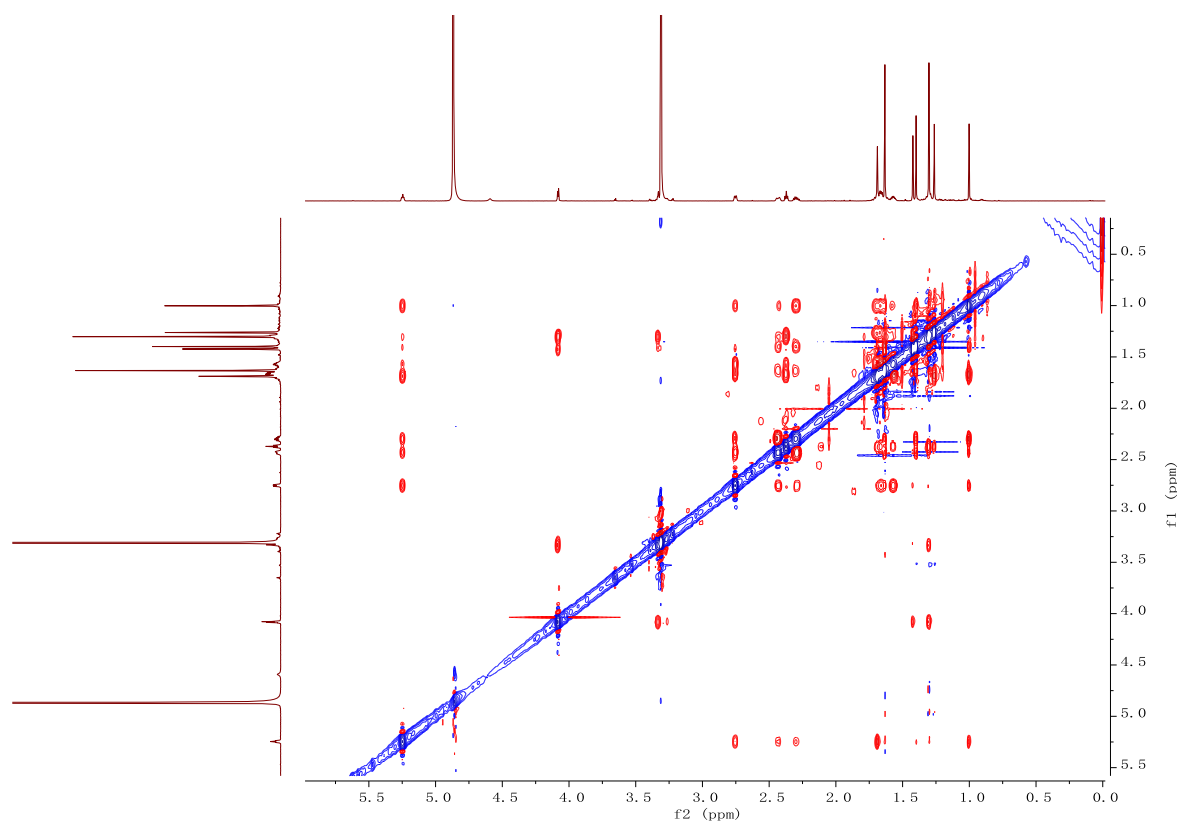
HMBC of compound **3** (800MHz, in CD₃OD)



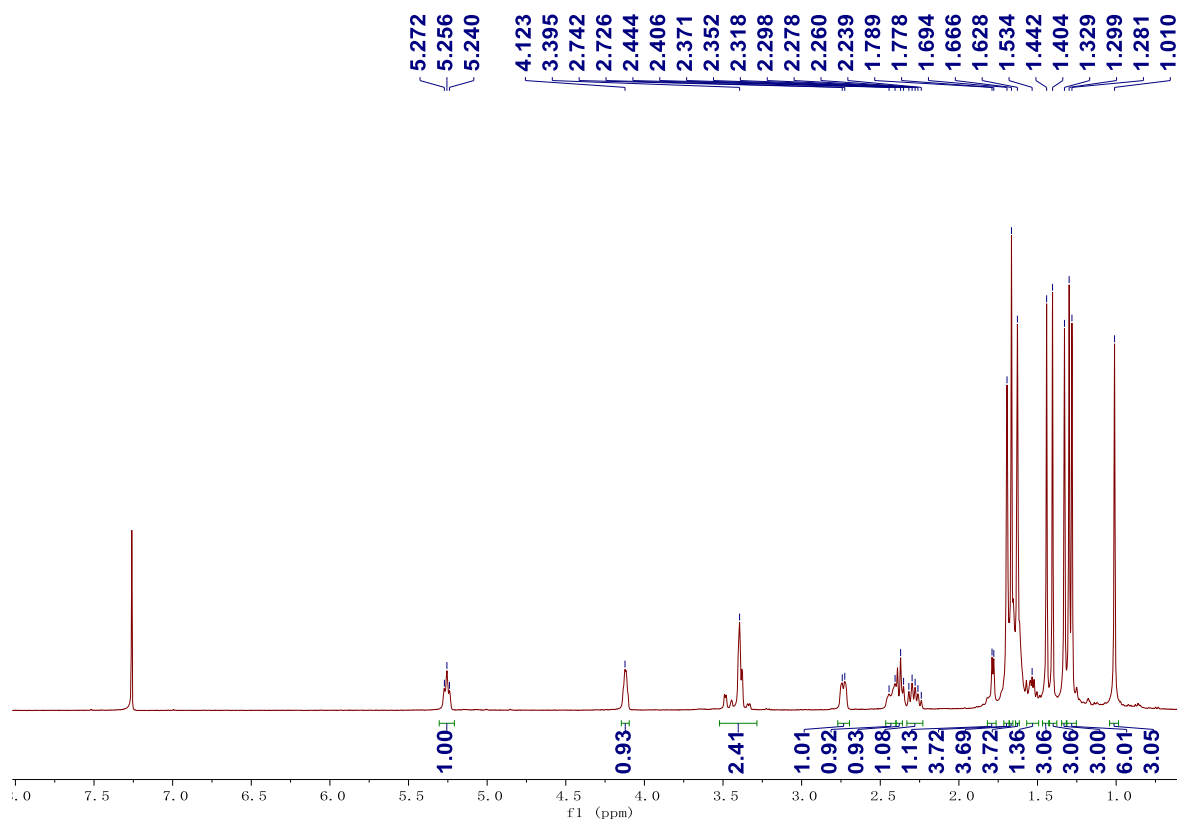
¹H-¹H COSY of compound **3** (800MHz, in CD₃OD)



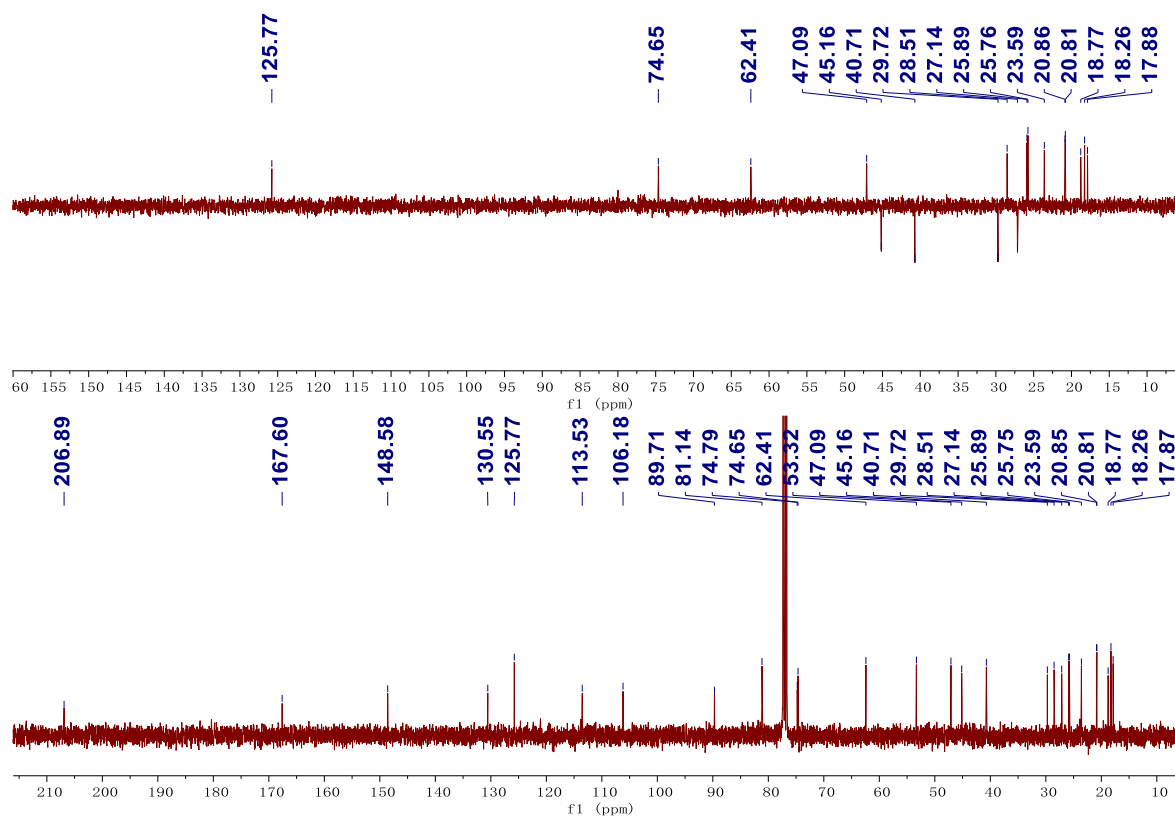
ROESY of compound **3** (800MHz, in CD₃OD)



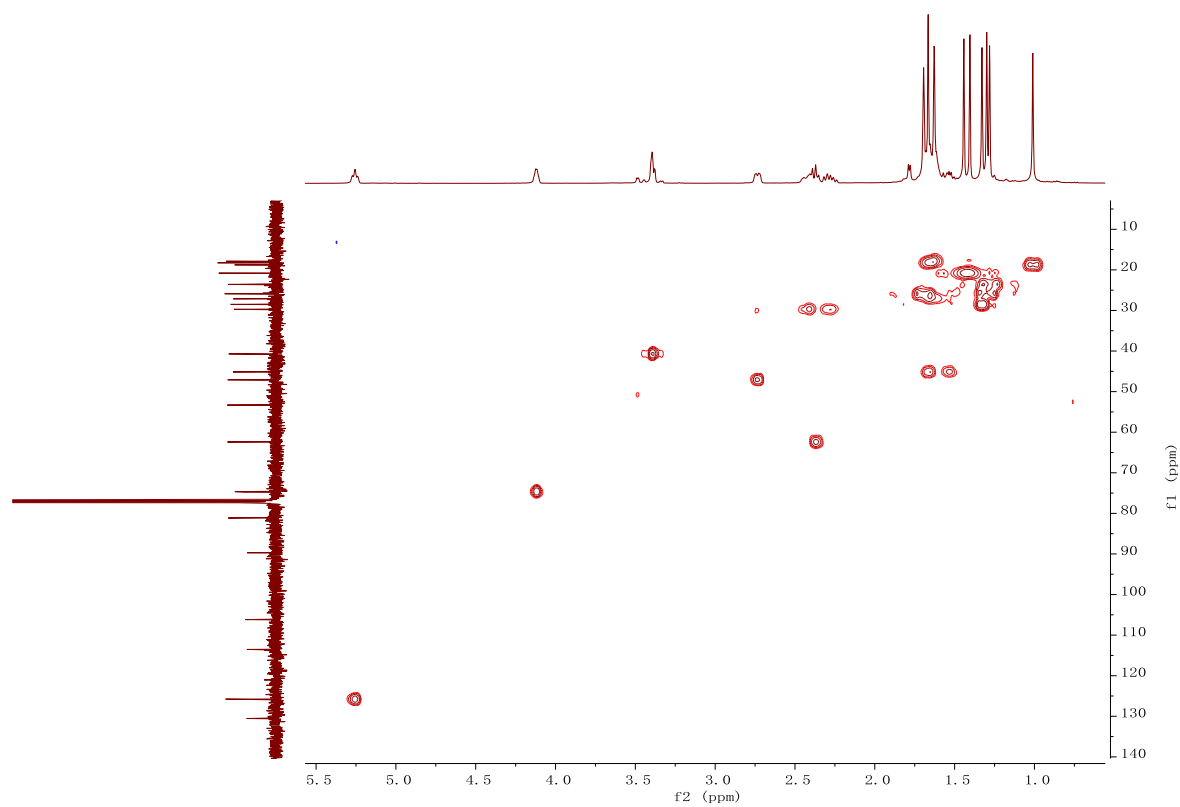
¹H NMR of compound **3** (400MHz, in CDCl₃)



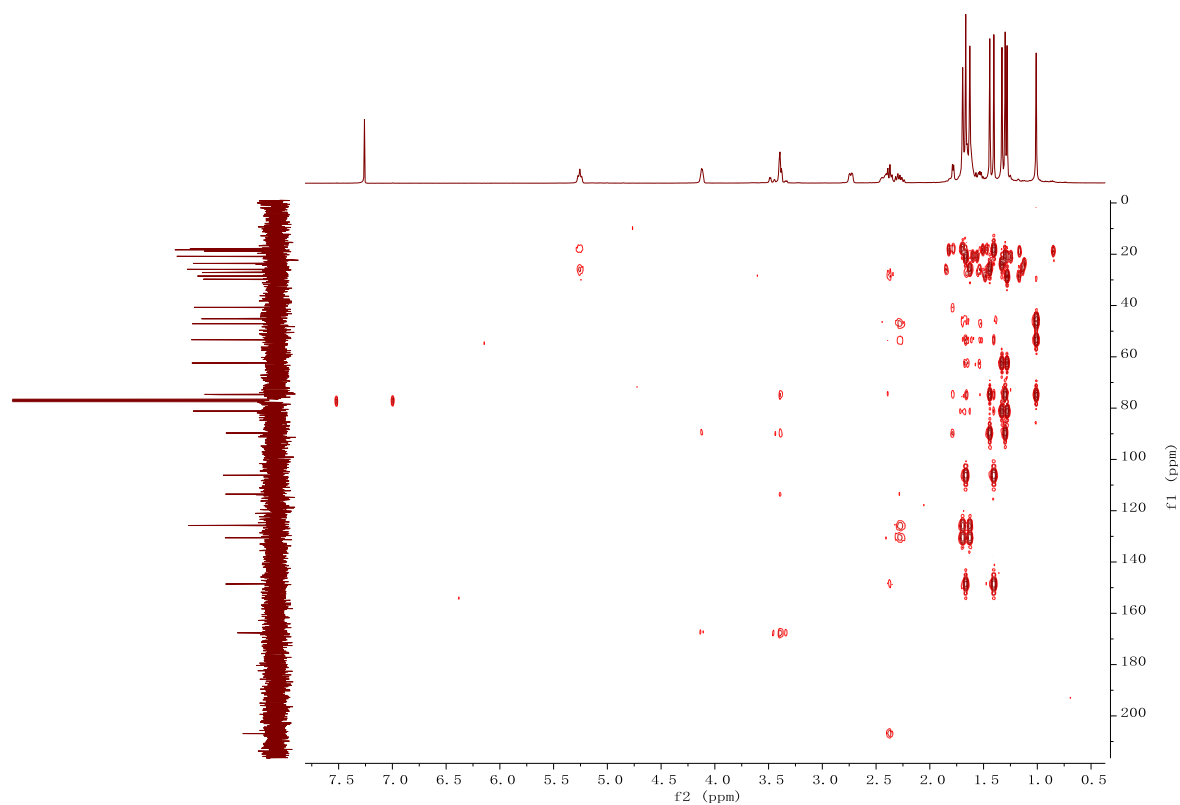
^{13}C NMR of compound **3** (100MHz, in CDCl_3)



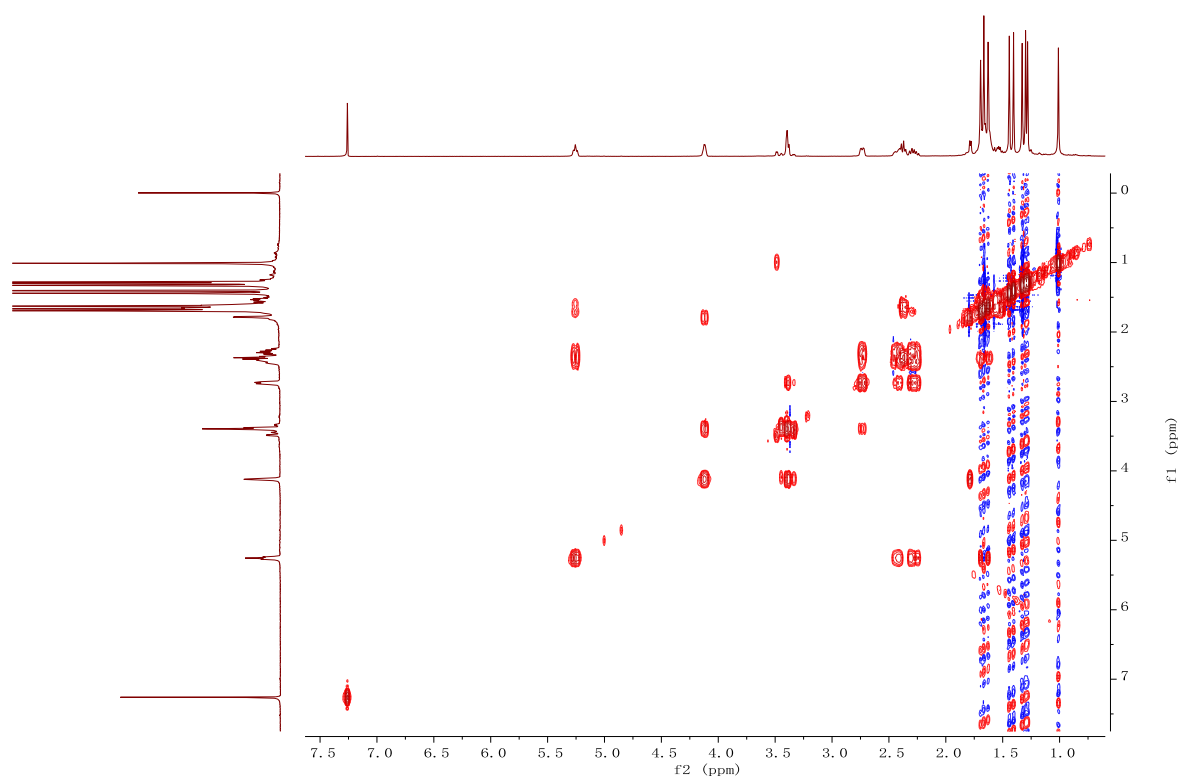
HSQC of compound **3** (400MHz, in CDCl_3)



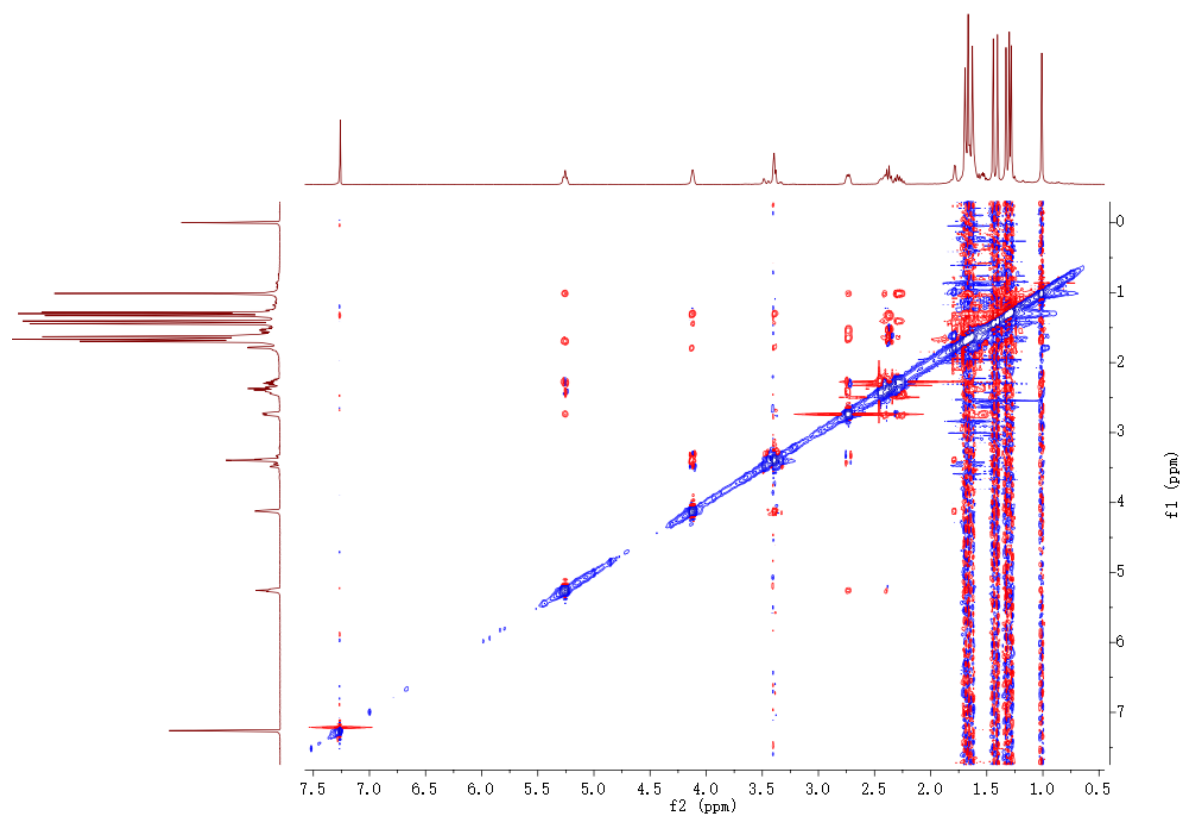
HMBC of compound **3** (400MHz, in CDCl₃)



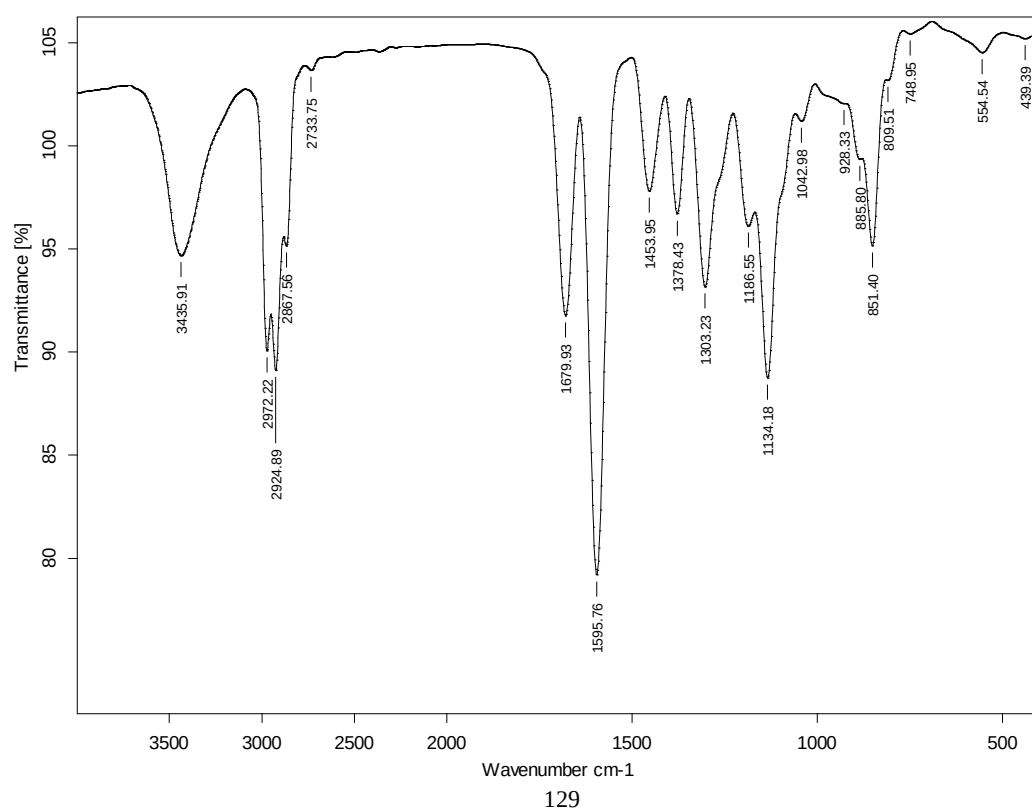
¹H-¹H COSY of compound **3** (400MHz, in CDCl₃)



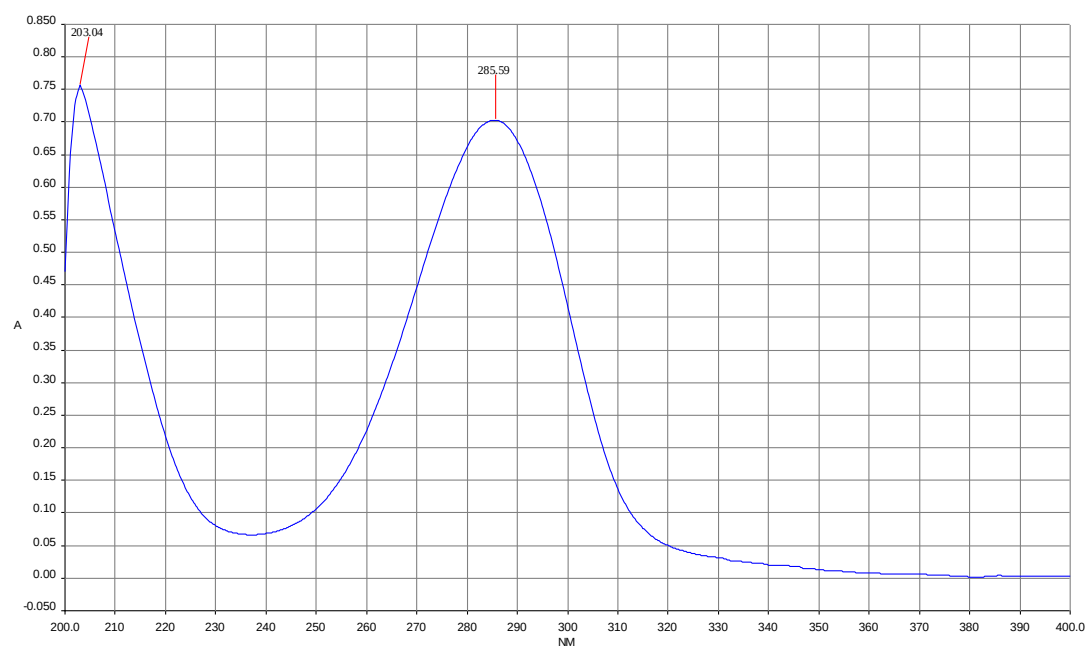
NOESY of compound **3** (400MHz, in CDCl₃)



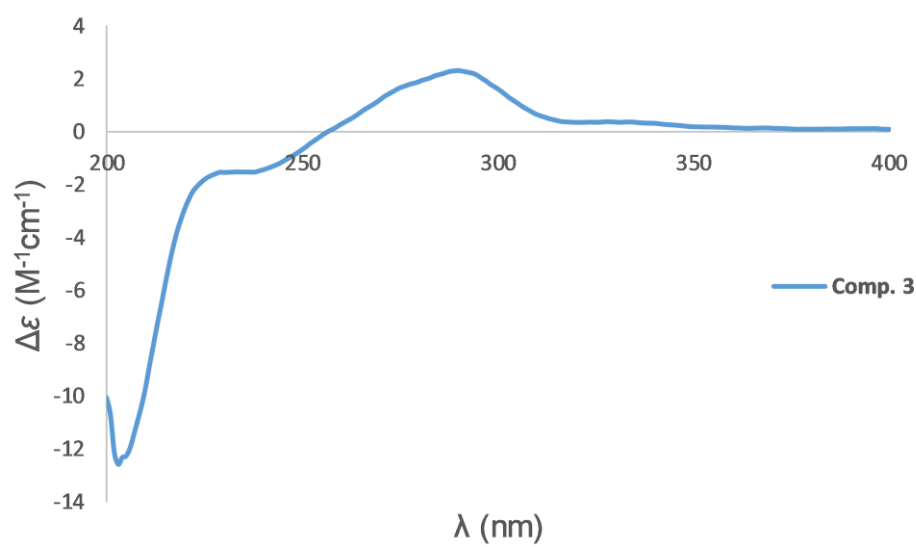
IR of compound **3**



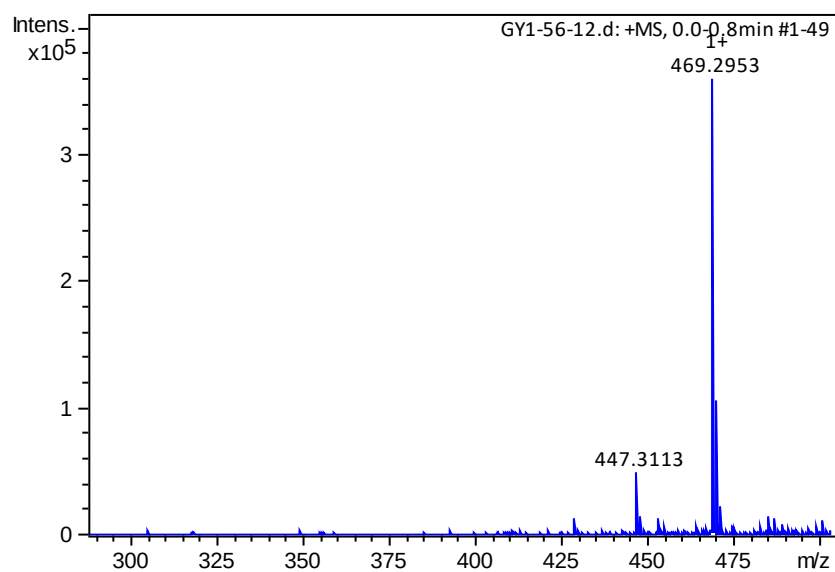
UV of compound 3



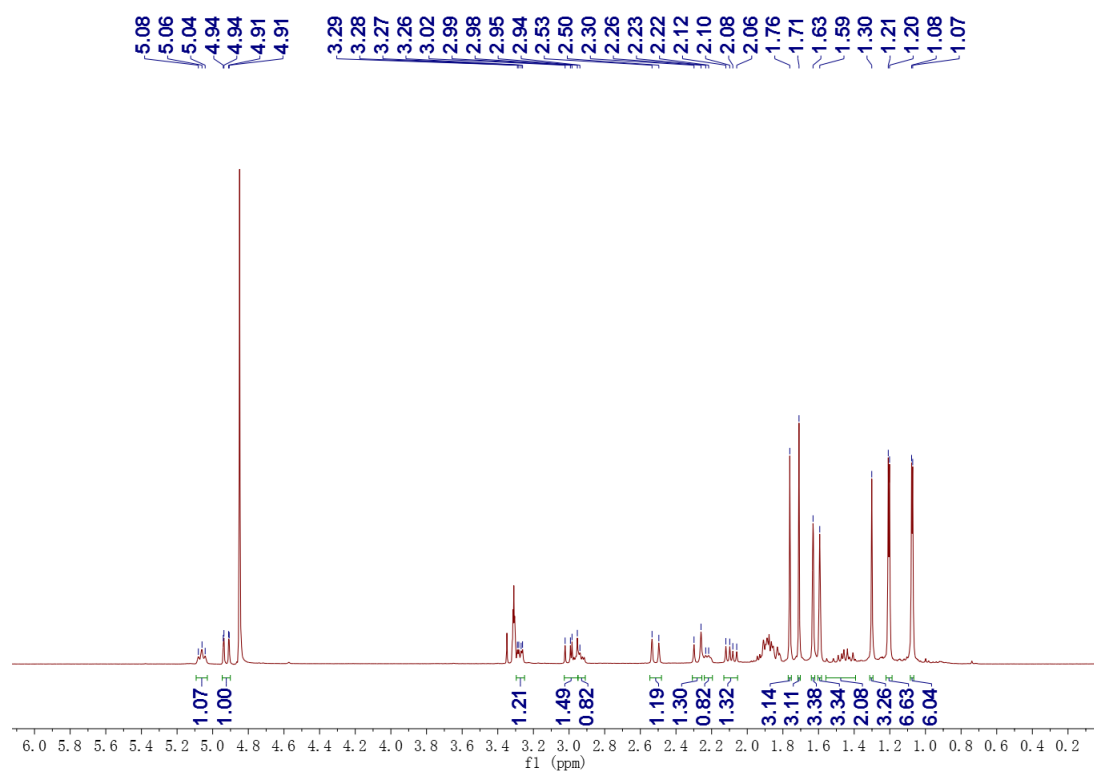
CD of compound 3



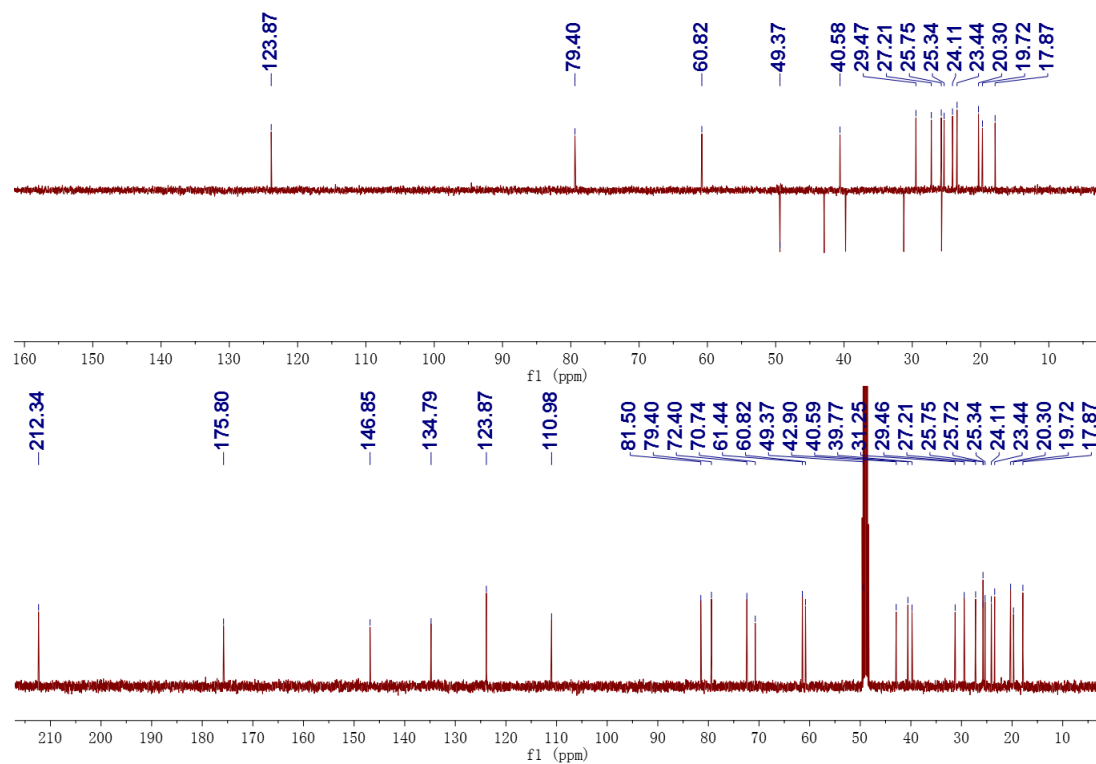
HRESIMS of compound 4



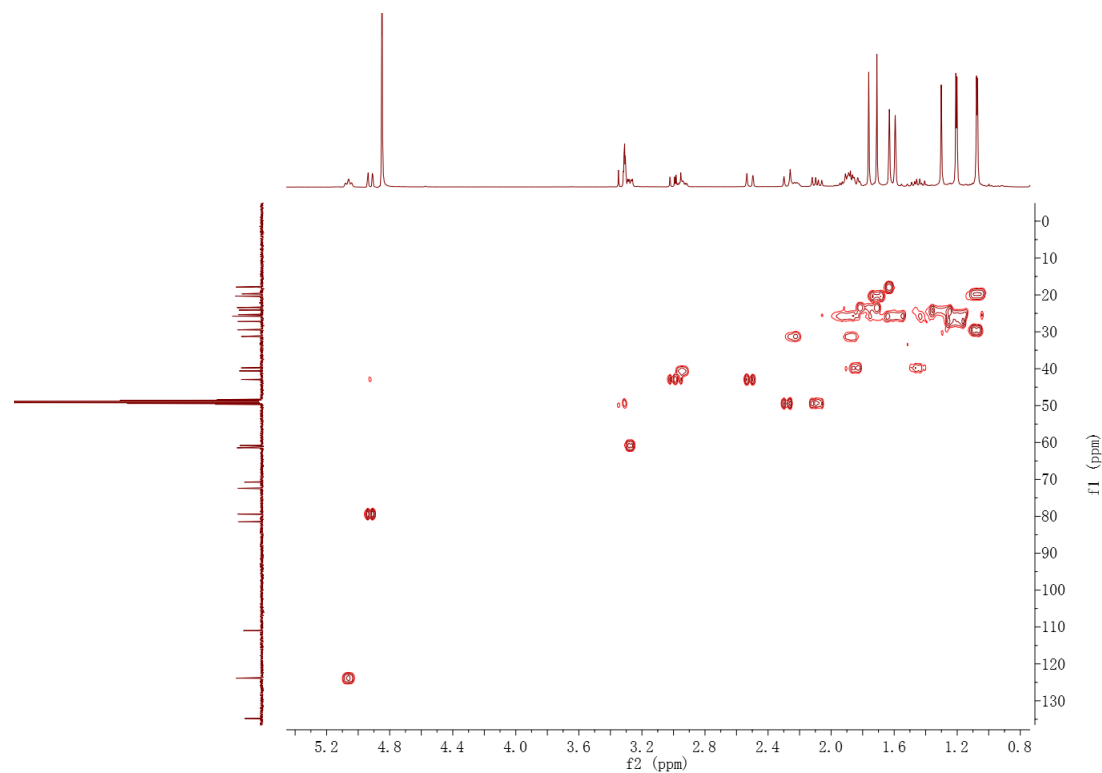
¹H NMR of compound 4 (400MHz, in CD₃OD)



