Supporting information

Lignan−Phloroglucinol Hybrids with an Unprecedented Beadlike Core from the Leaves of *Melicope chunii*

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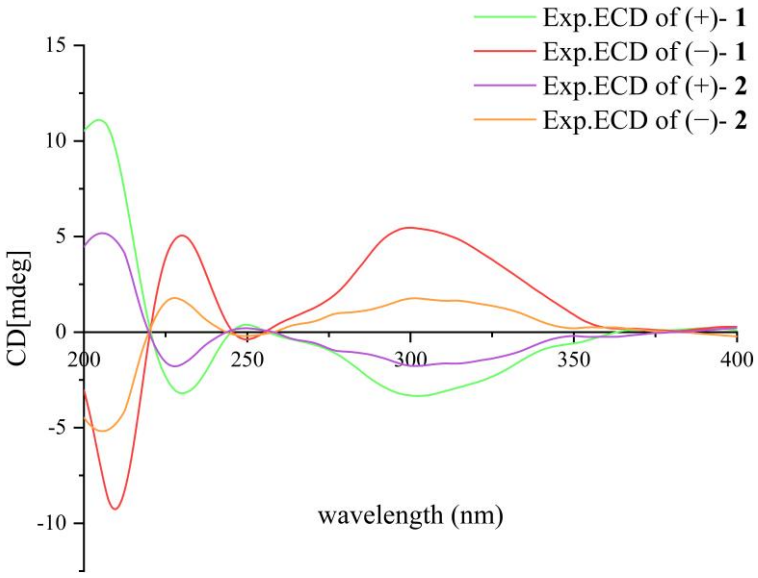


Figure S1. Experimental ECD spectra of (+)/(−)-**1** and (+)/(−)-**2.**

Table S1. ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR date of compounds **1**-**2** in $CDCl_3$

No.	**1**		**2**	
	δ_C	δ_H, mult (*J* in Hz)	δ_C	δ_H, mult (*J* in Hz)
1	131.8		129.6	
2	109.7	7.07 d (1.7)	108.1	6.90 d (1.6)
3	147.7		147.3	
4	148.9		147.9	
5	107.4	6.76 d (8.5)	107.7	6.77 d (8.1)
6	122.2	7.06 dd (8.5, 1.7)	122.2	7.00 dd (8.1, 1.6)
7	107.3		110.0	
8	96.4		97.6	
9	37.6	2.59 d (15.1) 1.94 d (15.1)	36.7	2.58 d (15.4) 2.05 d (15.4)
10	101.1	5.94 s	101.3	5.94 s
1′	131.5		133.2	
2′	109.0	7.63 d (1.8)	109.2	7.71 d (1.8)
3′	148.9		148.5	
4′	153.7		152.2	
5′	108.5	6.93 d (8.2)	108.1	6.90 d (8.3)
6′	127.2	7.85 dd (8.2, 1.8)	126.2	7.94 dd (8.4, 1.8)
7′	202.8		196.0	
8′	55.7	4.89 dd (8.7, 3.8)	55.3	4.64 dd (8.4,5.4)
9′	69.5	a 4.53 dd (8.7, 3.8) b 4.15 dd (8.7, 3.8)	68.6	4.38 m

10′	102.5	6.10 d (3.8)	102.0	6.04 d (2.1)
1″	112.8		112.1	
2″	48.6	a 2.01 d (19.0) b 1.12 d (19.0)	48.8	a 1.99 d (19.2) b 0.95 m
3″	92.8		92.6	
4″	215.4		215.8	
5″	62.4		62.6	
6″	125.4	5.58 d (5.9)	125.7	5.54 d (5.9)
7″	138.2	5.93 d (5.9)	137.9	5.91 d (5.9)
8″	90.4		90.3	
9″	29.3	1.23 s	29.3	1.22 s
10″	28.9	1.40 s	28.9	1.41 s
11″	30.5	a 2.15 dd (14.9, 7.5) b 2.06 m	30.5	a 2.07 m b 1.97 m
12″	119.1	5.00 t (7.6)	119.0	4.94 t (8.3)
13″	134.4		133.6	
14″	25.8	1.48 s	25.9	1.52 s
15″	17.5	1.31 s	17.3	1.23 s
7-OCH_3			48.7	3.14 s
7-OH		6.66 s		
1″OH		3.72 s		3.78 s

Table S2. ^{1}H NMR Spectroscopic Data for Compounds **3-6** (δ in ppm)

No	**3**[a]	**4**[b]	**5**[b]	**6**[b]
1				
2	6.84 d (1.7)	7.07 d (1.7)	6.88 d (1.7)	7.03 d (1.6)
3				
4				
5	6.77 m	6.85 d (8.1)	6.62 d (8.2)	6.85 d (7.9)
6	6.80 m	7.04 dd (8.1, 1.7)	6.95 dd (8.2, 1.7)	7.05 dd (7.9, 1.6)
7				
8				
9	a 2.22 d (14.9) b 1.88 d (14.9)	2.53 d (7.6)	a 3.26 d (14.7) b 2.01 d (14.7)	a 3.58 d (14.1) b 2.31 d (14.1)
10	a 6.01 s b 5.96 s	a 6.03 s b 6.01 s	a 5.96 s b 5.90 s	6.03 d (8.3) 6.01 d (8.3)
1'				
2'	7.66 d (2.0)	7.33 d (1.7)	7.59 d (1.8)	7.42 d (1.7)
3'				
4'				
5'	7.12 d (8.3)	6.84 d (8.3)	6.93 d (8.3)	6.81 d (8.2)
6'	7.87 dd (8.3, 2.0)	7.42 dd (8.3, 1.7)	7.79 dd (8.3, 1.8)	7.33 dd (8.2, 1.7)
7'				
8'	4.93 dd (8.7, 4.4)	4.08 t (8.3)	4.75 dd (8.9, 3.9)	3.87 dd (9.6, 7.9)
9'	a 4.34 dd (8.0, 4.3) b 4.04 dd (8.0, 4.3)	a 4.24 t (8.5) b 4.19 t (8.5)	a 4.44 t (8.9) b 4.12 dd (8.9, 3.9)	a 4.41 m b 3.68 t (9.6)
10'	6.18 s	6.05 s	6.11 s	6.04 s
1"				
2"				
3"	1.33 t (7.0)	3.23 d (1.4)		
4"				
5"				
6"				
7"	1.81 m	2.08 m	a 2.82 dd (13.5, 7.7) b 2.67 dd (13.5, 7.7)	a 2.71 dd (13.6, 6.8) b 2.67 dd (13.6, 6.8)
8"	4.72 m	4.84 m	4.70 m	4.69 m
9"				
10"	1.44 s	1.50 s	1.66 s	1.52 s
11"	1.60 s	1.61 s	1.58 s	1.41 s

12"	2.01 m	2.21 m	a 2.38 dd (13.6, 9.0) b 2.18 dd (13.6, 9.0)	a 2.39 dd (14.0, 6.7) b 2.16 dd (14.0, 6.7)
13"	5.07 m	5.13 m	4.50 m	4.54 m
14"				
15"	1.13 s	1.54 s	1.30 s	1.30 s
16"	1.38 s	1.70 s	1.39 s	1.53 s
7-OH	6.49 s	3.23 s	6.63 s	
7-OCH_3				3.13 s
1"-OH	6.54 s	2.43 s	4.67 s	2.50 s
2"-OH	5.39 s			
2"-OCH_3		3.14 s		
3"-OH				
6"-OCH_3	3.71 s	3.83 s		

[a] Recorded in DMSO-d_6. [b] Recorded in $CDCl_3$.

Table S3. ^{13}C NMR Spectroscopic Data for Compounds **3-6** (δ in ppm)

No	**3**[a]	**4**[b]	**5**[b]	**6**[b]
1	131.3	132.6	131.4	129.3
2	109.6	109.7	110.5	109.6
3	146.0	147.8	146.3	147.4
4	147.0	148.3	147.5	148.0
5	106.6	107.7	107.4	107.7
6	121.5	122.4	123.3	122.7
7	106.3	108.1	106.7	111.2
8	96.0	96.3	95.4	96.6
9	36.9	35.5	38.6	35.1
10	100.8	101.5	101.0	101.3
1'	130.9	130.0	130.7	132.9
2'	108.6	109.6	108.9	108.4
3'	148.1	148.5	149.0	148.6
4'	152.8	152.5	153.7	152.1
5'	108.3	108.7	108.5	107.9
6'	126.6	125.4	127.0	124.3
7'	200.9	195.4	202.3	195.0
8'	54.8	53.4	57.3	55.3
9'	68.5	68.0	68.7	68.9
10'	102.4	102.1	102.5	102.1
1"	111.0	110.5	99.8	98.4
2"	79.3	80.2	188.3	189.1
3"	53.3	53.3	151.7	151.9
4"	216.6	215.9	129.4	128.1
5"	60.6	62.0	196.6	196.8
6"	171.3	171.4	64.6	65.6

7"	22.0	23.0	23.1	22.8
8"	122.1	121.4	118.5	118.6
9"	132.1	133.1	133.8	133.9
10"	25.4	17.9	17.9	17.7
11"	17.3	25.9	25.9	25.9
12"	30.7	30.6	35.2	32.9
13"	120.0	119.1	118.8	118.8
14"	131.9	135.0	135.7	135.5
15"	16.8	26.1	17.5	17.6
16"	25.6	17.7	25.7	25.7
7-OCH_3				49.4
2"-OCH_3		52.8		
6"-OCH_3	51.7	50.3		

[a] Recorded in DMSO-d_6.

[b] Recorded in $CDCl_3$.

1 Single crystal X-ray data of 1–2

Table S4. Crystal data and structure refinement for **1**

CCDC number	2375875
Empirical formula	$C_{35}H_{36}O_{11}$
Formula weight	664.68
Temperature [K]	233.00
Crystal system	orthorhombic
Space group (number)	$P2_12_12_1$ (19)
a [Å]	10.5584(5)
b [Å]	11.0468(7)
c [Å]	29.2690(17)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	3413.8(3)
Z	4
ρ_{calc} [gcm^{-3}]	1.293
μ [mm^{-1}]	0.810
F (000)	1408
Crystal size [mm^3]	0.13×0.11×0.1
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	8.56 to 137.90 (0.83 Å)
Index ranges	−12 ≤ h ≤ 12, −13 ≤ k ≤ 13, −35 ≤ l ≤ 35
Reflections collected	53410
Independent reflections	6304R_{int} = 0.0959, R_{sigma} = 0.0369
Data / Restraints / Parameters	6304/0/439
Goodness-of-fit on F^2	1.008
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0728, wR_2 = 0.1954
Final *R* indexes [all data]	R_1 = 0.0929, wR_2 = 0.2167
Largest peak/hole [eÅ^{-3}]	0.39/−0.34
Flack X parameter	0.04(12)

Table S5. Crystal data and structure refinement for **2**

CCDC number	2375874
Empirical formula	$C_{36}H_{38}O_{11}$
Formula weight	646.66
Temperature [K]	150(2)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	12.1942(6)
b [Å]	18.9173(8)
c [Å]	13.9396(7)
α [°]	90
β [°]	95.265(4)
γ [°]	90
Volume [Å^3]	3202.0(3)
Z	4
ρ_{calc} [gcm^{-3}]	1.341
μ [mm^{-1}]	0.825
F (000)	1368
Crystal size [mm^3]	0.080×0.080×0.080
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	7.28 to 133.33 (0.84 Å)
Index ranges	−14 ≤ h ≤ 14, 0 ≤ k ≤ 22, 0 ≤ l ≤ 16
Reflections collected	5696
Independent reflections	5696R_{int} = 0.0941R_{sigma} = 0.0592
Data / Restraints / Parameters	5696/625/514
Goodness-of-fit on F^2	1.072
Final R indexes [I≥2σ(I)]	R_1 = 0.0702, wR_2 = 0.1696
Final R indexes [all data]	R_1 = 0.0983, wR_2 = 0.1957
Largest peak/hole [eÅ^{-3}]	0.46/−0.33
Extinction coefficient	0.0022(3)

Table S6. Cytotoxic activity (IC_{50} values in μM) of compounds **1–6** [a]

Compounds	IC_{50}(μM) [c]		
	HCT-116	HT-1080	HepG2
1	13.75 ± 0.12	12.70 ± 0.53	14.69 ± 0.96
2	4.32 ± 0.09	2.59 ± 0.07	3.68 ± 0.35
3	14.15 ± 1.35	22.11 ± 0.49	23.01 ± 0.23
4	＞50	＞50	＞50
5	＞100	＞100	＞100
6	＞100	＞100	＞100
Erastin[b]	10.42±0.56	5.50 ± 1.12	13.2± 1.09

[a] Cell viability was determined by the CCK8 assay after 48 h treatment.

[b] Positive control.

[c] IC_{50} values are indicated as the mean ± SD of three independent experiments.

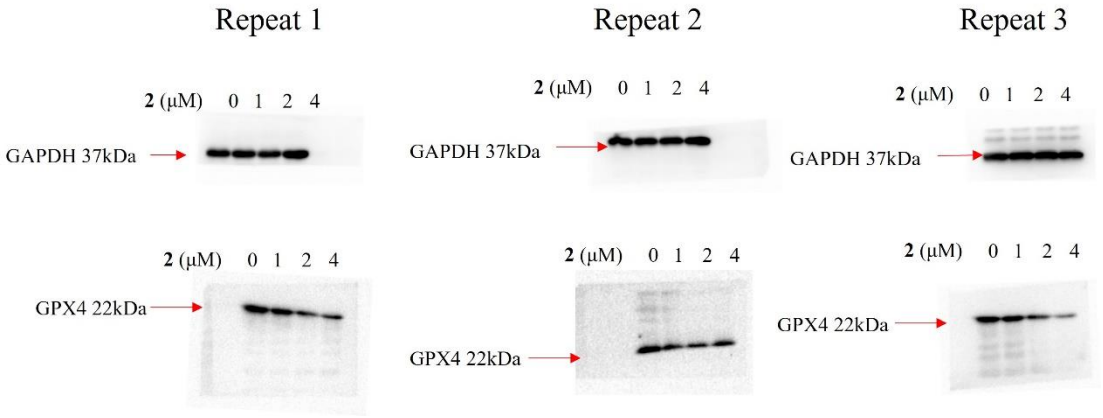


Figure S2. The raw images for all Western blot.

2. Computational Studies

The 3D structures of selected compounds were subjected to Schrödinger MacroModel 9.1 (Schrödinger. LLC, USA) to perform conformational analysis using the MMFF force field in gas phase. The conformers occurring in energy window of 3 kcal/mol were chosen, and then the conformers were initially optimized at B3LYP/6-31g (d, p) level in MeOH using the CPCM polarizable conductor calculation model by Gaussian 09 program package[1]. The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the B3LYP/6-31g (d, p) level for all optimized stable conformers. Rotatory strengths for a total of 60 excited states were calculated. ECD spectra were generated using the program SpecDis 1.7.1[2]with UV correction and a half-bandwidth of σ = 0.30 eV.

References

1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09 Rev*. A.01, Gaussian Inc., Wallingford, CT, 2009

2 T. Bruhn, A. Schaumlöffel, Y. Hemberger and G. Bringmann, SpecDis: quantifying the comparison of calculated and experimental electronic circular dichroism spectra, *Chirality*, 2013, **25**, 243-249

2.1 ECD spectra calculation of **1**

Table S7. Energies of the optimized conformers of compound **1**

Boltzmann distributions of the optimized **1** at the B3LYP-D3/6-31+G(d) level in the gas phase.

conformer	Energy (Hartree)	Energy (kcal/mol)	Population (%)
1	-2183.383878	-1370094.058	15.08
2	-2183.384008	-1370094.14	17.32
3	-2183.384756	-1370094.609	38.24
4	-2183.382701	-1370093.319	4.34
5	-2183.383574	-1370093.867	10.93
6	-2183.383813	-1370094.017	14.09

Table S8. Standard orientation of conformation **1**A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.914699	-1.746544	-0.419207
2	6	0	-4.117536	-2.584938	0.360328
3	6	0	-2.766632	-2.738160	0.132733
4	6	0	-2.215384	-2.016331	-0.947446
5	6	0	-3.016574	-1.170726	-1.721321
6	6	0	-4.391048	-1.015857	-1.465149
7	8	0	-6.200010	-1.741191	0.080226
8	6	0	-6.237153	-2.833109	1.010301
9	8	0	-4.883350	-3.135627	1.368847
10	6	0	-0.746868	-2.168340	-1.287623
11	6	0	0.248340	-1.150855	-0.620808
12	6	0	1.536371	-2.042638	-0.400423
13	6	0	1.117052	-3.429273	-0.927945
14	8	0	-0.311309	-3.440751	-0.849005
15	6	0	0.401970	0.191513	-1.368799
16	6	0	0.087407	1.262161	-0.315451
17	6	0	0.172671	0.511963	1.019760
18	8	0	-0.276649	-0.799490	0.680941
19	6	0	2.812455	-1.554727	-1.068977
20	6	0	3.971437	-1.103471	-0.245980
21	8	0	2.878235	-1.531293	-2.294520
22	6	0	4.050133	-1.313325	1.151893
23	6	0	5.176964	-0.857105	1.795507
24	6	0	6.206185	-0.202393	1.120061
25	6	0	6.156424	0.018383	-0.245476
26	6	0	5.022085	-0.454461	-0.916577
27	8	0	5.468324	-0.900060	3.143216
28	6	0	6.831264	-0.470871	3.249222

29	8	0	7.175076	0.176072	2.011370
30	6	0	0.993866	2.520771	-0.397293
31	6	0	0.986942	3.153394	-1.760259
32	6	0	1.961161	3.087946	-2.682917
33	6	0	1.789709	3.744236	-4.030971
34	6	0	3.272120	2.362444	-2.506133
35	8	0	1.499100	0.488768	1.501456
36	8	0	-0.524401	-2.031196	-2.681179
37	6	0	-1.383633	1.689146	-0.332422
38	6	0	-1.986940	1.653329	1.112802
39	6	0	-0.823107	1.148611	1.984359
40	8	0	-2.002462	2.032938	-1.314146
41	6	0	-3.243632	0.833914	1.176536
42	6	0	-4.284197	1.623862	1.424813
43	6	0	-3.847912	3.062879	1.564185
44	8	0	-2.394064	2.970975	1.490517
45	6	0	-4.203916	3.663842	2.925912
46	6	0	-4.353104	3.937402	0.410860
47	1	0	-2.149895	-3.383830	0.744385
48	1	0	-2.568529	-0.612795	-2.534516
49	1	0	-5.002209	-0.336756	-2.048917
50	1	0	-6.790039	-2.531468	1.900605
51	1	0	-6.688462	-3.708504	0.522039
52	1	0	1.651187	-2.098005	0.678230
53	1	0	1.480483	-4.253435	-0.310686
54	1	0	1.441728	-3.560010	-1.964144
55	1	0	-0.283284	0.258851	-2.213265
56	1	0	1.402142	0.318930	-1.775894
57	1	0	3.267860	-1.810811	1.709634
58	1	0	6.957085	0.532844	-0.765708
59	1	0	4.931196	-0.321940	-1.988343
60	1	0	6.925283	0.244016	4.067623
61	1	0	7.481892	-1.344455	3.388628
62	1	0	0.657312	3.248417	0.353699
63	1	0	1.995950	2.206393	-0.099878
64	1	0	0.072926	3.683400	-2.023761
65	1	0	0.817666	4.239264	-4.122222
66	1	0	2.575747	4.491907	-4.209037
67	1	0	1.872998	3.002687	-4.838191
68	1	0	3.334147	1.511815	-3.199287
69	1	0	4.114869	3.026528	-2.743683
70	1	0	3.424916	1.974434	-1.497220
71	1	0	1.496035	0.093959	2.388361

72	1	0	-1.059550	-2.710332	-3.124219
73	1	0	-1.148544	0.445374	2.757386
74	1	0	-0.350078	2.010635	2.463995
75	1	0	-3.234825	-0.235393	1.024039
76	1	0	-5.320730	1.314359	1.512201
77	1	0	-3.762635	4.661885	3.023768
78	1	0	-5.291198	3.755732	3.034211
79	1	0	-3.822547	3.031552	3.733901
80	1	0	-5.448747	3.990710	0.420968
81	1	0	-3.956879	4.954444	0.509219
82	1	0	-4.024537	3.520420	-0.544279

Table S9. Standard orientation of conformation **1**B

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.537590	-2.403215	0.265265
2	6	0	3.560422	-3.170383	-0.369397
3	6	0	2.232702	-3.121572	-0.002800
4	6	0	1.896462	-2.262985	1.065806
5	6	0	2.877556	-1.489891	1.693530
6	6	0	4.226553	-1.544790	1.298628
7	8	0	5.753608	-2.607173	-0.352439
8	6	0	5.550184	-3.749465	-1.196178
9	8	0	4.138477	-3.884531	-1.400647
10	6	0	0.461481	-2.176768	1.542008
11	6	0	-0.456089	-1.108456	0.827068
12	6	0	-1.815951	-1.896054	0.675061
13	6	0	-1.573930	-3.194643	1.459992
14	8	0	-0.169759	-3.425077	1.314280
15	6	0	-0.452939	0.286961	1.499632
16	6	0	-0.035154	1.248611	0.379388
17	6	0	-0.300891	0.450078	-0.898474
18	8	0	0.049051	-0.879013	-0.509934
19	6	0	-3.089698	-1.195811	1.103026
20	6	0	-4.199840	-0.993110	0.127581
21	8	0	-3.210074	-0.811657	2.263191
22	6	0	-5.256412	-0.141554	0.535361
23	6	0	-6.287890	0.052581	-0.350417
24	6	0	-6.319525	-0.567431	-1.602510
25	6	0	-5.310108	-1.412580	-2.021734
26	6	0	-4.241945	-1.612004	-1.131329
27	8	0	-7.393032	0.862591	-0.216929
28	6	0	-8.235365	0.555116	-1.332778

29	8	0	-7.440051	-0.177198	-2.284070
30	6	0	-0.725896	2.638401	0.421440
31	6	0	-0.486316	3.378252	1.707396
32	6	0	0.381320	4.380542	1.917939
33	6	0	0.517538	5.007663	3.283134
34	6	0	1.300987	4.956877	0.871521
35	8	0	-1.658637	0.540107	-1.264775
36	8	0	0.391611	-1.859712	2.922829
37	6	0	1.481163	1.440806	0.291029
38	6	0	1.958819	1.311783	-1.197017
39	6	0	0.680960	0.922896	-1.963880
40	8	0	2.219488	1.678206	1.219217
41	6	0	3.113542	0.363140	-1.337269
42	6	0	4.208870	1.033248	-1.682989
43	6	0	3.917166	2.509034	-1.820216
44	8	0	2.471224	2.573346	-1.640160
45	6	0	4.232672	3.053917	-3.214792
46	6	0	4.596949	3.337893	-0.723525
47	1	0	1.477940	-3.716002	-0.501608
48	1	0	2.592203	-0.818091	2.493831
49	1	0	4.979000	-0.922182	1.769413
50	1	0	6.041838	-3.583081	-2.155327
51	1	0	5.931614	-4.646690	-0.688246
52	1	0	-1.847910	-2.153522	-0.380682
53	1	0	-2.091620	-4.058711	1.038302
54	1	0	-1.839471	-3.072710	2.514727
55	1	0	0.248524	0.324879	2.331719
56	1	0	-1.434586	0.538470	1.897608
57	1	0	-5.224604	0.332688	1.509050
58	1	0	-5.343951	-1.897657	-2.991225
59	1	0	-3.447090	-2.282113	-1.437271
60	1	0	-9.068555	-0.078253	-1.001705
61	1	0	-8.583813	1.480762	-1.793198
62	1	0	-0.399248	3.226835	-0.442045
63	1	0	-1.797901	2.456079	0.287166
64	1	0	-1.073155	3.028555	2.557123
65	1	0	-0.177767	4.568898	4.006134
66	1	0	1.538969	4.877847	3.667784
67	1	0	0.331861	6.090410	3.240751
68	1	0	1.092823	6.026066	0.721391
69	1	0	2.343050	4.880123	1.208726
70	1	0	1.241845	4.454356	-0.095374
71	1	0	-1.805329	0.004132	-2.060906

72	1	0	0.861598	-2.565159	3.397875
73	1	0	0.861192	0.157285	-2.724896
74	1	0	0.275634	1.815604	-2.448441
75	1	0	3.006504	-0.696604	-1.153282
76	1	0	5.198083	0.615420	-1.840199
77	1	0	3.894086	4.092623	-3.298525
78	1	0	5.312490	3.027446	-3.403458
79	1	0	3.727241	2.457848	-3.981057
80	1	0	5.688169	3.271713	-0.814012
81	1	0	4.306538	4.390702	-0.813100
82	1	0	4.298632	2.970374	0.261468

Table S10. Standard orientation of conformation **1**C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.006864	-1.722279	0.503562
2	6	0	4.240825	-2.560369	-0.306618
3	6	0	2.887618	-2.737144	-0.112671
4	6	0	2.297669	-2.028795	0.955963
5	6	0	3.067849	-1.182502	1.760199
6	6	0	4.448322	-1.015087	1.547461
7	8	0	6.321483	-1.759764	0.091575
8	6	0	6.296678	-2.446234	-1.168452
9	8	0	5.056435	-3.159129	-1.245678
10	6	0	0.819515	-2.188794	1.245290
11	6	0	-0.155856	-1.175934	0.539127
12	6	0	-1.407247	-2.088626	0.220900
13	6	0	-1.025721	-3.454222	0.821756
14	8	0	0.404568	-3.468000	0.803138
15	6	0	-0.370442	0.146827	1.306967
16	6	0	-0.047327	1.246475	0.285412
17	6	0	-0.056459	0.515697	-1.062817
18	8	0	0.428502	-0.783531	-0.725507
19	6	0	-2.754460	-1.605241	0.726178
20	6	0	-3.858001	-1.305017	-0.229843
21	8	0	-2.932693	-1.465427	1.933139
22	6	0	-4.986433	-0.627703	0.296137
23	6	0	-6.007742	-0.333688	-0.573462
24	6	0	-5.966239	-0.703643	-1.920514
25	6	0	-4.892515	-1.390692	-2.454047
26	6	0	-3.829408	-1.676664	-1.582365
27	8	0	-7.205924	0.293082	-0.311757
28	6	0	-7.808451	0.518628	-1.590285

29	8	0	-7.121917	-0.315642	-2.542254
30	6	0	-0.994300	2.476574	0.349535
31	6	0	-1.103307	3.054045	1.732241
32	6	0	-2.143756	2.931470	2.573409
33	6	0	-2.090158	3.532807	3.956493
34	6	0	-3.421635	2.189875	2.266436
35	8	0	-1.364860	0.453454	-1.587170
36	8	0	0.548472	-2.048718	2.630547
37	6	0	1.408165	1.716554	0.366677
38	6	0	2.071825	1.708217	-1.053301
39	6	0	0.951571	1.201344	-1.978532
40	8	0	1.976887	2.070429	1.374876
41	6	0	3.337301	0.899368	-1.070518
42	6	0	4.380098	1.700734	-1.268169
43	6	0	3.937496	3.137489	-1.412190
44	8	0	2.483124	3.032270	-1.400178
45	6	0	4.345072	3.755285	-2.751743
46	6	0	4.386560	4.004005	-0.229969
47	1	0	2.298339	-3.394044	-0.739355
48	1	0	2.589752	-0.629876	2.559968
49	1	0	5.038529	-0.346091	2.163585
50	1	0	6.342408	-1.707768	-1.981839
51	1	0	7.125970	-3.153320	-1.212649
52	1	0	-1.403605	-2.179363	-0.861668
53	1	0	-1.365753	-4.300325	0.221034
54	1	0	-1.396477	-3.545426	1.847085
55	1	0	0.287647	0.213906	2.172562
56	1	0	-1.384777	0.236865	1.686704
57	1	0	-5.017307	-0.360299	1.345169
58	1	0	-4.874343	-1.691020	-3.496084
59	1	0	-2.975726	-2.210898	-1.982049
60	1	0	-8.860194	0.231643	-1.553852
61	1	0	-7.678183	1.569806	-1.878937
62	1	0	-0.627734	3.242587	-0.347592
63	1	0	-1.963287	2.147590	-0.029768
64	1	0	-0.223096	3.589117	2.085624
65	1	0	-1.139009	4.041750	4.142457
66	1	0	-2.903853	4.257103	4.104171
67	1	0	-2.218464	2.755868	4.723461
68	1	0	-3.517320	1.308349	2.915198
69	1	0	-4.294228	2.827428	2.465082
70	1	0	-3.486799	1.843083	1.233092
71	1	0	-1.331494	0.007493	-2.448670