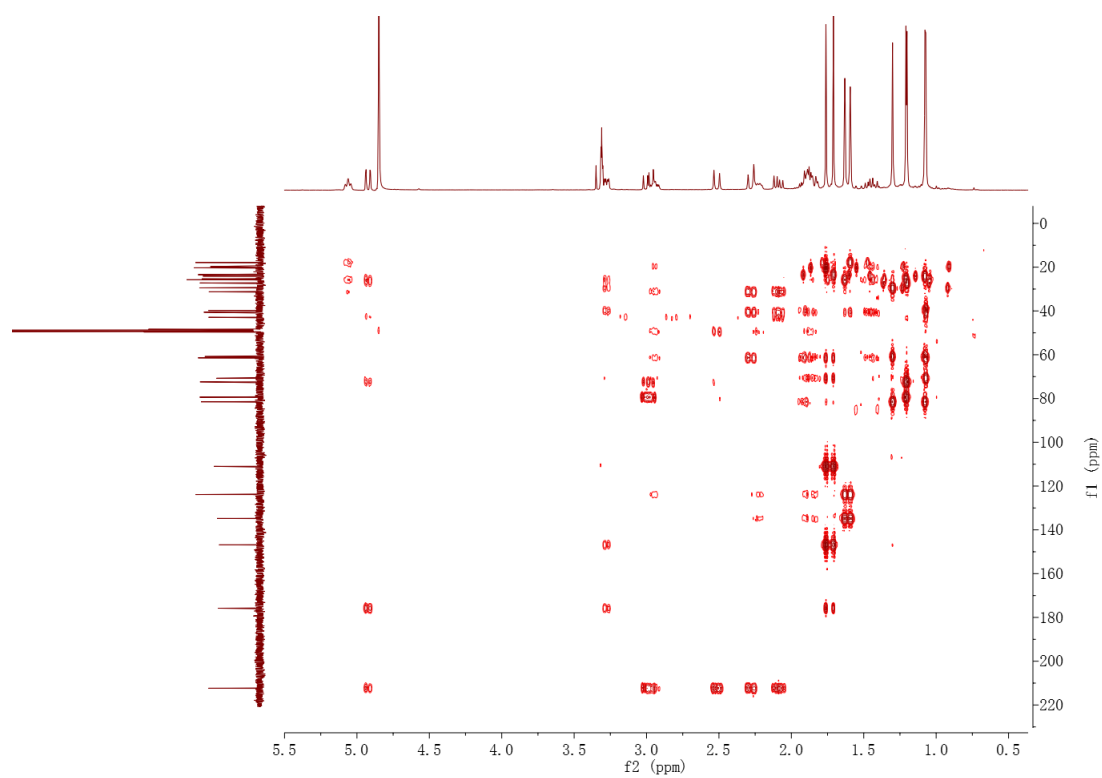
^{13}C NMR of compound **4** (100MHz, in CD_3OD)



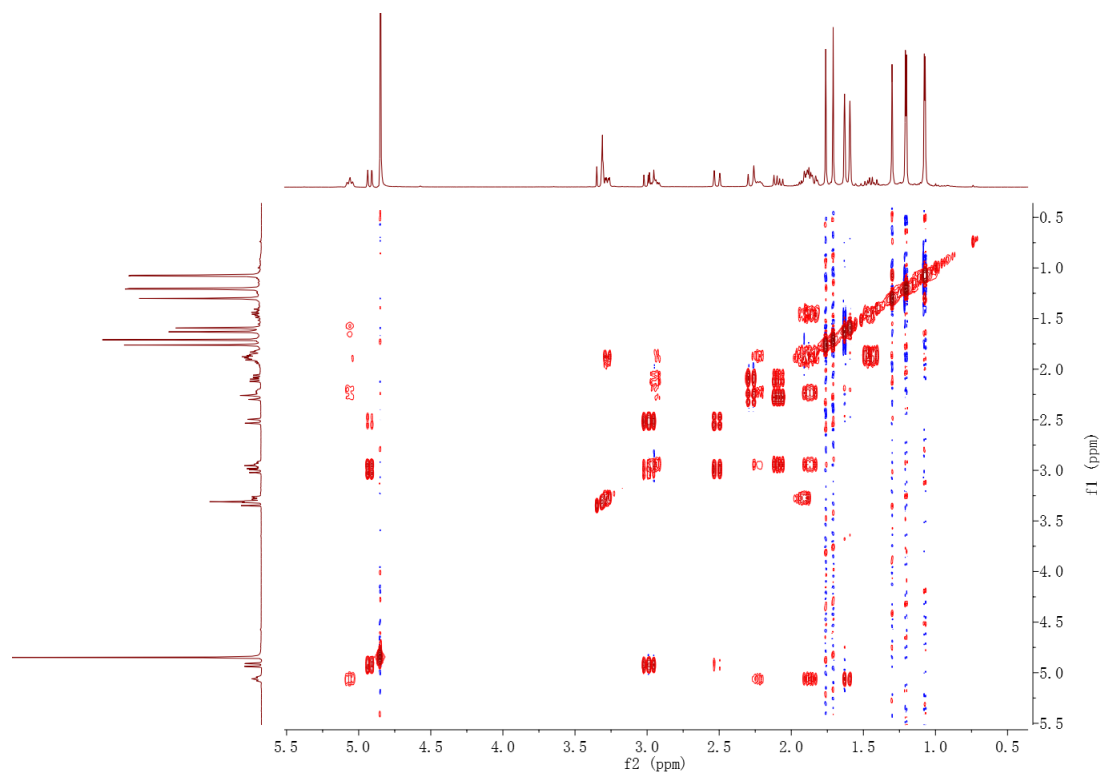
HSQC of compound **4** (400MHz, in CD_3OD)



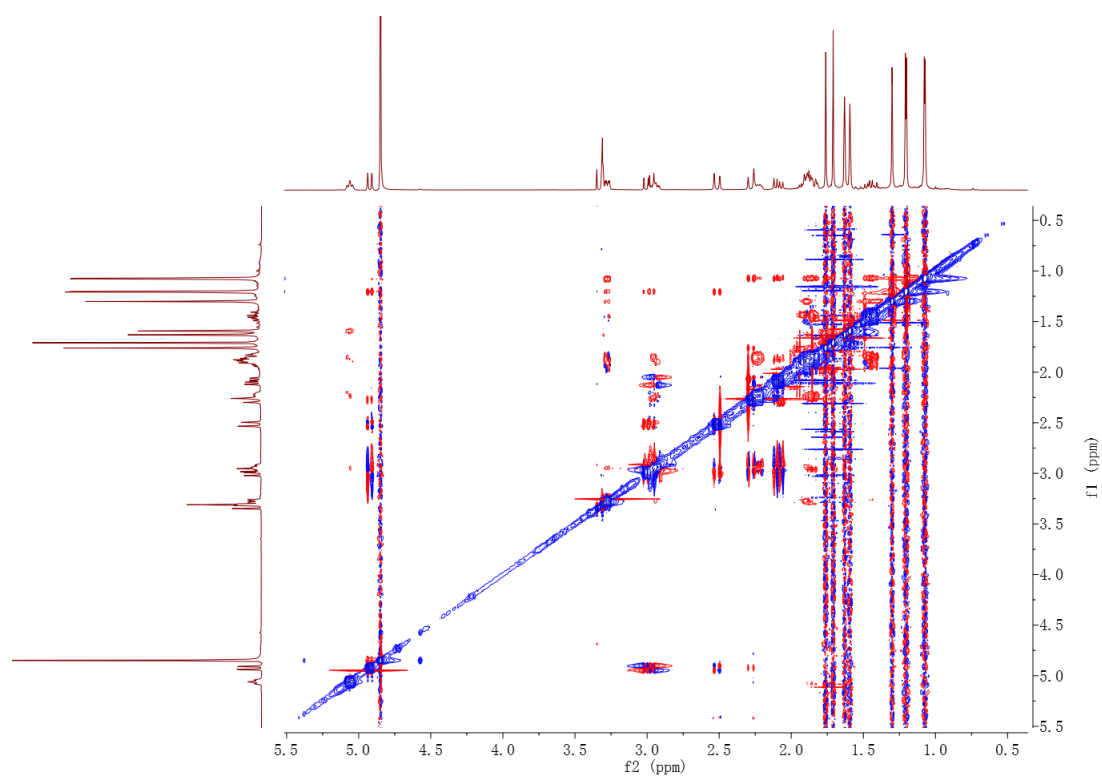
HMBC of compound **4** (400MHz, in CD₃OD)



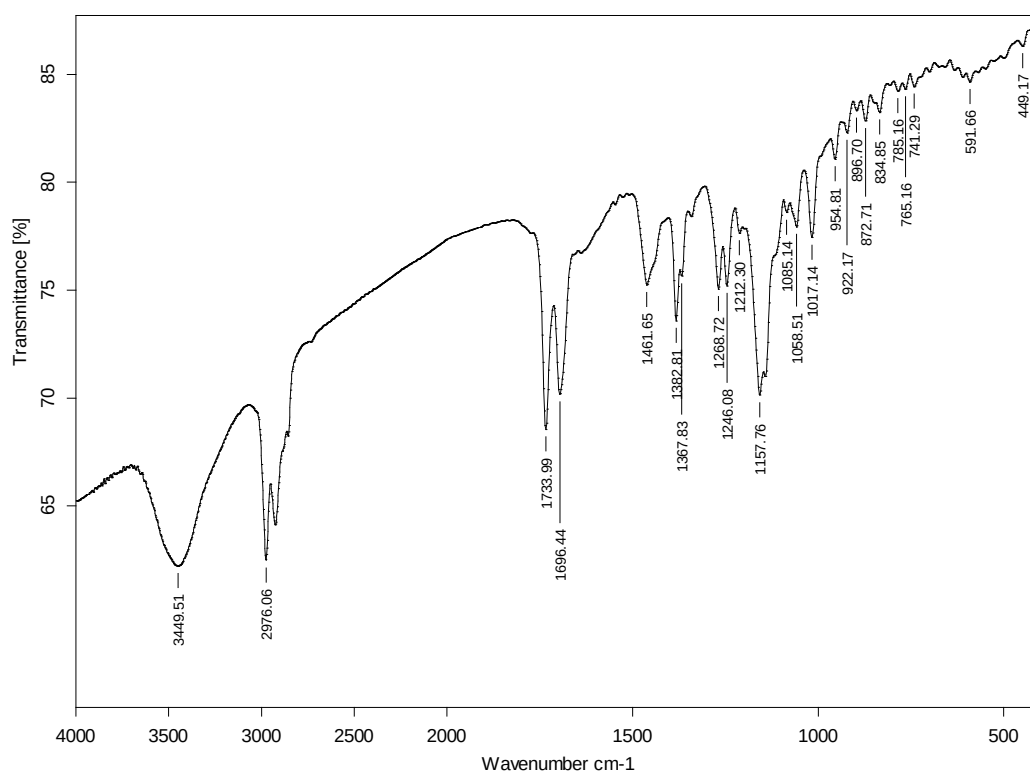
¹H-¹H COSY of compound **4** (400MHz, in CD₃OD)



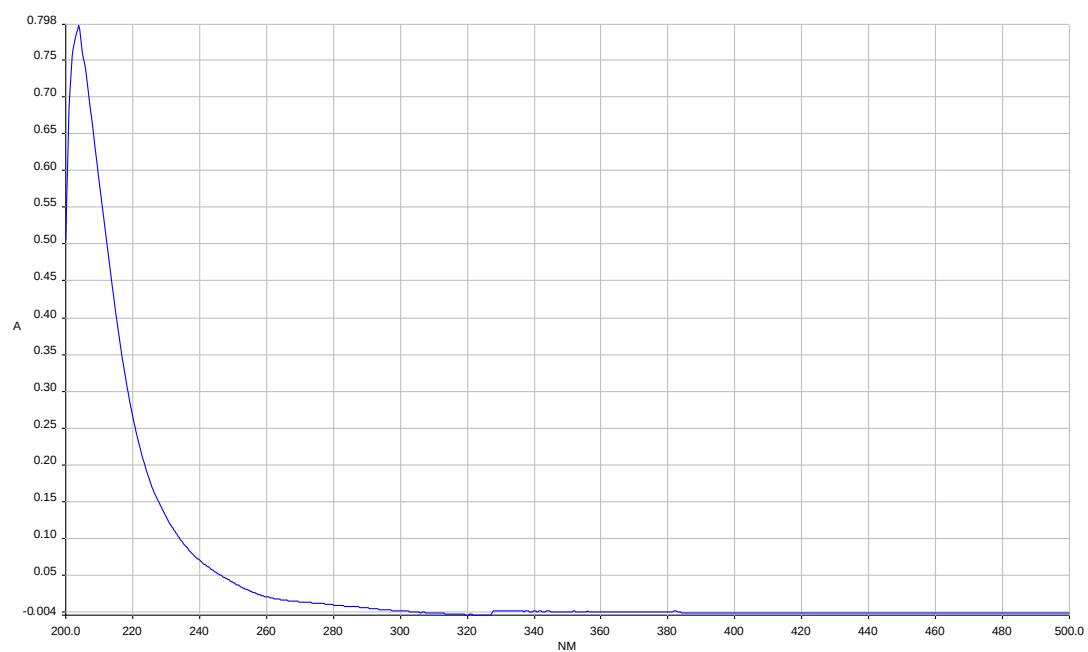
NOESY of compound **4** (400MHz, in CD₃OD)



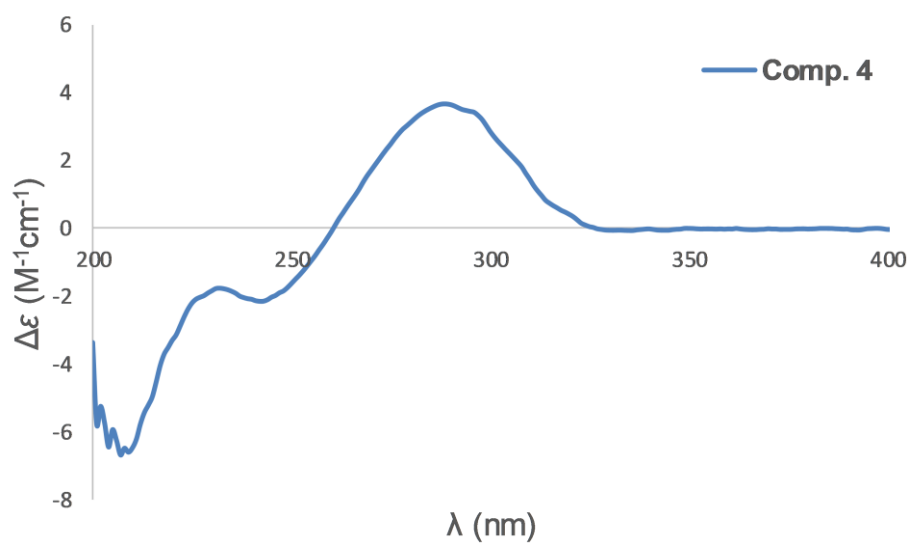
IR of compound **4**



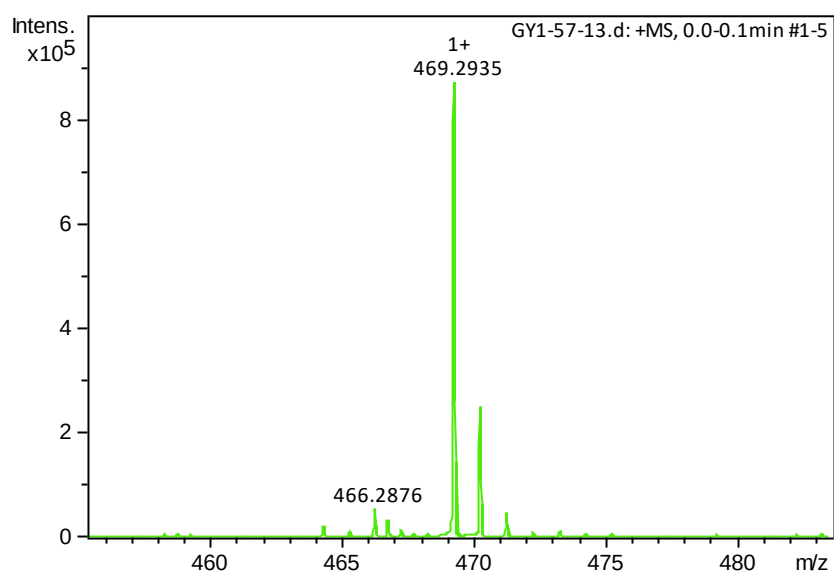
UV of compound **4**



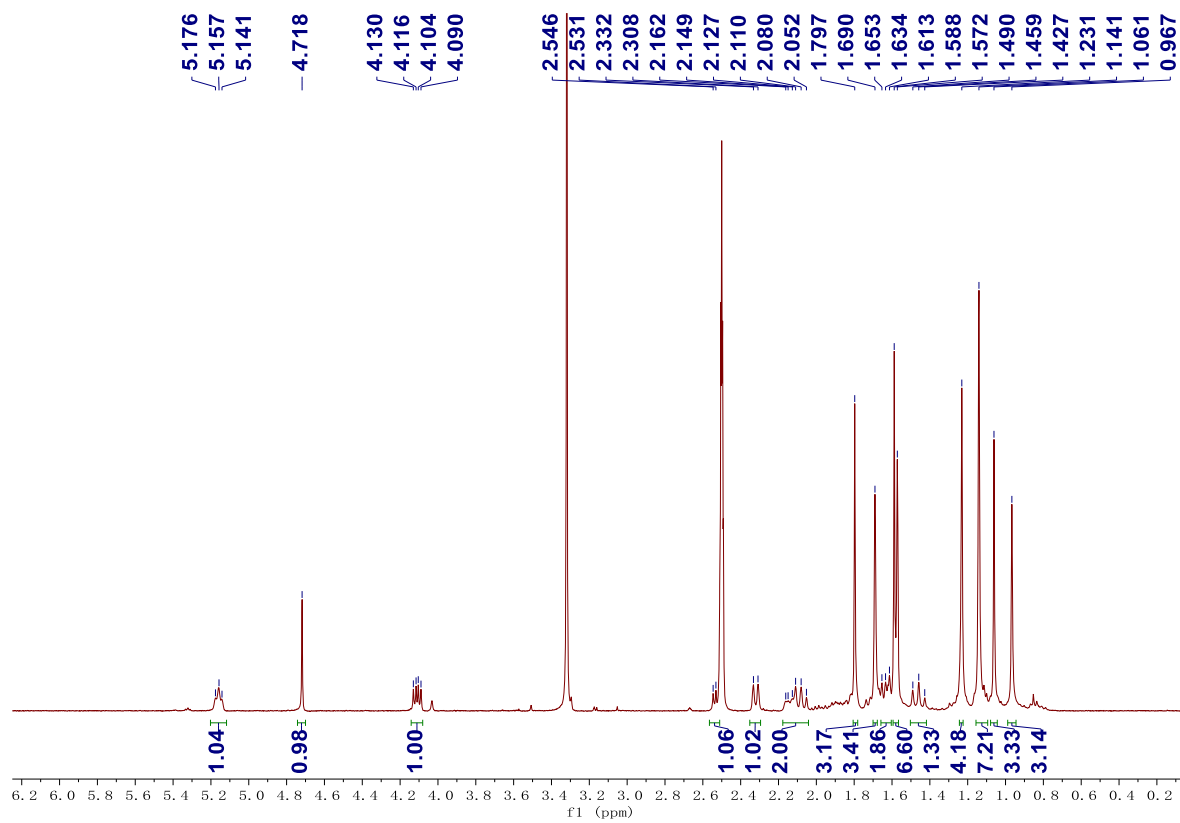
CD of compound **4**



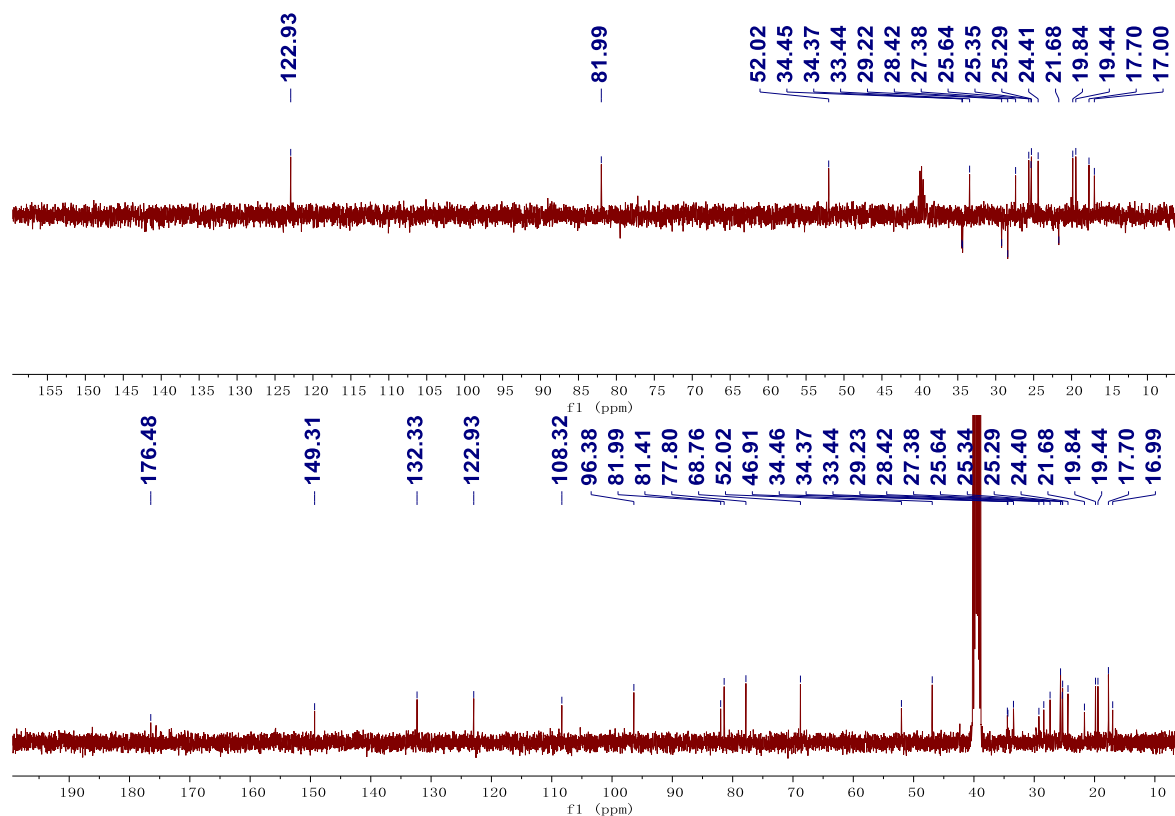
HRESIMS of compound 5



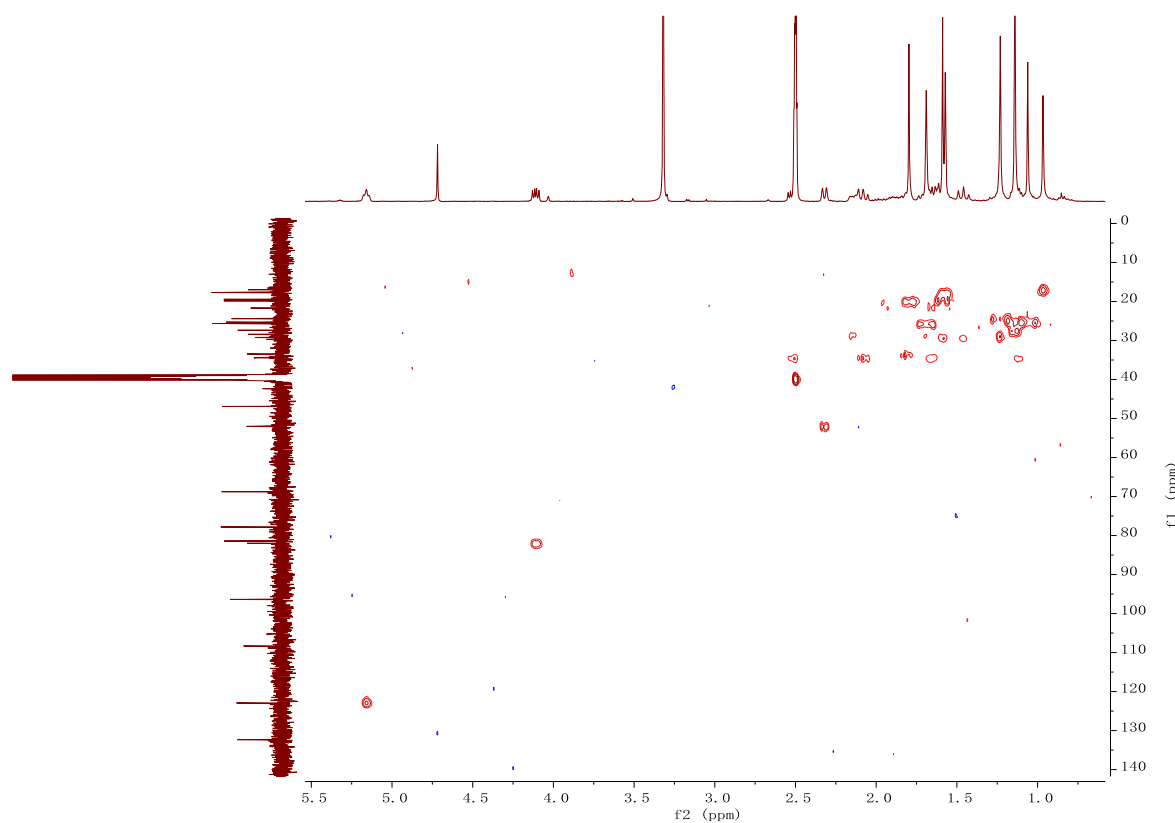
¹H NMR of compound 5 (400MHz, in DMSO-d₆)



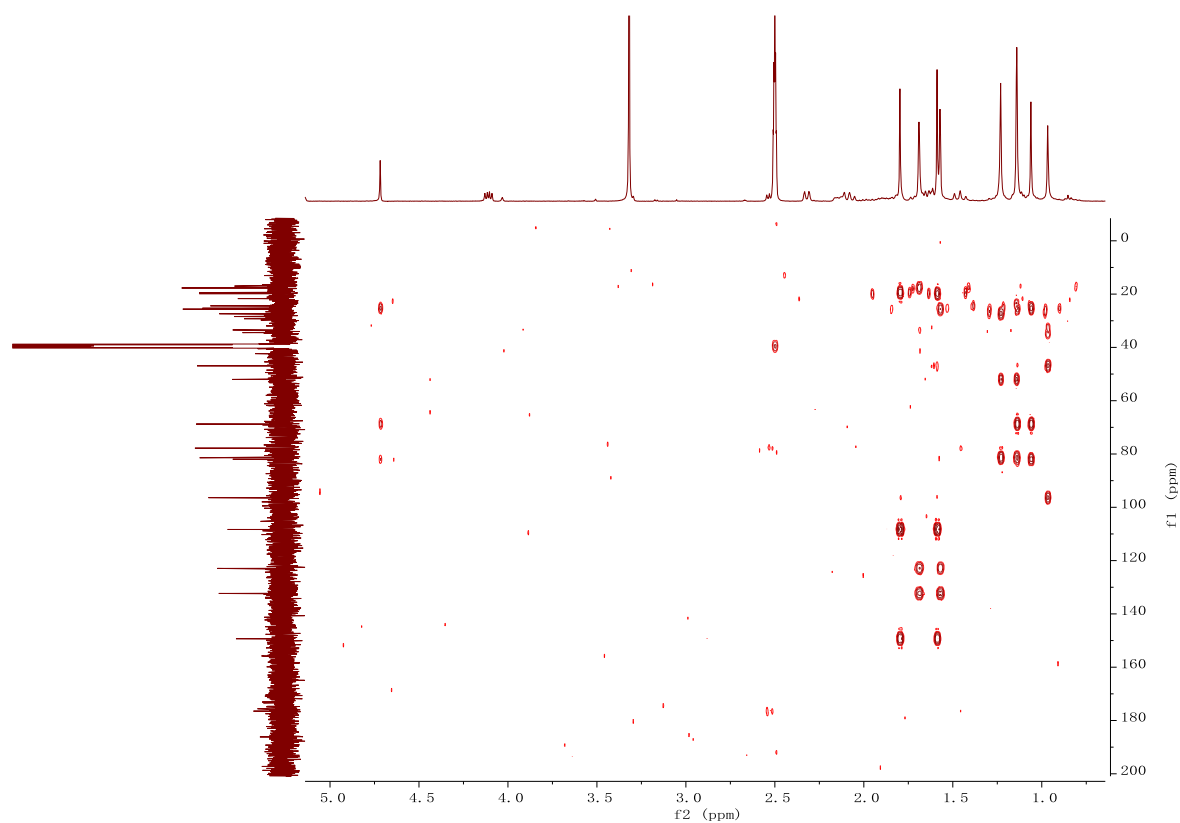
^{13}C NMR of compound 5 (100MHz, in $\text{DMSO}-d_6$)



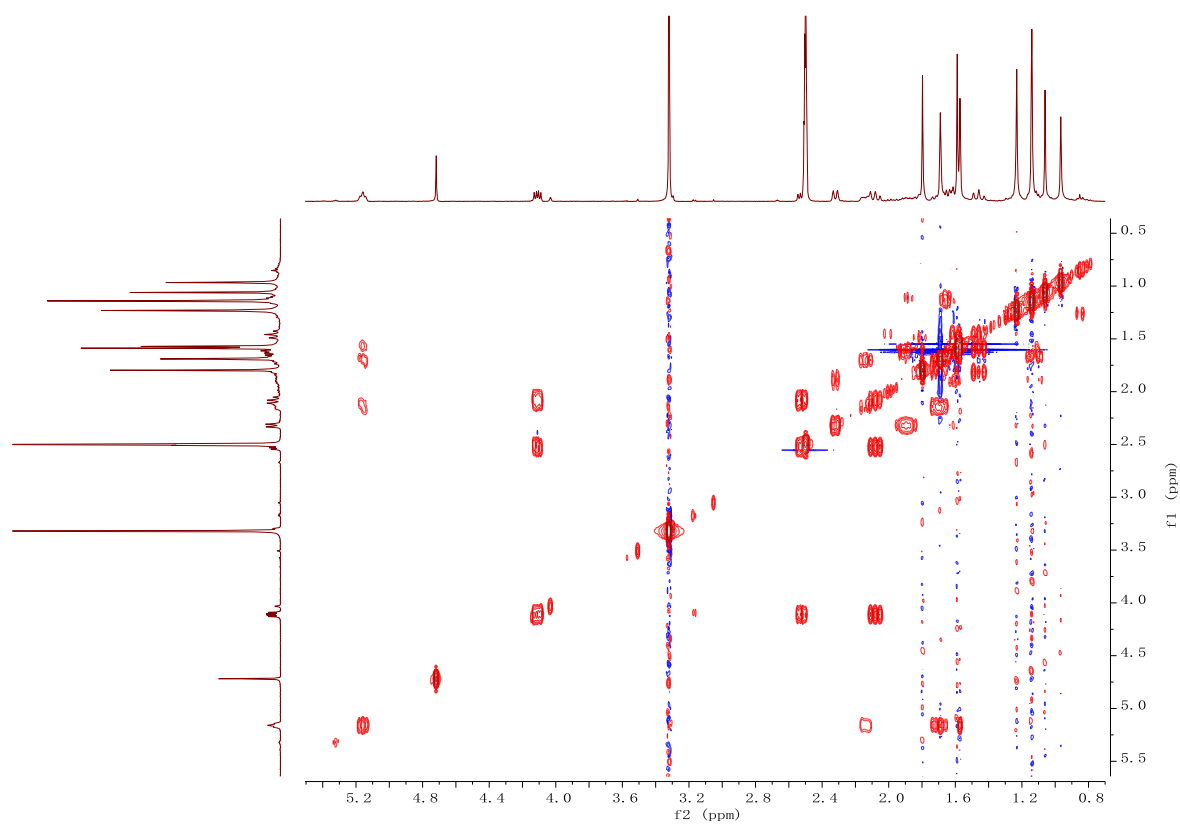
HSQC of compound 5 (400MHz, in $\text{DMSO}-d_6$)