72	1	0	1.069807	-2.726549	3.091863
73	1	0	1.320152	0.529863	-2.760408
74	1	0	0.470993	2.064271	-2.448808
75	1	0	3.331774	-0.170918	-0.924296
76	1	0	5.423282	1.404040	-1.311530
77	1	0	3.898815	4.750173	-2.858434
78	1	0	5.435027	3.858537	-2.812943
79	1	0	4.004046	3.127899	-3.581341
80	1	0	5.481179	4.066171	-0.193258
81	1	0	3.986336	5.018761	-0.335048
82	1	0	4.021140	3.574818	0.706164

Table S11. Standard orientation of conformation **1**D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.097699	-2.890917	-0.614873
2	6	0	3.922578	-2.155959	0.553986
3	6	0	2.687844	-2.001568	1.146786
4	6	0	1.588554	-2.617237	0.511412
5	6	0	1.765988	-3.350387	-0.665941
6	6	0	3.036290	-3.507161	-1.250032
7	8	0	5.429463	-2.889910	-0.966476
8	6	0	6.048327	-1.930452	-0.091823
9	8	0	5.141008	-1.680845	0.986166
10	6	0	0.217308	-2.470857	1.137307
11	6	0	-0.634134	-1.219323	0.694722
12	6	0	-2.092747	-1.822628	0.629469
13	6	0	-1.917040	-3.262140	1.142080
14	8	0	-0.570100	-3.595534	0.794122
15	6	0	-0.376248	0.057560	1.531490
16	6	0	0.029572	1.115147	0.496911
17	6	0	-0.482745	0.540954	-0.826261
18	8	0	-0.264175	-0.860763	-0.657851
19	6	0	-3.185703	-1.078965	1.372759
20	6	0	-4.356492	-0.529564	0.628691
21	8	0	-3.100092	-0.938202	2.589358
22	6	0	-4.636544	-0.867719	-0.717983
23	6	0	-5.749401	-0.297283	-1.292732
24	6	0	-6.573631	0.588475	-0.599234
25	6	0	-6.323048	0.938266	0.715751
26	6	0	-5.201883	0.353906	1.319279
27	8	0	-6.208331	-0.433167	-2.585972
28	6	0	-7.490835	0.206998	-2.601613

29	8	0	-7.574557	1.029091	-1.424949
30	6	0	-0.464538	2.553908	0.807955
31	6	0	0.010280	3.064689	2.139272
32	6	0	1.018813	3.919727	2.370519
33	6	0	1.387776	4.311465	3.779812
34	6	0	1.883602	4.540988	1.303364
35	8	0	-1.849870	0.834009	-1.000483
36	8	0	0.307800	-2.369378	2.550979
37	6	0	1.537776	1.144289	0.233104
38	6	0	1.819941	1.175363	-1.308486
39	6	0	0.422575	1.047405	-1.942832
40	8	0	2.403893	1.163426	1.076701
41	6	0	2.814908	0.133396	-1.731305
42	6	0	3.937045	0.722013	-2.135873
43	6	0	3.831191	2.224745	-2.021126
44	8	0	2.436425	2.422971	-1.646016
45	6	0	4.057485	2.945923	-3.351204
46	6	0	4.733160	2.784742	-0.914174
47	1	0	2.566878	-1.419837	2.051259
48	1	0	0.903160	-3.811564	-1.130841
49	1	0	3.176845	-4.082552	-2.158937
50	1	0	6.976335	-2.347980	0.302379
51	1	0	6.220551	-0.997499	-0.644790
52	1	0	-2.305846	-1.874019	-0.435003
53	1	0	-2.569016	-3.981441	0.642080
54	1	0	-2.059881	-3.312407	2.225796
55	1	0	0.412941	-0.100388	2.265373
56	1	0	-1.265375	0.358199	2.083359
57	1	0	-4.021341	-1.552653	-1.288232
58	1	0	-6.964091	1.632012	1.248820
59	1	0	-4.960298	0.582401	2.351334
60	1	0	-7.572078	0.837016	-3.488291
61	1	0	-8.281188	-0.554367	-2.563722
62	1	0	-0.161007	3.220423	-0.005777
63	1	0	-1.559405	2.516557	0.788207
64	1	0	-0.517738	2.659698	3.002929
65	1	0	0.728607	3.845833	4.519650
66	1	0	2.420903	4.012183	4.005743
67	1	0	1.338814	5.401622	3.912865
68	1	0	1.818590	5.637764	1.344510
69	1	0	2.935302	4.277672	1.476962
70	1	0	1.636833	4.218463	0.290424
71	1	0	-2.141879	0.472099	-1.852741

72	1	0	0.725487	-3.187938	2.866740
73	1	0	0.411231	0.382763	-2.812273
74	1	0	0.084752	2.040760	-2.251626
75	1	0	2.589284	-0.923382	-1.690597
76	1	0	4.829882	0.225599	-2.502843
77	1	0	3.848381	4.015446	-3.238303
78	1	0	5.097238	2.831474	-3.679994
79	1	0	3.397504	2.540018	-4.124199
80	1	0	5.789582	2.616133	-1.157728
81	1	0	4.572277	3.863503	-0.809149
82	1	0	4.503721	2.297993	0.036961

Table S12. Standard orientation of conformation **1**E

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-4.254213	-2.697016	-0.239790
2	6	0	-3.171272	-3.399962	0.288841
3	6	0	-1.881029	-3.208160	-0.156134
4	6	0	-1.696678	-2.269198	-1.193524
5	6	0	-2.783288	-1.560545	-1.714339
6	6	0	-4.092138	-1.761226	-1.239704
7	8	0	-5.402795	-3.045352	0.439436
8	6	0	-5.040512	-4.203864	1.204307
9	8	0	-3.611881	-4.215804	1.312481
10	6	0	-0.310385	-2.024667	-1.752083
11	6	0	0.553165	-0.915930	-1.032894
12	6	0	1.987862	-1.575188	-1.019627
13	6	0	1.808856	-2.851709	-1.857082
14	8	0	0.443962	-3.218791	-1.636954
15	6	0	0.376525	0.507715	-1.614573
16	6	0	-0.043993	1.360850	-0.410699
17	6	0	0.372688	0.517470	0.796644
18	8	0	0.120364	-0.813336	0.344337
19	6	0	3.151667	-0.733355	-1.504566
20	6	0	4.300959	-0.448735	-0.596659
21	8	0	3.146772	-0.303222	-2.654730
22	6	0	4.470870	-1.093932	0.653043
23	6	0	5.578856	-0.750754	1.394099
24	6	0	6.501822	0.198753	0.956569
25	6	0	6.359209	0.846833	-0.257641
26	6	0	5.244158	0.497218	-1.030062
27	8	0	5.944130	-1.202453	2.644579
28	6	0	7.263119	-0.685425	2.862779

29	8	0	7.474314	0.367959	1.907042
30	6	0	0.522489	2.806022	-0.406018
31	6	0	0.139514	3.594517	-1.626538
32	6	0	-0.816033	4.532282	-1.722117
33	6	0	-1.090713	5.219465	-3.036722
34	6	0	-1.705426	4.975533	-0.588208
35	8	0	1.737072	0.710885	1.093123
36	8	0	-0.361216	-1.628895	-3.113073
37	6	0	-1.562546	1.407838	-0.220176
38	6	0	-1.930956	1.153031	1.282737
39	6	0	-0.577861	0.834468	1.945389
40	8	0	-2.376571	1.628067	-1.087270
41	6	0	-2.994614	0.104776	1.436395
42	6	0	-4.116735	0.662897	1.881547
43	6	0	-3.937255	2.149018	2.082149
44	8	0	-2.513417	2.340975	1.830940
45	6	0	-4.215329	2.599790	3.517564
46	6	0	-4.741345	2.970188	1.066876
47	1	0	-1.043135	-3.751863	0.261111
48	1	0	-2.612827	-0.825275	-2.491175
49	1	0	-4.927670	-1.188301	-1.625801
50	1	0	-5.479596	-4.131996	2.200039
51	1	0	-5.372738	-5.106753	0.672403
52	1	0	2.125219	-1.878027	0.015350
53	1	0	2.429073	-3.683640	-1.517058
54	1	0	1.990149	-2.653264	-2.917932
55	1	0	-0.384491	0.526182	-2.393393
56	1	0	1.299552	0.871328	-2.062785
57	1	0	3.777516	-1.837456	1.026216
58	1	0	7.076960	1.588611	-0.590811
59	1	0	5.085195	0.963766	-1.995801
60	1	0	7.331261	-0.276263	3.871510
61	1	0	8.001442	-1.479634	2.689612
62	1	0	0.204185	3.312440	0.510869
63	1	0	1.612438	2.709549	-0.347745
64	1	0	0.693477	3.342052	-2.531021
65	1	0	-0.414569	4.876166	-3.826479
66	1	0	-2.122958	5.030525	-3.363563
67	1	0	-0.984303	6.309625	-2.942545
68	1	0	-1.572599	6.049192	-0.391499
69	1	0	-2.758711	4.831011	-0.862574
70	1	0	-1.541123	4.431281	0.343383
71	1	0	1.968422	0.172350	1.867191

72	1	0	-0.794823	-2.349315	-3.600097
73	1	0	-0.641280	0.010273	2.662637
74	1	0	-0.221801	1.729272	2.463529
75	1	0	-2.815752	-0.931870	1.187619
76	1	0	-5.057257	0.156019	2.071968
77	1	0	-3.951756	3.656622	3.636500
78	1	0	-5.277951	2.480657	3.760328
79	1	0	-3.624659	2.009980	4.225493
80	1	0	-5.816882	2.806798	1.207527
81	1	0	-4.534290	4.038194	1.198395
82	1	0	-4.466216	2.677508	0.050623

Table S12. Standard orientation of conformation **1**F

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.865135	-2.115228	-0.234097
2	6	0	4.322135	-1.540305	0.911567
3	6	0	2.983710	-1.645463	1.222727
4	6	0	2.167170	-2.358774	0.318632
5	6	0	2.714077	-2.931948	-0.833507
6	6	0	4.086510	-2.826005	-1.127052
7	8	0	6.218492	-1.864015	-0.279970
8	6	0	6.460767	-0.913183	0.771946
9	8	0	5.318536	-0.923708	1.634199
10	6	0	0.693223	-2.496598	0.636538
11	6	0	-0.248939	-1.331026	0.159954
12	6	0	-1.576228	-2.108835	-0.205273
13	6	0	-1.238359	-3.578939	0.109148
14	8	0	0.186841	-3.656393	0.005966
15	6	0	-0.325773	-0.131424	1.130487
16	6	0	0.040230	1.086324	0.271428
17	6	0	-0.116247	0.582309	-1.167549
18	8	0	0.284043	-0.784654	-1.069697
19	6	0	-2.843504	-1.654999	0.497376
20	6	0	-3.986633	-1.105751	-0.286024
21	8	0	-2.921378	-1.740002	1.719789
22	6	0	-5.014064	-0.468078	0.453495
23	6	0	-6.078272	0.037657	-0.251586
24	6	0	-6.171168	-0.078241	-1.641231
25	6	0	-5.192526	-0.707829	-2.386462
26	6	0	-4.090332	-1.216676	-1.680763
27	8	0	-7.164801	0.741662	0.218611
28	6	0	-8.061019	0.851588	-0.891907

29	8	0	-7.313397	0.533775	-2.080893
30	6	0	-0.781866	2.364121	0.595290
31	6	0	-0.744955	2.721884	2.054258
32	6	0	-1.728833	2.539937	2.950804
33	6	0	-1.527847	2.909595	4.400066
34	6	0	-3.081541	1.946848	2.641729
35	8	0	-1.455957	0.694992	-1.593755
36	8	0	0.481403	-2.579537	2.038390
37	6	0	1.536063	1.416649	0.313299
38	6	0	2.103227	1.590070	-1.137190
39	6	0	0.882749	1.334055	-2.039601
40	8	0	2.197259	1.558363	1.316771
41	6	0	3.283242	0.699299	-1.405384
42	6	0	4.375471	1.440024	-1.571294
43	6	0	4.061505	2.909135	-1.414891
44	8	0	2.608493	2.918039	-1.292798
45	6	0	4.426673	3.735295	-2.649885
46	6	0	4.675701	3.497996	-0.139070
47	1	0	2.578298	-1.191006	2.117477
48	1	0	2.062800	-3.473302	-1.508779
49	1	0	4.513286	-3.276142	-2.017083
50	1	0	7.344856	-1.216398	1.335266
51	1	0	6.576070	0.087049	0.334034
52	1	0	-1.664091	-1.999447	-1.282341
53	1	0	-1.653253	-4.281063	-0.616966
54	1	0	-1.563050	-3.844052	1.119559
55	1	0	0.367266	-0.246457	1.962700
56	1	0	-1.314635	-0.025947	1.569223
57	1	0	-4.936010	-0.389038	1.530837
58	1	0	-5.274137	-0.800673	-3.463993
59	1	0	-3.315772	-1.721812	-2.245354
60	1	0	-8.877111	0.125822	-0.779733
61	1	0	-8.430824	1.875308	-0.962982
62	1	0	-0.392113	3.198505	-0.003831
63	1	0	-1.800082	2.178925	0.248247
64	1	0	0.199574	3.130188	2.410639
65	1	0	-0.527236	3.314423	4.582050
66	1	0	-2.266605	3.656902	4.722955
67	1	0	-1.665290	2.032178	5.047810
68	1	0	-3.203856	0.984651	3.158209
69	1	0	-3.883378	2.605155	3.003570
70	1	0	-3.247145	1.770065	1.577005
71	1	0	-1.511106	0.407028	-2.519045