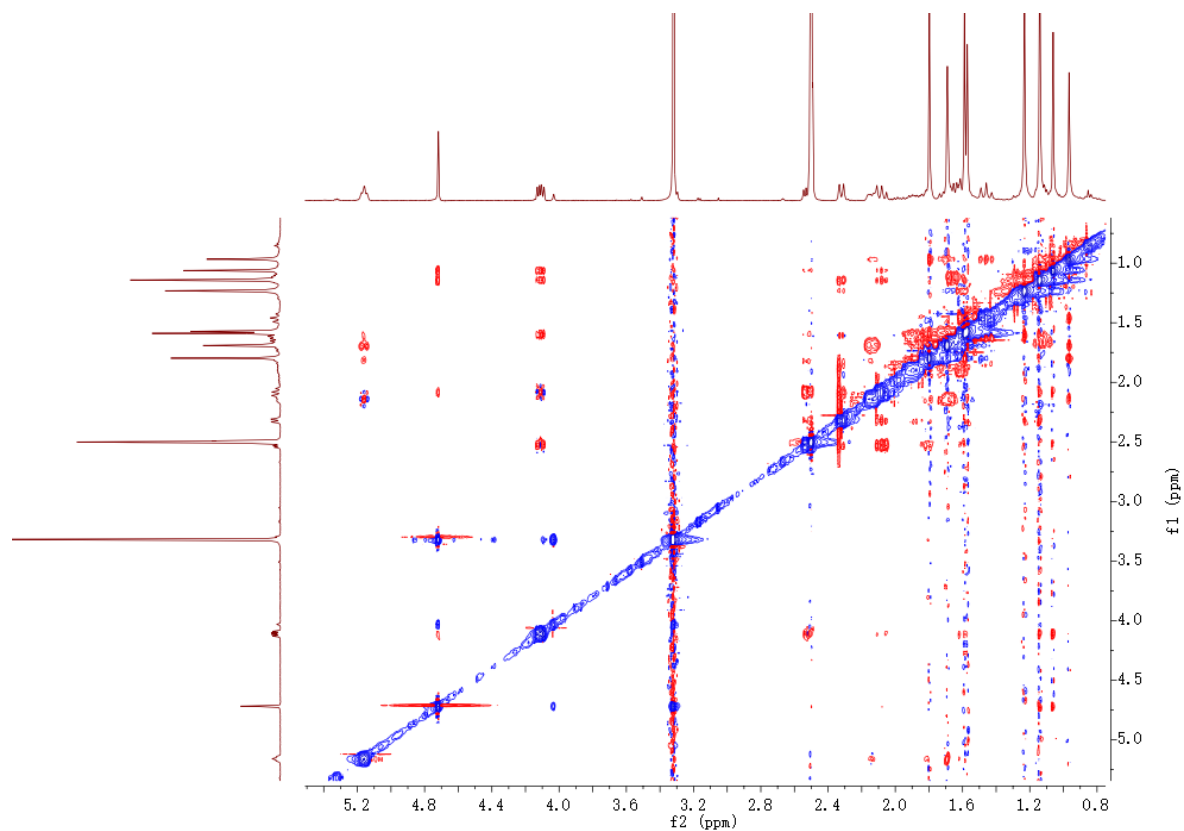
HMBC of compound 5 (400MHz, in DMSO- d_6)



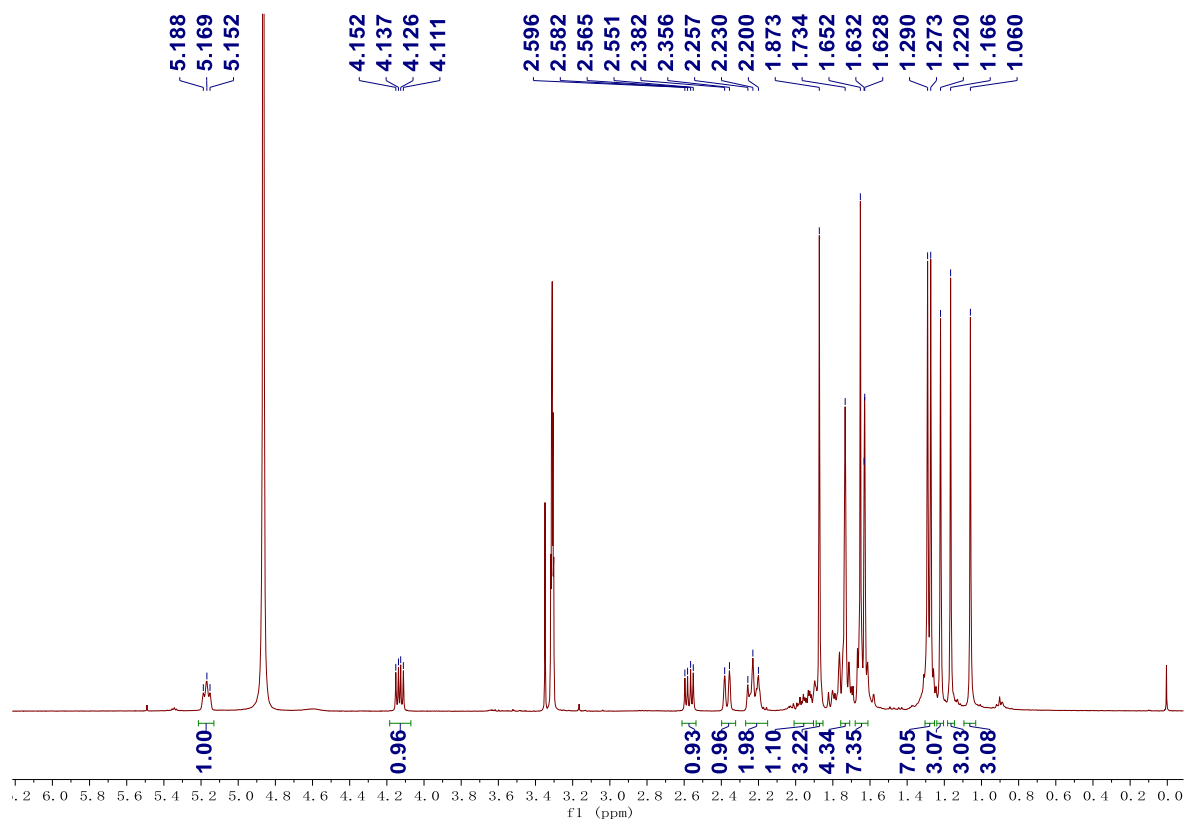
^1H - ^1H COSY of compound 5 (400MHz, in DMSO- d_6)



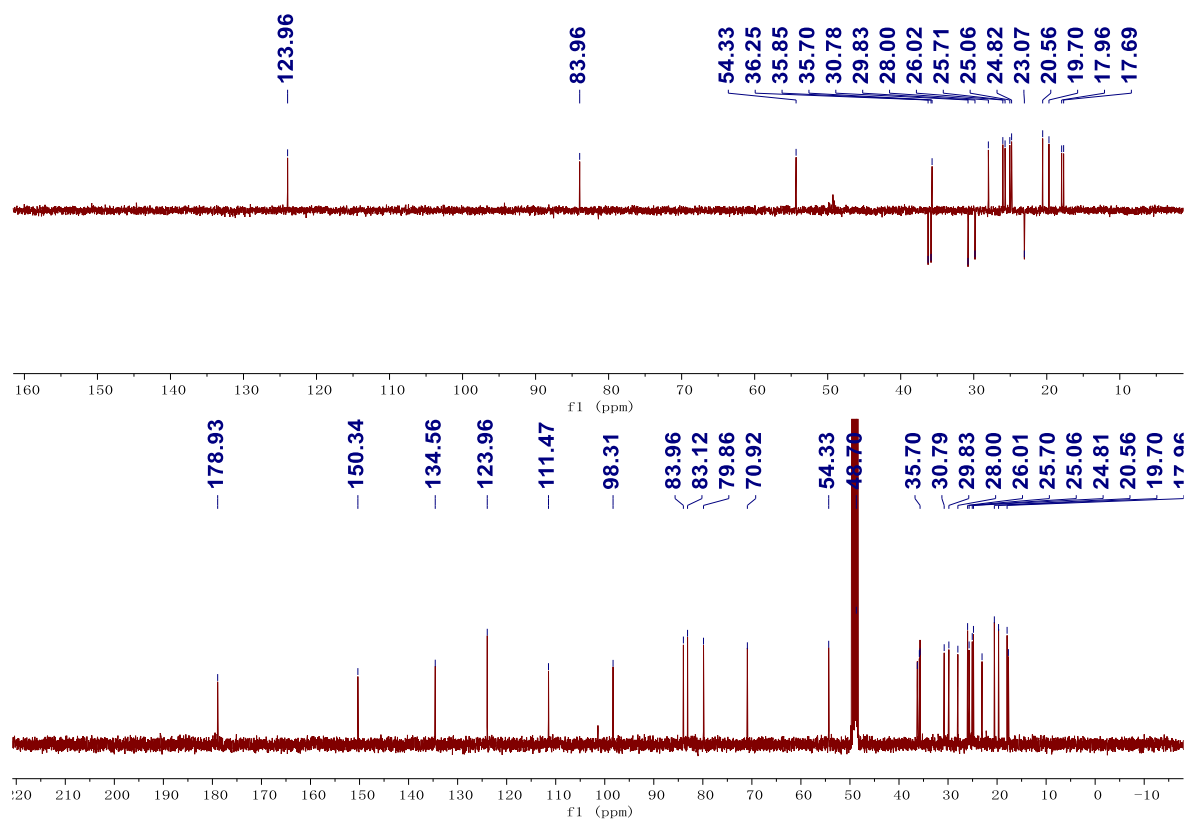
NOESY of compound 5 (400MHz, in DMSO-*d*₆)



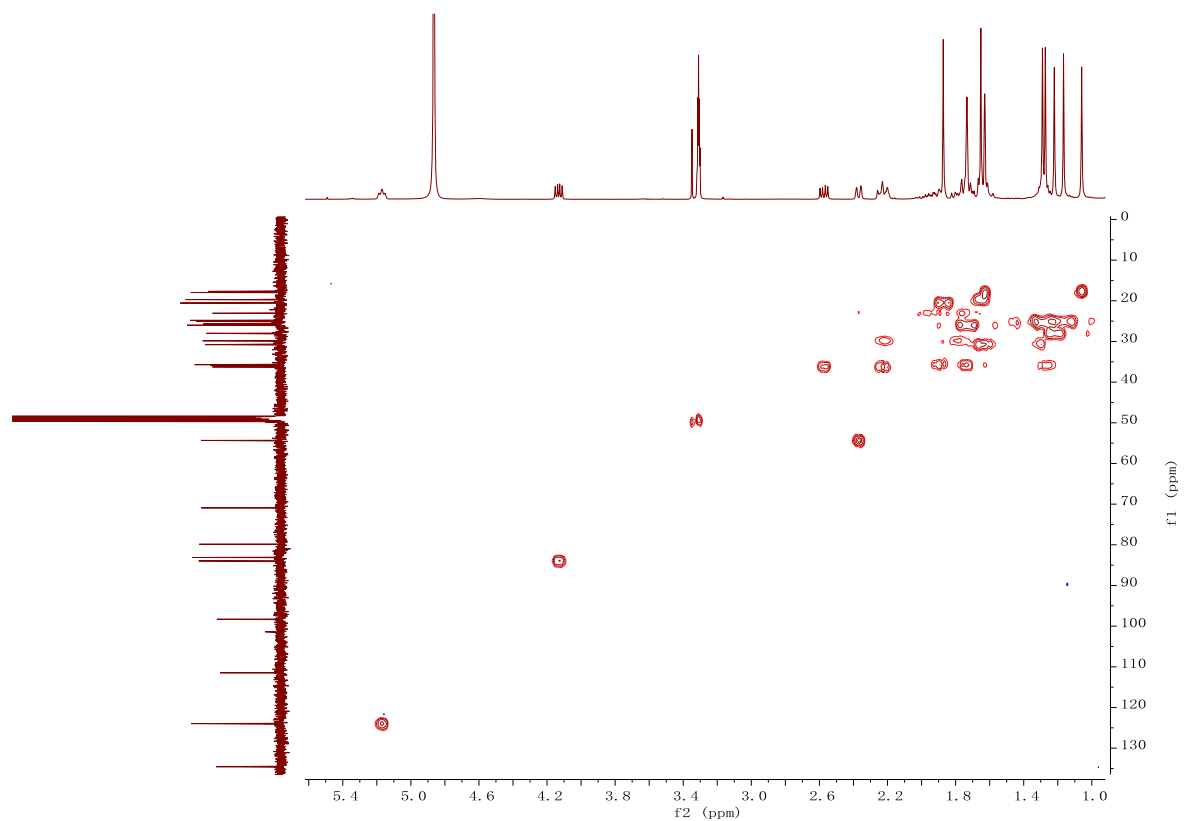
¹H NMR of compound 5 (400MHz, in CD₃OD)



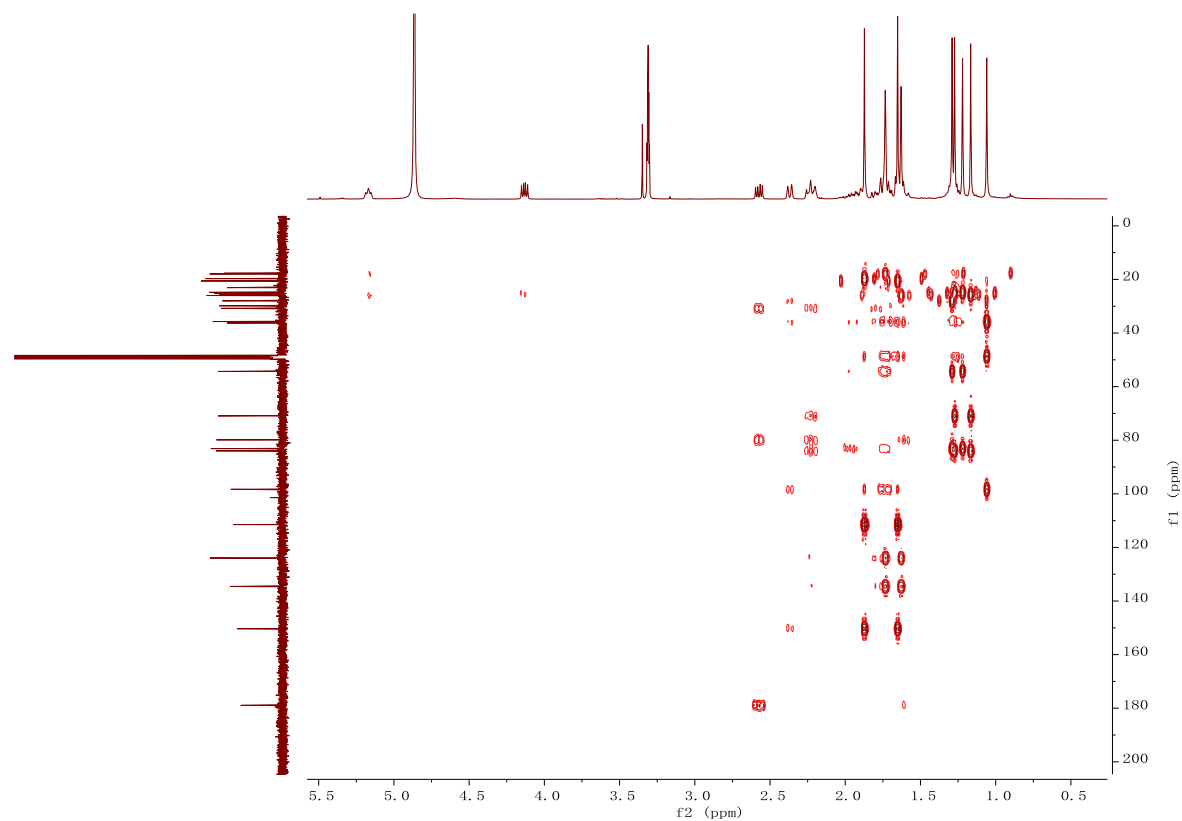
^{13}C NMR of compound 5 (100MHz, in CD_3OD)



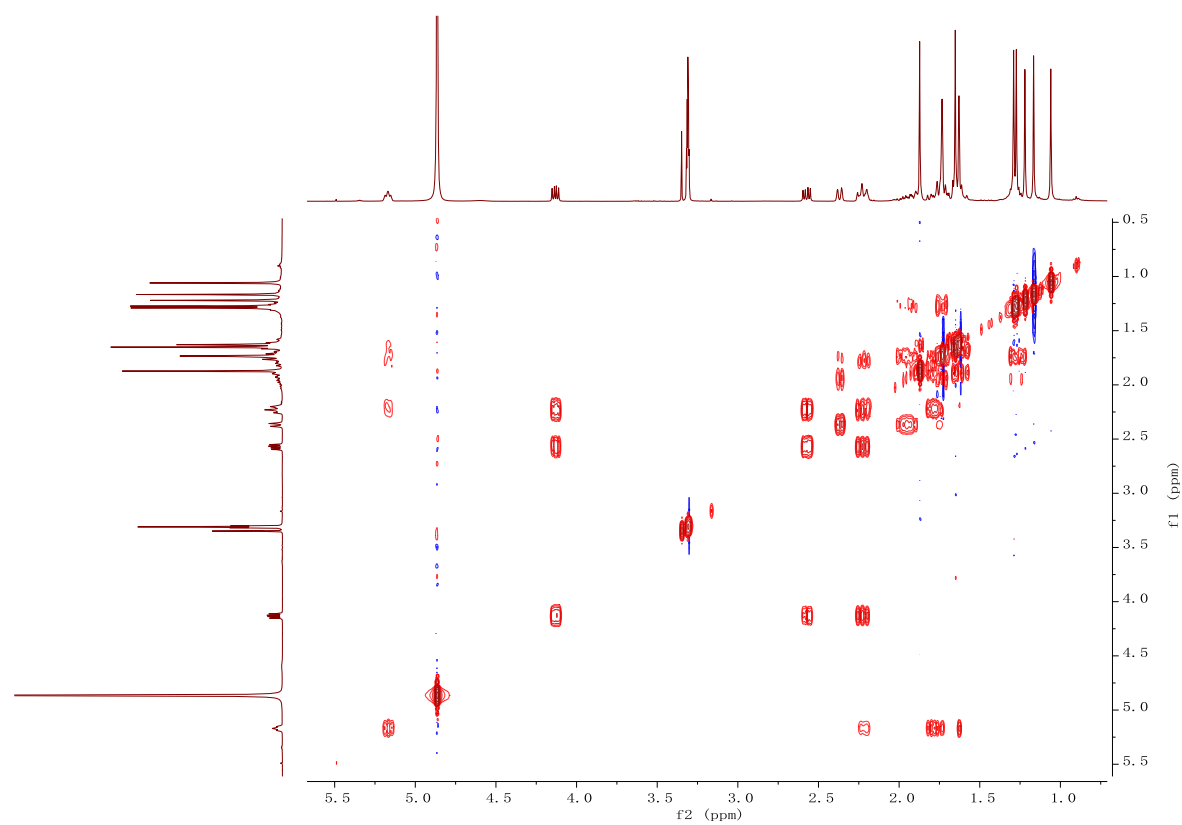
HSQC of compound 5 (400MHz, in CD_3OD)



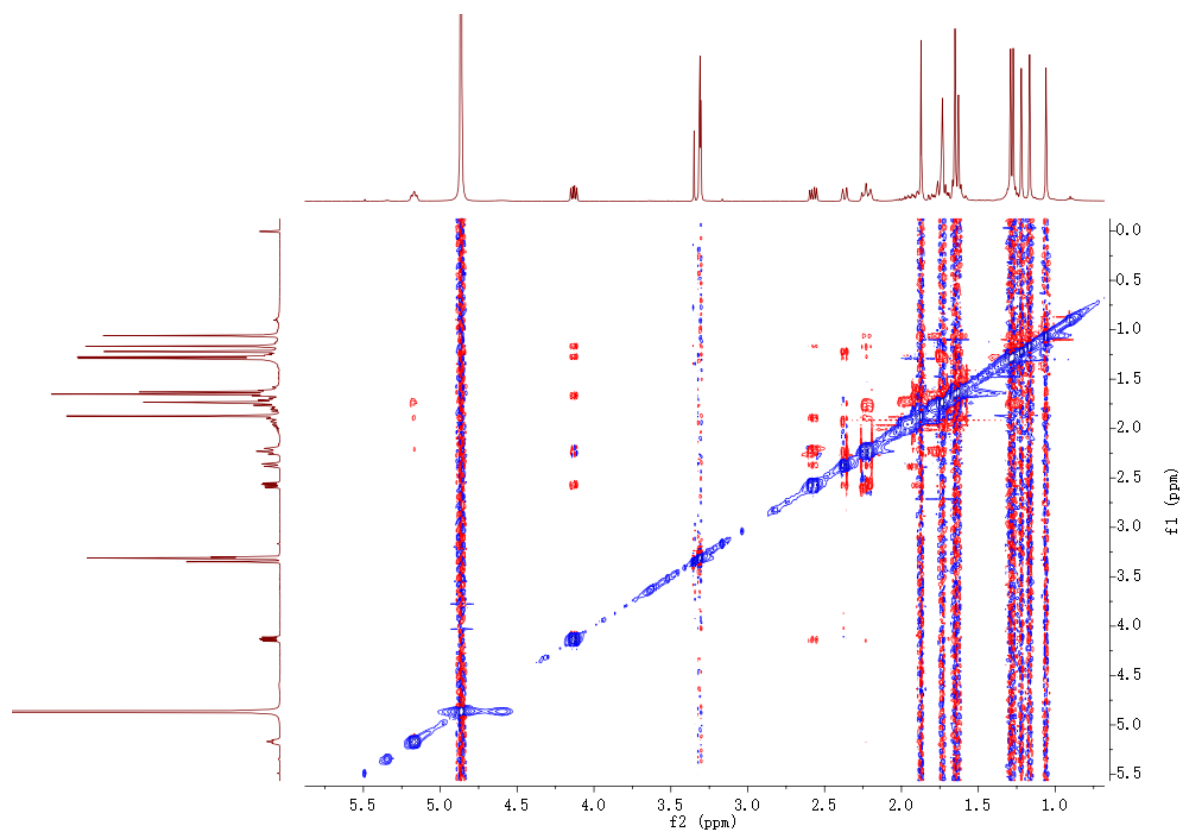
HMBC of compound 5 (400MHz, in CD₃OD)



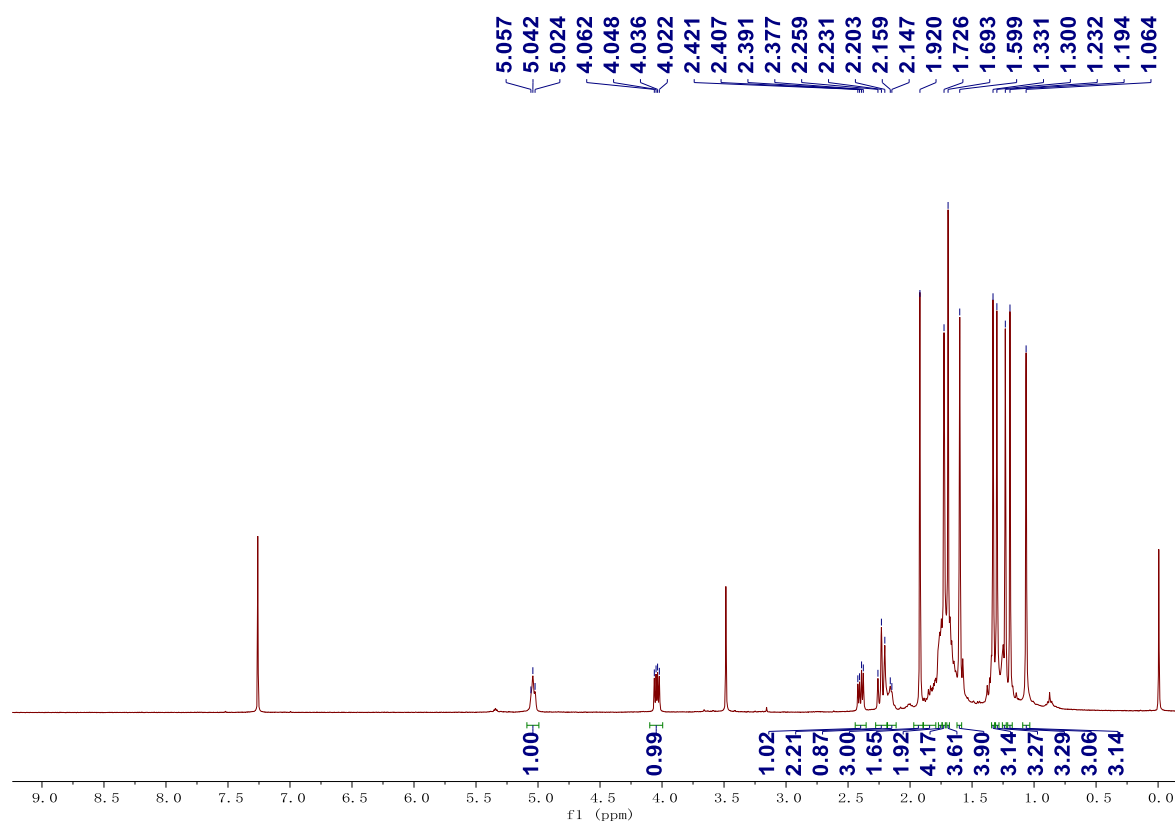
¹H-¹H COSY of compound 5 (400MHz, in CD₃OD)



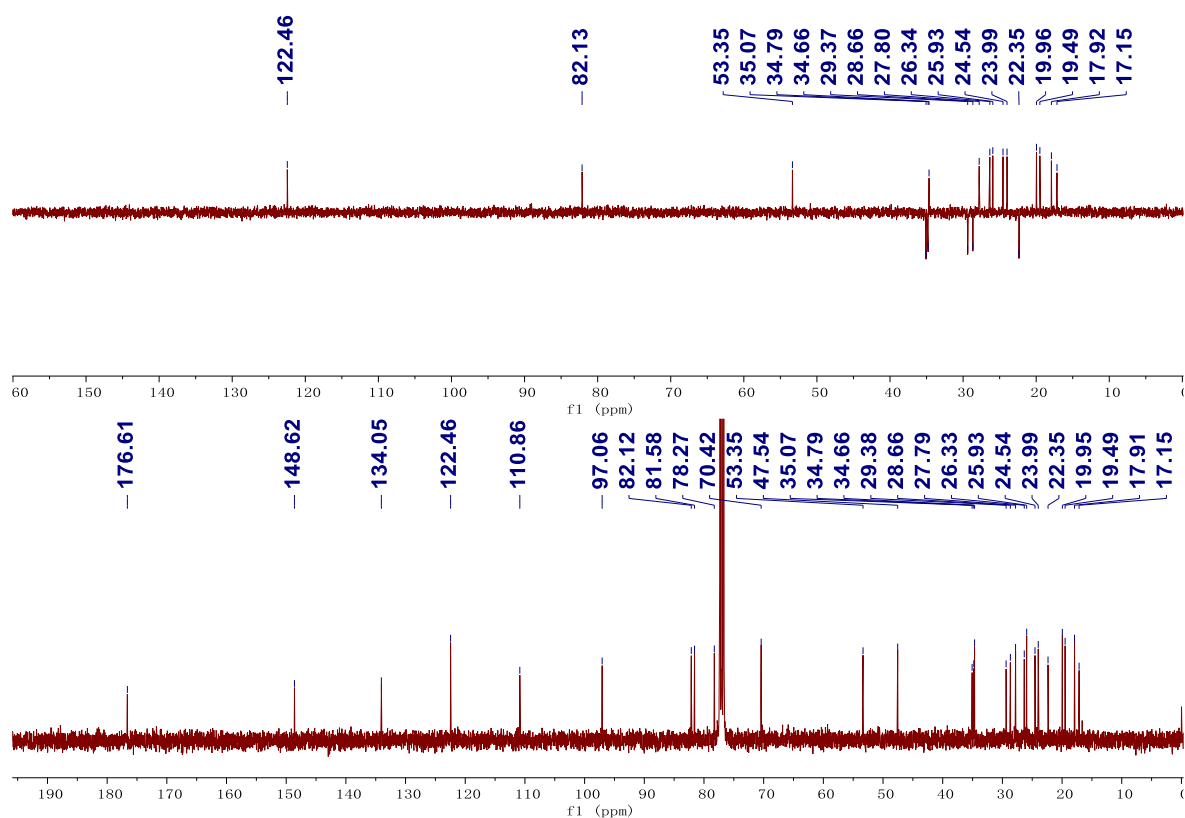
NOESY of compound 5 (400MHz, in CD₃OD)



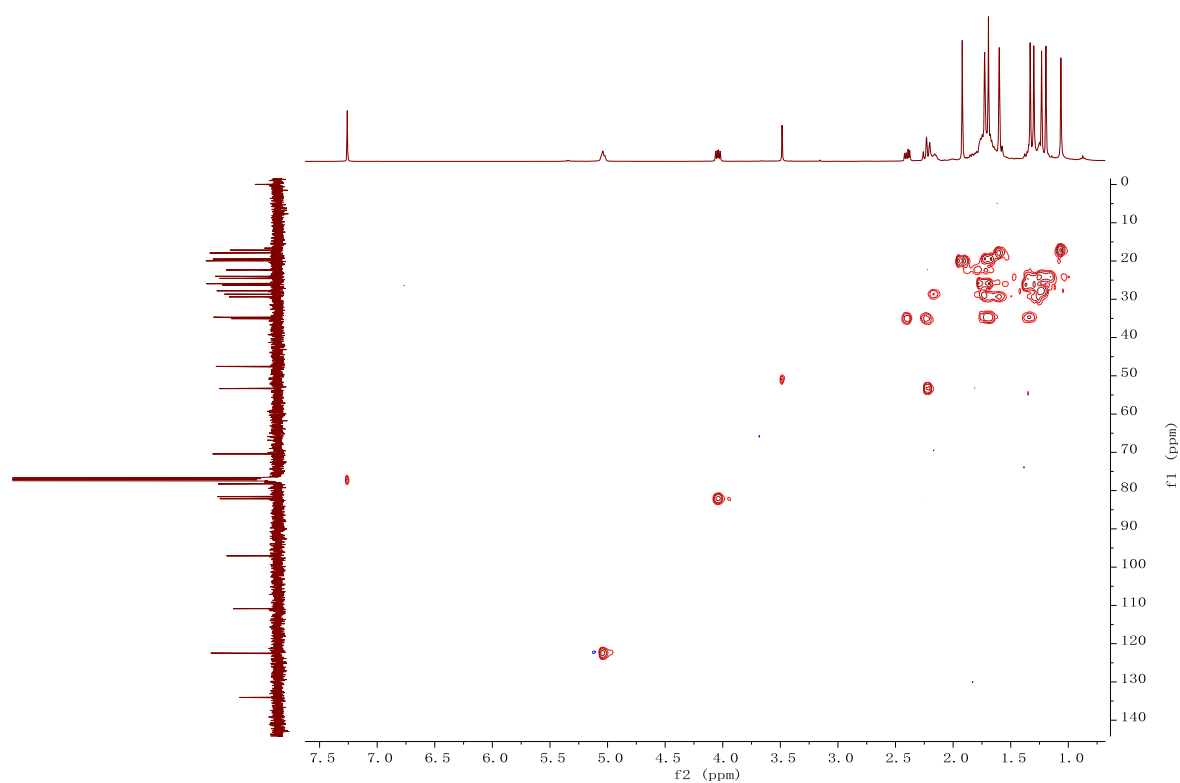
¹H NMR of compound 5 (400MHz, in CDCl₃)



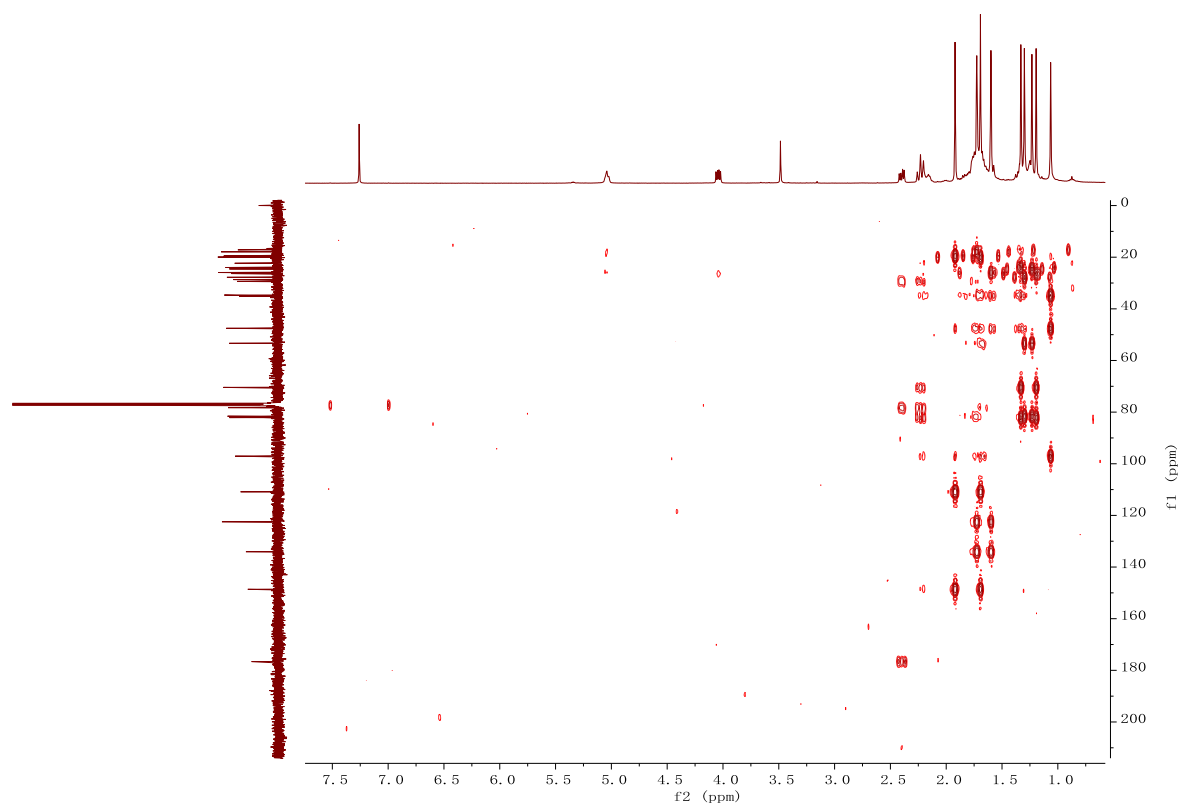
^{13}C NMR of compound 5 (100MHz, in CDCl_3)



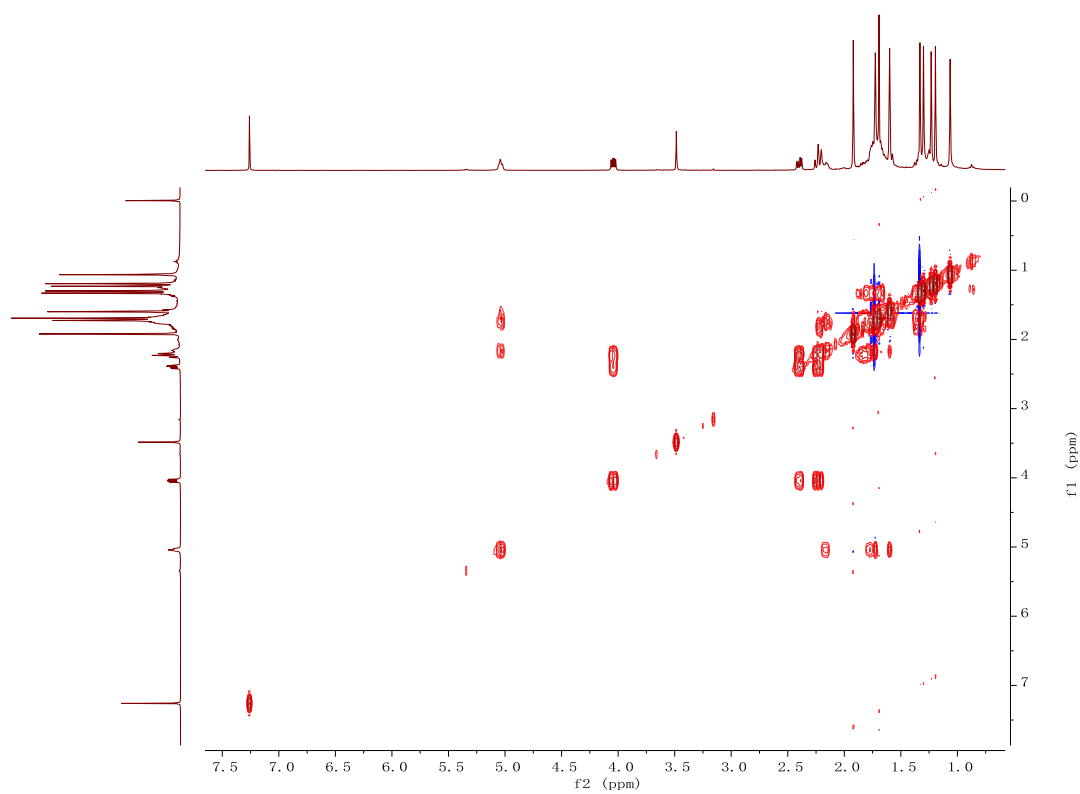
HSQC of compound 5 (400MHz, in CDCl_3)