72	1	0	0.969639	-3.357839	2.354465
73	1	0	1.137560	0.778653	-2.947741
74	1	0	0.449039	2.297776	-2.322179
75	1	0	3.188383	-0.376081	-1.457640
76	1	0	5.373900	1.074198	-1.789471
77	1	0	4.064431	4.762674	-2.533846
78	1	0	5.514398	3.767088	-2.784748
79	1	0	3.973744	3.304004	-3.548146
80	1	0	5.771346	3.470541	-0.192356
81	1	0	4.363384	4.541520	-0.018816
82	1	0	4.344566	2.927528	0.732224

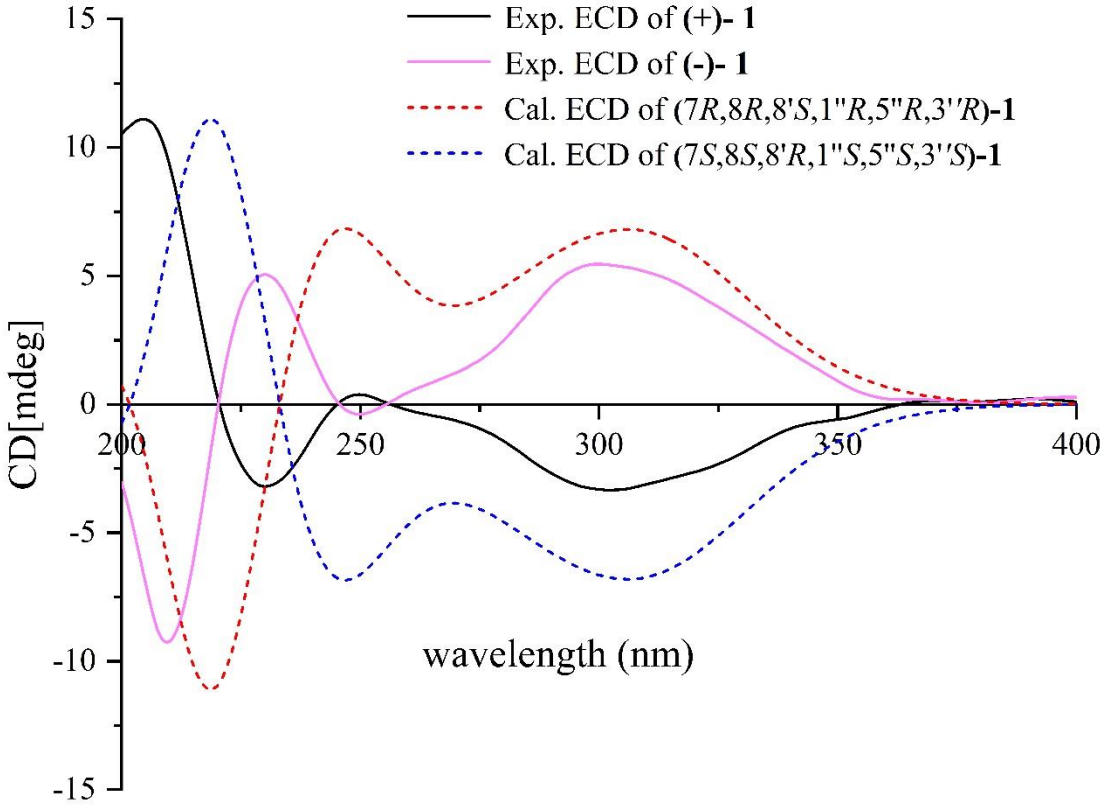


Figure S3. Computational methods for ECD of compound **1.**
b3lyp/6-31+g (d, p) scrf = (solvent = methanol)

2.2 ECD spectra calculation of **2**

Table S13. Energies of the optimized conformers of compound **2.**
Boltzmann distributions of the optimized **2** at the B3LYP-D3/6-31+G(d) level in the gas phase.

conformers	Energy (Hartree)	Energy (kcal/mol)	Population (%)
1	-2222.680731	-1394753.205	8.36
2	-2222.681485	-1394753.679	18.58
3	-2222.681211	-1394753.506	13.89
4	-2222.681485	-1394753.678	18.57
5	-2222.682223	-1394754.142	40.6

Table S14. Standard orientation of conformation **2**A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.316994	-1.568485	2.079549
2	6	0	-4.249416	-1.558176	0.689235
3	6	0	-3.118978	-1.954768	0.006136
4	6	0	-2.019546	-2.382720	0.778630
5	6	0	-2.093714	-2.398281	2.174225
6	6	0	-3.253653	-1.991340	2.854731
7	8	0	-5.570921	-1.160209	2.482910
8	6	0	-6.180709	-0.628225	1.298344
9	8	0	-5.465401	-1.152639	0.174781
10	6	0	-0.727300	-2.736389	0.075278
11	6	0	0.302577	-1.545787	-0.050103
12	6	0	1.683378	-2.277349	0.136596
13	6	0	1.293618	-3.758728	0.287752
14	8	0	-0.041729	-3.731172	0.804379
15	6	0	0.070723	-0.686286	-1.298849
16	6	0	0.518950	0.720942	-0.852740
17	6	0	0.066737	0.722575	0.622794
18	8	0	0.159615	-0.645139	1.056668
19	6	0	2.725787	-2.079344	-0.952255
20	6	0	4.001906	-1.375081	-0.639995
21	8	0	2.520642	-2.539870	-2.072134
22	6	0	4.209310	-0.683132	0.577268
23	6	0	5.411720	-0.033594	0.734004
24	6	0	6.402303	-0.054515	-0.247017
25	6	0	6.231626	-0.733710	-1.440982
26	6	0	5.007069	-1.389833	-1.620905
27	8	0	5.863074	0.681412	1.824276
28	6	0	7.064190	1.322526	1.381832
29	8	0	7.497716	0.645590	0.188921

30	8	0	1.906190	0.922022	-1.024905
31	6	0	0.940930	1.566750	1.559135
32	8	0	-0.948140	-3.155246	-1.263140
33	6	0	-0.303938	1.805202	-1.511783
34	6	0	-1.660109	1.932502	-0.770649
35	6	0	-1.413193	1.209333	0.574992
36	8	0	0.077879	2.466414	-2.455677
37	6	0	-1.553830	-4.438852	-1.407181
38	6	0	-2.167487	3.344636	-0.707951
39	6	0	-3.249807	3.474964	-1.470312
40	6	0	-3.601037	2.168483	-2.139697
41	8	0	-2.646810	1.235578	-1.555392
42	6	0	-3.381991	2.220683	-3.656539
43	6	0	-5.004838	1.674784	-1.786361
44	6	0	0.983589	3.018590	1.168330
45	6	0	0.371202	4.055620	1.764654
46	6	0	0.525541	5.455996	1.222563
47	6	0	-0.504847	3.954589	2.987669
48	1	0	-3.071550	-1.929134	-1.075281
49	1	0	-1.226877	-2.719042	2.739050
50	1	0	-3.313267	-2.005797	3.937843
51	1	0	-7.221649	-0.949863	1.250020
52	1	0	-6.089113	0.467928	1.307737
53	1	0	2.048417	-1.930513	1.100592
54	1	0	1.909037	-4.294227	1.013255
55	1	0	1.323192	-4.268659	-0.680339
56	1	0	0.618095	-1.027945	-2.175800
57	1	0	-0.993839	-0.688745	-1.541916
58	1	0	3.452977	-0.624894	1.348787
59	1	0	7.008358	-0.751181	-2.197922
60	1	0	4.806498	-1.923883	-2.543091
61	1	0	6.852343	2.372738	1.139500
62	1	0	7.832784	1.226851	2.149798
63	1	0	2.021230	1.368429	-1.884025
64	1	0	0.562353	1.422508	2.575768
65	1	0	1.954346	1.155584	1.525557
66	1	0	-2.079311	0.349079	0.631914
67	1	0	-1.637961	1.863400	1.419990
68	1	0	-2.515320	-4.489961	-0.882217
69	1	0	-1.710674	-4.571804	-2.479640
70	1	0	-0.898917	-5.230495	-1.028149
71	1	0	-1.666046	4.109974	-0.129688
72	1	0	-3.823129	4.382503	-1.630150

73	1	0	-3.564303	1.233135	-4.094558
74	1	0	-4.070248	2.937085	-4.121189
75	1	0	-2.355281	2.523819	-3.879462
76	1	0	-5.133928	1.646831	-0.700659
77	1	0	-5.764936	2.337284	-2.217402
78	1	0	-5.161623	0.663603	-2.174406
79	1	0	1.587089	3.229307	0.286313
80	1	0	1.131110	5.476313	0.311171
81	1	0	-0.453178	5.902340	0.992976
82	1	0	0.997611	6.114411	1.965299
83	1	0	-1.530265	4.275696	2.753436
84	1	0	-0.557209	2.945238	3.401442
85	1	0	-0.142337	4.626672	3.777571

Table S15. Standard orientation of conformation **2**B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.536798	-1.820383	1.657549
2	6	0	-4.296629	-1.753175	0.288234
3	6	0	-3.066665	-2.055565	-0.257039
4	6	0	-2.047862	-2.448437	0.635338
5	6	0	-2.294462	-2.520578	2.009117
6	6	0	-3.553617	-2.207577	2.548611
7	8	0	-5.855595	-1.506790	1.910262
8	6	0	-6.350929	-0.976742	0.672495
9	8	0	-5.462701	-1.405745	-0.364980
10	6	0	-0.661016	-2.707283	0.088084
11	6	0	0.301454	-1.459354	0.110147
12	6	0	1.696845	-2.115256	0.424944
13	6	0	1.377803	-3.619481	0.521374
14	8	0	-0.007850	-3.678214	0.876860
15	6	0	0.154503	-0.567155	-1.127675
16	6	0	0.479416	0.841507	-0.590262
17	6	0	-0.127686	0.765515	0.827220
18	8	0	-0.014965	-0.611629	1.223340
19	6	0	2.827280	-1.848798	-0.555379
20	6	0	4.050165	-1.122455	-0.112111
21	8	0	2.742706	-2.279894	-1.702546
22	6	0	5.130939	-1.078259	-1.028247
23	6	0	6.254450	-0.388194	-0.644682
24	6	0	6.346501	0.251944	0.594379
25	6	0	5.309724	0.223927	1.506875
26	6	0	4.154288	-0.478625	1.129672

27	8	0	7.444436	-0.233663	-1.324109
28	6	0	8.185167	0.736976	-0.578368
29	8	0	7.581133	0.831022	0.724429
30	8	0	1.865522	1.112357	-0.605575
31	6	0	0.600778	1.611910	1.879297
32	8	0	-0.694752	-3.101658	-1.275126
33	6	0	-0.321651	1.912260	-1.295843
34	6	0	-1.754581	1.945950	-0.705114
35	6	0	-1.617172	1.183671	0.634824
36	8	0	0.128228	2.634122	-2.162109
37	6	0	-1.194611	-4.415125	-1.518943
38	6	0	-2.335001	3.329998	-0.649671
39	6	0	-3.341261	3.437908	-1.513181
40	6	0	-3.558541	2.142315	-2.256153
41	8	0	-2.616232	1.235195	-1.614696
42	6	0	-3.202439	2.262432	-3.742570
43	6	0	-4.961663	1.567690	-2.053440
44	6	0	0.617770	3.078035	1.543204
45	6	0	-0.103034	4.064460	2.102951
46	6	0	0.041885	5.489479	1.626826
47	6	0	-1.100861	3.878863	3.218055
48	1	0	-2.886686	-1.987949	-1.322707
49	1	0	-1.487182	-2.812982	2.669382
50	1	0	-3.747488	-2.267454	3.614328
51	1	0	-7.349912	-1.371291	0.482694
52	1	0	-6.346697	0.121902	0.723634
53	1	0	1.945572	-1.761245	1.422415
54	1	0	1.934906	-4.128055	1.310581
55	1	0	1.550083	-4.114150	-0.439865
56	1	0	0.807486	-0.848292	-1.952067
57	1	0	-0.877631	-0.612894	-1.481657
58	1	0	5.048376	-1.576109	-1.987130
59	1	0	5.383935	0.726871	2.464848
60	1	0	3.317562	-0.481076	1.816671
61	1	0	9.218818	0.405073	-0.472275
62	1	0	8.115932	1.714287	-1.074682
63	1	0	2.044318	1.616291	-1.420916
64	1	0	0.122640	1.413997	2.843668
65	1	0	1.629788	1.243594	1.940622
66	1	0	-2.239649	0.290316	0.589596
67	1	0	-1.965155	1.793028	1.471416
68	1	0	-2.207592	-4.541359	-1.117790
69	1	0	-1.211037	-4.526956	-2.605065

70	1	0	-0.540833	-5.175710	-1.079100
71	1	0	-1.932958	4.095444	0.001700
72	1	0	-3.941226	4.322735	-1.700206
73	1	0	-3.290030	1.284523	-4.228953
74	1	0	-3.881646	2.960770	-4.246384
75	1	0	-2.177071	2.624606	-3.857958
76	1	0	-5.189003	1.498081	-0.985665
77	1	0	-5.712268	2.205680	-2.535112
78	1	0	-5.027389	0.563392	-2.482809
79	1	0	1.302360	3.347342	0.739970
80	1	0	0.738982	5.570370	0.787081
81	1	0	-0.926942	5.901599	1.308545
82	1	0	0.401625	6.138835	2.437289
83	1	0	-2.113440	4.136748	2.874917
84	1	0	-1.130267	2.859300	3.608504
85	1	0	-0.874668	4.555516	4.053384