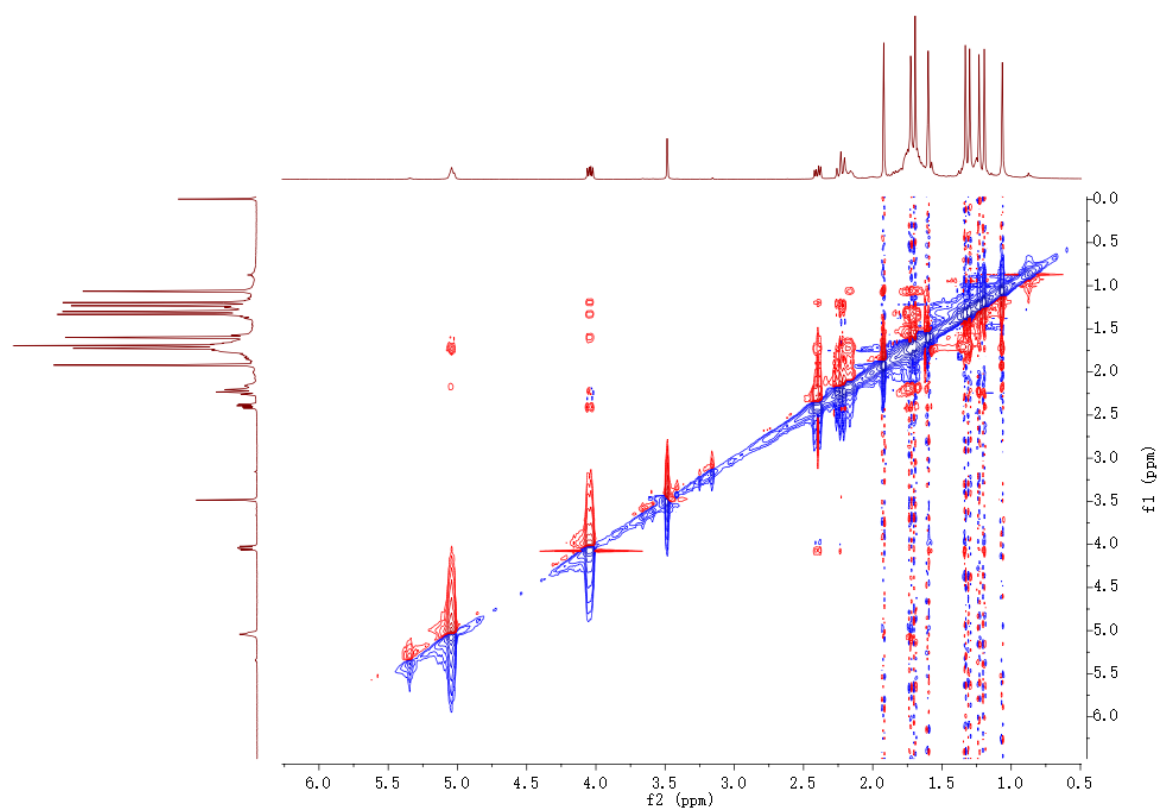
HMBC of compound 5 (400MHz, in CDCl₃)



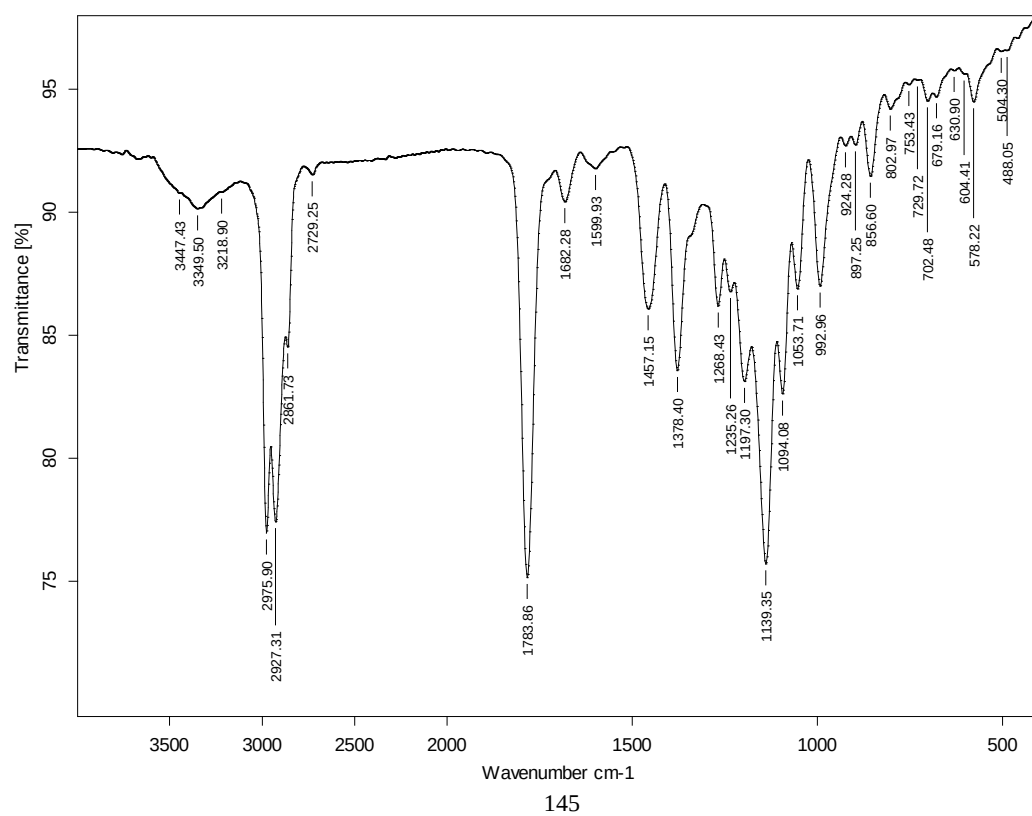
¹H-¹H COSY of compound 5 (400MHz, in CDCl₃)



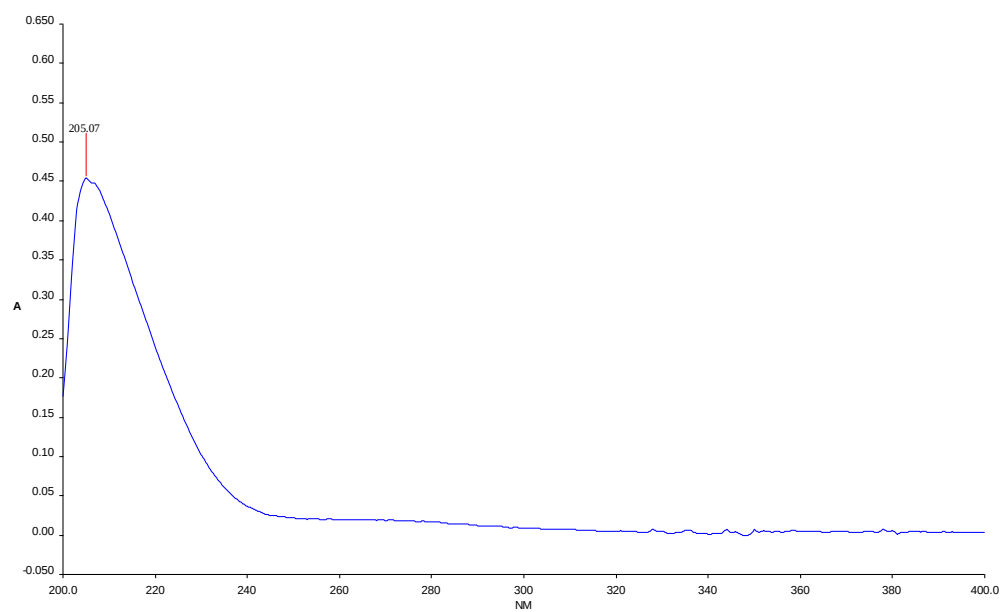
NOESY of compound 5 (400MHz, in CDCl₃)



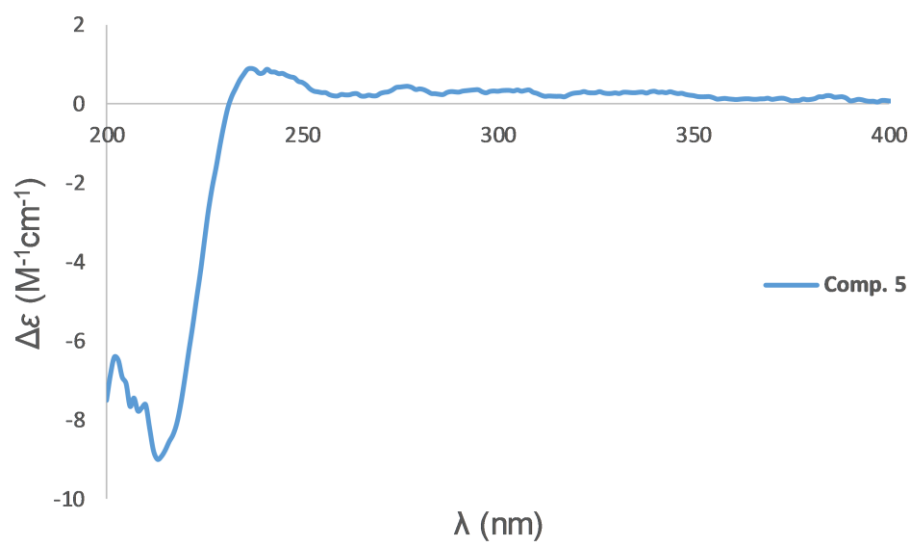
IR of compound 5



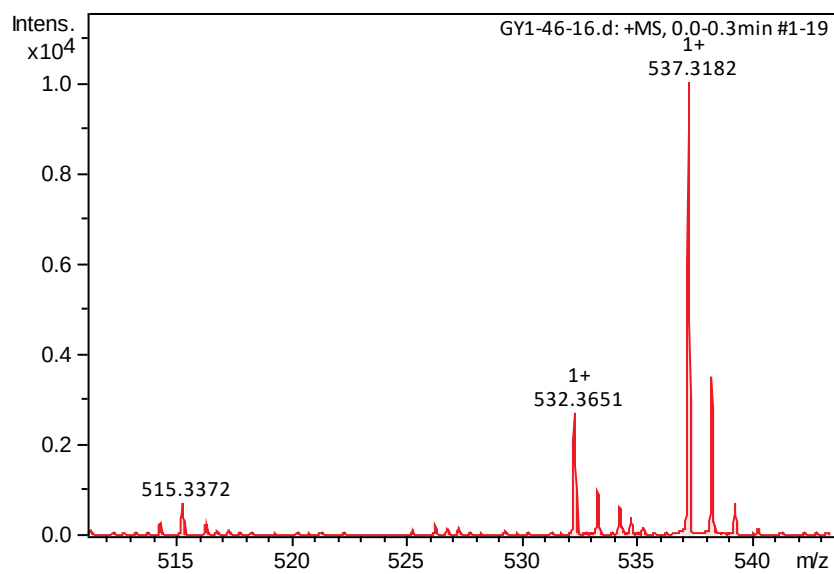
UV of compound 5



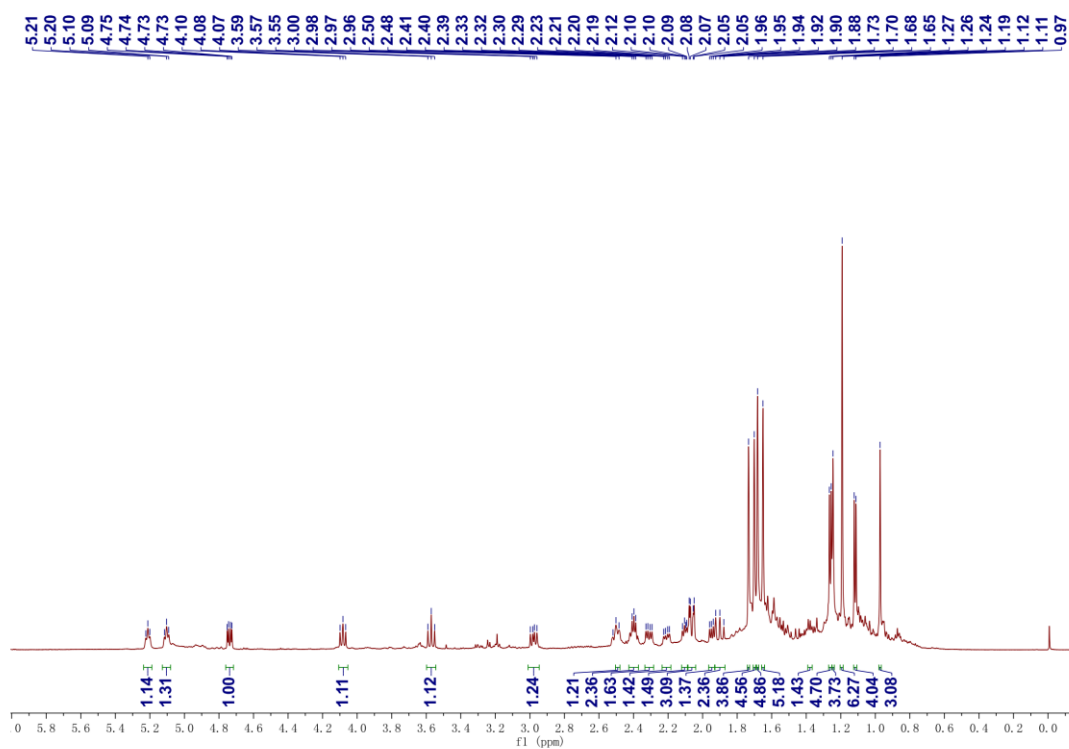
CD of compound 5



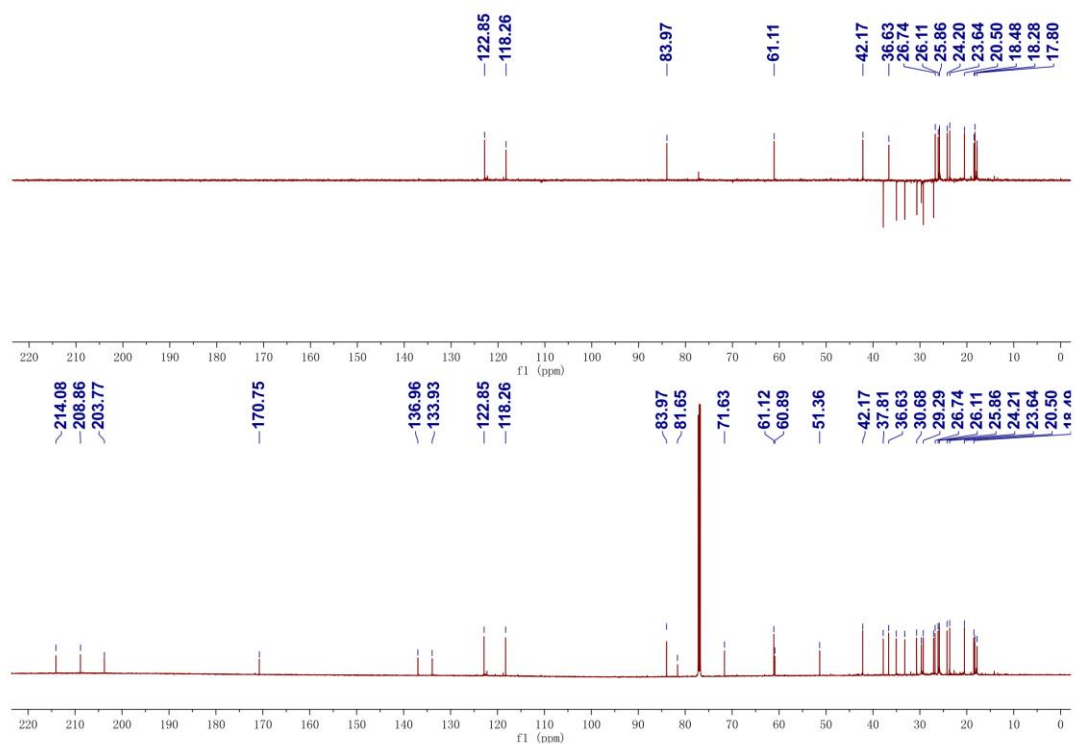
HRESIMS of compound **6**



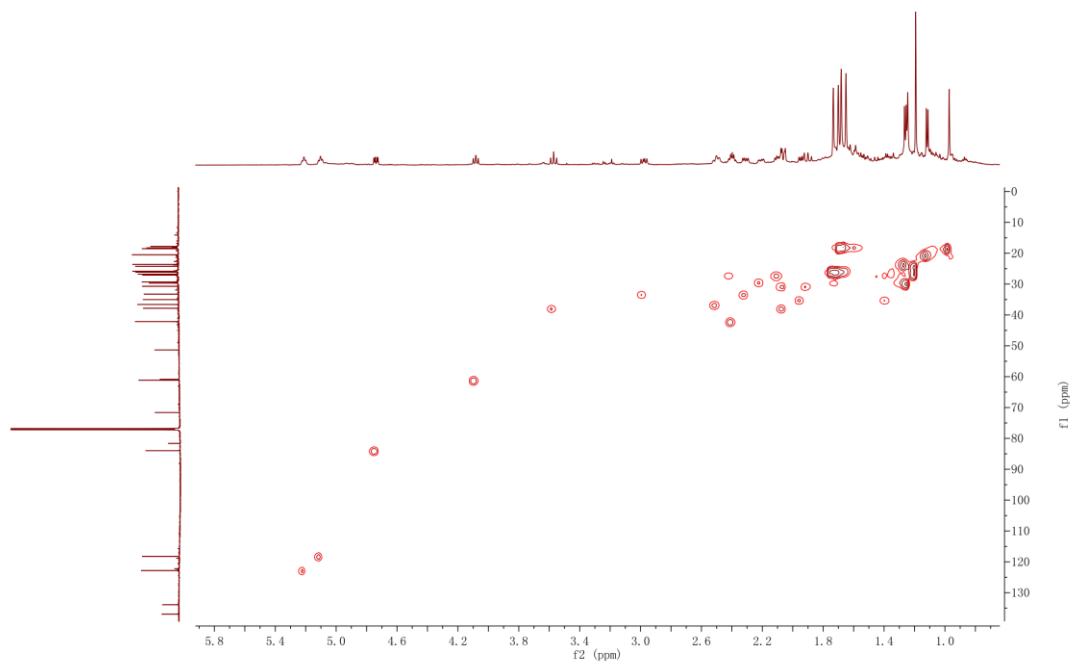
^1H NMR of compound **6** (600MHz, in CDCl_3)



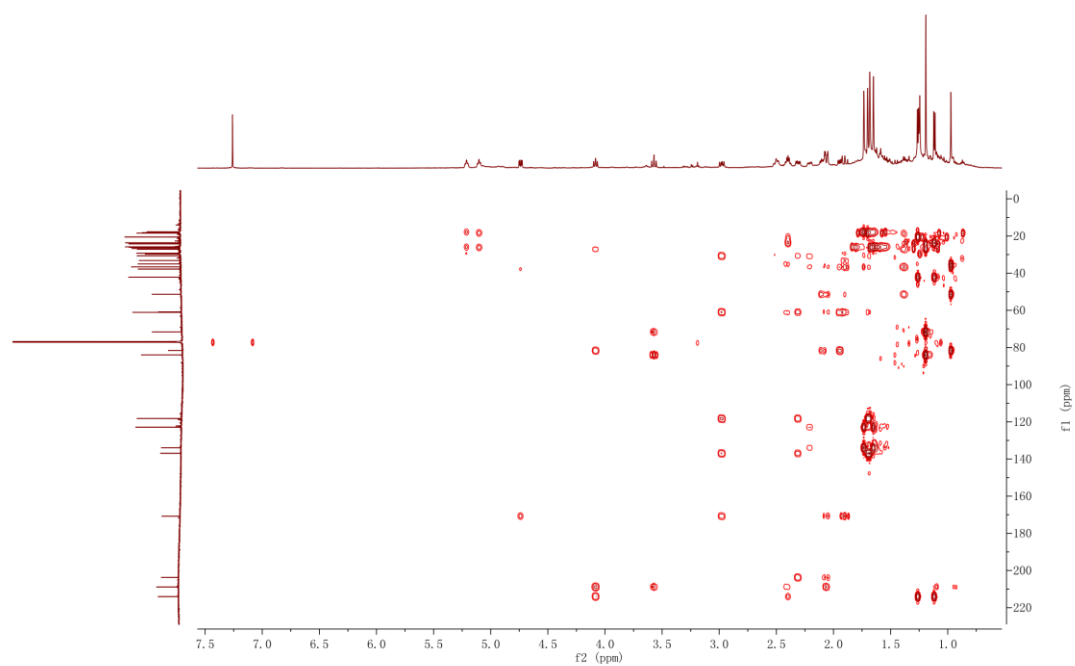
^{13}C NMR of compound **6** (150MHz, in CDCl_3)



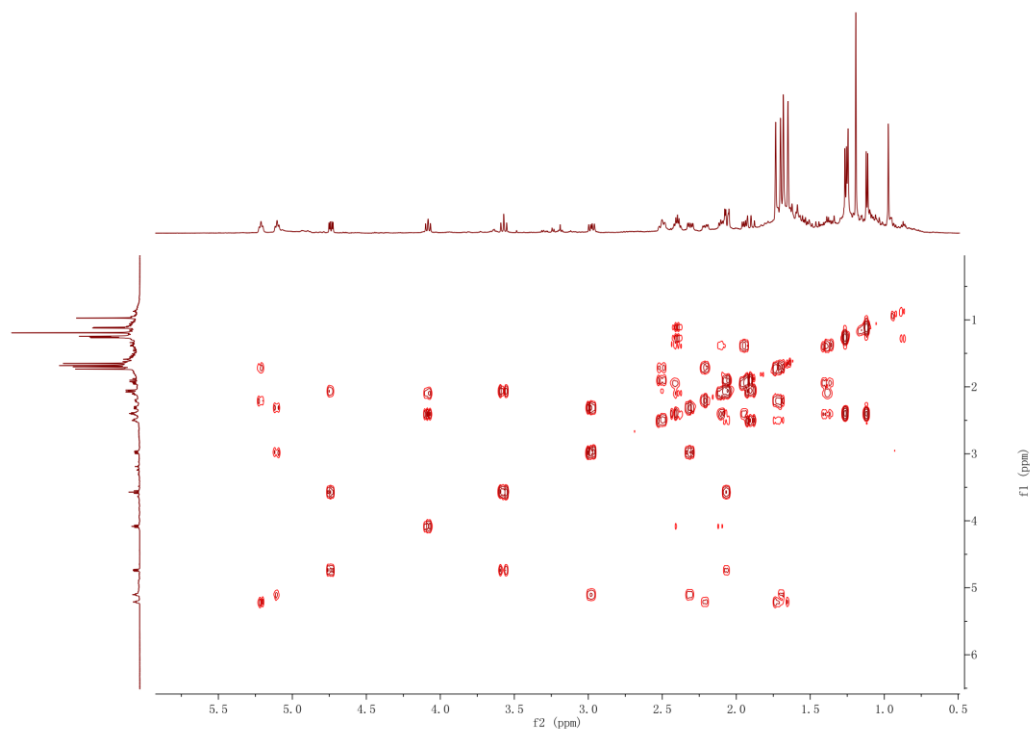
HSQC of compound **6** (600MHz, in CDCl_3)



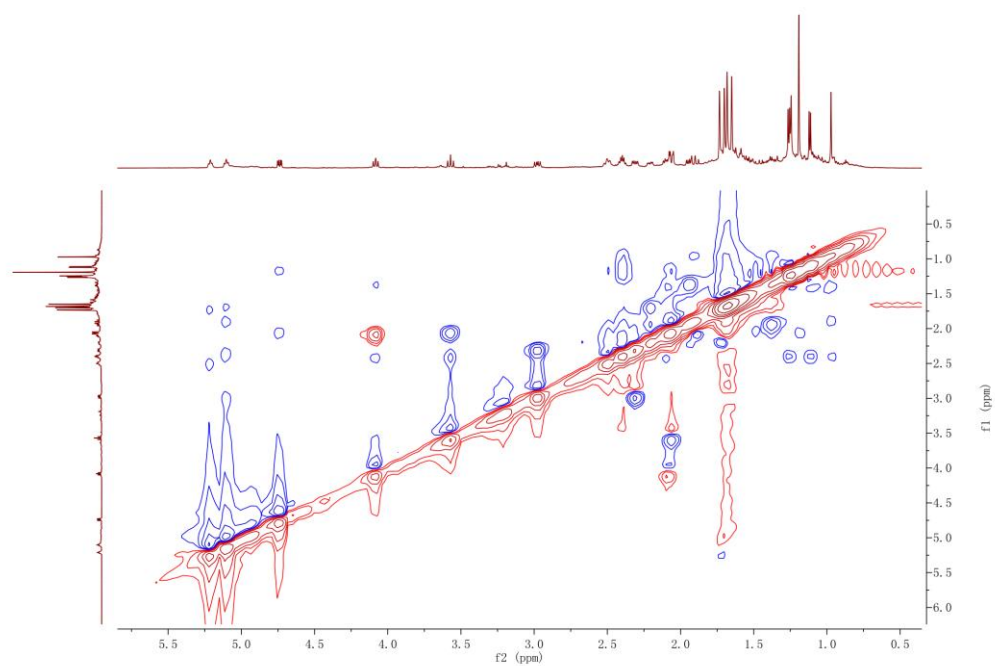
HMBC of compound **6** (600MHz, in CDCl₃)



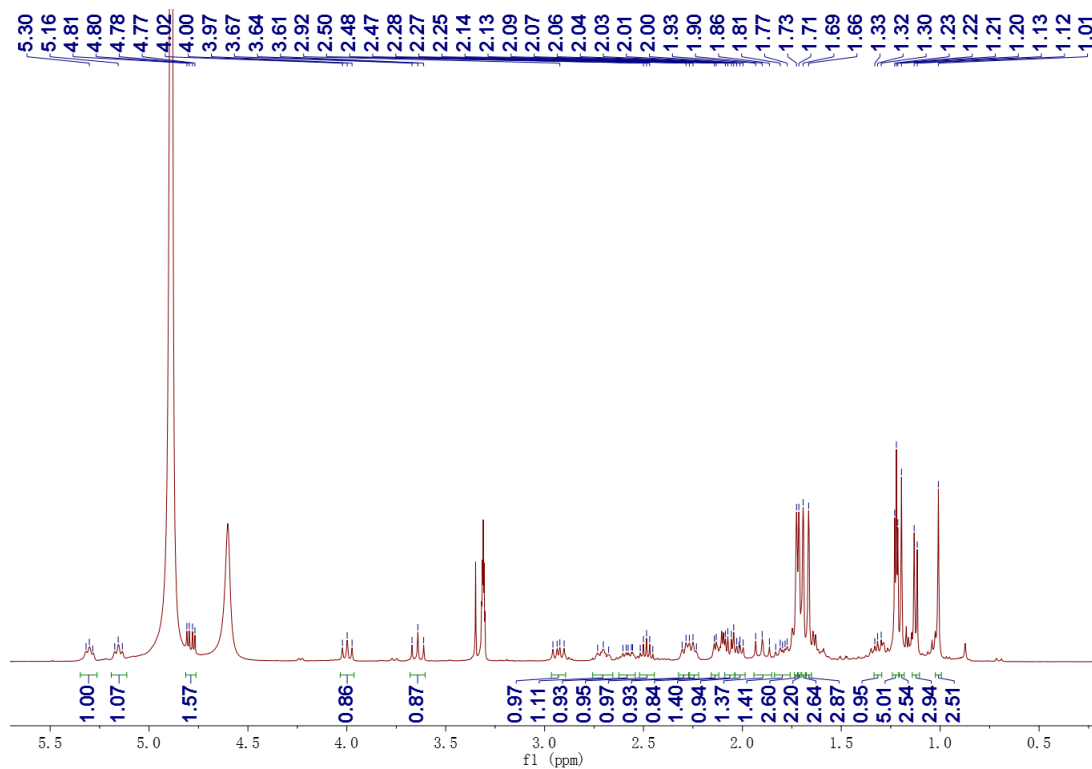
¹H-¹H COSY of compound **6** (600MHz, in CDCl₃)



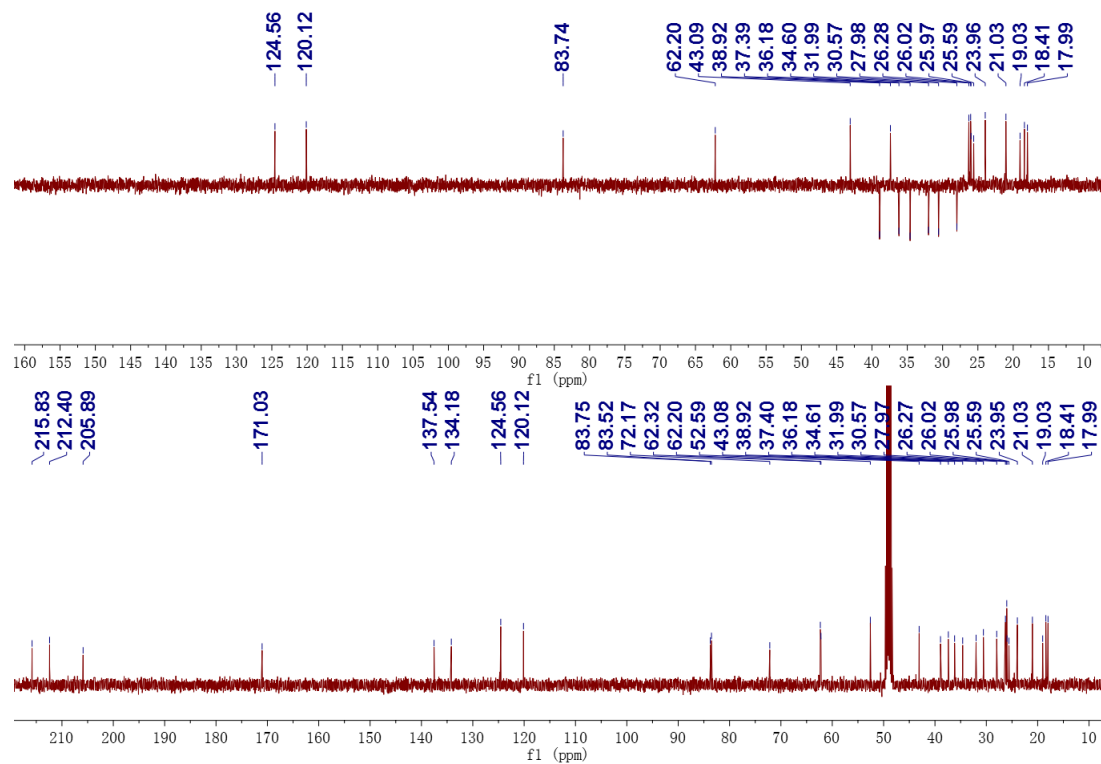
ROESY of compound **6** (600MHz, in CDCl₃)



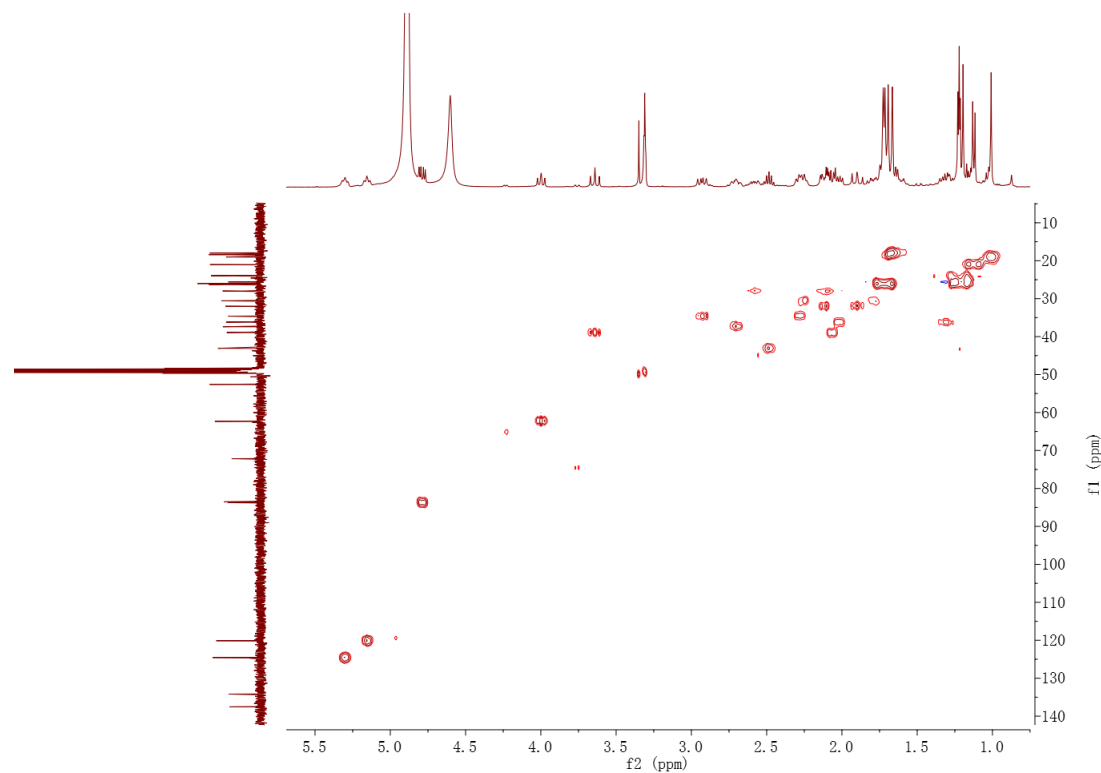
¹H NMR of compound **6** (400MHz, in CD₃OD)



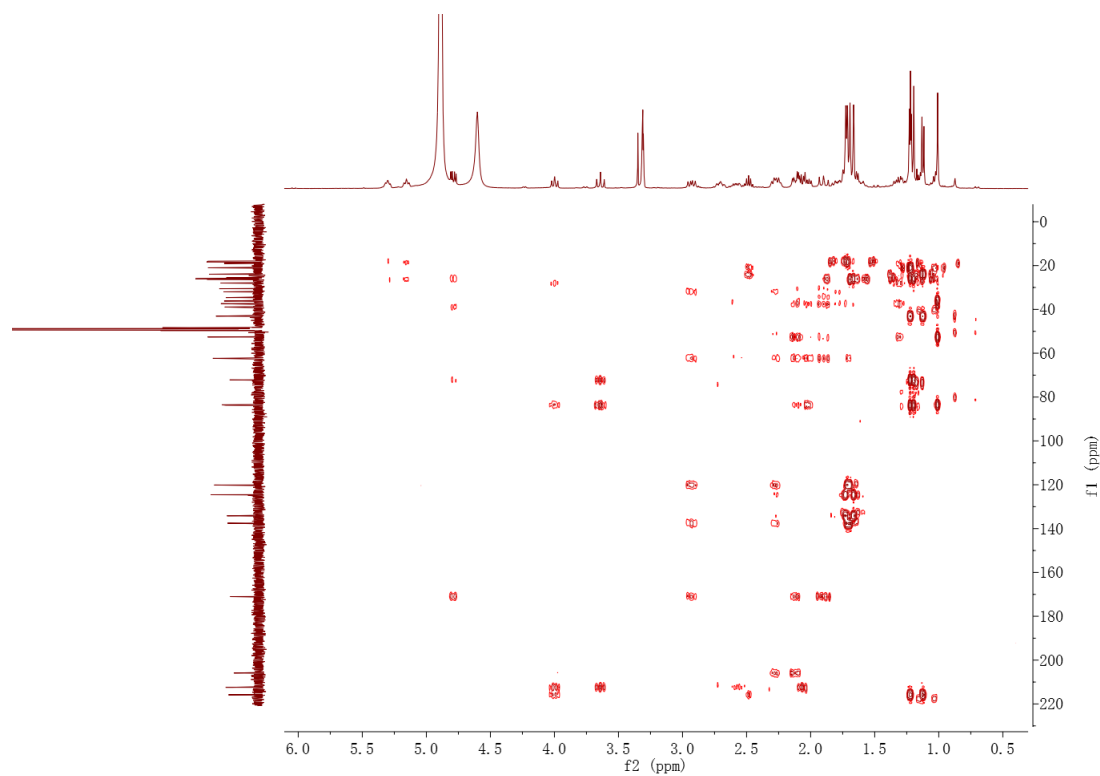
^{13}C NMR of compound **6** (100MHz, in CD_3OD)



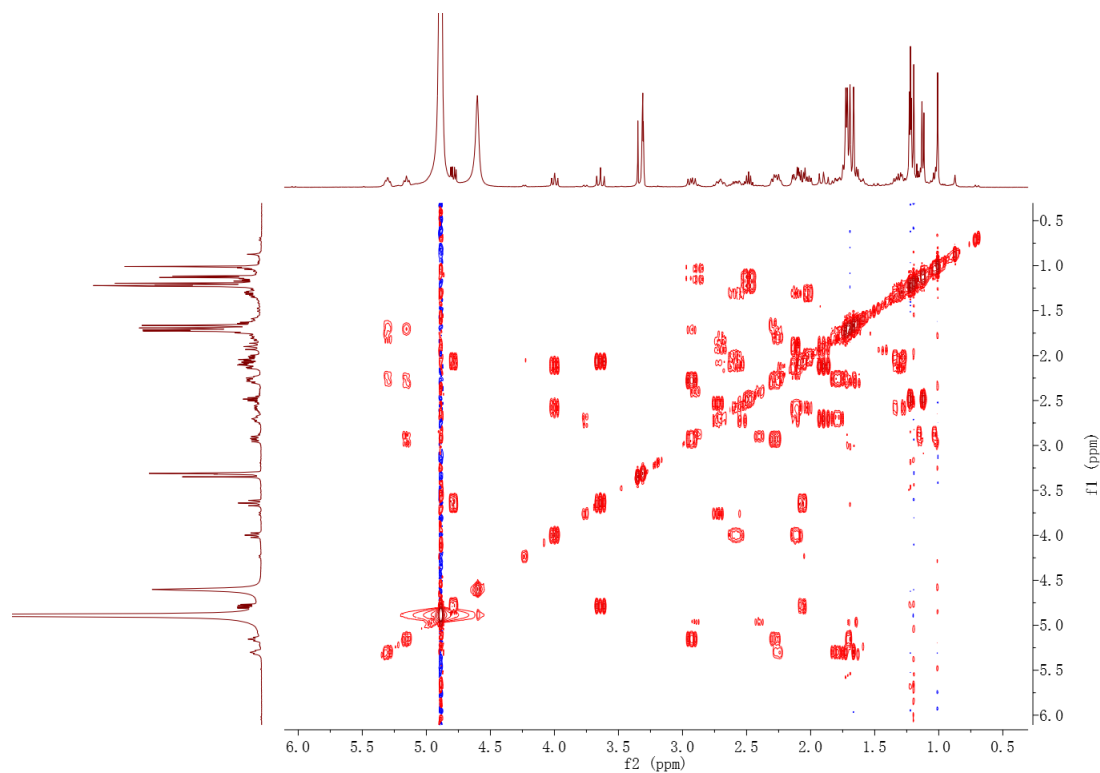
HSQC of compound **6** (400MHz, in CD_3OD)



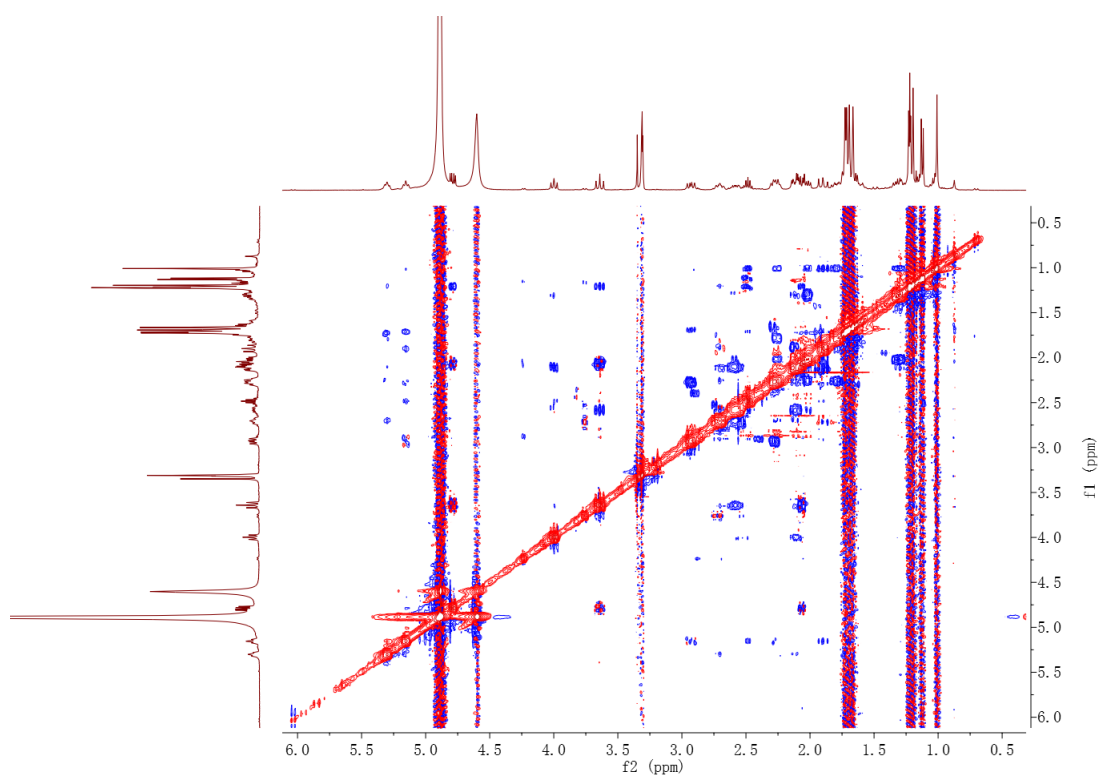
HMBC of compound **6** (400MHz, in CD₃OD)



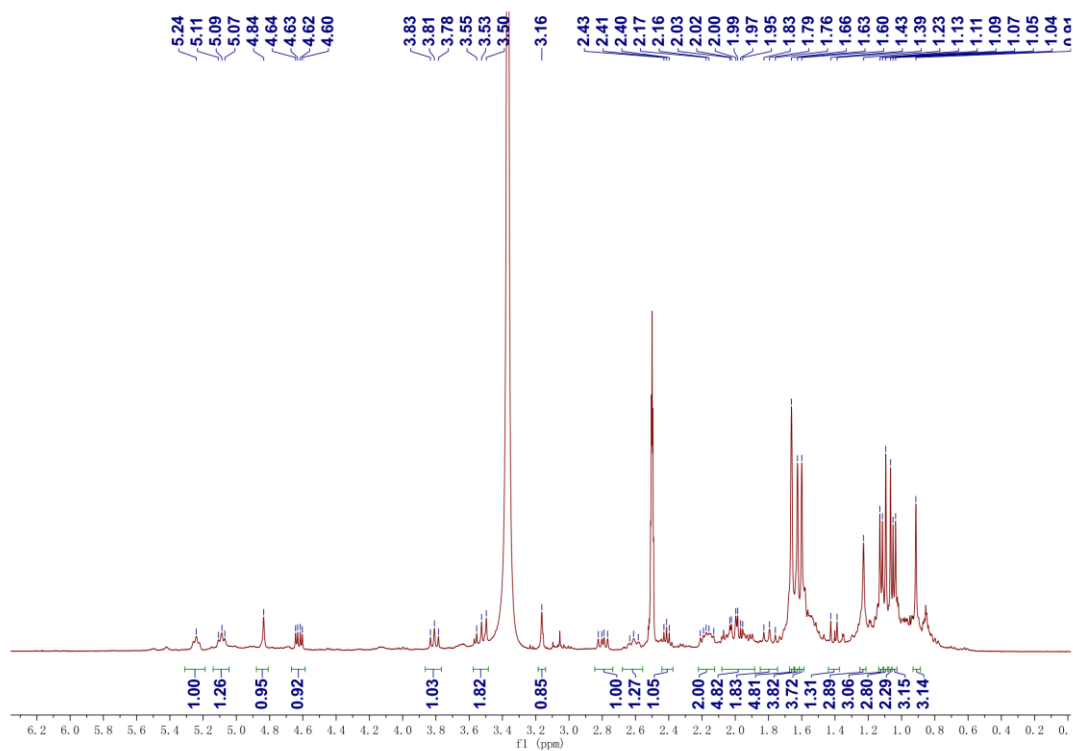
¹H-¹H COSY of compound **6** (400MHz, in CD₃OD)



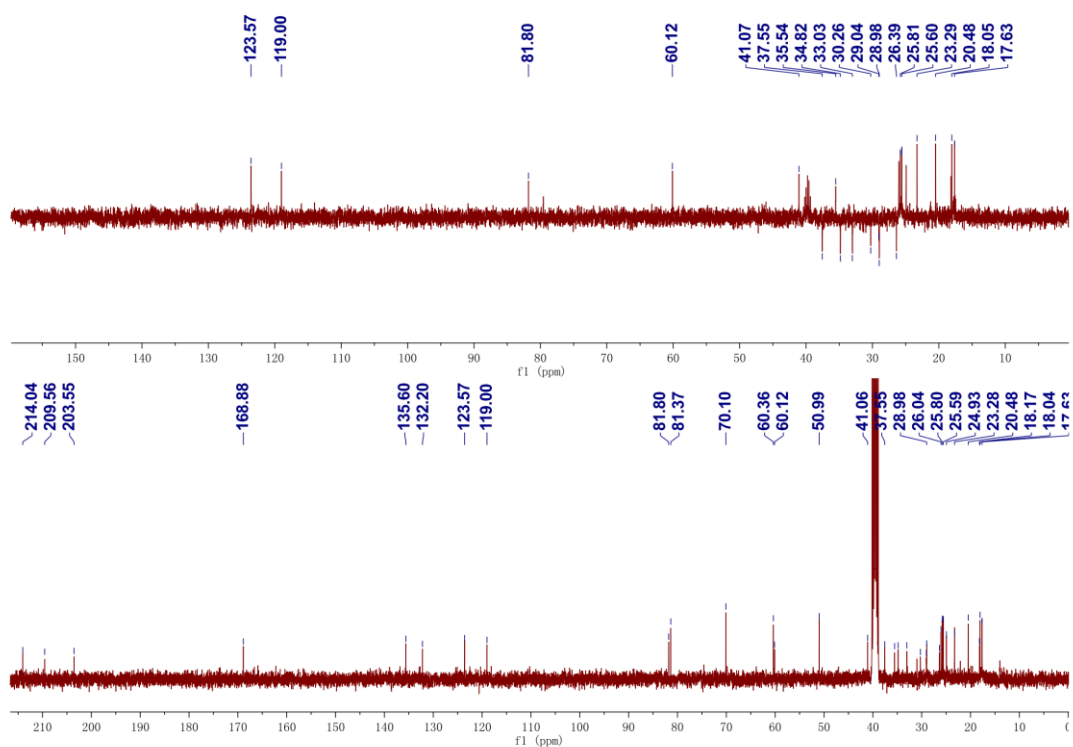
NOESY of compound **6** (400MHz, in CD₃OD)



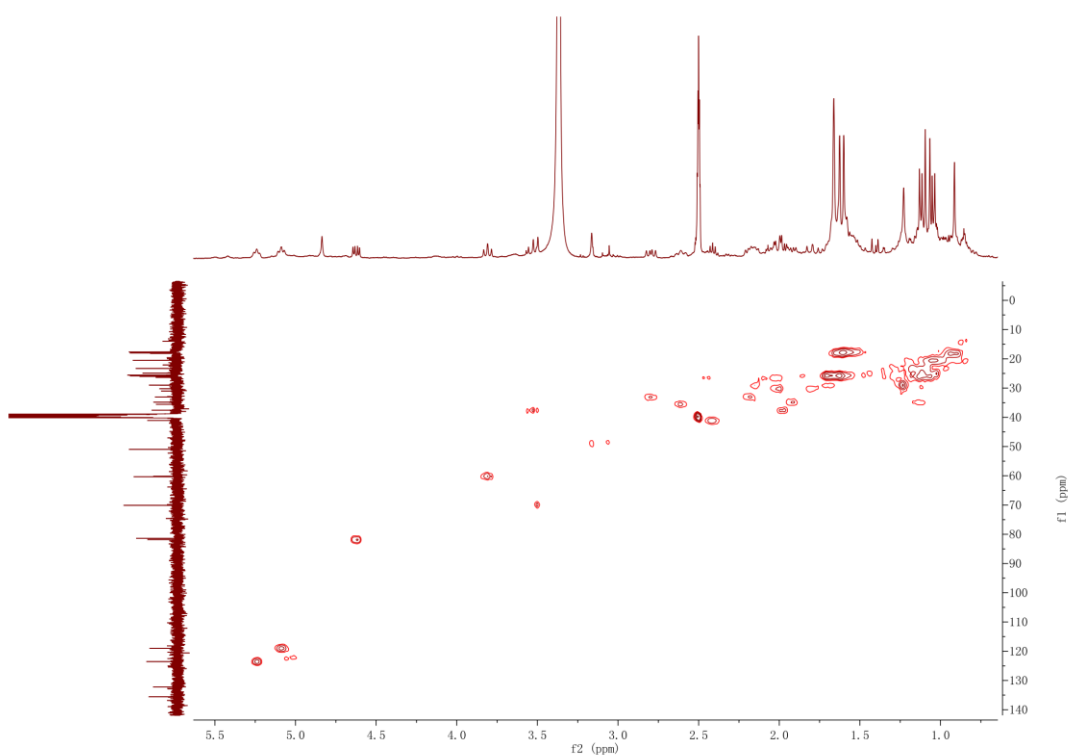
¹H NMR of compound **6** (400MHz, in DMSO-*d*₆)



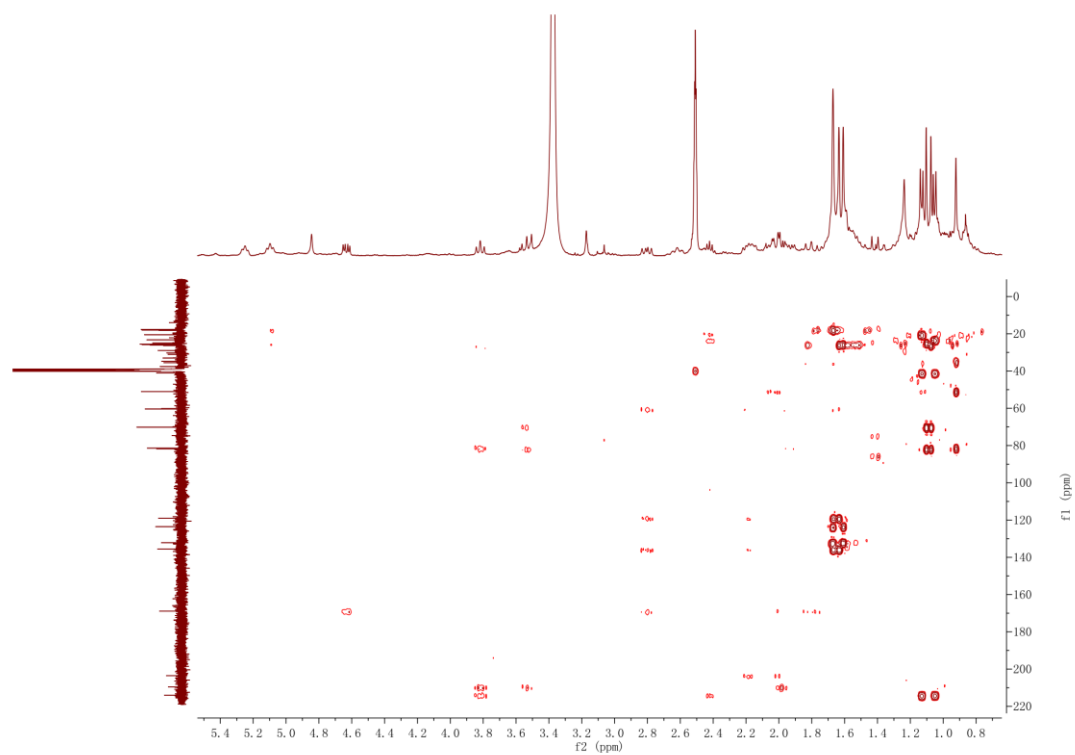
^{13}C NMR of compound **6** (100MHz, in $\text{DMSO}-d_6$)



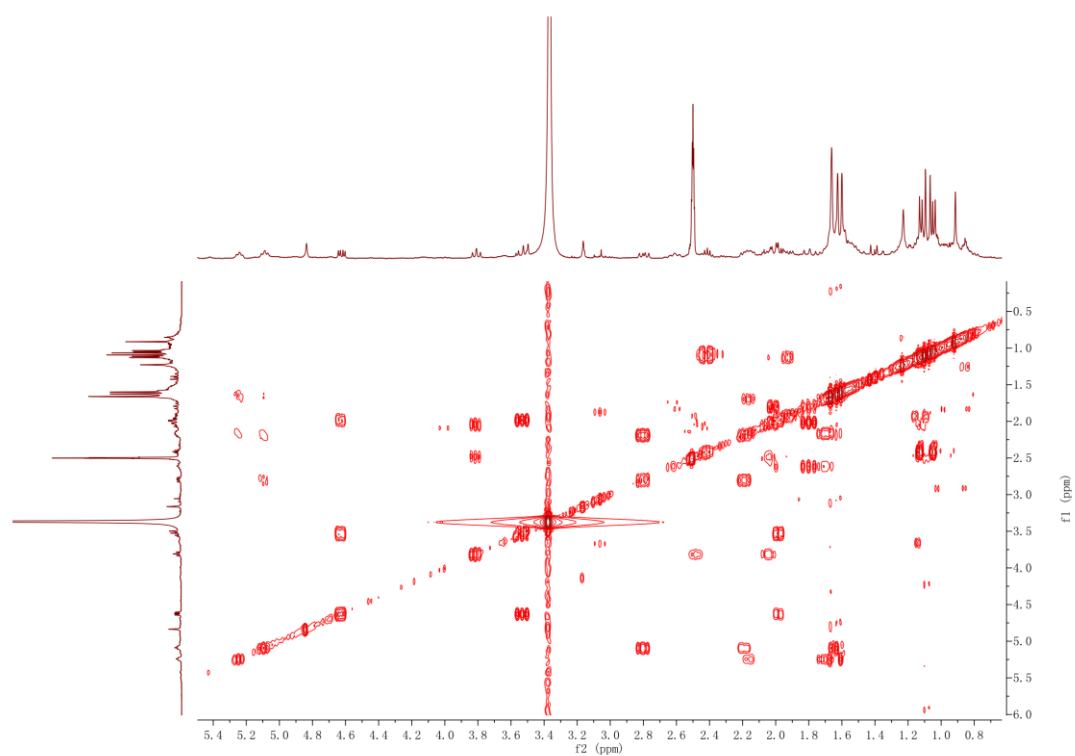
HSQC of compound **6** (400MHz, in $\text{DMSO}-d_6$)



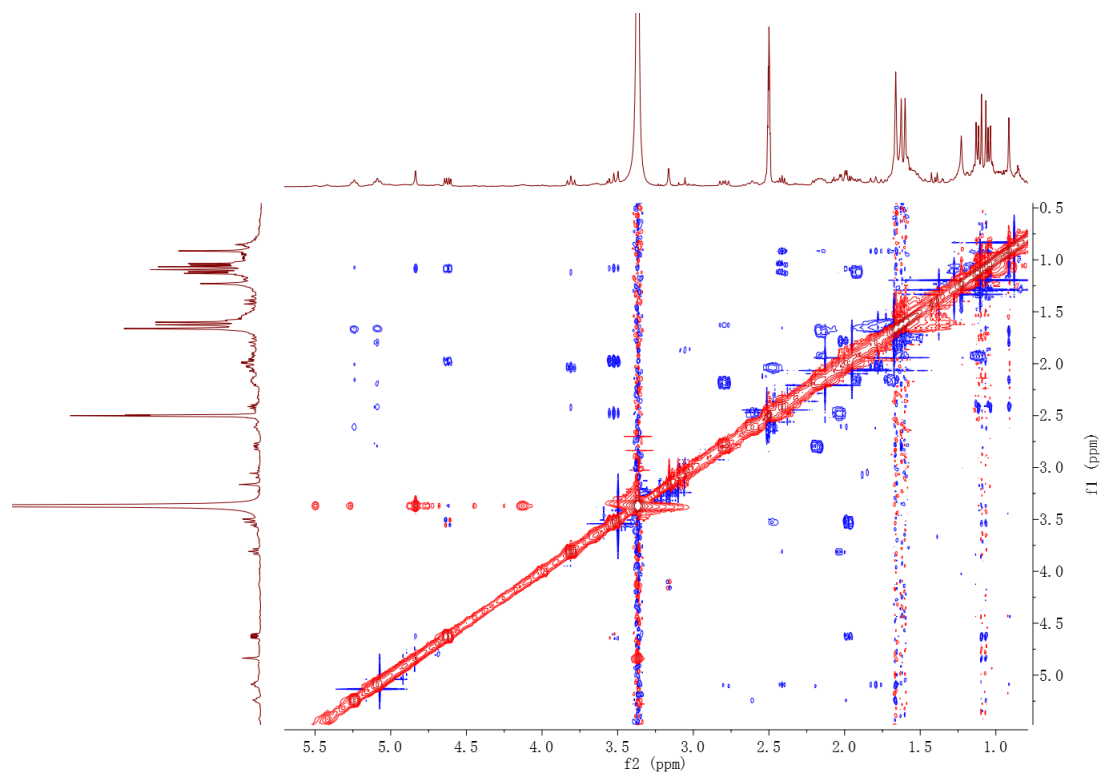
HMBC of compound **6** (400MHz, in DMSO-*d*₆)



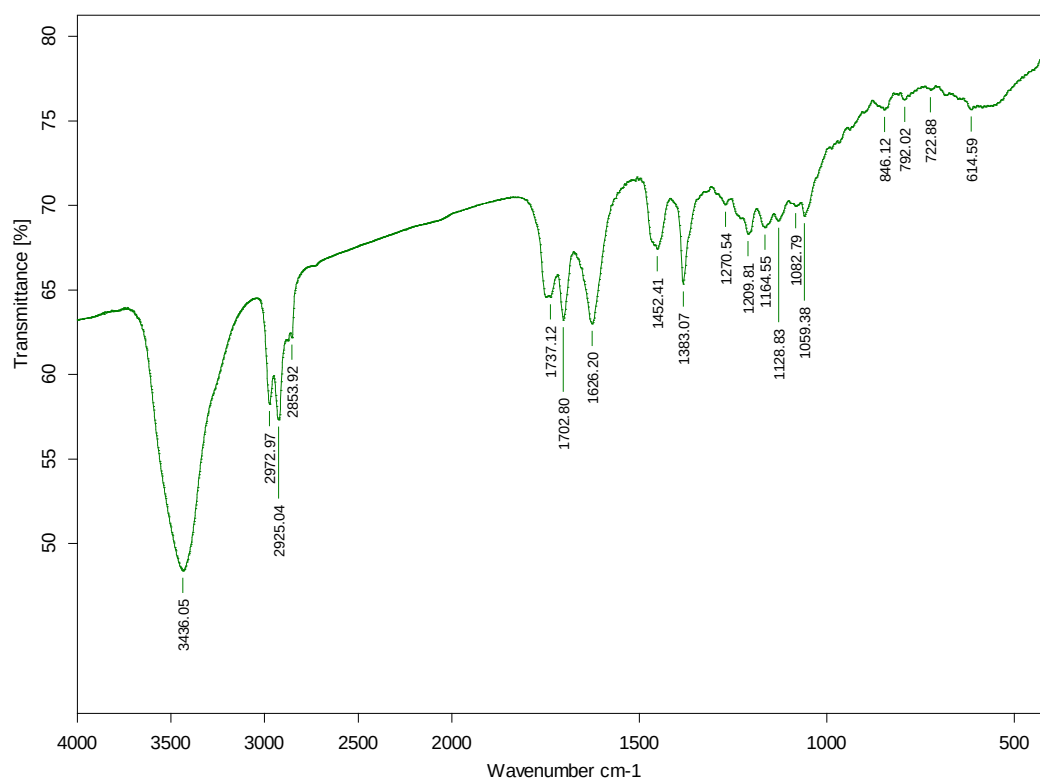
¹H-¹H COSY of compound **6** (400MHz, in DMSO-*d*₆)



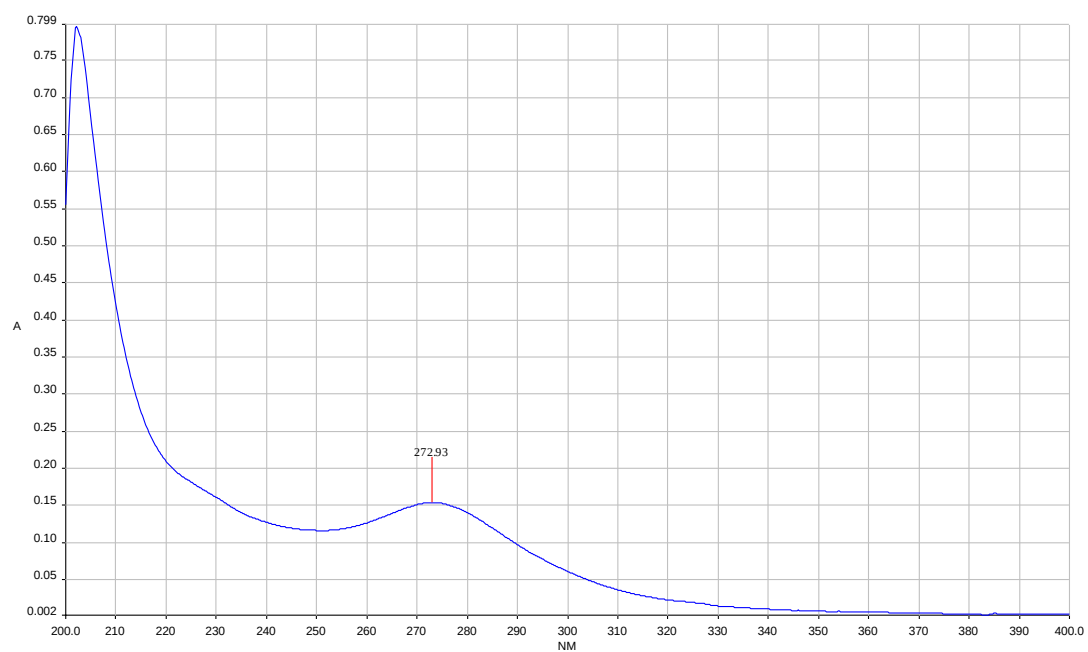
NOESY of compound **6** (400MHz, in DMSO-*d*₆)



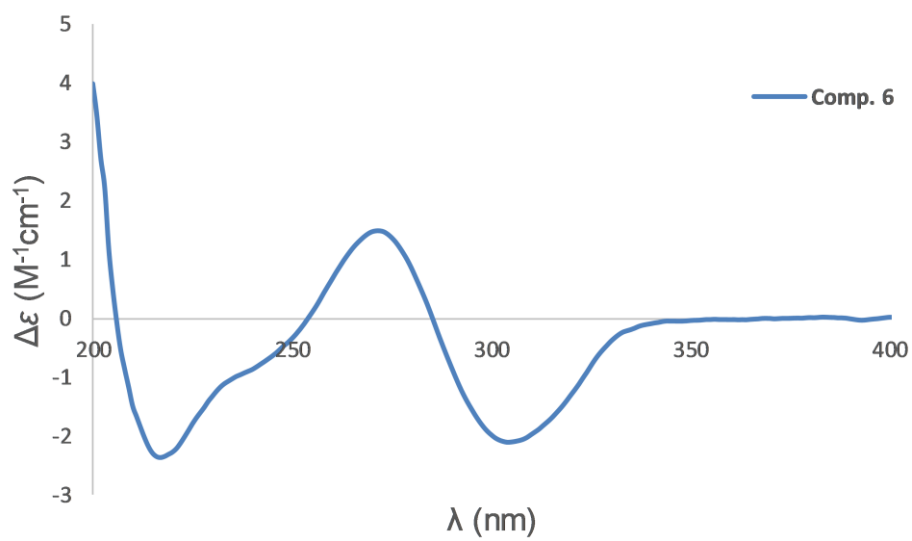
IR of compound **6**



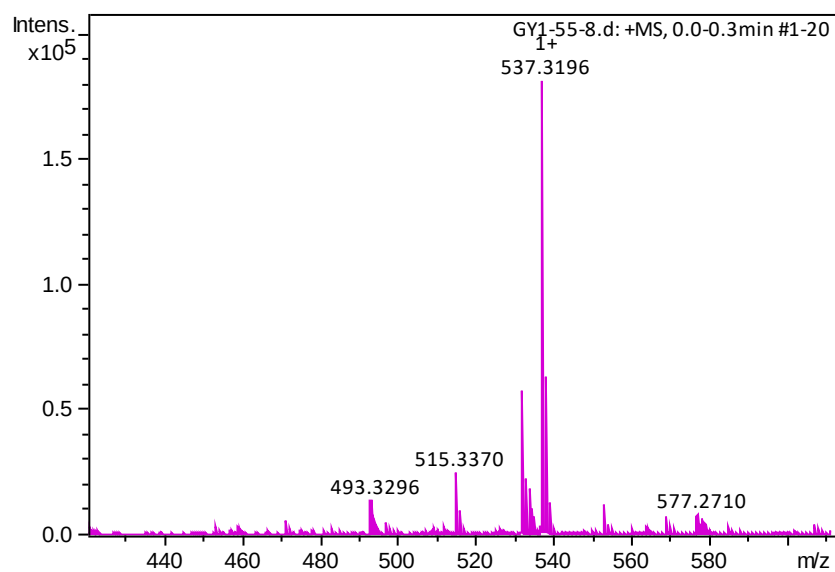
UV of compound **6**



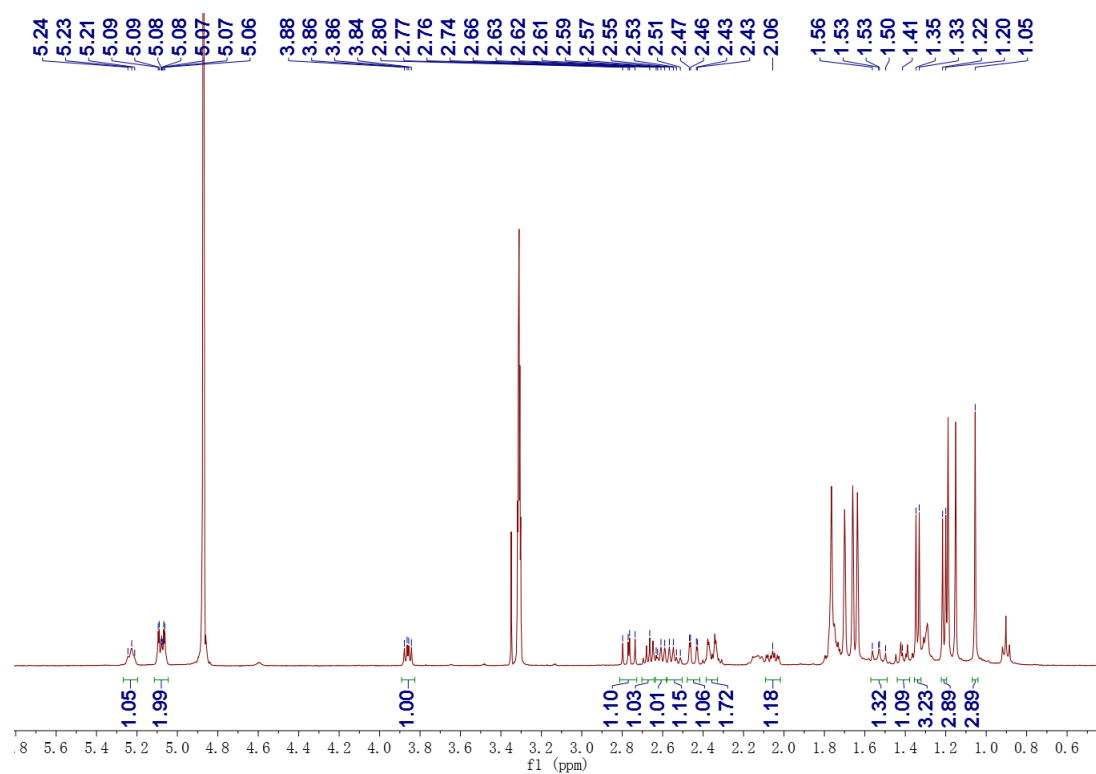
CD of compound **6**



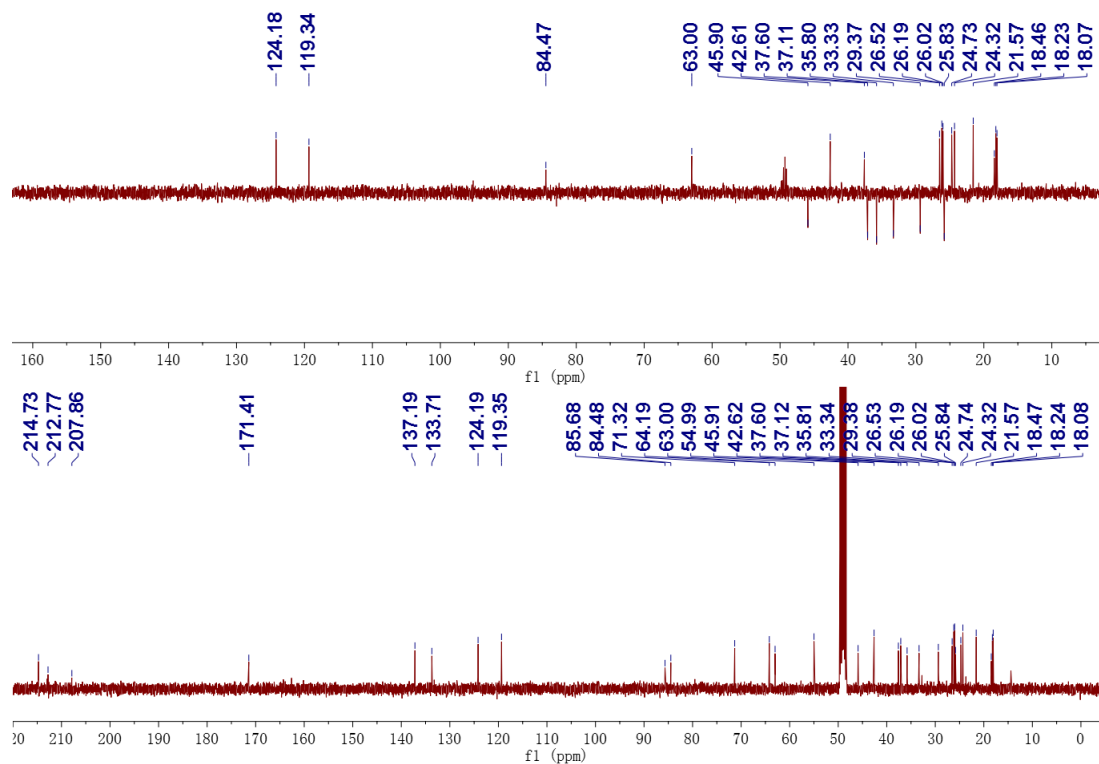
HRESIMS of compound 7



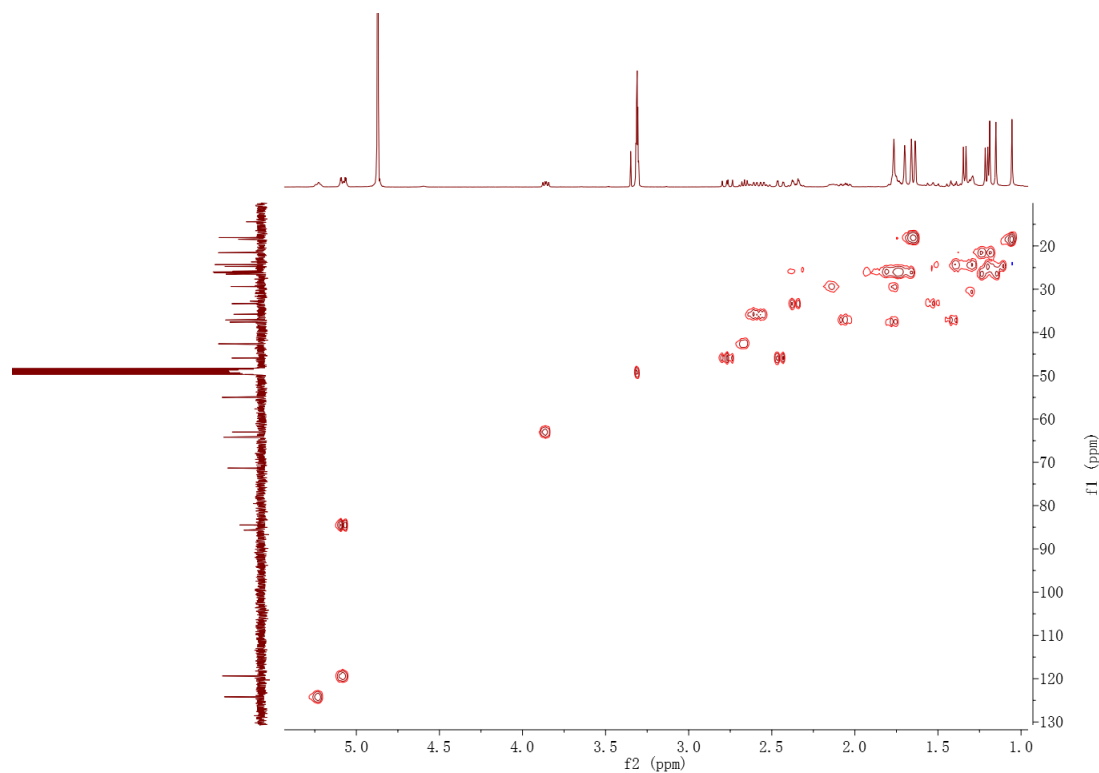
¹H NMR of compound 7 (400MHz, in CD₃OD)