Table S15. Standard orientation of conformation **2**C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.247924	1.213865	-2.056414
2	6	0	-4.158664	1.475849	-0.692278
3	6	0	-3.003573	1.955561	-0.111273
4	6	0	-1.901421	2.178721	-0.962432
5	6	0	-1.997020	1.919736	-2.332432
6	6	0	-3.181805	1.431746	-2.908669
7	8	0	-5.521871	0.783220	-2.360645
8	6	0	-6.137188	0.527417	-1.090132
9	8	0	-5.378843	1.225595	-0.096279
10	6	0	-0.585098	2.608879	-0.353341
11	6	0	0.408299	1.425985	-0.026024
12	6	0	1.808028	2.066383	-0.351787
13	6	0	1.462838	3.506434	-0.771873
14	8	0	0.118655	3.429405	-1.260132
15	6	0	0.166064	0.810786	1.359507
16	6	0	0.540724	-0.672120	1.163893
17	6	0	0.059503	-0.909576	-0.285047
18	8	0	0.231085	0.348981	-0.956825
19	6	0	2.856472	2.035832	0.748335
20	6	0	4.102170	1.238932	0.564347
21	8	0	2.682783	2.705083	1.763319
22	6	0	4.264226	0.313434	-0.494623
23	6	0	5.444956	-0.391096	-0.537919

24	6	0	6.456857	-0.207128	0.403586
25	6	0	6.330087	0.698853	1.442286
26	6	0	5.127771	1.414558	1.507956
27	8	0	5.852960	-1.321075	-1.471855
28	6	0	7.047022	-1.897251	-0.931856
29	8	0	7.523407	-1.012424	0.097501
30	8	0	1.919039	-0.906039	1.358446
31	6	0	0.864269	-1.976898	-1.036911
32	8	0	-0.766395	3.271085	0.889351
33	6	0	-0.312138	-1.598922	1.999846
34	6	0	-1.677263	-1.814067	1.297399
35	6	0	-1.441855	-1.288304	-0.137022
36	8	0	0.065942	-2.121595	3.028438
37	6	0	-1.316113	4.585027	0.806434
38	6	0	-2.185621	-3.222558	1.426679
39	6	0	-3.273446	-3.246730	2.192070
40	6	0	-3.622778	-1.860525	2.677677
41	8	0	-2.656706	-1.017805	1.986650
42	6	0	-3.420581	-1.711202	4.190068
43	6	0	-5.019292	-1.410724	2.243727
44	6	0	0.406154	-2.144474	-2.457666
45	6	0	-0.204312	-3.206598	-3.008111
46	6	0	-0.619966	-3.192187	-4.459363
47	6	0	-0.544415	-4.482782	-2.278060
48	1	0	-2.938979	2.141557	0.953593
49	1	0	-1.128374	2.087672	-2.957271
50	1	0	-3.257645	1.232659	-3.972353
51	1	0	-7.160186	0.905710	-1.099813
52	1	0	-6.100912	-0.552048	-0.883145
53	1	0	2.149943	1.535258	-1.237050
54	1	0	2.082108	3.875966	-1.591517
55	1	0	1.525501	4.186845	0.083300
56	1	0	0.750261	1.275521	2.152038
57	1	0	-0.890864	0.908604	1.616954
58	1	0	3.491107	0.125720	-1.227828
59	1	0	7.122829	0.841369	2.168790
60	1	0	4.961737	2.125219	2.310017
61	1	0	6.814518	-2.873129	-0.484476
62	1	0	7.800851	-1.975990	-1.716228
63	1	0	2.021520	-1.257142	2.262331
64	1	0	1.918087	-1.682457	-1.008179
65	1	0	0.791426	-2.913869	-0.473730
66	1	0	-2.062013	-0.405178	-0.282308

67	1	0	-1.732454	-2.020689	-0.894088
68	1	0	-2.283233	4.584616	0.289304
69	1	0	-1.449413	4.913936	1.839147
70	1	0	-0.635480	5.267215	0.286267
71	1	0	-1.693019	-4.065244	0.953840
72	1	0	-3.853356	-4.122251	2.465574
73	1	0	-3.601646	-0.673240	4.490613
74	1	0	-4.117258	-2.356433	4.738725
75	1	0	-2.397612	-1.985271	4.462438
76	1	0	-5.136600	-1.533765	1.163027
77	1	0	-5.790429	-2.000468	2.753462
78	1	0	-5.168820	-0.353992	2.485734
79	1	0	0.576104	-1.273754	-3.089912
80	1	0	-0.361074	-2.246614	-4.946262
81	1	0	-0.138289	-4.008180	-5.016629
82	1	0	-1.704571	-3.342217	-4.558720
83	1	0	-0.105231	-5.349986	-2.790124
84	1	0	-0.196748	-4.496804	-1.242306
85	1	0	-1.632040	-4.643726	-2.270442

Table S15. Standard orientation of conformation **2**D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.536863	-1.820453	1.657532
2	6	0	-4.296704	-1.753140	0.288225
3	6	0	-3.066738	-2.055489	-0.257074
4	6	0	-2.047938	-2.448445	0.635265
5	6	0	-2.294531	-2.520688	2.009040
6	6	0	-3.553679	-2.207717	2.548562
7	8	0	-5.855665	-1.506878	1.910281
8	6	0	-6.351025	-0.976767	0.672552
9	8	0	-5.462778	-1.405654	-0.364958
10	6	0	-0.661103	-2.707273	0.087963
11	6	0	0.301366	-1.459351	0.110079
12	6	0	1.696760	-2.115262	0.424833
13	6	0	1.377708	-3.619498	0.521189
14	8	0	-0.007921	-3.678238	0.876716
15	6	0	0.154404	-0.567081	-1.127686
16	6	0	0.479414	0.841522	-0.590205
17	6	0	-0.127684	0.765491	0.827278
18	8	0	-0.015069	-0.611674	1.223321
19	6	0	2.827202	-1.848779	-0.555472
20	6	0	4.050098	-1.122493	-0.112178

21	8	0	2.742603	-2.279826	-1.702659
22	6	0	5.130874	-1.078255	-1.028310
23	6	0	6.254404	-0.388259	-0.644678
24	6	0	6.346489	0.251752	0.594449
25	6	0	5.309712	0.223673	1.506946
26	6	0	4.154247	-0.478793	1.129669
27	8	0	7.444412	-0.233733	-1.324072
28	6	0	8.185096	0.736906	-0.578302
29	8	0	7.581152	0.830739	0.724559
30	8	0	1.865548	1.112271	-0.605488
31	6	0	0.600870	1.611803	1.879365
32	8	0	-0.694863	-3.101608	-1.275236
33	6	0	-0.321558	1.912403	-1.295695
34	6	0	-1.754487	1.946112	-0.705003
35	6	0	-1.617146	1.183758	0.634903
36	8	0	0.128384	2.634312	-2.161889
37	6	0	-1.194734	-4.415071	-1.519082
38	6	0	-2.334964	3.330122	-0.649507
39	6	0	-3.341205	3.438044	-1.513039
40	6	0	-3.558412	2.142490	-2.256097
41	8	0	-2.616074	1.235370	-1.614697
42	6	0	-3.202288	2.262723	-3.742503
43	6	0	-4.961519	1.567799	-2.053459
44	6	0	0.618003	3.077931	1.543279
45	6	0	-0.102836	4.064394	2.102915
46	6	0	0.042201	5.489400	1.626792
47	6	0	-1.100813	3.878851	3.217896
48	1	0	-2.886775	-1.987792	-1.322741
49	1	0	-1.487249	-2.813160	2.669274
50	1	0	-3.747554	-2.267677	3.614274
51	1	0	-7.349989	-1.371355	0.482727
52	1	0	-6.346858	0.121876	0.723767
53	1	0	1.945476	-1.761322	1.422336
54	1	0	1.934849	-4.128120	1.310342
55	1	0	1.549966	-4.114114	-0.440083
56	1	0	0.807325	-0.848223	-1.952125
57	1	0	-0.877752	-0.612741	-1.481617
58	1	0	5.048303	-1.576023	-1.987234
59	1	0	5.383945	0.726504	2.464978
60	1	0	3.317517	-0.481278	1.816665
61	1	0	9.218794	0.405117	-0.472331
62	1	0	8.115704	1.714270	-1.074496
63	1	0	2.044406	1.616166	-1.420840

64	1	0	0.122734	1.413925	2.843745
65	1	0	1.629844	1.243385	1.940654
66	1	0	-2.239677	0.290440	0.589624
67	1	0	-1.965096	1.793102	1.471515
68	1	0	-2.207619	-4.541378	-1.117711
69	1	0	-1.211405	-4.526784	-2.605212
70	1	0	-0.540827	-5.175673	-1.079465
71	1	0	-1.932983	4.095554	0.001920
72	1	0	-3.941203	4.322861	-1.700009
73	1	0	-3.289842	1.284845	-4.228955
74	1	0	-3.881509	2.961075	-4.246280
75	1	0	-2.176930	2.624937	-3.857844
76	1	0	-5.188904	1.498117	-0.985699
77	1	0	-5.712125	2.205786	-2.535131
78	1	0	-5.027192	0.563521	-2.482883
79	1	0	1.302721	3.347196	0.740140
80	1	0	0.739411	5.570256	0.787138
81	1	0	-0.926567	5.901555	1.308375
82	1	0	0.401853	6.138751	2.437298
83	1	0	-2.113370	4.136598	2.874586
84	1	0	-1.130179	2.859334	3.608471
85	1	0	-0.874796	4.555633	4.053168

Table S16. Standard orientation of conformation **2**E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.444188	-1.632164	1.522634
2	6	0	-4.189578	-1.694284	0.155601
3	6	0	-2.951321	-2.038132	-0.344763
4	6	0	-1.939026	-2.332546	0.592216
5	6	0	-2.200346	-2.274503	1.963658
6	6	0	-3.468337	-1.923921	2.457024
7	8	0	-5.767115	-1.304551	1.730775
8	6	0	-6.255130	-0.902710	0.442736
9	8	0	-5.348826	-1.415283	-0.540432
10	6	0	-0.540778	-2.612752	0.087367
11	6	0	0.400164	-1.347821	0.022615
12	6	0	1.798818	-1.950355	0.416677
13	6	0	1.507452	-3.449183	0.613717
14	8	0	0.118125	-3.506416	0.958148
15	6	0	0.257286	-0.566238	-1.289720
16	6	0	0.524537	0.892620	-0.867652
17	6	0	-0.102690	0.915544	0.543638

18	8	0	0.057587	-0.416845	1.058288
19	6	0	2.949608	-1.720973	-0.548150
20	6	0	4.128659	-0.913541	-0.128298
21	8	0	2.915710	-2.242310	-1.660040
22	6	0	5.231811	-0.887594	-1.018138
23	6	0	6.314290	-0.123582	-0.657707
24	6	0	6.345114	0.606076	0.534130
25	6	0	5.285577	0.597725	1.420374
26	6	0	4.171197	-0.179071	1.066083
27	8	0	7.515092	0.034627	-1.316878
28	6	0	8.191774	1.089063	-0.626128
29	8	0	7.550183	1.246471	0.652362
30	8	0	1.899246	1.213132	-0.889243
31	6	0	0.579486	1.894068	1.508125
32	8	0	-0.547047	-3.115492	-1.240405
33	6	0	-0.297641	1.876302	-1.669039
34	6	0	-1.724641	1.969024	-1.068627
35	6	0	-1.599043	1.259550	0.299141
36	8	0	0.139035	2.520931	-2.600419
37	6	0	-1.020730	-4.453395	-1.384413
38	6	0	-2.248143	3.378452	-1.053645
39	6	0	-3.274256	3.492882	-1.892448
40	6	0	-3.566108	2.176739	-2.571585
41	8	0	-2.625961	1.263381	-1.936834
42	6	0	-3.276188	2.221975	-4.076020
43	6	0	-4.977257	1.661309	-2.279684
44	6	0	-0.013762	1.842336	2.887150
45	6	0	-0.725335	2.791210	3.517210
46	6	0	-1.272309	2.553963	4.904076
47	6	0	-1.061349	4.144813	2.941094
48	1	0	-2.758666	-2.070764	-1.409872
49	1	0	-1.397557	-2.491740	2.657569
50	1	0	-3.673056	-1.880345	3.521461
51	1	0	-7.246168	-1.328966	0.281289
52	1	0	-6.267380	0.195304	0.388381
53	1	0	2.010788	-1.521406	1.392888
54	1	0	2.063501	-3.890863	1.442847
55	1	0	1.699836	-4.006480	-0.308550
56	1	0	0.940094	-0.894008	-2.071873
57	1	0	-0.763420	-0.676626	-1.663580
58	1	0	5.196518	-1.455013	-1.940613
59	1	0	5.311971	1.170237	2.341070
60	1	0	3.316866	-0.169066	1.731076

61	1	0	9.236166	0.814222	-0.472955
62	1	0	8.091206	2.024527	-1.192725
63	1	0	2.071708	1.661605	-1.737558
64	1	0	1.643931	1.640443	1.540526
65	1	0	0.516077	2.898074	1.073780
66	1	0	-2.184187	0.341536	0.263008
67	1	0	-1.996623	1.869300	1.114052
68	1	0	-2.038435	-4.564653	-0.990861
69	1	0	-1.016138	-4.653223	-2.457937
70	1	0	-0.362510	-5.163927	-0.873376
71	1	0	-1.808572	4.156830	-0.439401
72	1	0	-3.848122	4.391566	-2.094239
73	1	0	-3.418987	1.228025	-4.514023
74	1	0	-3.954474	2.921907	-4.578797
75	1	0	-2.245472	2.541708	-4.252990
76	1	0	-5.155968	1.650313	-1.200234
77	1	0	-5.729141	2.301605	-2.756133
78	1	0	-5.093253	0.640859	-2.658011
79	1	0	0.140345	0.896789	3.405845
80	1	0	-1.014332	1.557805	5.277504
81	1	0	-0.885007	3.297890	5.614647
82	1	0	-2.367427	2.650009	4.915764
83	1	0	-0.720303	4.945939	3.611199
84	1	0	-0.617469	4.321781	1.958436
85	1	0	-2.150263	4.262311	2.844312