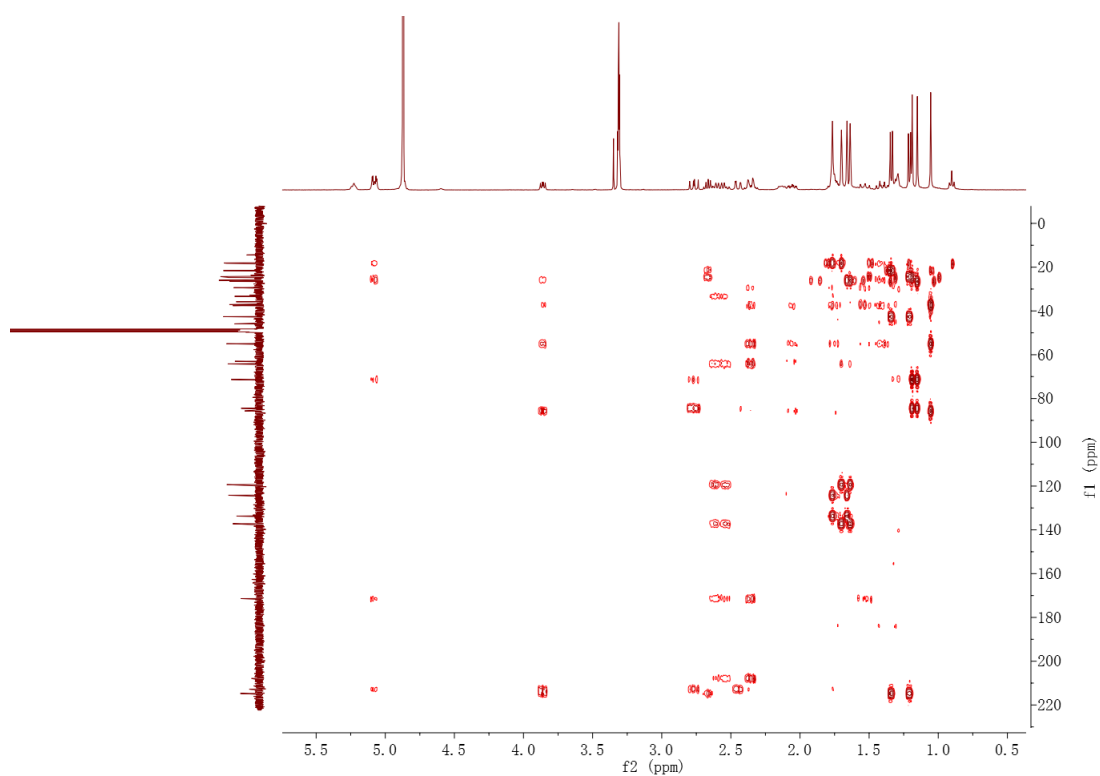
^{13}C NMR of compound 7 (100MHz, in CD_3OD)



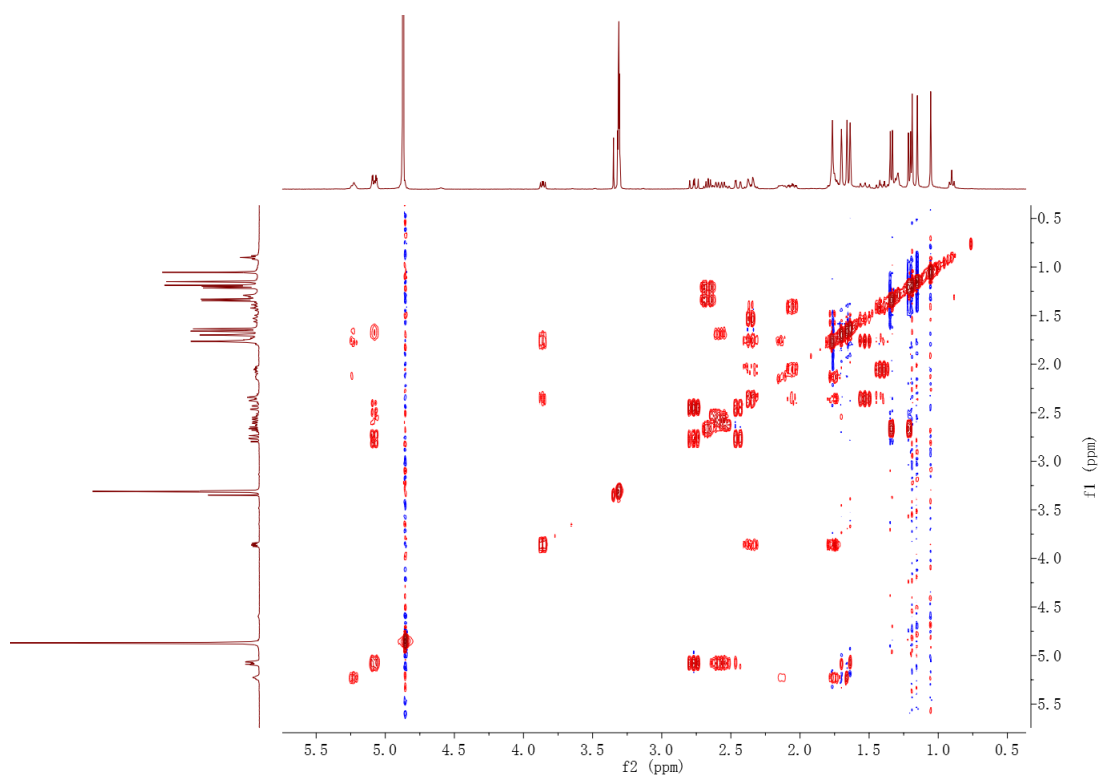
HSQC of compound 7 (400MHz, in CD_3OD)



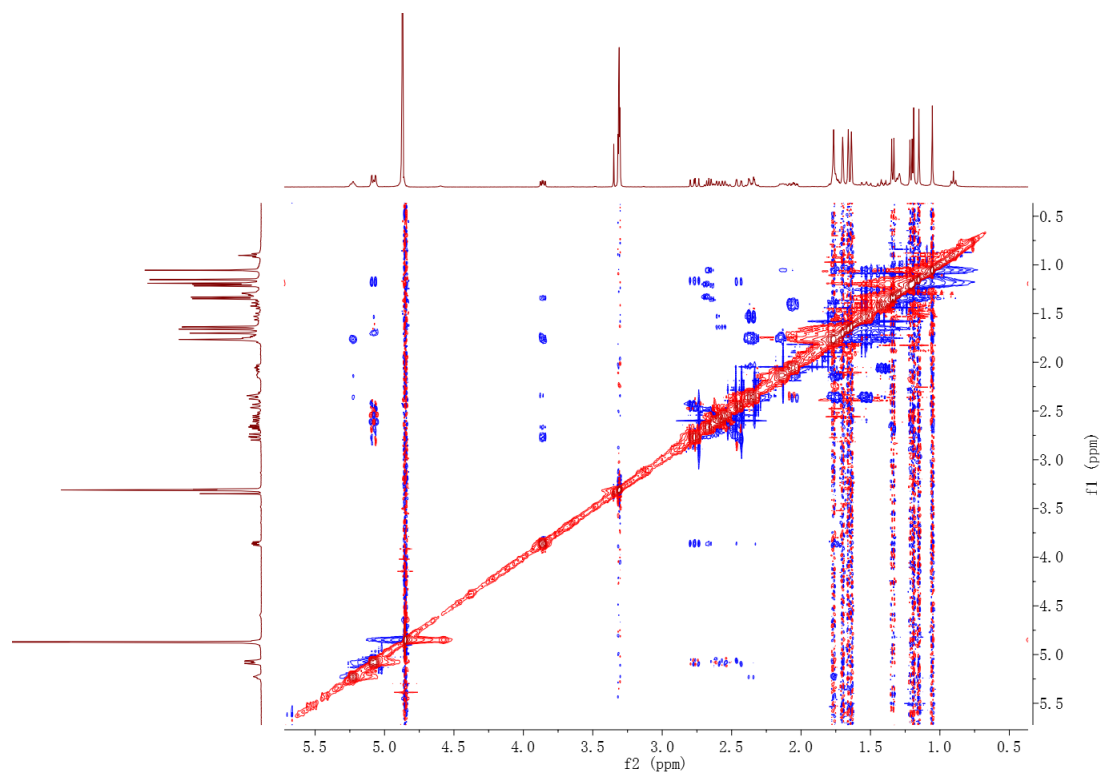
HMBC of compound 7 (400MHz, in CD₃OD)



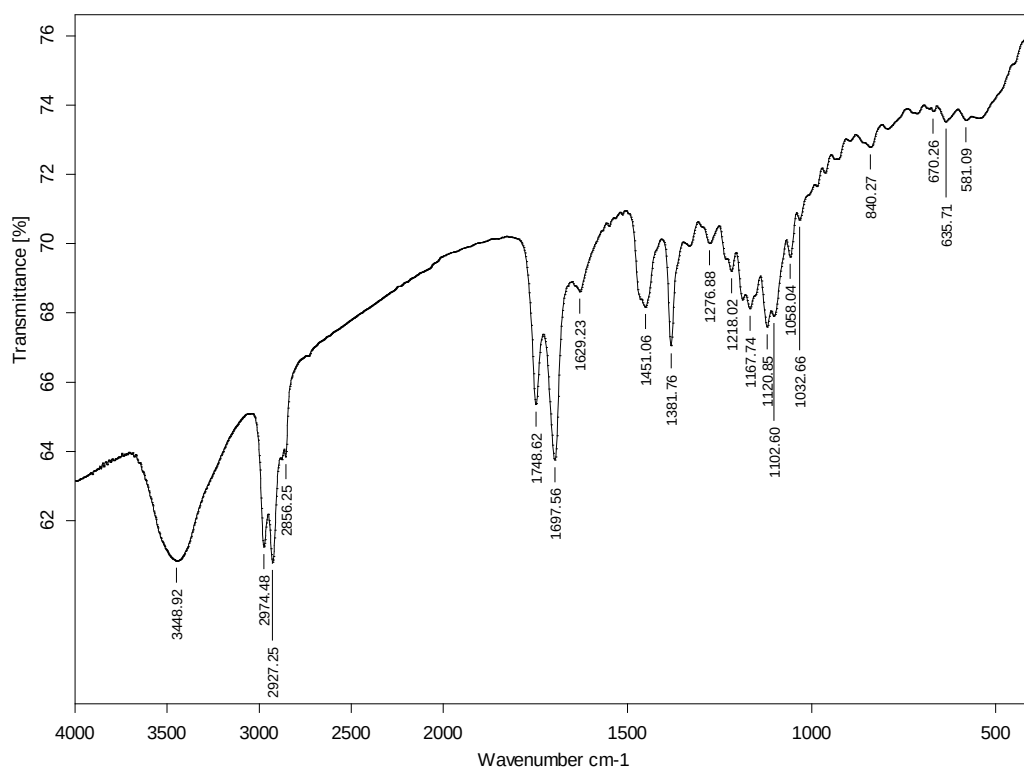
¹H-¹H COSY of compound 7 (400MHz, in CD₃OD)



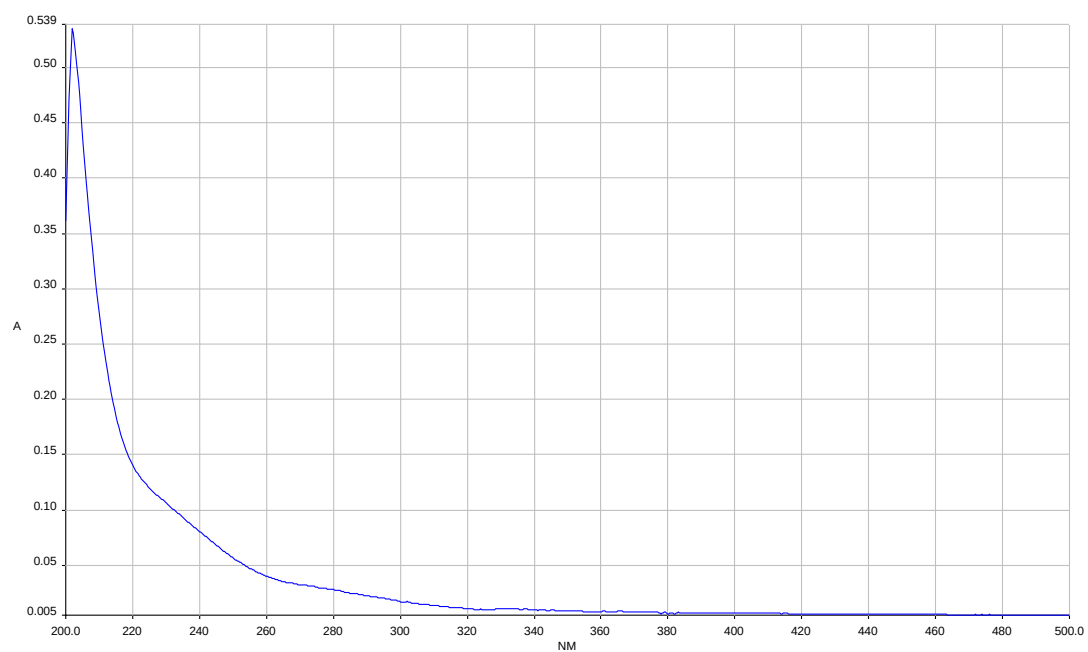
NOESY of compound **7** (400MHz, in CD₃OD)



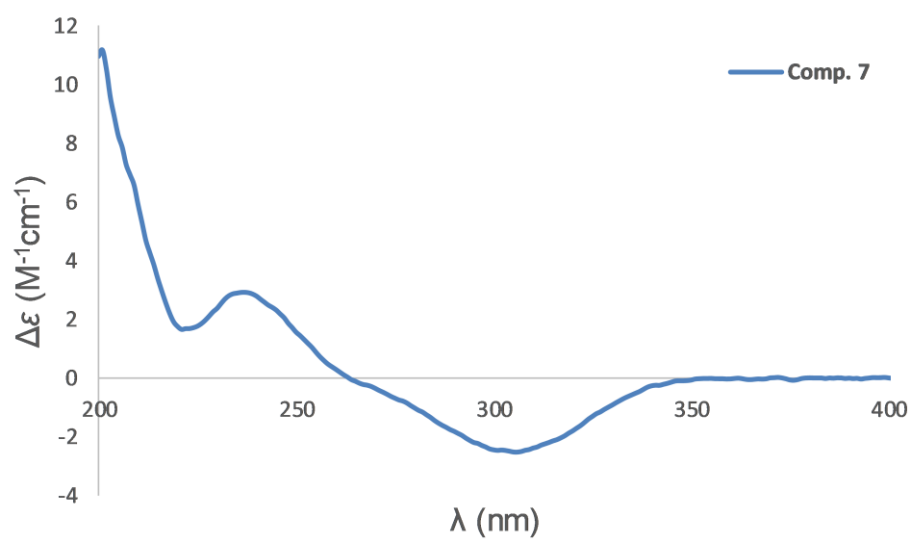
IR of compound **7**



UV of compound 7

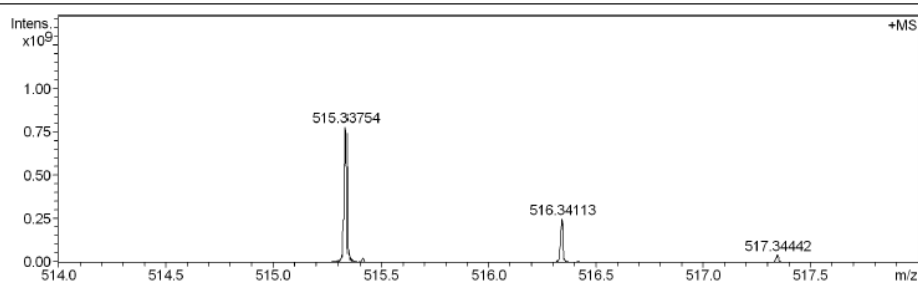


CD of compound 7

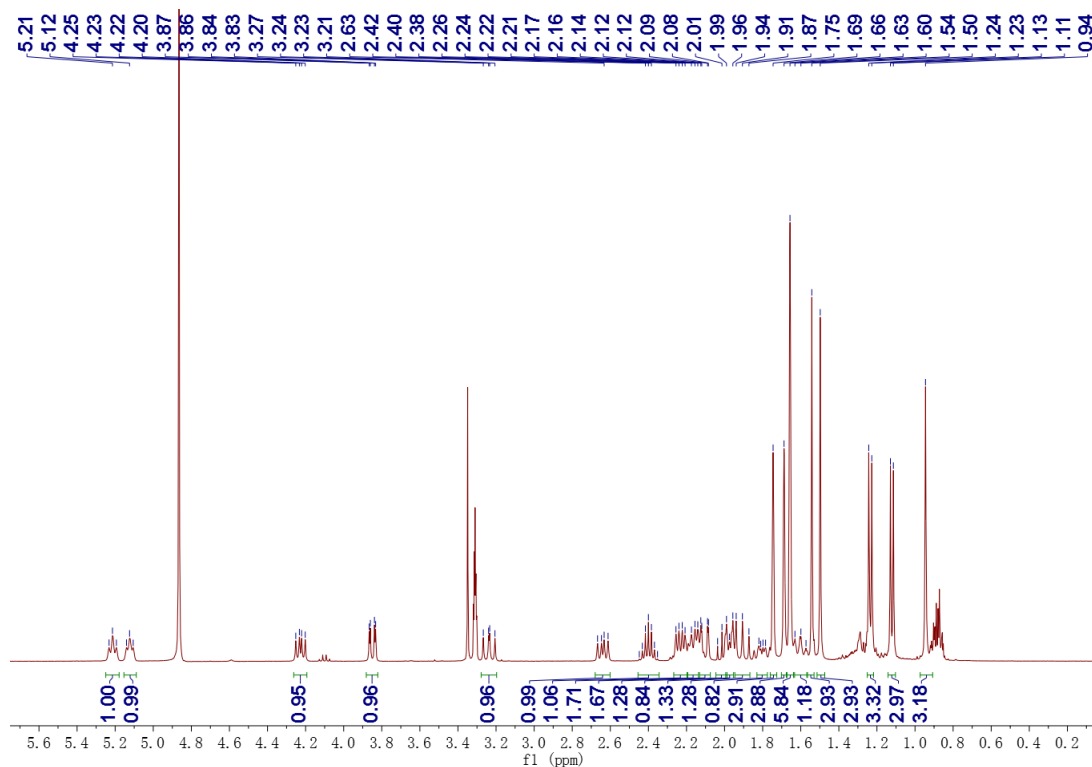


HRESIMS of compound 8

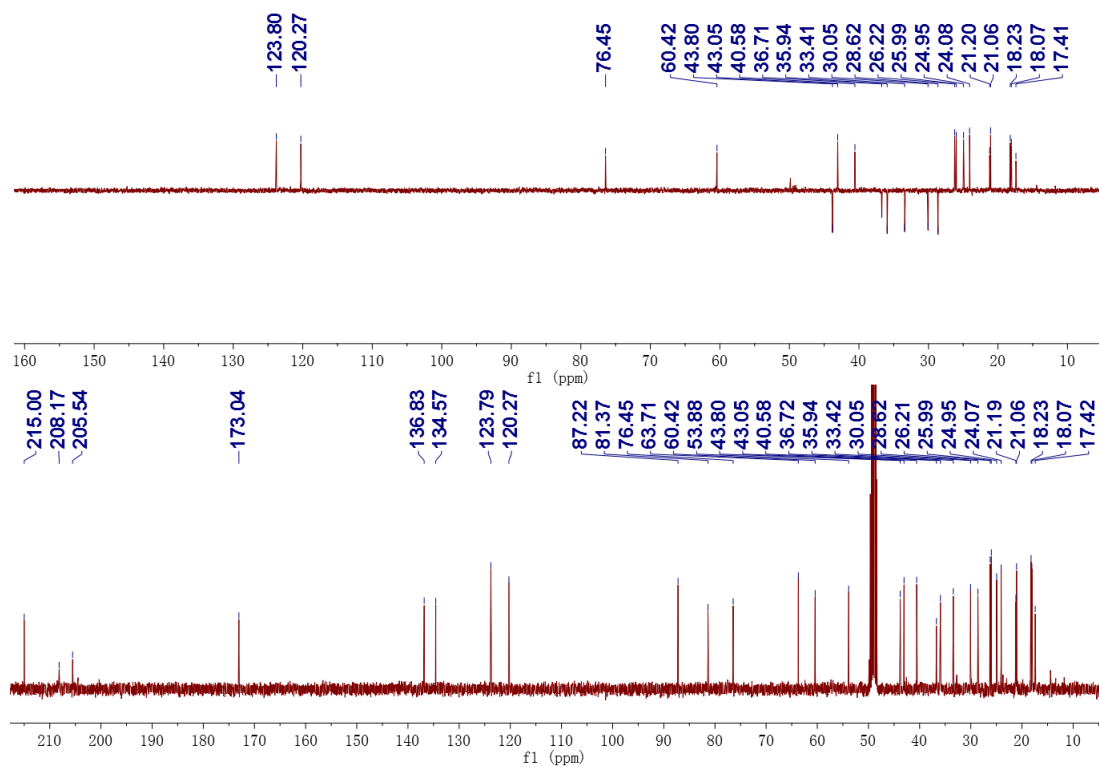
Mass Spectrum SmartFormula Report					
Analysis Info				Acquisition Date	10/21/2016 5:45:50 PM
Analysis Name	D:\Data\test\GY 1-47-17 APCI poss_000003.d				
Method	20160104_P			Operator	
Sample Name	Sample			Instrument	solariX
Comment					
Acquisition Parameter					
Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	147.5 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	3000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Jan 4 08:26:07 2016
Source Accumulation	0.001 sec	n/a	n/a	Data Acquisition Size	1048576
Ion Accumulation Time	0.100 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



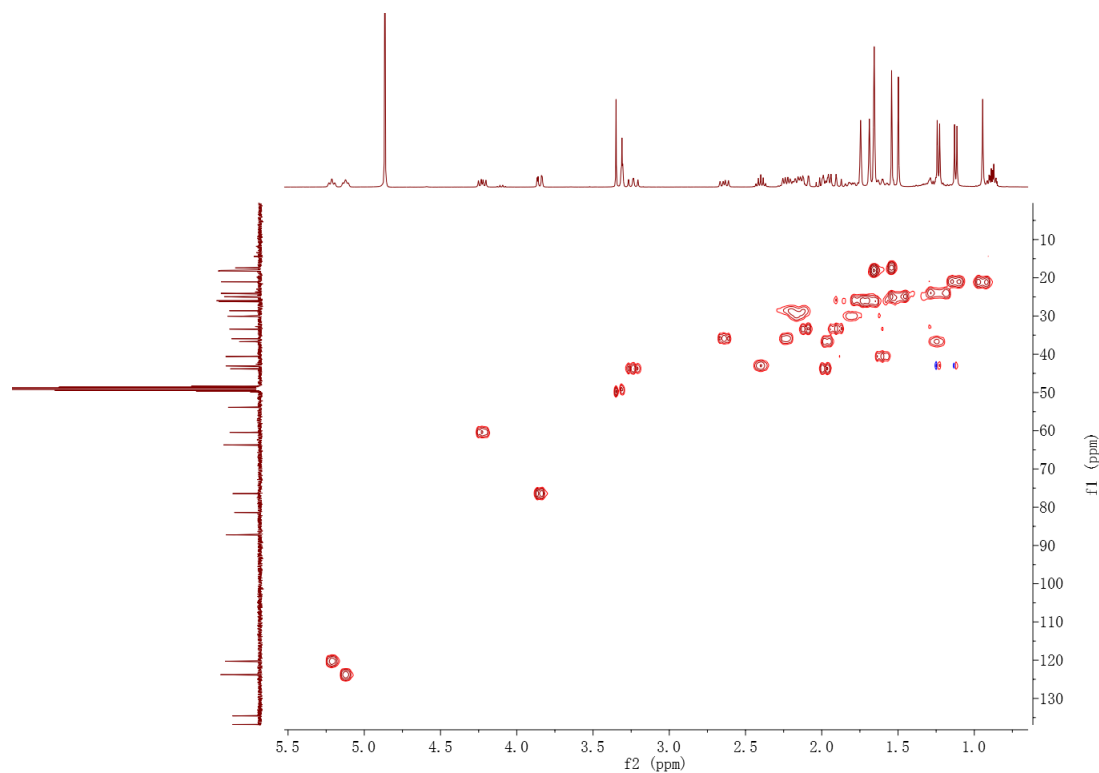
¹H NMR of compound 8 (400MHz, in CD₃OD)



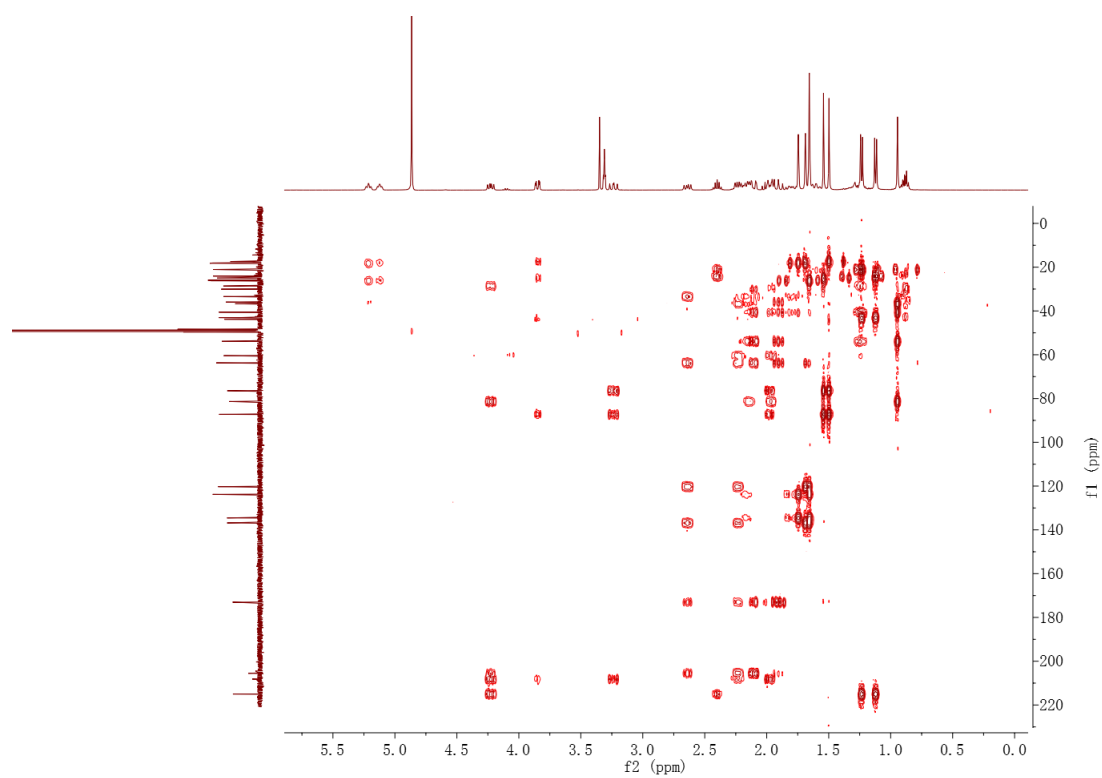
^{13}C NMR of compound **8** (100MHz, in CD_3OD)



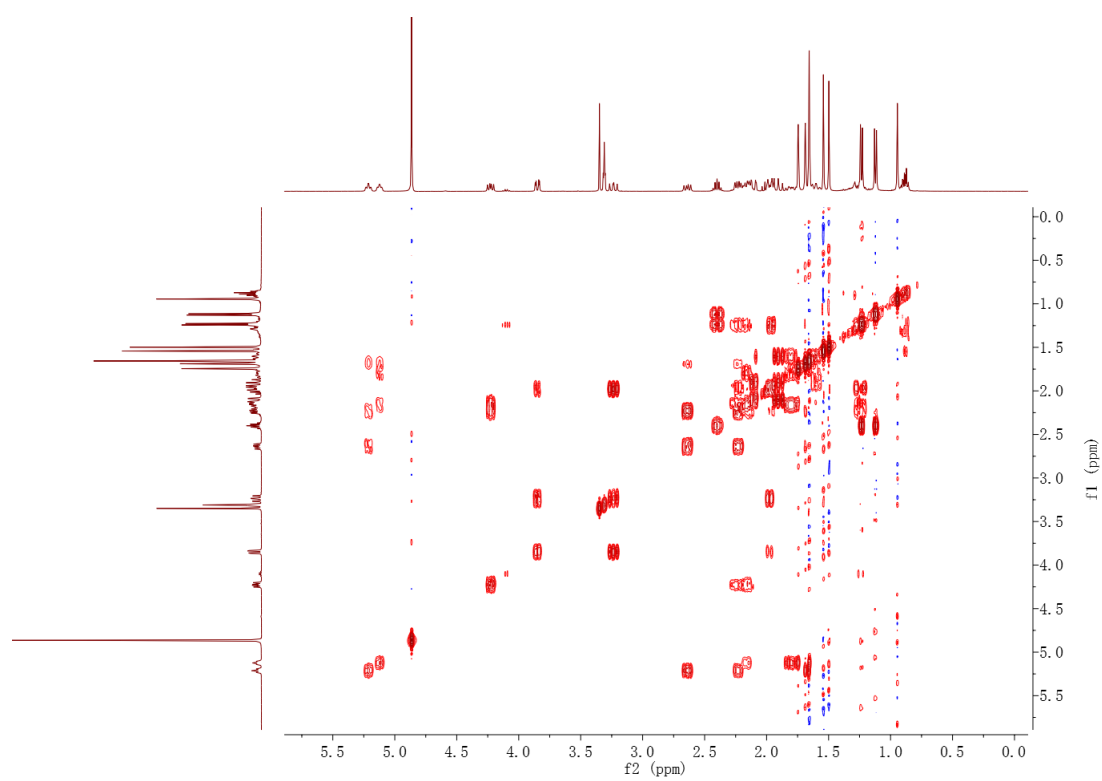
HSQC of compound **8** (400MHz, in CD_3OD)



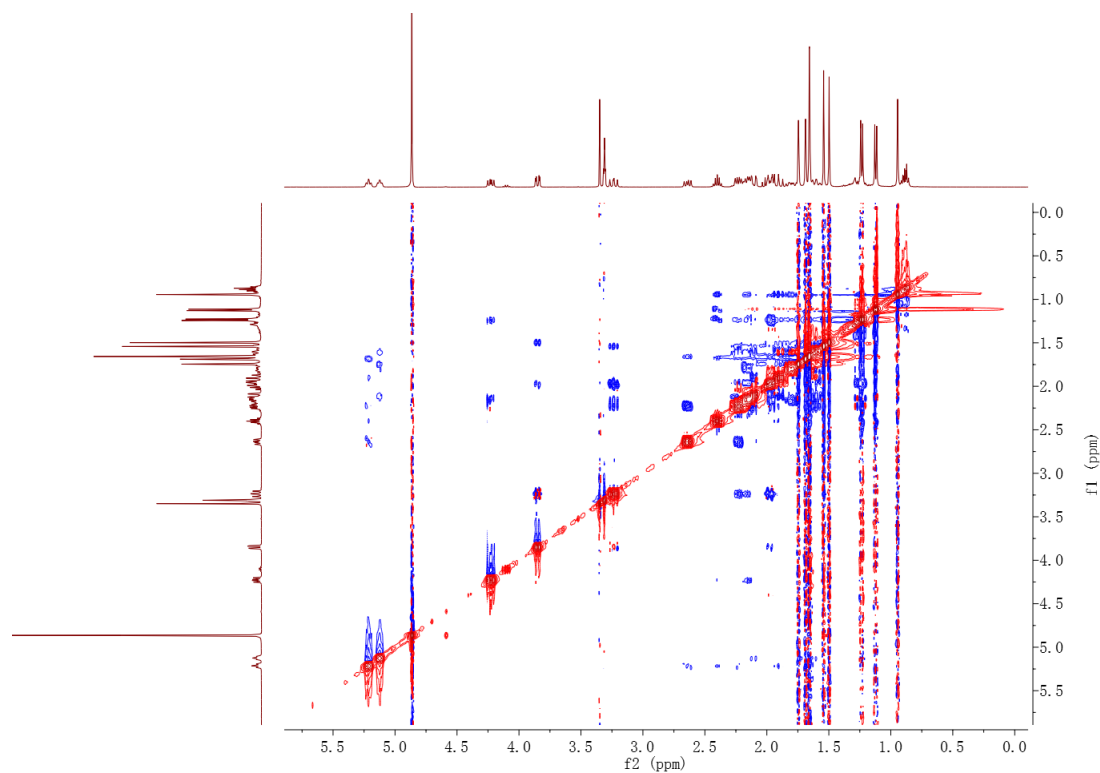
HMBC of compound **8** (400MHz, in CD₃OD)