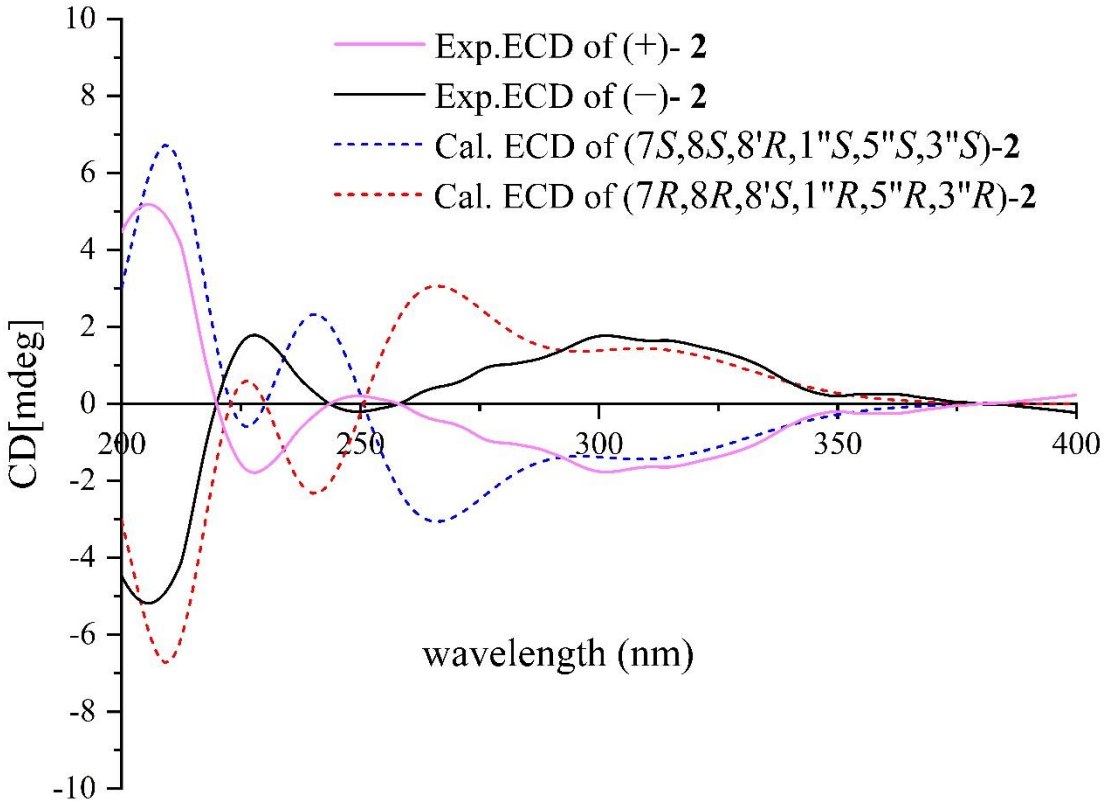


Figure S4. Computational methods for ECD of compound **2.**
b3lyp/6-31+g(d, p) scrf = (solvent = methanol)

2.3. ECD spectra calculation of **3**

Table S17. Energies of the optimized conformers of compound **3**

Boltzmann distributions of the optimized **3** at the B3LYP-D3/6-31+G(d) level in the gas phase.

conformer	Energy (Hartree)	Energy (kcal/mol)	Population (%)
1	-2412.401795	-1513804.803	48.94
2	-2412.402969	-1513805.54	51.06

Table S18. Standard orientation of conformation **3**A

Atomic	Center	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.195012	-3.365294	1.444798
2	6	0	-0.868312	-3.551698	0.953498
3	6	0	0.176190	-2.735801	1.323298
4	6	0	-0.148907	-1.696000	2.230098
5	6	0	-1.448706	-1.508896	2.707198
6	6	0	-2.515309	-2.346493	2.315998
7	8	0	-3.036015	-4.334792	0.922398
8	6	0	-2.199817	-5.180494	0.065498
9	8	0	-0.837715	-4.639898	0.082898
10	6	0	0.942096	-0.798603	2.748998
11	6	0	1.230600	0.599296	2.081998
12	6	0	2.753201	0.783991	2.318798
13	6	0	3.290797	-0.585410	2.767098
14	8	0	2.177494	-1.523307	2.720198
15	6	0	3.518002	1.390889	1.141398
16	6	0	3.839000	0.597688	-0.079202
17	8	0	3.901606	2.537988	1.255798
18	6	0	3.192196	-0.630810	-0.376902
19	6	0	3.559195	-1.239211	-1.552702
20	6	0	4.538196	-0.680614	-2.430802
21	6	0	5.178800	0.507084	-2.146302
22	6	0	4.800302	1.139485	-0.944302
23	8	0	3.080091	-2.436810	-2.081402
24	6	0	3.761291	-2.609212	-3.365802
25	8	0	4.708094	-1.497115	-3.531202
26	6	0	0.320903	1.728799	2.586098
27	6	0	-0.550195	2.169001	1.394598
28	6	0	0.180303	1.568299	0.167898
29	8	0	0.986800	0.478097	0.655698
30	6	0	-1.913097	1.429105	1.373598
31	6	0	-2.080700	0.604906	0.088298
32	6	0	-0.894499	0.985102	-0.820702

33	8	0	-2.708697	1.464207	2.273598
34	6	0	-0.736391	3.692202	1.356298
35	6	0	-1.785789	4.146805	0.390898
36	6	0	-1.557987	4.876104	-0.713502
37	6	0	-2.687786	5.295307	-1.604802
38	6	0	-0.199986	5.320500	-1.156402
39	8	0	1.024806	2.470696	-0.488902
40	6	0	-3.459299	0.838010	-0.545502
41	6	0	-3.875002	-0.283489	-1.445602
42	6	0	-5.132803	-0.471485	-1.874702
43	6	0	-5.484006	-1.605284	-2.789902
44	6	0	-6.270800	0.420918	-1.484502
45	8	0	0.701997	-0.467003	4.121898
46	8	0	-1.315396	1.987203	-1.729902
47	6	0	-0.267902	-0.110000	-1.703802
48	8	0	0.634999	0.069498	-2.489502
49	8	0	-0.840706	-1.331698	-1.501102
50	6	0	-0.263309	-2.440100	-2.254002
51	1	0	1.195190	-2.875704	0.963098
52	1	0	-1.657004	-0.694396	3.410698
53	1	0	-3.526508	-2.189890	2.684398
54	1	0	-2.171920	-6.184994	0.508598
55	1	0	-2.581817	-5.100393	-0.960302
56	1	0	2.876403	1.508891	3.172498
57	1	0	3.651597	-0.573711	3.809198
58	1	0	4.050295	-1.031513	2.103698
59	1	0	2.428795	-1.060908	0.278598
60	1	0	5.924001	0.938282	-2.809102
61	1	0	5.270905	2.095084	-0.681302
62	1	0	4.344788	-3.537613	-3.316402
63	1	0	3.010991	-2.528609	-4.164202
64	1	0	0.919706	2.578297	2.971798
65	1	0	-0.298997	1.406100	3.452198
66	1	0	-1.988803	-0.483595	0.366998
67	1	0	-1.015190	4.047302	2.373598
68	1	0	0.250211	4.157699	1.127398
69	1	0	-2.800790	3.853208	0.661598
70	1	0	-3.664286	5.241810	-1.106802
71	1	0	-2.565083	6.324507	-1.965402
72	1	0	-2.742088	4.640308	-2.487602
73	1	0	0.594112	4.629598	-0.822002
74	1	0	-0.119986	5.401400	-2.247102
75	1	0	0.040817	6.308999	-0.740702

76	1	0	1.706104	1.974994	-1.030502
77	1	0	-4.206499	0.982712	0.266798
78	1	0	-3.444096	1.790810	-1.126602
79	1	0	-3.068404	-0.949991	-1.758602
80	1	0	-6.226408	-2.268782	-2.326002
81	1	0	-5.914505	-1.233283	-3.729502
82	1	0	-4.615908	-2.221587	-3.053402
83	1	0	-6.410100	0.431718	-0.393902
84	1	0	-6.085797	1.457418	-1.799302
85	1	0	-7.224801	0.113621	-1.928102
86	1	0	0.799895	-1.264103	4.690598
87	1	0	-0.590894	2.667401	-1.864202
88	1	0	0.835191	-2.383703	-2.230302
89	1	0	-0.631311	-3.318299	-1.707802
90	1	0	-0.639409	-2.393199	-3.278102

Table S19. Standard orientation of conformation **3**B

Atomic Number	Center Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.610598	-1.028202	2.372194
2	6	0	3.179001	0.327499	2.268294
3	6	0	1.854802	0.689202	2.364494
4	6	0	0.942800	-0.374197	2.579394
5	6	0	1.364197	-1.702198	2.682094
6	6	0	2.724197	-2.064200	2.573594
7	8	0	4.988998	-1.099504	2.243494
8	6	0	5.452401	0.279495	2.061194
9	8	0	4.278902	1.156797	2.054194
10	6	0	-0.520400	-0.068894	2.756994
11	6	0	-1.521400	-0.183192	1.546494
12	6	0	-2.596698	0.880210	1.894394
13	6	0	-1.993697	1.758309	3.003694
14	8	0	-0.648197	1.265406	3.263894
15	6	0	-3.138797	1.672211	0.705894
16	6	0	-2.340895	2.744009	0.042194
17	8	0	-4.272397	1.432313	0.340694
18	6	0	-0.943194	2.889107	0.246194
19	6	0	-0.328893	3.893106	-0.462106
20	6	0	-1.045891	4.756107	-1.347306
21	6	0	-2.405291	4.631509	-1.542706
22	6	0	-3.038893	3.595810	-0.825806
23	8	0	1.020708	4.240603	-0.456306
24	6	0	1.156010	5.343403	-1.410306

25	8	0	-0.183189	5.666705	-1.923206
26	6	0	-2.033003	-1.606791	1.287294
27	6	0	-1.485003	-2.033192	-0.082706
28	6	0	-1.026501	-0.698893	-0.728006
29	8	0	-0.812799	0.232106	0.344494
30	6	0	-0.153905	-2.823795	0.050894
31	6	0	0.984796	-2.128097	-0.704206
32	6	0	0.324098	-0.979196	-1.486606
33	8	0	-0.039207	-3.836495	0.687994
34	6	0	-2.458105	-2.865491	-0.929106
35	6	0	-3.827404	-2.265888	-1.004606
36	6	0	-4.970705	-2.908886	-0.723606
37	6	0	-6.295004	-2.218184	-0.852906
38	6	0	-5.046808	-4.337486	-0.281706
39	8	0	-1.947600	-0.129792	-1.617806
40	6	0	1.775995	-3.117998	-1.573906
41	6	0	3.171795	-2.635001	-1.820206
42	6	0	3.628496	-2.141202	-2.981906
43	6	0	5.058197	-1.708104	-3.127206
44	6	0	2.794197	-1.989200	-4.213006
45	8	0	-1.092201	-0.932293	3.745894
46	8	0	-0.020102	-1.460995	-2.780006
47	6	0	1.139401	0.305703	-1.696906
48	8	0	0.874102	1.161903	-2.511006
49	8	0	2.191501	0.395801	-0.837906
50	6	0	2.979603	1.620799	-0.920306
51	1	0	1.514003	1.721802	2.293694
52	1	0	0.626396	-2.493896	2.857094
53	1	0	3.043995	-3.100901	2.647294
54	1	0	6.069101	0.544794	2.930294
55	1	0	5.929001	0.345294	1.074694
56	1	0	-3.481299	0.327011	2.323394
57	1	0	-2.549097	1.675210	3.952994
58	1	0	-1.849095	2.818108	2.736394
59	1	0	-0.379596	2.228106	0.912794
60	1	0	-2.958090	5.283710	-2.213506
61	1	0	-4.117893	3.446312	-0.960006
62	1	0	1.522712	6.221002	-0.862206
63	1	0	1.760309	4.990102	-2.257306
64	1	0	-3.144403	-1.642889	1.286494
65	1	0	-1.732804	-2.310992	2.093294
66	1	0	1.683797	-1.681198	0.061294
67	1	0	-2.050505	-2.960391	-1.962606

68	1	0	-2.497107	-3.899691	-0.514606
69	1	0	-3.834002	-1.219288	-1.329106
70	1	0	-6.191302	-1.134484	-1.007706
71	1	0	-6.862805	-2.614783	-1.705106
72	1	0	-6.912004	-2.353882	0.044294
73	1	0	-5.560309	-4.953685	-1.032006
74	1	0	-4.053208	-4.781688	-0.119706
75	1	0	-5.603508	-4.437385	0.659094
76	1	0	-1.836298	0.860308	-1.652006
77	1	0	1.815593	-4.103898	-1.058006
78	1	0	1.229994	-3.300097	-2.525506
79	1	0	3.827295	-2.713602	-0.952906
80	1	0	5.534196	-2.201705	-3.985306
81	1	0	5.122999	-0.625104	-3.295506
82	1	0	5.664897	-1.939205	-2.243306
83	1	0	1.739597	-1.764298	-3.968706
84	1	0	3.146398	-1.181201	-4.864306
85	1	0	2.796395	-2.914000	-4.805006
86	1	0	-0.729601	-0.723294	4.636394
87	1	0	-0.700001	-0.852494	-3.199006
88	1	0	2.317305	2.493401	-0.829506
89	1	0	3.648703	1.528498	-0.054506
90	1	0	3.521503	1.630798	-1.868606

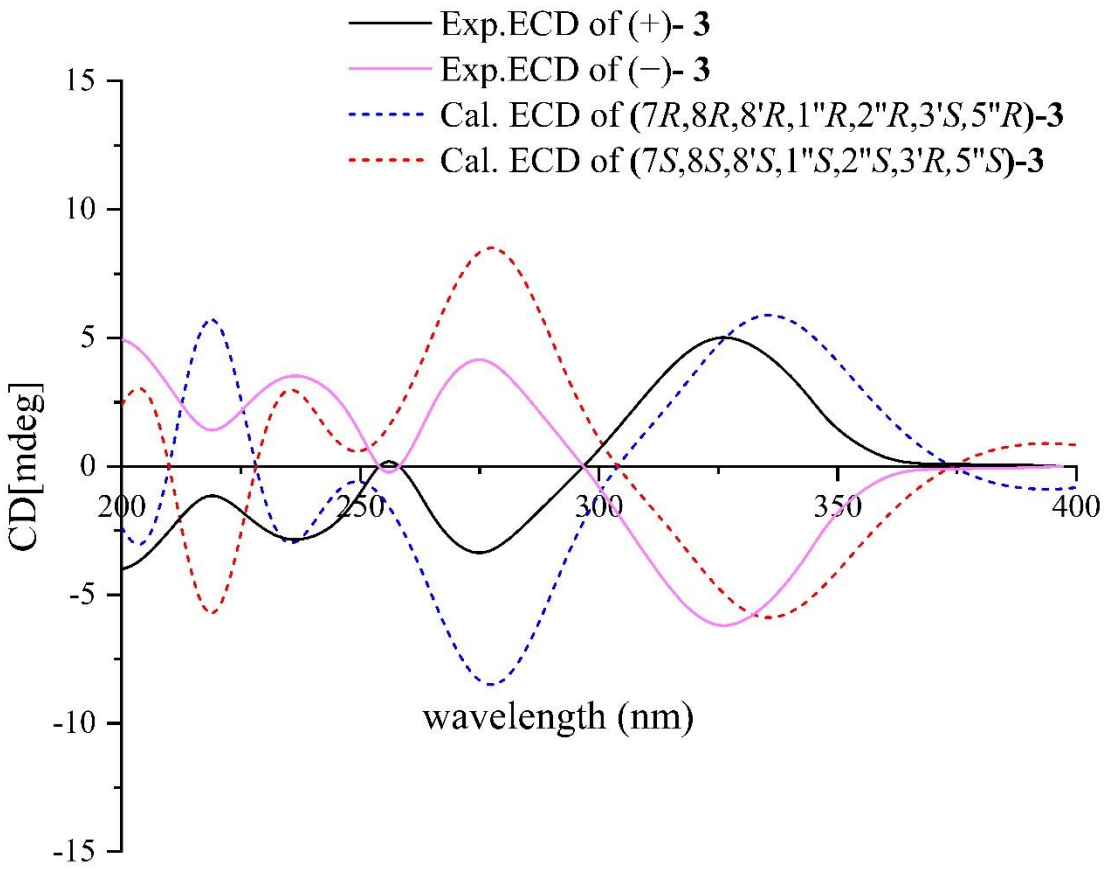


Figure S5. Computational methods for ECD of compound **3.**

b3lyp/6-31+g(d, p) scrf = (solvent = methanol)

2.4 ECD spectra calculation of **4**

Table S20. Energies of the optimized conformers of compound **4**

Boltzmann distributions of the optimized **4** at the B3LYP-D3/6-31+G(d) level in the gas phase

conformer	Energy (Hartree)	Energy (kcal/mol)	Population (%)
1	-2451.839479	-1538552.489	0.3
2	-2451.843185	-1538554.815	14.99
3	-2451.838663	-1538551.977	0.12
4	-2451.839812	-1538552.699	0.42
5	-2451.844814	-1538555.837	84.17

Table S21. Standard orientation of conformation **4**A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.957115	-2.191356	-1.364065
2	6	0	4.052451	-1.709928	-2.307617
3	6	0	2.691753	-1.794408	-2.129972
4	6	0	2.235064	-2.384965	-0.934490
5	6	0	3.142838	-2.877252	0.004704
6	6	0	4.533608	-2.788371	-0.194981
7	8	0	6.244970	-1.933146	-1.787449
8	6	0	6.105655	-1.534297	-3.157739
9	8	0	4.748407	-1.121755	-3.349325
10	6	0	0.745161	-2.469135	-0.677894
11	6	0	0.055733	-1.101470	-0.249197
12	6	0	-1.338569	-1.203439	-0.911683
13	6	0	-0.996322	-1.951529	-2.219683
14	8	0	0.087636	-2.814182	-1.913311
15	6	0	-2.403596	-1.940963	-0.124563
16	6	0	-3.831512	-1.635391	-0.399115
17	8	0	-2.111086	-2.797552	0.712844
18	6	0	-4.795479	-2.201483	0.473666
19	6	0	-6.115970	-1.937998	0.204326
20	6	0	-6.510575	-1.157458	-0.887793
21	6	0	-5.592261	-0.600691	-1.758698
22	6	0	-4.237505	-0.851948	-1.491852
23	8	0	-7.229439	-2.322074	0.913080
24	6	0	-8.352154	-1.948802	0.106166
25	8	0	-7.870405	-1.039264	-0.902949
26	8	0	0.524900	-3.465043	0.273859
27	6	0	0.104799	-0.773565	1.254407
28	6	0	1.147013	0.349471	1.404463

29	6	0	1.428883	0.836065	-0.044955
30	8	0	0.681239	0.007202	-0.924316
31	6	0	2.434777	-0.120272	2.143576
32	6	0	2.133139	-0.709539	3.497438
33	6	0	2.793774	-1.709512	4.102494
34	6	0	3.995216	-2.415200	3.525922
35	6	0	2.369336	-2.201073	5.464965
36	6	0	0.647550	1.607402	2.117920
37	6	0	1.058058	2.840579	1.308922
38	6	0	0.927449	2.347799	-0.154049
39	8	0	0.041413	1.636940	3.168219
40	6	0	0.331017	4.126967	1.719706
41	6	0	0.697935	5.304960	0.861762
42	6	0	-0.121959	6.080471	0.135984
43	6	0	0.429198	7.194215	-0.720305
44	6	0	-1.619983	5.922811	0.058265
45	6	0	-0.538751	2.440034	-0.595212
46	8	0	-1.330211	1.848042	0.322961
47	8	0	-0.966066	2.997486	-1.580224
48	6	0	-2.751662	2.008312	0.160057
49	8	0	1.790910	3.104587	-0.975572
50	8	0	2.785745	0.802932	-0.350937
51	6	0	1.718609	2.930768	-2.407980
52	1	0	2.000259	-1.411876	-2.868724
53	1	0	2.759782	-3.351324	0.899352
54	1	0	5.238805	-3.172948	0.533960
55	1	0	6.772699	-0.695309	-3.360166
56	1	0	6.320341	-2.395565	-3.807329
57	1	0	-1.678100	-0.193180	-1.129059
58	1	0	-0.700103	-1.225444	-2.989072
59	1	0	-1.820865	-2.559614	-2.605793
60	1	0	-4.479629	-2.810684	1.312191
61	1	0	-5.906177	-0.001686	-2.606344
62	1	0	-3.500255	-0.439930	-2.171227
63	1	0	-8.765404	-2.838515	-0.384986
64	1	0	-9.093057	-1.439712	0.723896
65	1	0	-0.420372	-3.432430	0.535826
66	1	0	0.383861	-1.650731	1.837649
67	1	0	-0.870826	-0.440224	1.612039
68	1	0	2.947401	-0.832858	1.496292
69	1	0	3.112539	0.739448	2.235688
70	1	0	1.298308	-0.259081	4.031419
71	1	0	4.843550	-2.350918	4.221778

72	1	0	4.316458	-2.001868	2.568706
73	1	0	3.788027	-3.485685	3.385007
74	1	0	3.179064	-2.081209	6.198879
75	1	0	1.489894	-1.664081	5.834610
76	1	0	2.129189	-3.273535	5.435664
77	1	0	2.140972	2.970869	1.459777
78	1	0	-0.745622	3.942465	1.722038
79	1	0	0.600028	4.316830	2.767573
80	1	0	1.766486	5.516870	0.810301
81	1	0	0.007295	8.166524	-0.429132
82	1	0	1.519872	7.259512	-0.651759
83	1	0	0.162130	7.038894	-1.775537
84	1	0	-2.116798	6.887475	0.228024
85	1	0	-1.915548	5.578262	-0.942004
86	1	0	-2.017783	5.214057	0.788664
87	1	0	-3.202545	1.382656	0.929125
88	1	0	-3.022464	3.056853	0.304047
89	1	0	-3.064861	1.685857	-0.833680
90	1	0	3.012488	1.657030	-0.763886
91	1	0	1.489976	1.894026	-2.674258
92	1	0	0.965984	3.595526	-2.830831
93	1	0	2.711875	3.193006	-2.781157

Table S22. Standard orientation of conformation **4**B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.696449	-0.553948	-0.281041
2	6	0	4.991184	0.004874	-1.344362
3	6	0	3.756284	-0.460614	-1.733972
4	6	0	3.227598	-1.548532	-1.010540
5	6	0	3.941203	-2.115258	0.048808
6	6	0	5.198790	-1.620632	0.438510
7	8	0	6.868950	0.148056	-0.085832
8	6	0	6.994949	0.977918	-1.249147
9	8	0	5.699532	1.082136	-1.845991
10	6	0	1.833704	-2.037534	-1.317846
11	6	0	0.704438	-1.180405	-0.646064
12	6	0	-0.524283	-1.457665	-1.576357
13	6	0	0.151778	-1.943789	-2.899099
14	8	0	1.559183	-1.860696	-2.704555
15	6	0	-1.488222	-2.494054	-1.039748
16	6	0	-2.928661	-2.191433	-0.901858
17	8	0	-1.052423	-3.605250	-0.713733

18	6	0	-3.728340	-3.151983	-0.230571
19	6	0	-5.058062	-2.857162	-0.069285
20	6	0	-5.621889	-1.672516	-0.555503
21	6	0	-4.871452	-0.730638	-1.232843
22	6	0	-3.506622	-1.009503	-1.391995
23	8	0	-6.041783	-3.617783	0.520861
24	6	0	-7.192354	-2.770929	0.597775
25	8	0	-6.958420	-1.648437	-0.275363
26	8	0	1.718099	-3.378018	-0.920797
27	6	0	0.573598	-1.384769	0.864955
28	6	0	0.367639	0.021845	1.420400
29	6	0	1.061568	0.939784	0.394887
30	8	0	1.006668	0.215085	-0.824746
31	6	0	0.829813	0.213929	2.899809
32	6	0	2.184790	-0.362530	3.209564
33	6	0	2.437762	-1.569142	3.743015
34	6	0	1.386312	-2.583953	4.115693
35	6	0	3.857689	-2.023101	3.973997
36	6	0	-1.090287	0.459489	1.333646
37	6	0	-1.189219	1.930562	0.934077
38	6	0	0.157147	2.253981	0.214650
39	8	0	-2.045120	-0.252293	1.572738
40	6	0	-2.568551	2.270301	0.327791
41	6	0	-2.744519	3.710144	-0.068772
42	6	0	-3.262594	4.698901	0.678011
43	6	0	-3.351967	6.107627	0.146528
44	6	0	-3.759011	4.525531	2.091237
45	6	0	0.112299	2.573021	-1.290508
46	8	0	-0.868221	1.923620	-1.945634
47	8	0	0.906370	3.307866	-1.833589
48	6	0	-0.816763	2.019820	-3.381765
49	8	0	0.887075	3.269250	0.884828
50	8	0	2.371422	1.263379	0.708167
51	6	0	0.369744	4.598589	0.882202
52	1	0	3.199986	-0.003978	-2.541283
53	1	0	3.516827	-2.964195	0.570653
54	1	0	5.750508	-2.055916	1.264531
55	1	0	7.687234	0.500339	-1.958360
56	1	0	7.338882	1.969280	-0.950726
57	1	0	-1.009480	-0.499617	-1.728652
58	1	0	-0.135719	-2.976427	-3.130731
59	1	0	-0.101001	-1.304620	-3.748862
60	1	0	-3.282820	-4.067146	0.140019

61	1	0	-5.315537	0.184117	-1.609443
62	1	0	-2.896636	-0.276395	-1.903876
63	1	0	-7.312691	-2.402804	1.624568
64	1	0	-8.071592	-3.316522	0.252347
65	1	0	0.768269	-3.627363	-0.854354
66	1	0	1.508017	-1.794206	1.250530
67	1	0	-0.235777	-2.056831	1.149981
68	1	0	0.838333	1.289529	3.112883
69	1	0	0.060024	-0.232554	3.537444
70	1	0	3.028387	0.257832	2.921310
71	1	0	0.363902	-2.218599	3.993494
72	1	0	1.511059	-2.909209	5.157606
73	1	0	1.491371	-3.483562	3.492586
74	1	0	4.028369	-2.263760	5.032798
75	1	0	4.580567	-1.259919	3.671182
76	1	0	4.070551	-2.939538	3.405162
77	1	0	-1.112176	2.476511	1.886493
78	1	0	-2.741348	1.630106	-0.537239
79	1	0	-3.307411	1.970721	1.075842
80	1	0	-2.395077	3.967574	-1.068569
81	1	0	-2.769606	6.800249	0.771441
82	1	0	-2.979426	6.180334	-0.880320
83	1	0	-4.388921	6.471043	0.161991
84	1	0	-4.797352	4.872191	2.183993
85	1	0	-3.715950	3.491241	2.440860
86	1	0	-3.164967	5.139585	2.783640
87	1	0	-1.675283	1.451288	-3.740805
88	1	0	0.117862	1.585650	-3.745654
89	1	0	-0.885055	3.063158	-3.698185
90	1	0	2.457681	2.234375	0.677242
91	1	0	-0.581379	4.651976	1.422154
92	1	0	1.119786	5.202217	1.396881
93	1	0	0.235277	4.971184	-0.137073

Table S23. Standard orientation of conformation **4**C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.736133	0.411975	0.463299
2	6	0	-5.175169	0.260530	-0.804880
3	6	0	-4.036042	0.936771	-1.191233
4	6	0	-3.457354	1.813775	-0.246249
5	6	0	-4.032752	1.973798	1.017814
6	6	0	-5.187063	1.264384	1.399827