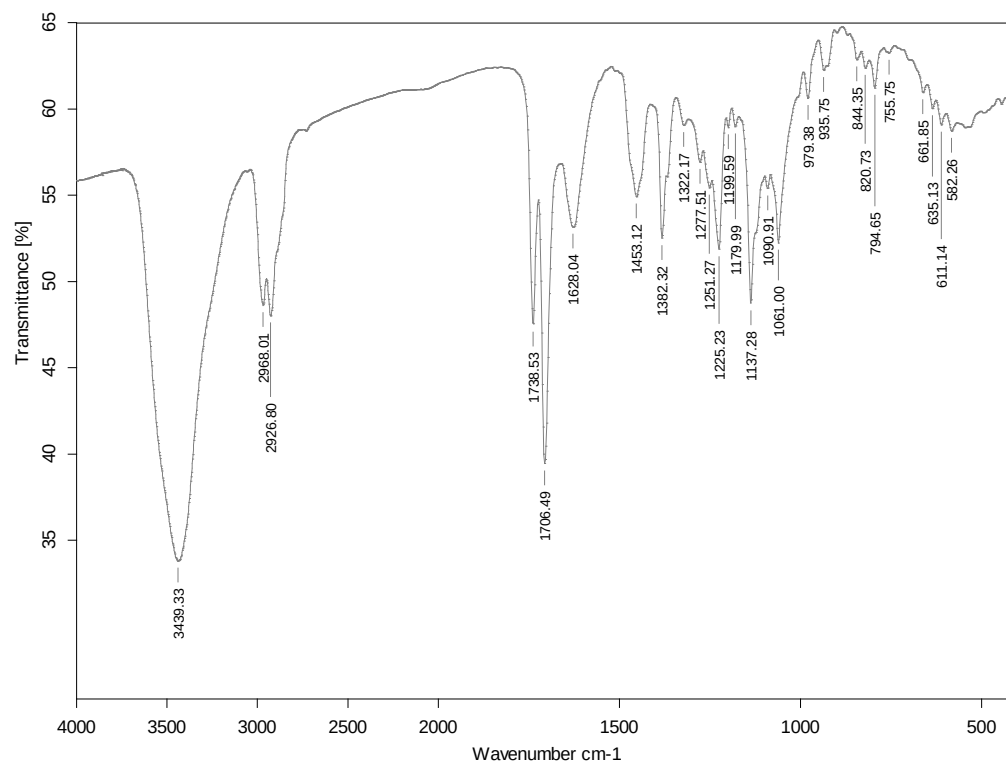
¹H-¹H COSY of compound **8** (400MHz, in CD₃OD)



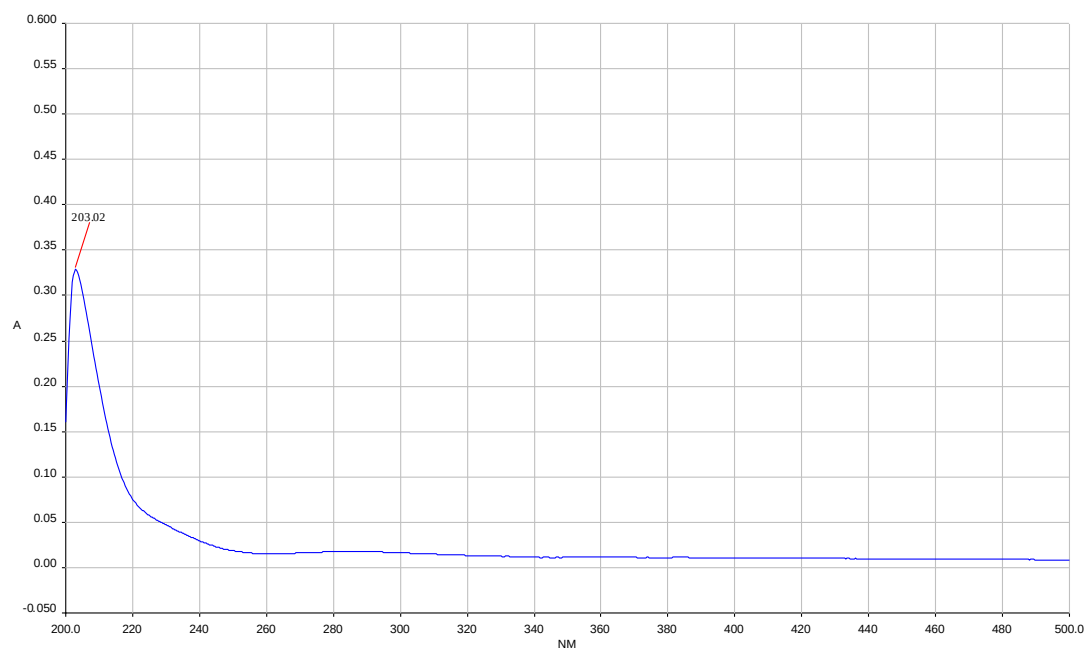
NOESY of compound **8** (400MHz, in CD₃OD)



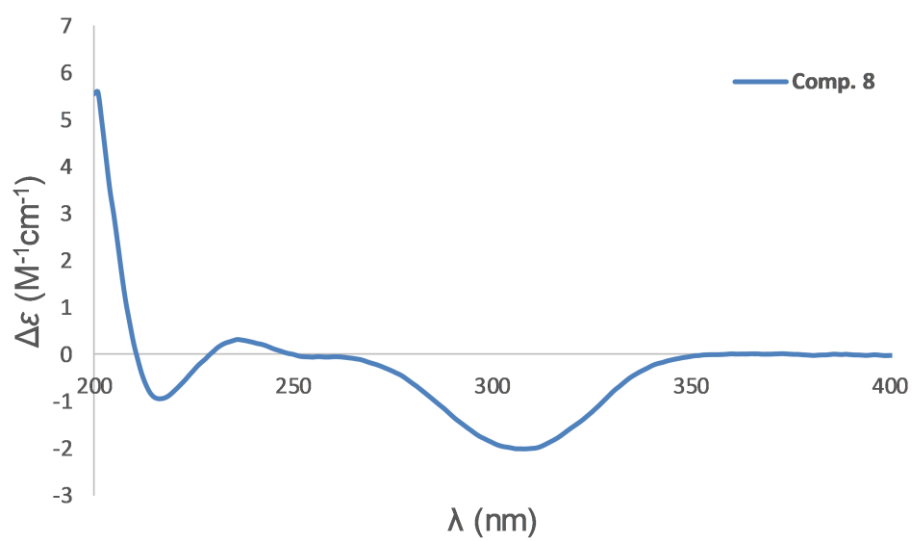
IR of compound **8**



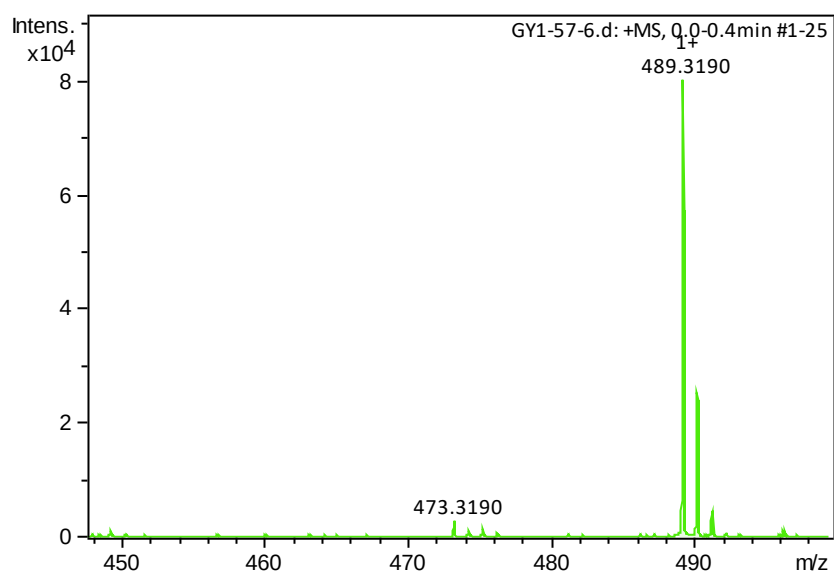
UV of compound **8**



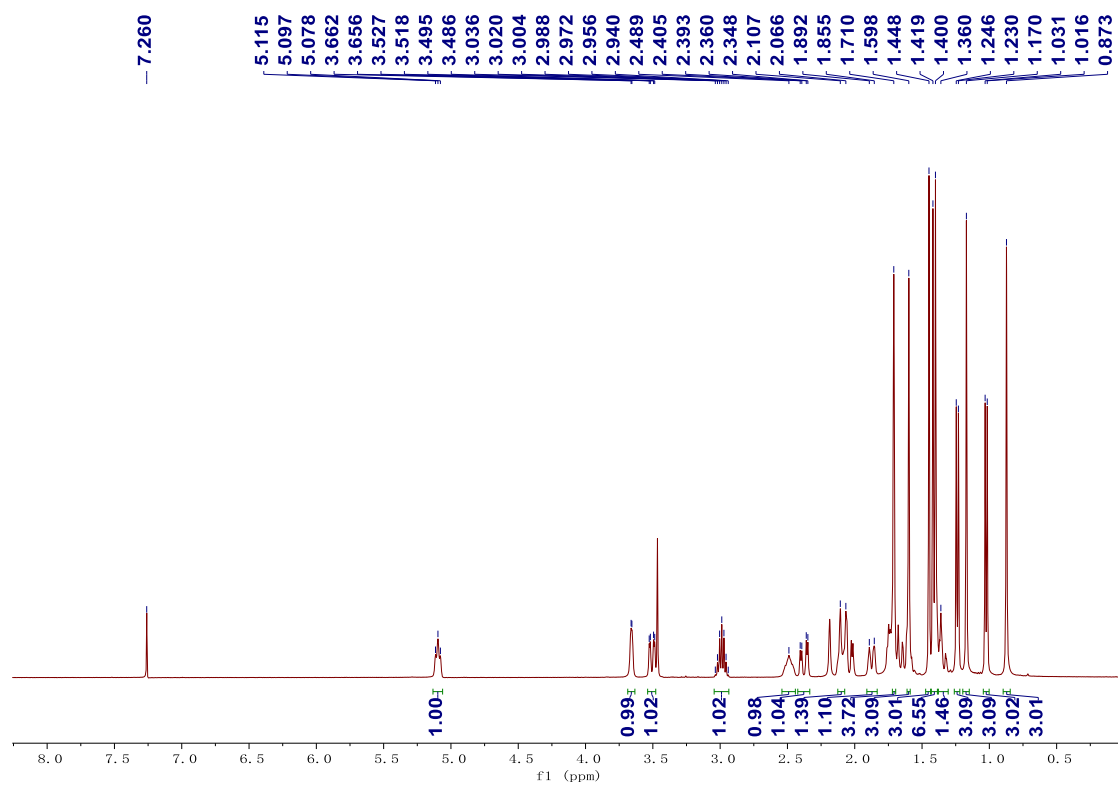
CD of compound **8**



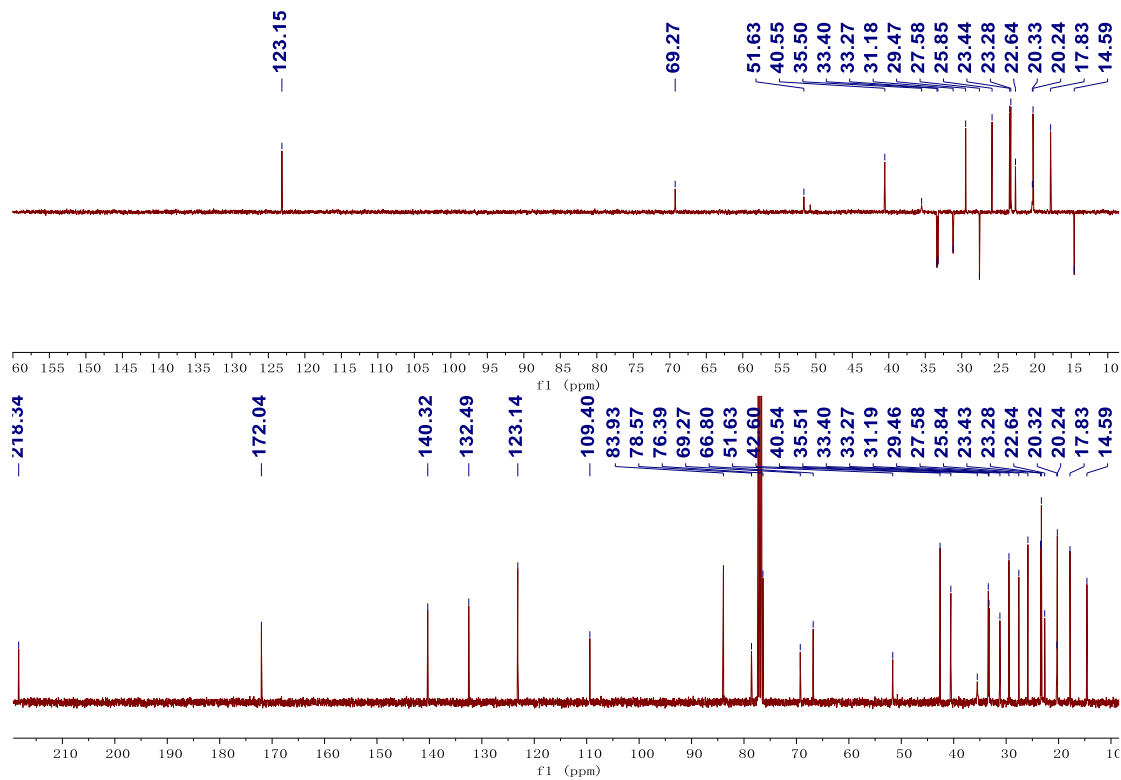
HRESIMS of compound **9**



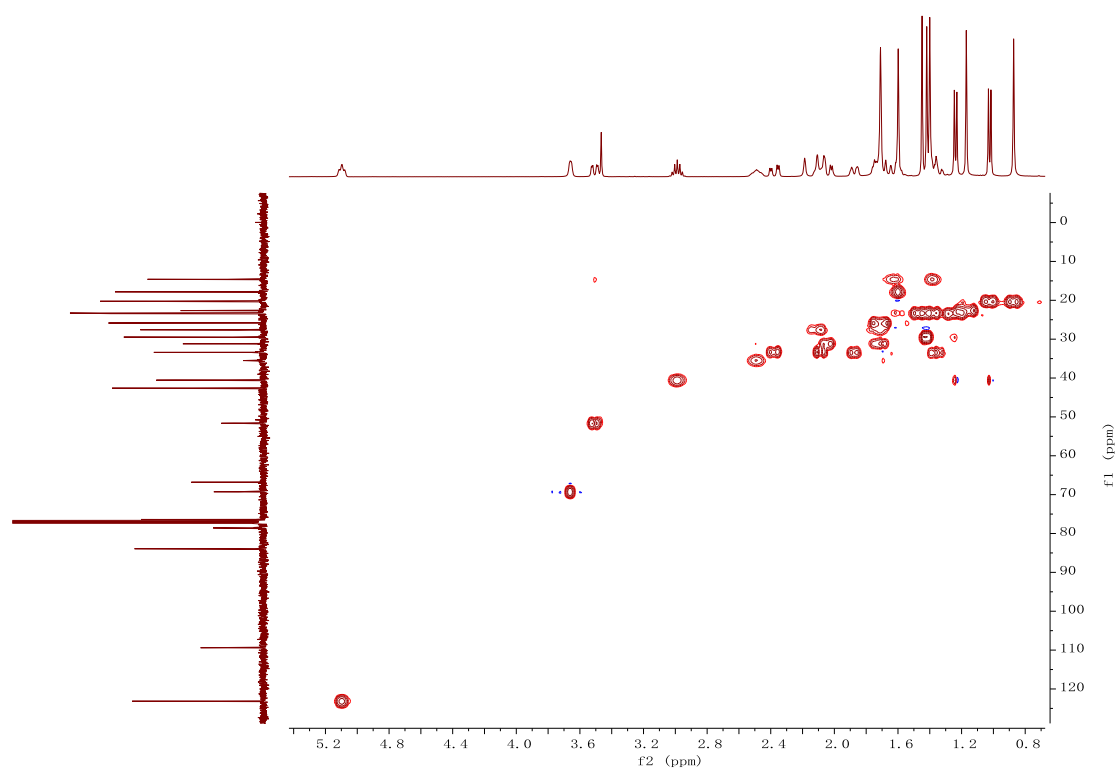
¹H NMR of compound **9** (400MHz, in CDCl₃)



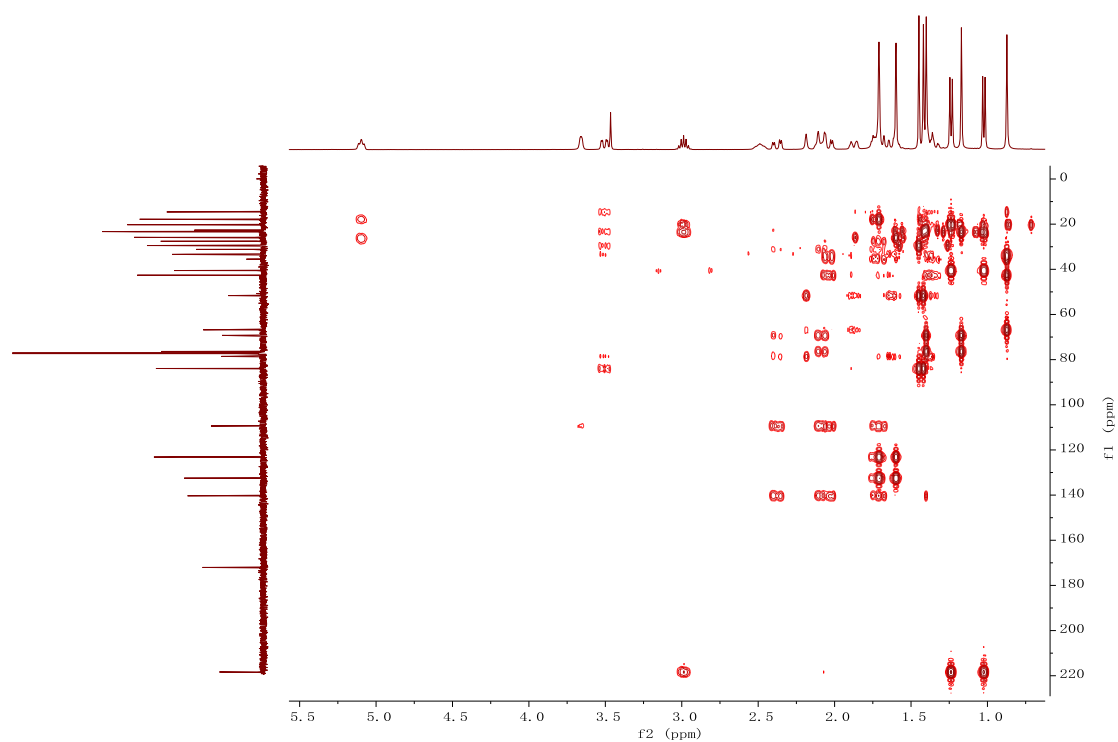
^{13}C NMR of compound **9** (100MHz, in CDCl_3)



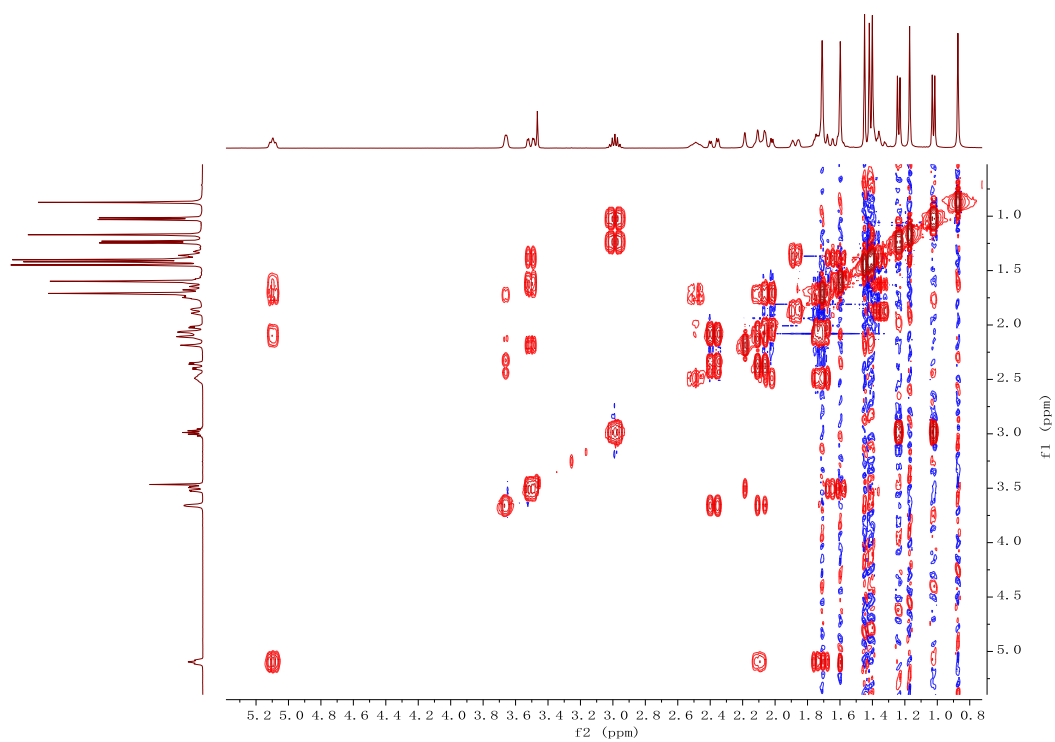
HSQC of compound **9** (400MHz, in CDCl_3)



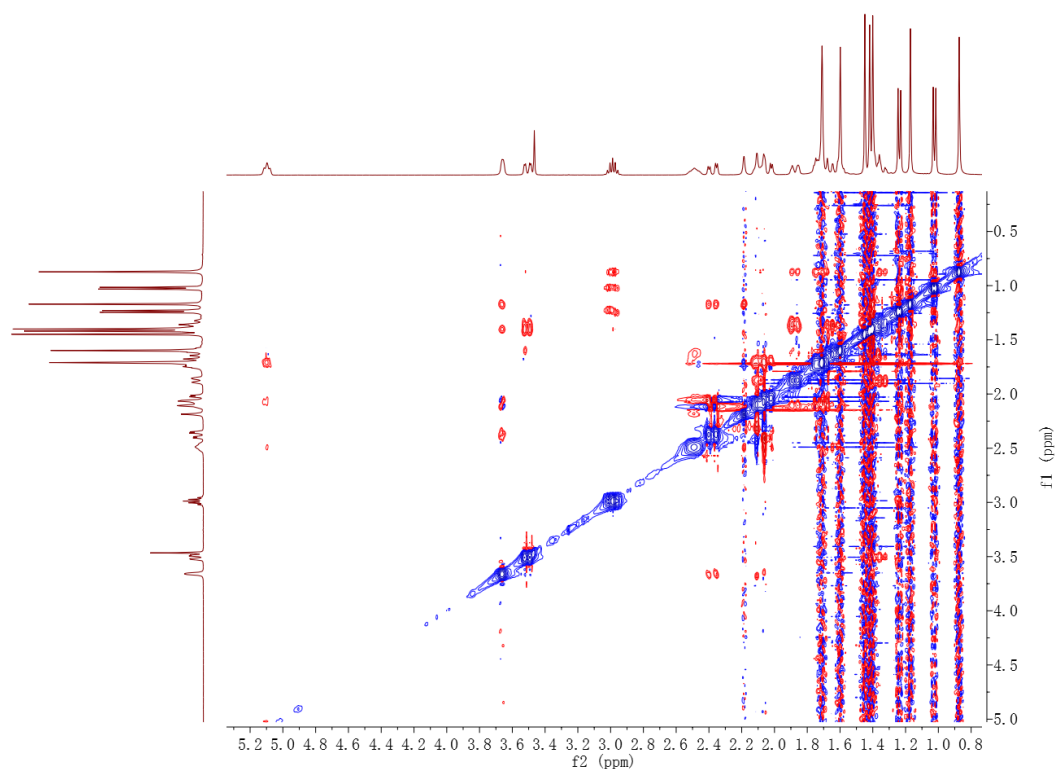
HMBC of compound **9** (400MHz, in CDCl₃)



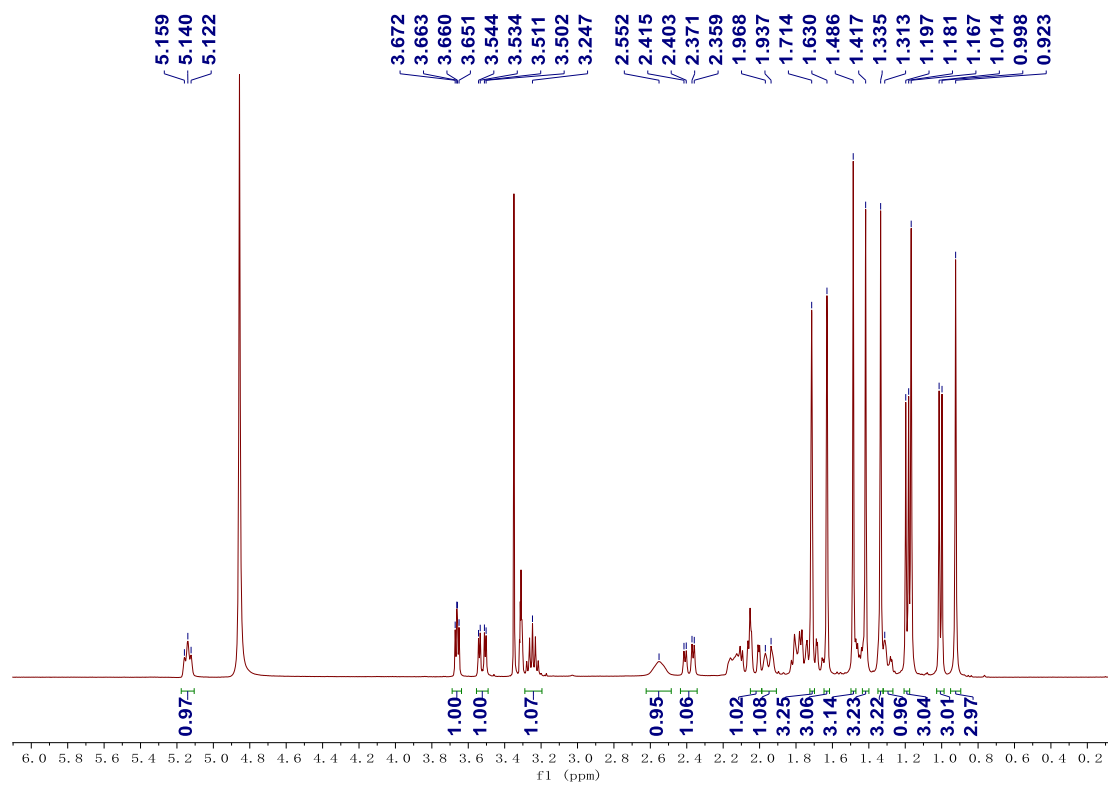
¹H–¹H COSY of compound **9** (400MHz, in CDCl₃)



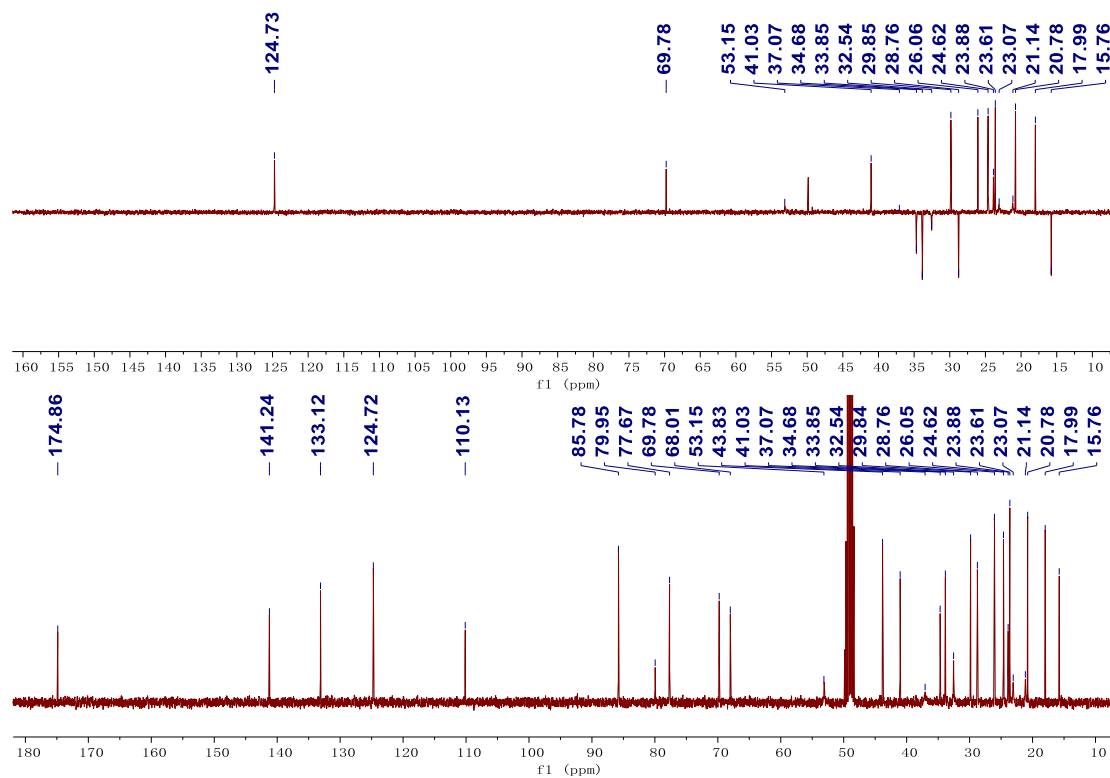
NOESY of compound **9** (400MHz, in CDCl₃)



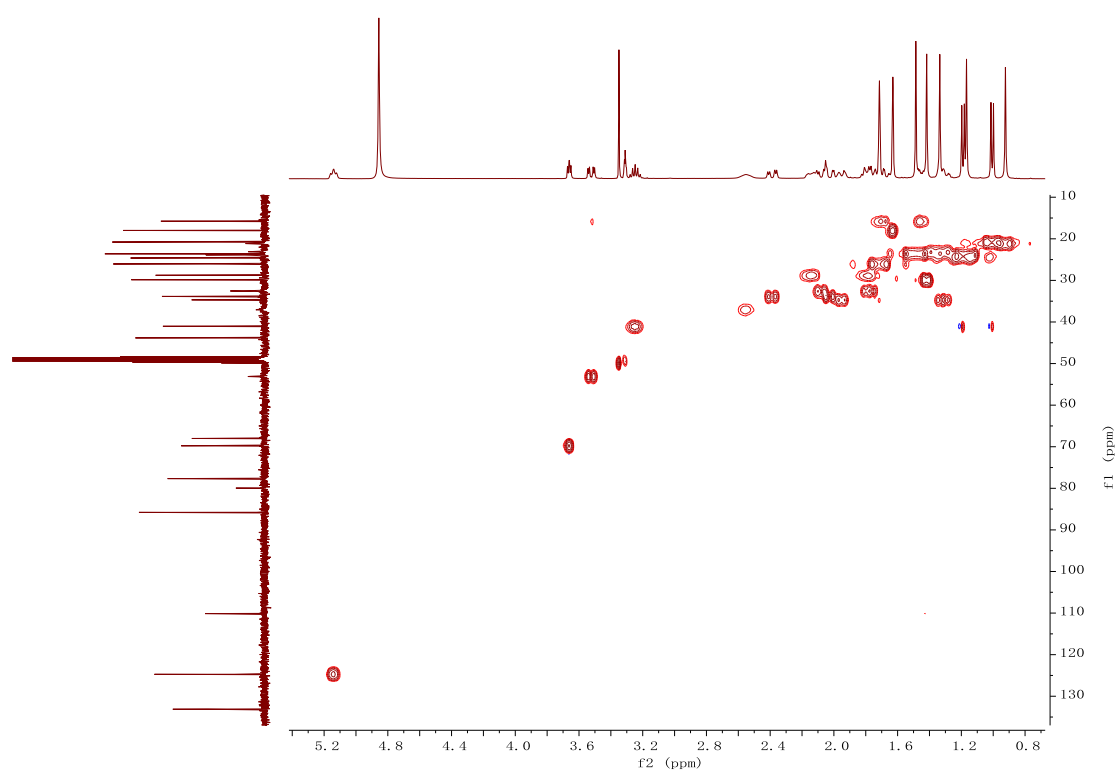
¹H NMR of compound **9** (400MHz, in CD₃OD)



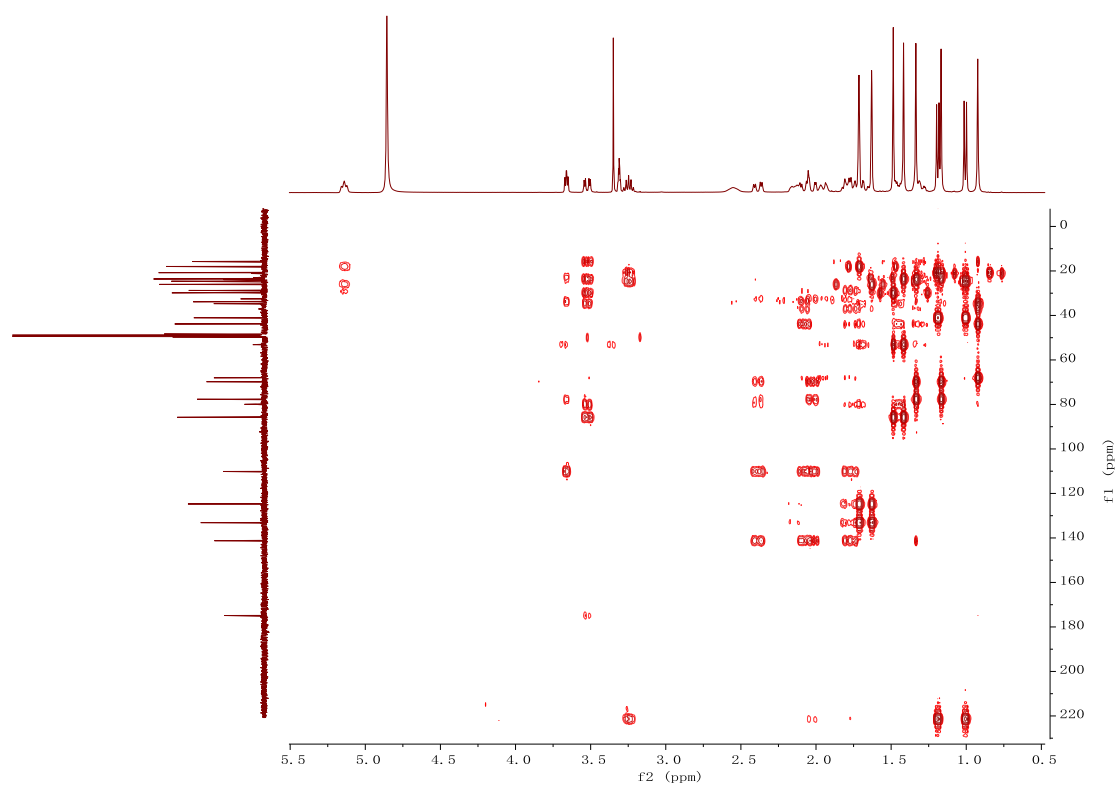
^{13}C NMR of compound **9** (100MHz, in CD_3OD)



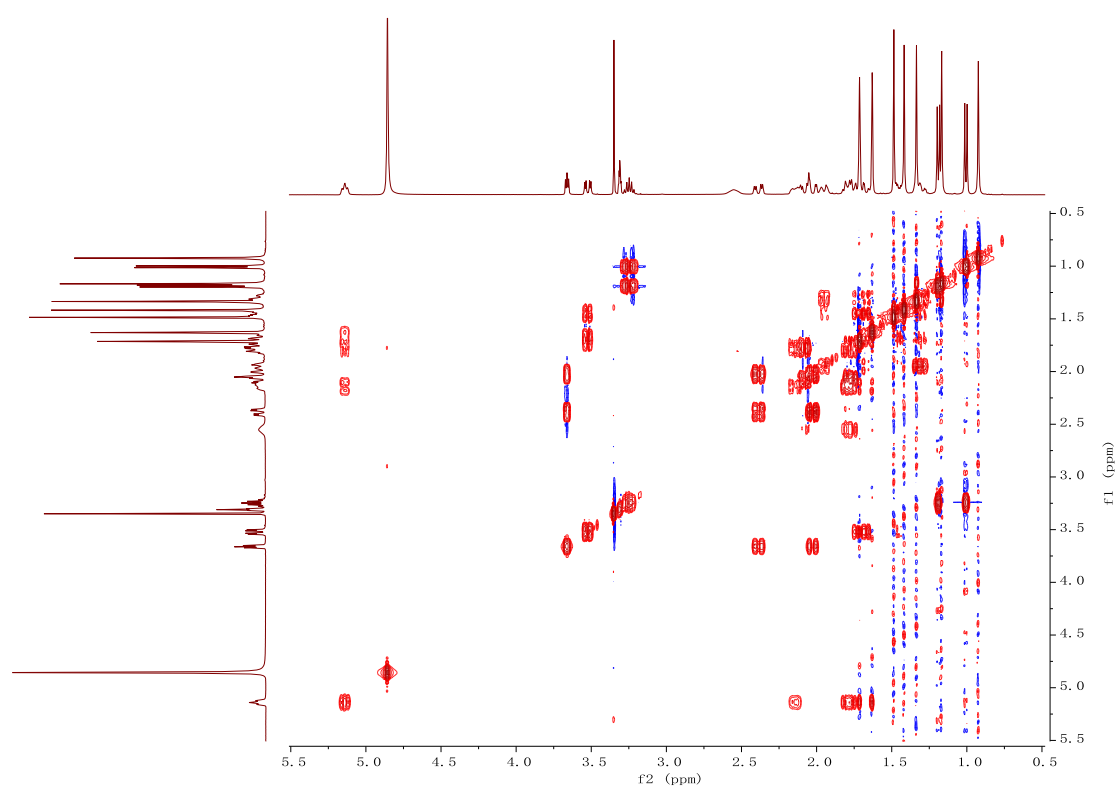
HSQC of compound **9** (400MHz, in CD_3OD)



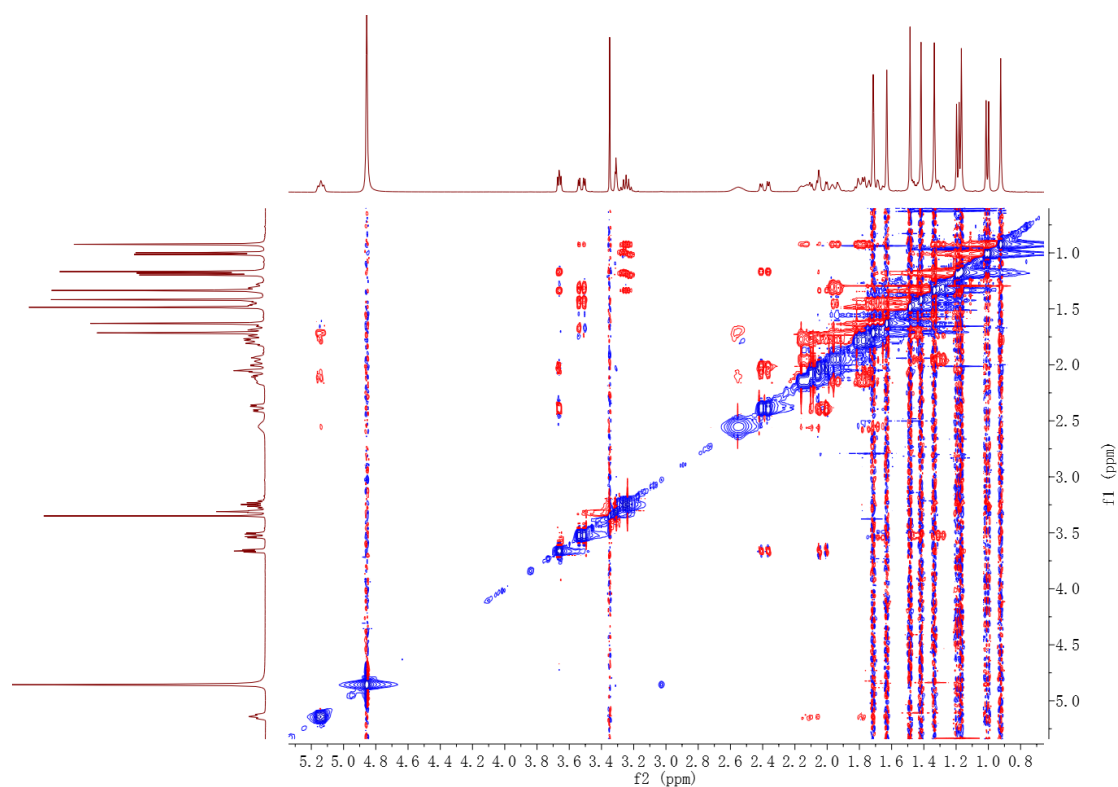
HMBC of compound **9** (400MHz, in CD₃OD)



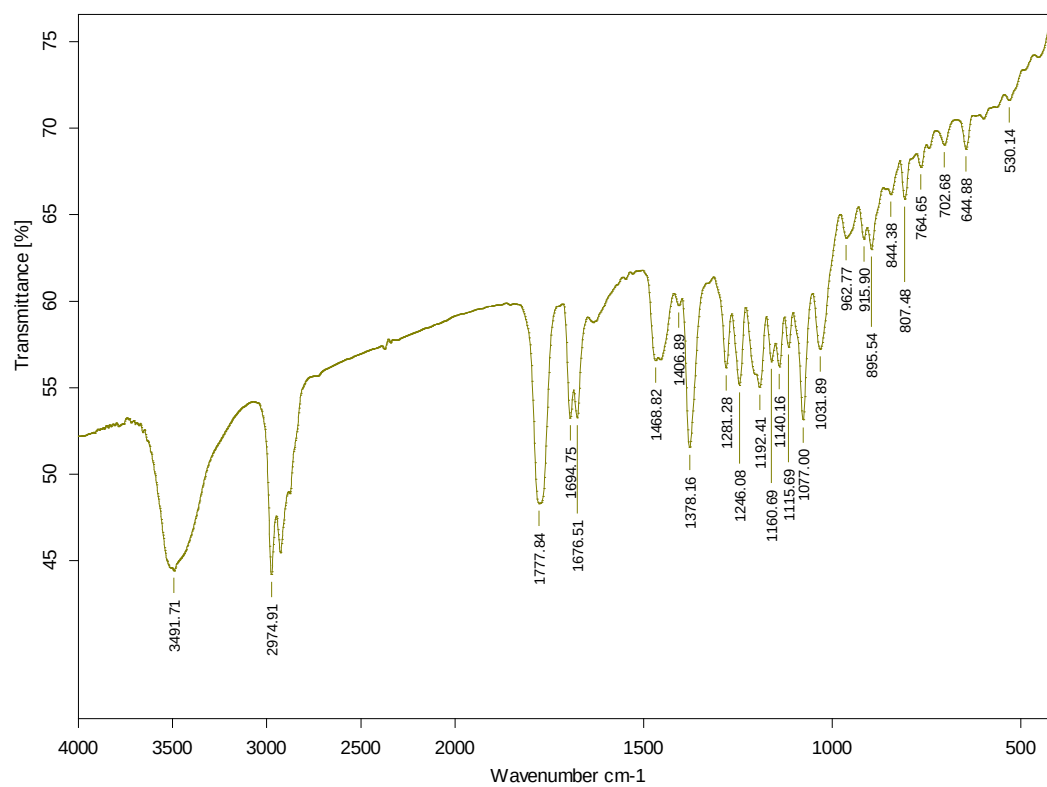
¹H-¹H COSY of compound **9** (400MHz, in CD₃OD)



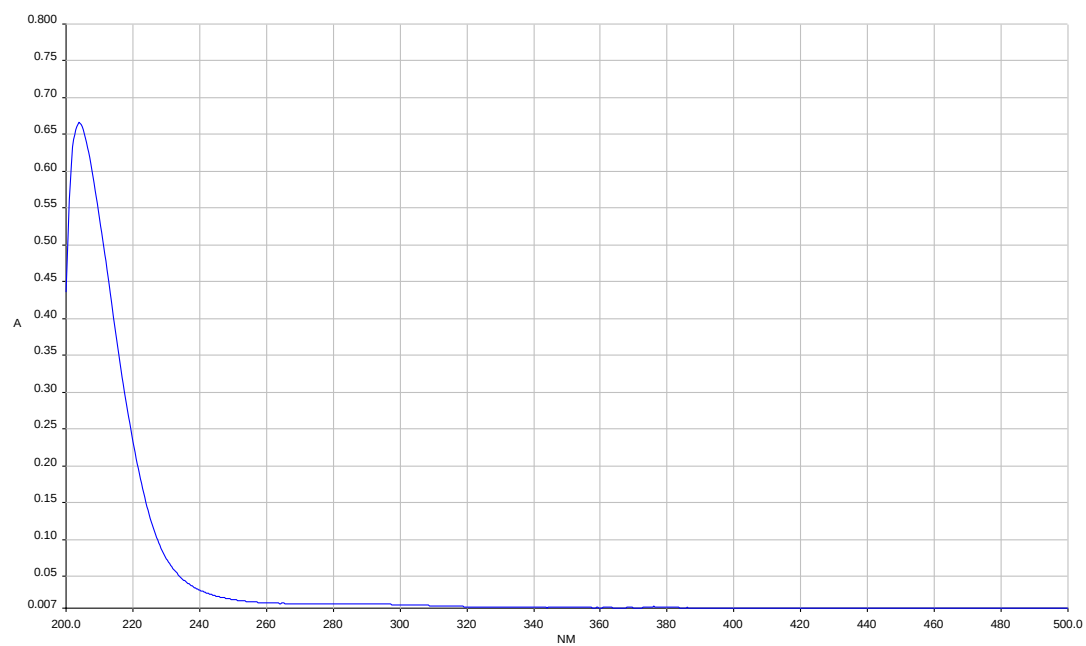
NOESY of compound **9** (400MHz, in CD₃OD)



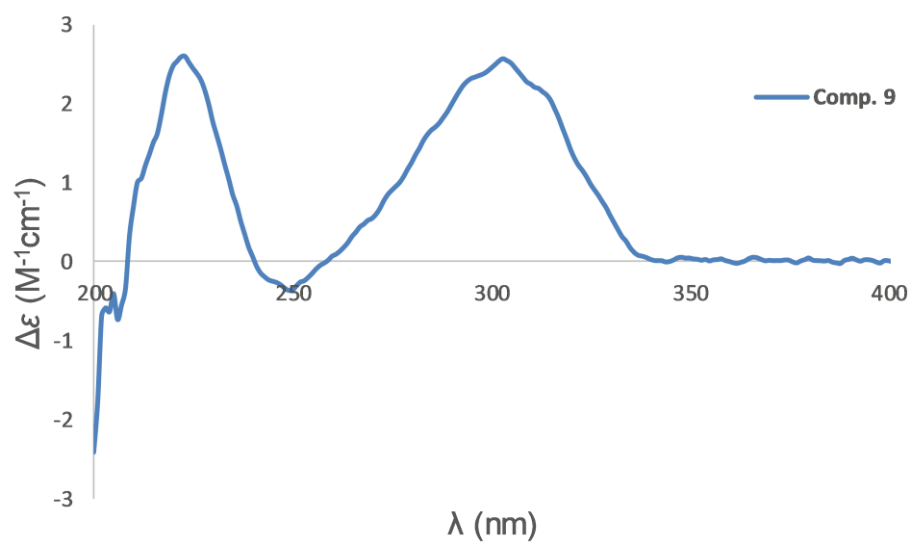
IR of compound **9**



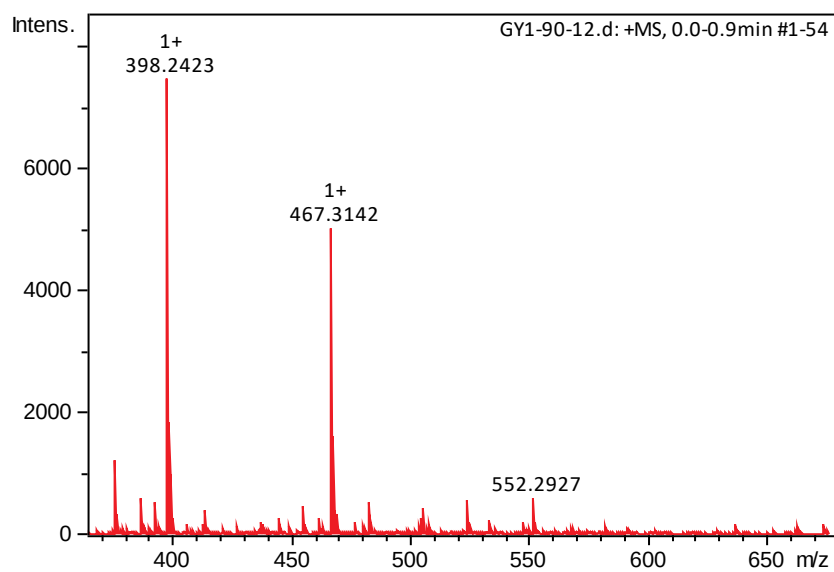
UV of compound **9**



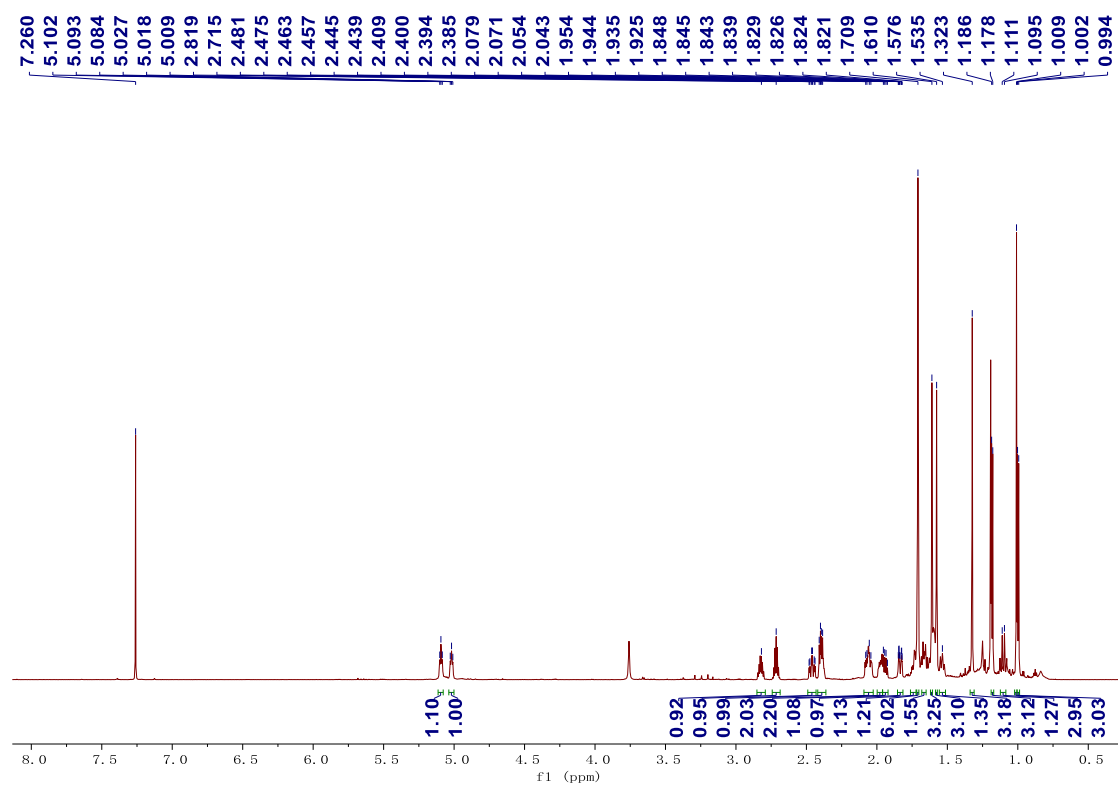
CD of compound **9**



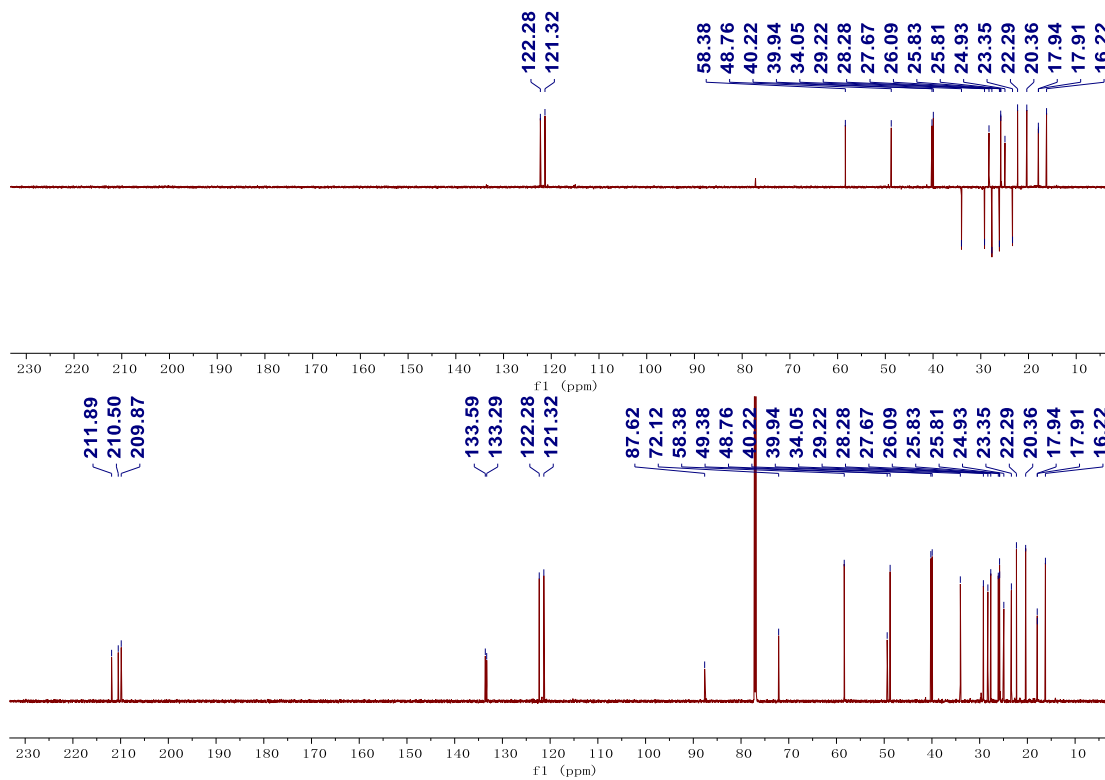
HRESIMS of compound **10**



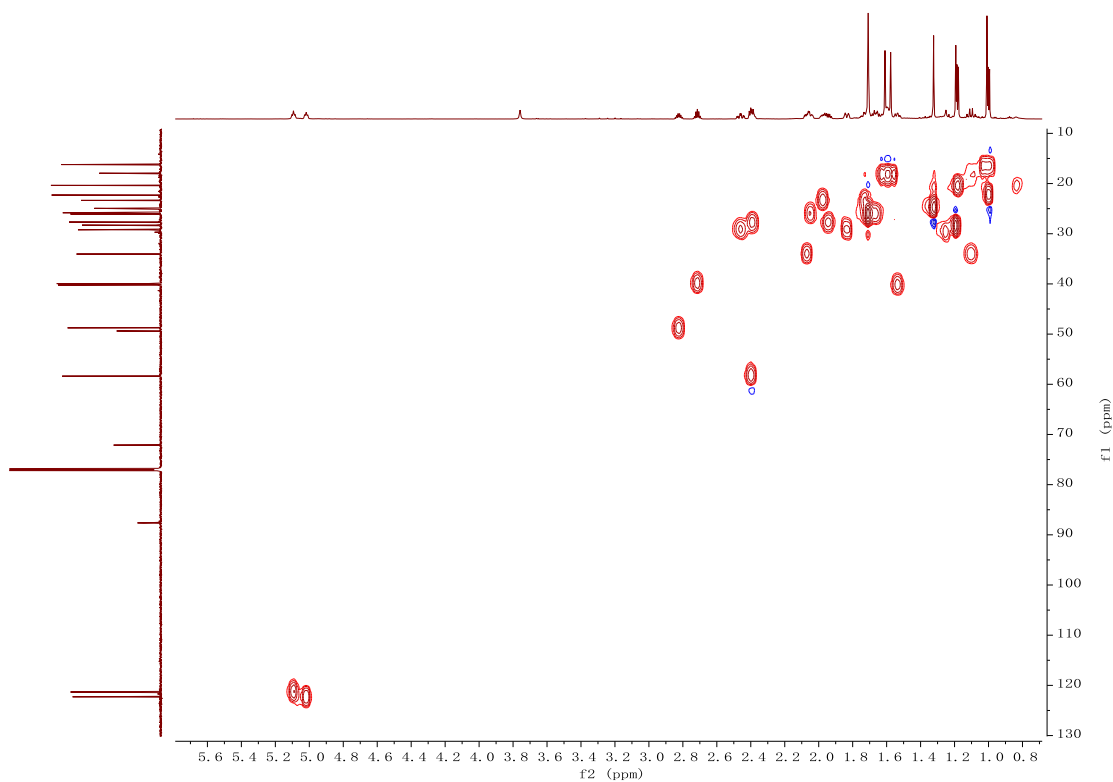
¹H NMR of compound **10** (800MHz, in CDCl₃)



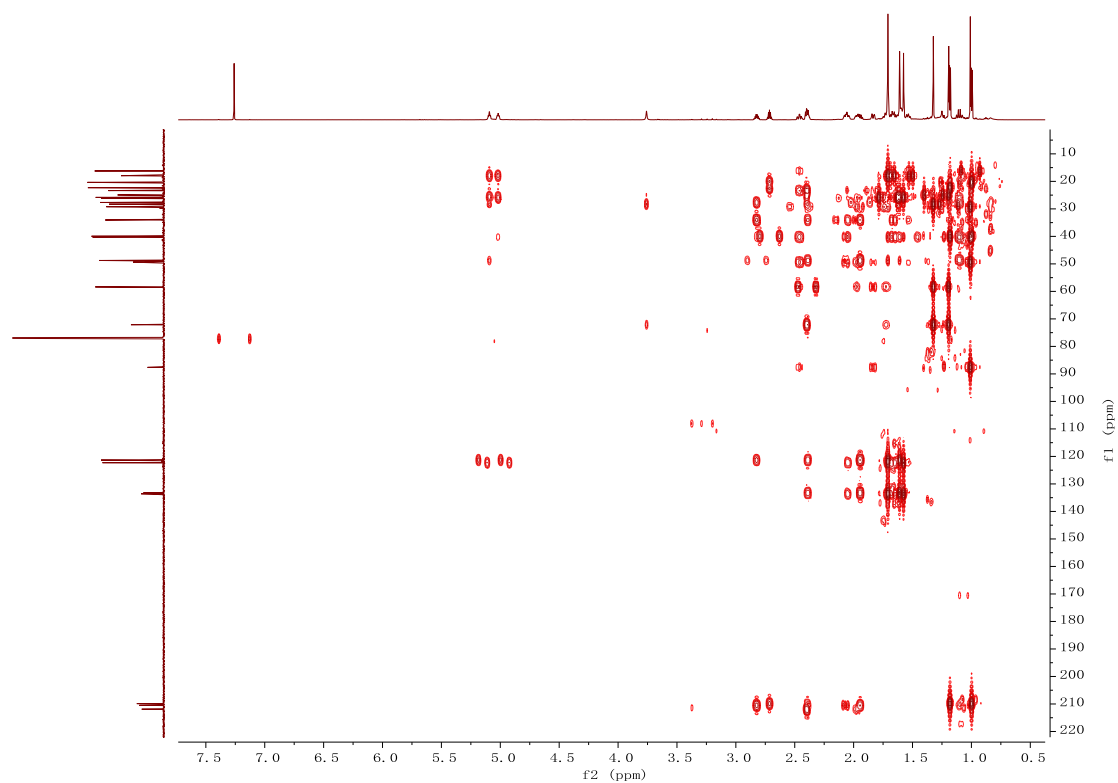
^{13}C NMR of compound **10** (200MHz, in CDCl_3)



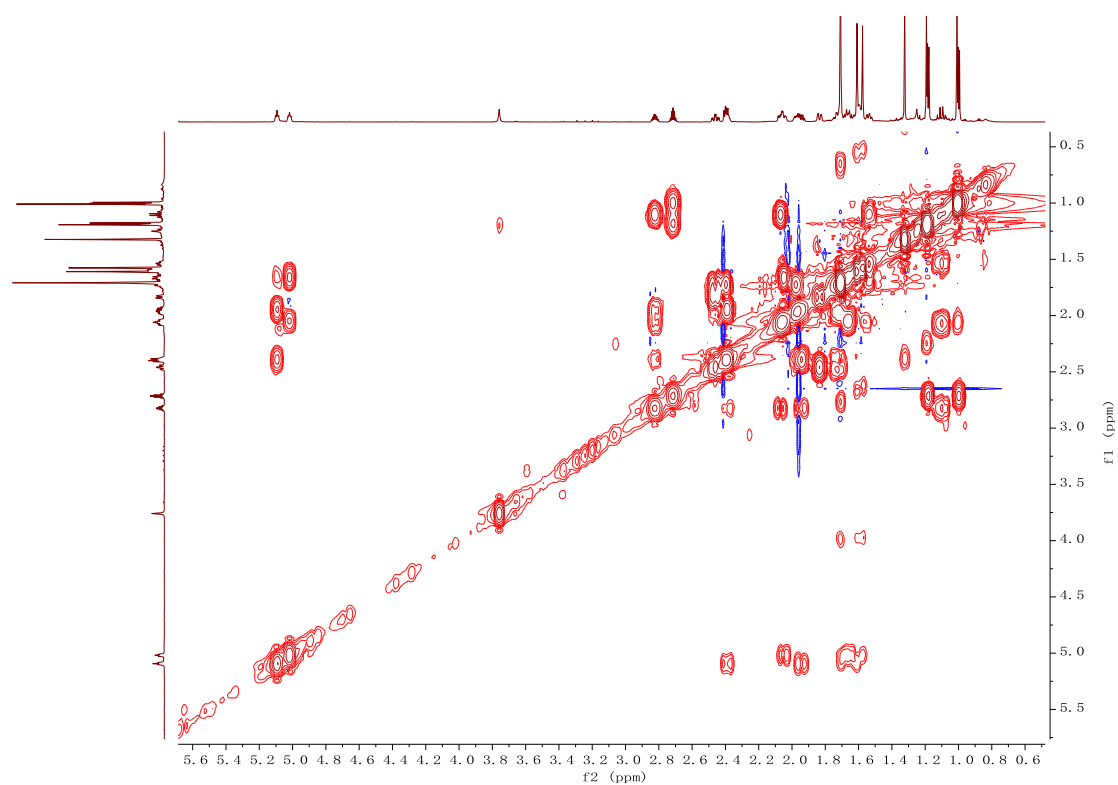
HSQC of compound **10** (800MHz, in CDCl_3)



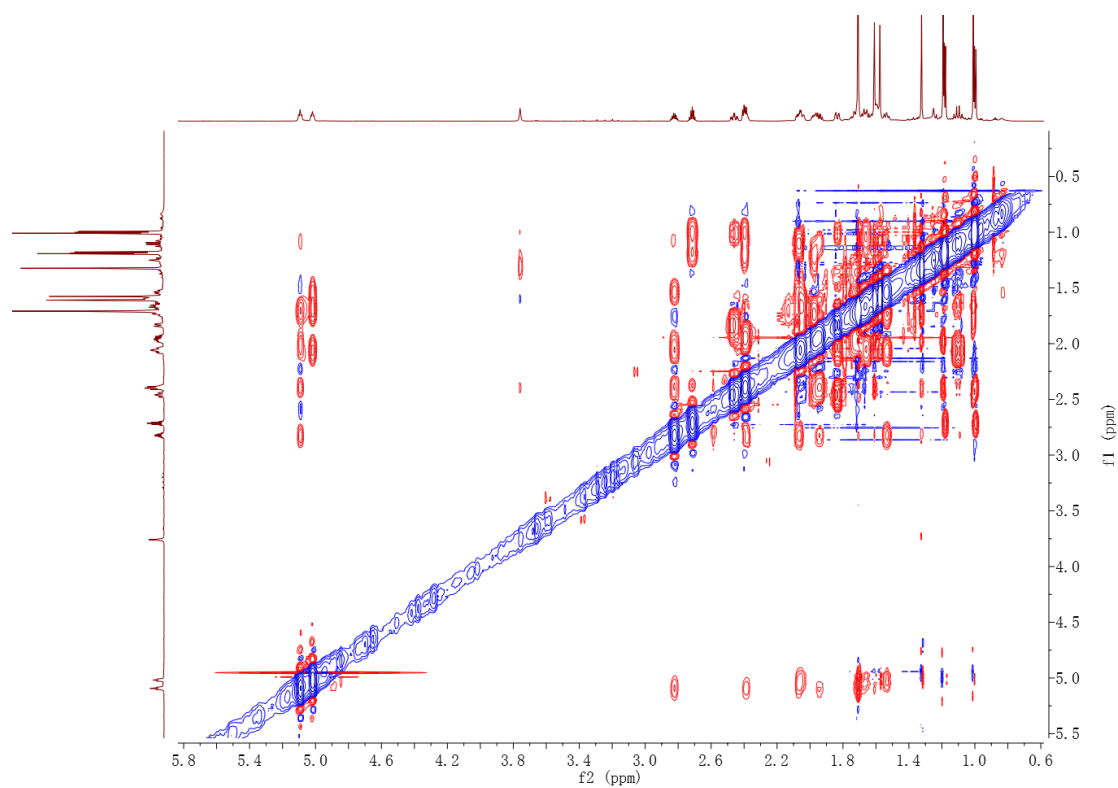
HMBC of compound **10** (800MHz, in CDCl₃)



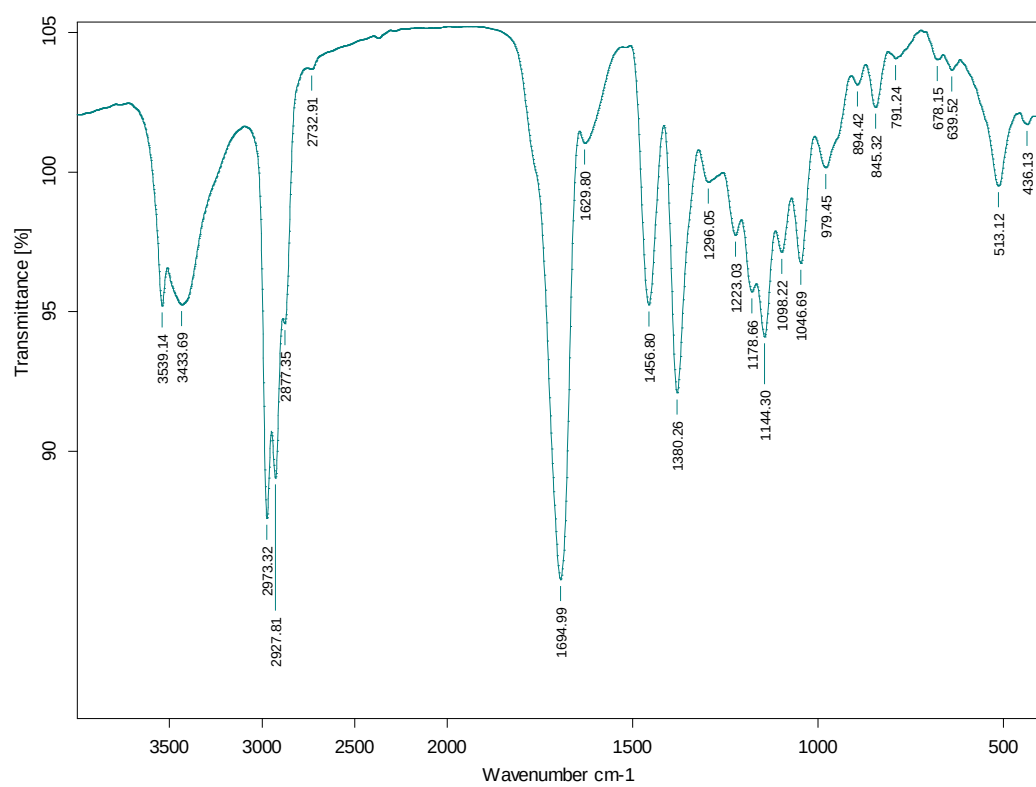
¹H-¹H COSY of compound **10** (800MHz, in CDCl₃)



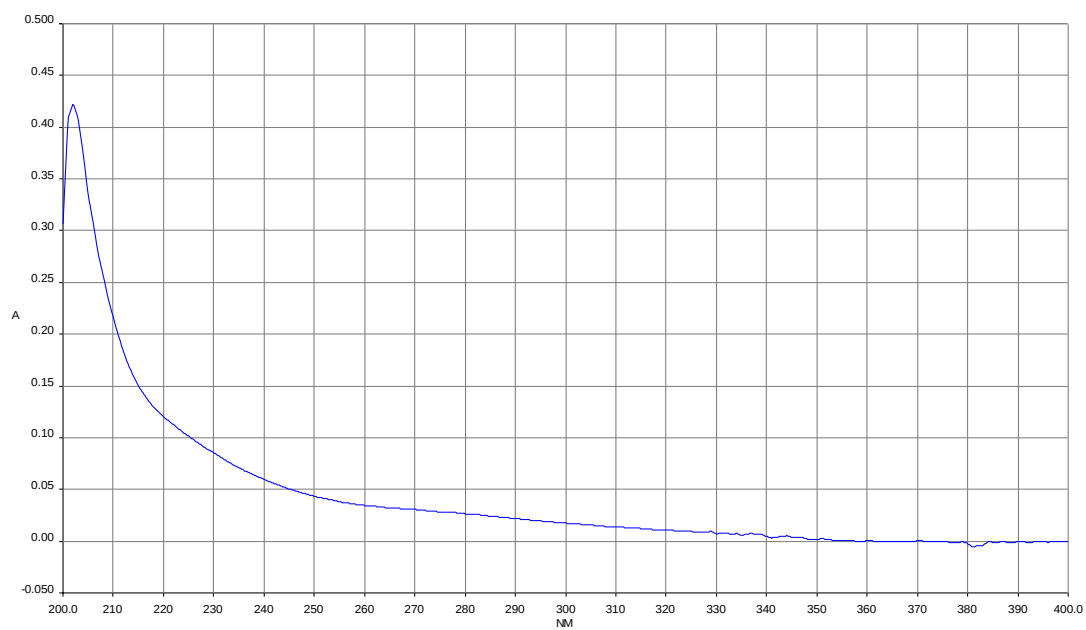
ROESY of compound **10** (800MHz, in CDCl₃)



IR of compound **10**



UV of compound **10**



CD of compound **10**