7	8	0	-6.827660	-0.417014	0.585508
8	6	0	-7.082939	-0.900084	-0.741711
9	8	0	-5.898416	-0.671662	-1.517753
10	6	0	-2.168877	2.528584	-0.585575
11	6	0	-0.874449	1.669871	-0.315863
12	6	0	0.157140	2.336543	-1.281076
13	6	0	-0.747253	2.968836	-2.371710
14	8	0	-2.108892	2.749549	-1.982657
15	6	0	1.021926	3.368064	-0.568703
16	6	0	2.420127	3.051717	-0.214720
17	8	0	0.516695	4.449810	-0.242474
18	6	0	3.026614	1.820033	-0.570022
19	6	0	4.302555	1.602956	-0.111839
20	6	0	4.990048	2.535665	0.663099
21	6	0	4.429576	3.756598	1.005475
22	6	0	3.128339	3.996024	0.554720
23	8	0	5.109521	0.505636	-0.326648
24	6	0	6.207682	0.667070	0.575115
25	8	0	6.230084	2.052570	0.974361
26	8	0	-2.128691	3.722026	0.152974
27	6	0	-0.510416	1.515020	1.166146
28	6	0	-0.369548	0.007943	1.414234
29	6	0	-0.999785	-0.671052	0.171270
30	8	0	-1.092969	0.335185	-0.820323
31	6	0	-1.027012	-0.381651	2.772977
32	6	0	-0.967720	-1.836434	3.143727
33	6	0	-0.176300	-2.410982	4.065223
34	6	0	-0.243500	-3.898741	4.311327
35	6	0	0.842147	-1.684181	4.907350
36	6	0	1.077787	-0.475503	1.413729
37	6	0	1.165348	-1.809355	0.707879
38	6	0	0.006135	-1.828756	-0.328008
39	8	0	2.001533	0.103607	1.951244
40	6	0	2.585964	-2.207588	0.277074
41	6	0	2.598072	-3.445605	-0.574782
42	6	0	3.226879	-3.622573	-1.748774
43	6	0	3.116497	-4.933303	-2.489734
44	6	0	4.093938	-2.591275	-2.426467
45	6	0	0.543917	-1.447141	-1.717355
46	8	0	-0.018132	-2.125621	-2.720569
47	8	0	1.396611	-0.594737	-1.890586
48	6	0	0.451860	-1.798362	-4.041143
49	8	0	-0.540684	-3.121523	-0.243786

50	8	0	-2.262941	-1.229528	0.406734
51	6	0	-1.653145	-3.532257	-1.049548
52	1	0	-3.595516	0.810734	-2.171574
53	1	0	-3.587775	2.679188	1.708626
54	1	0	-5.627994	1.384593	2.383502
55	1	0	-7.917679	-0.334549	-1.177996
56	1	0	-7.290094	-1.970311	-0.703339
57	1	0	0.758525	1.538729	-1.703349
58	1	0	-0.608628	2.485218	-3.341810
59	1	0	-0.561812	4.043237	-2.471765
60	1	0	2.520916	1.052789	-1.139097
61	1	0	4.971063	4.479001	1.606366
62	1	0	2.626636	4.922205	0.811440
63	1	0	7.139811	0.426720	0.062869
64	1	0	6.048909	0.044891	1.465229
65	1	0	-1.267706	4.174331	0.001589
66	1	0	0.410478	2.031804	1.443777
67	1	0	-1.310852	1.930376	1.781826
68	1	0	-2.076308	-0.074223	2.700489
69	1	0	-0.553832	0.245681	3.534174
70	1	0	-1.637721	-2.476144	2.572813
71	1	0	-0.985405	-4.384333	3.669687
72	1	0	0.732138	-4.370796	4.126123
73	1	0	-0.500224	-4.113110	5.358407
74	1	0	1.845569	-2.093352	4.724944
75	1	0	0.633842	-1.830474	5.976504
76	1	0	0.887842	-0.611513	4.709826
77	1	0	0.814184	-2.528649	1.462104
78	1	0	3.069714	-1.368831	-0.221454
79	1	0	3.153875	-2.378929	1.202154
80	1	0	2.004523	-4.275404	-0.190898
81	1	0	2.492631	-5.654429	-1.951984
82	1	0	2.681218	-4.783385	-3.488590
83	1	0	4.106643	-5.384568	-2.646710
84	1	0	5.136922	-2.938320	-2.462694
85	1	0	4.080449	-1.618217	-1.934688
86	1	0	3.781899	-2.446964	-3.470282
87	1	0	1.519349	-2.014162	-4.121451
88	1	0	0.274067	-0.741129	-4.252713
89	1	0	-0.124442	-2.431541	-4.715451
90	1	0	-2.923710	-0.598325	0.069484
91	1	0	-2.352110	-4.040897	-0.379792
92	1	0	-1.295925	-4.225464	-1.817988

93	1	0	-2.164517	-2.695741	-1.521880

Table S24. Standard orientation of conformation **4**D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.458747	-3.403545	-0.540647
2	6	0	3.611397	-3.087585	-1.600005
3	6	0	2.253772	-2.942561	-1.437192
4	6	0	1.740187	-3.120458	-0.137118
5	6	0	2.589074	-3.455604	0.920380
6	6	0	3.977195	-3.600961	0.736990
7	8	0	5.763786	-3.434750	-0.988900
8	6	0	5.657647	-3.416626	-2.418597
9	8	0	4.363848	-2.899777	-2.746377
10	6	0	0.258933	-2.915996	0.103313
11	6	0	-0.215847	-1.397888	0.136403
12	6	0	-1.632811	-1.474044	-0.481151
13	6	0	-1.451543	-2.599179	-1.525947
14	8	0	-0.466068	-3.477800	-1.005480
15	6	0	-2.765535	-1.789601	0.475304
16	6	0	-4.136630	-1.336295	0.127843
17	8	0	-2.575305	-2.423884	1.515789
18	6	0	-5.130165	-1.441099	1.134368
19	6	0	-6.400653	-1.036871	0.805115
20	6	0	-6.720606	-0.555527	-0.468963
21	6	0	-5.773958	-0.454470	-1.471757
22	6	0	-4.467383	-0.851109	-1.147879
23	8	0	-7.519126	-0.989746	1.602459
24	6	0	-8.607553	-0.660851	0.731217
25	8	0	-8.038846	-0.204795	-0.512394
26	8	0	-0.082865	-3.574742	1.286098
27	6	0	-0.068343	-0.683616	1.492292
28	6	0	1.136706	0.265701	1.339669
29	6	0	1.422953	0.302746	-0.185379
30	8	0	0.533339	-0.615196	-0.810028
31	6	0	2.332883	-0.200950	2.230391
32	6	0	3.525083	0.715891	2.286905
33	6	0	3.851912	1.568993	3.273309
34	6	0	5.100881	2.411876	3.172613
35	6	0	3.061106	1.782169	4.539293
36	6	0	0.850311	1.723727	1.700481
37	6	0	1.371975	2.628939	0.587625
38	6	0	1.125299	1.790333	-0.690322

39	8	0	0.324208	2.100745	2.725708
40	6	0	0.843592	4.066951	0.644839
41	6	0	1.319303	4.909033	-0.505163
42	6	0	0.573852	5.575066	-1.400116
43	6	0	1.223143	6.333657	-2.531678
44	6	0	-0.933455	5.624387	-1.406528
45	6	0	-0.328484	1.965628	-1.144832
46	8	0	-1.161385	1.767998	-0.101151
47	8	0	-0.710941	2.283845	-2.247632
48	6	0	-2.552228	2.074268	-0.311506
49	8	0	2.053439	2.178480	-1.681374
50	8	0	2.744170	-0.009787	-0.487000
51	6	0	1.915390	1.633719	-3.012613
52	1	0	1.608228	-2.685622	-2.266337
53	1	0	2.159398	-3.620601	1.900672
54	1	0	4.636143	-3.855339	1.560331
55	1	0	6.426220	-2.761396	-2.830528
56	1	0	5.746991	-4.444689	-2.799573
57	1	0	-1.827880	-0.525561	-0.976775
58	1	0	-1.107316	-2.166283	-2.474865
59	1	0	-2.365057	-3.174265	-1.710818
60	1	0	-4.873608	-1.822198	2.115685
61	1	0	-6.031384	-0.086738	-2.458843
62	1	0	-3.711359	-0.793988	-1.922551
63	1	0	-9.197732	0.143872	1.171959
64	1	0	-9.210622	-1.556881	0.539828
65	1	0	-1.006180	-3.333338	1.515891
66	1	0	0.092324	-1.405957	2.292525
67	1	0	-0.970491	-0.120866	1.737005
68	1	0	2.647853	-1.179772	1.861781
69	1	0	1.912983	-0.346920	3.229597
70	1	0	4.185237	0.660278	1.424682
71	1	0	5.779560	2.210622	4.013496
72	1	0	4.856172	3.482784	3.219488
73	1	0	5.647019	2.225169	2.242045
74	1	0	2.744959	2.830916	4.620262
75	1	0	2.160852	1.169224	4.599886
76	1	0	3.687250	1.572110	5.417986
77	1	0	2.465919	2.637963	0.708099
78	1	0	-0.246417	4.047084	0.714047
79	1	0	1.192619	4.487516	1.597660
80	1	0	2.402240	4.941631	-0.629596
81	1	0	0.954287	7.399109	-2.502604

82	1	0	0.879925	5.949279	-3.502915
83	1	0	2.314693	6.254974	-2.501444
84	1	0	-1.383516	5.162052	-0.524836
85	1	0	-1.328686	5.113390	-2.295021
86	1	0	-1.283322	6.664742	-1.451015
87	1	0	-3.061659	1.740687	0.591561
88	1	0	-2.673800	3.150913	-0.451222
89	1	0	-2.934525	1.548924	-1.187383
90	1	0	3.078789	0.687181	-1.082026
91	1	0	2.922303	1.649947	-3.437541
92	1	0	1.242457	2.252000	-3.606020
93	1	0	1.546224	0.603834	-2.986065

Table S25. Standard orientation of conformation **4**E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.882713	-0.250508	-0.197373
2	6	0	5.391682	-1.150101	0.743770
3	6	0	4.248152	-1.890203	0.527616
4	6	0	3.571010	-1.678349	-0.690365
5	6	0	4.070859	-0.778397	-1.635417
6	6	0	5.251048	-0.052335	-1.409554
7	8	0	7.059739	0.303557	0.264668
8	6	0	7.115992	-0.067951	1.648636
9	8	0	6.251452	-1.194455	1.826589
10	6	0	2.244720	-2.361663	-0.917807
11	6	0	1.006216	-1.485962	-0.504006
12	6	0	-0.134430	-2.088140	-1.394407
13	6	0	0.651746	-2.801429	-2.533139
14	8	0	2.037483	-2.548047	-2.309605
15	6	0	-1.028236	-3.046294	-0.633678
16	6	0	-2.454477	-2.735244	-0.411234
17	8	0	-0.530217	-4.078253	-0.164433
18	6	0	-3.173587	-3.595906	0.459787
19	6	0	-4.482503	-3.277061	0.713395
20	6	0	-5.102266	-2.163817	0.134186
21	6	0	-4.432232	-1.322722	-0.732398
22	6	0	-3.087770	-1.623218	-0.992056
23	8	0	-5.396061	-3.946801	1.497099
24	6	0	-6.533574	-3.084213	1.584655
25	8	0	-6.403472	-2.095322	0.545094
26	8	0	2.230079	-3.574199	-0.207630
27	6	0	0.795211	-1.366692	1.009973

28	6	0	0.506060	0.116094	1.262858
29	6	0	1.115398	0.842207	0.050099
30	8	0	1.206835	-0.143125	-0.973977
31	6	0	1.054594	0.562026	2.650272
32	6	0	0.826393	2.003390	3.012706
33	6	0	-0.093352	2.496640	3.859486
34	6	0	-0.191753	3.983392	4.102721
35	6	0	-1.103975	1.671348	4.615356
36	6	0	-0.976470	0.460083	1.186823
37	6	0	-1.179626	1.787577	0.458101
38	6	0	0.063555	1.945145	-0.468331
39	8	0	-1.860670	-0.194968	1.698357
40	6	0	-2.626435	1.969301	-0.043585
41	6	0	-3.038079	3.399514	-0.237790
42	6	0	-3.443532	4.004519	-1.365775
43	6	0	-3.831245	5.463341	-1.360842
44	6	0	-3.542757	3.336598	-2.714424
45	6	0	-0.199909	1.618833	-1.948933
46	8	0	0.732886	2.158904	-2.741506
47	8	0	-1.109019	0.922513	-2.359671
48	6	0	0.695547	1.742758	-4.120311
49	8	0	0.737048	3.183011	-0.326600
50	8	0	2.356755	1.387613	0.327591
51	6	0	0.064751	4.371006	-0.731074
52	1	0	3.892482	-2.617900	1.246195
53	1	0	3.523264	-0.635411	-2.558156
54	1	0	5.646022	0.637615	-2.147964
55	1	0	8.137677	-0.348731	1.907387
56	1	0	6.751750	0.770253	2.261183
57	1	0	-0.691232	-1.250472	-1.798250
58	1	0	0.462787	-3.881072	-2.529053
59	1	0	0.400923	-2.396593	-3.516525
60	1	0	-2.683384	-4.453903	0.903652
61	1	0	-4.917599	-0.459496	-1.173875
62	1	0	-2.539907	-0.954256	-1.642586
63	1	0	-7.443953	-3.661760	1.418419
64	1	0	-6.538905	-2.576753	2.557905
65	1	0	1.314727	-3.934898	-0.184386
66	1	0	-0.005909	-1.998284	1.395515
67	1	0	1.715737	-1.653020	1.524027
68	1	0	0.609027	-0.110707	3.388974
69	1	0	2.131062	0.362814	2.629508
70	1	0	1.479264	2.708864	2.502066

71	1	0	-0.043015	4.219801	5.165660
72	1	0	-1.191091	4.359086	3.838431
73	1	0	0.549811	4.541343	3.521873
74	1	0	-2.123984	1.975810	4.342388
75	1	0	-1.005717	1.838523	5.697036
76	1	0	-1.022686	0.600127	4.423157
77	1	0	-0.996338	2.521937	1.257897
78	1	0	-3.256334	1.519908	0.735158
79	1	0	-2.778782	1.378060	-0.942391
80	1	0	-3.006251	4.006456	0.670719
81	1	0	-3.187858	6.042801	-2.039157
82	1	0	-3.757922	5.903752	-0.360979
83	1	0	-4.861618	5.599675	-1.718077
84	1	0	-2.939251	3.882543	-3.454315
85	1	0	-4.578408	3.363308	-3.081662
86	1	0	-3.204360	2.299880	-2.711373
87	1	0	0.852758	0.662860	-4.179585
88	1	0	1.511118	2.279434	-4.604031
89	1	0	-0.265249	2.002585	-4.571037
90	1	0	2.430723	2.232267	-0.151914
91	1	0	-0.730134	4.633395	-0.027077
92	1	0	-0.364846	4.271416	-1.733612
93	1	0	0.826236	5.153909	-0.736601

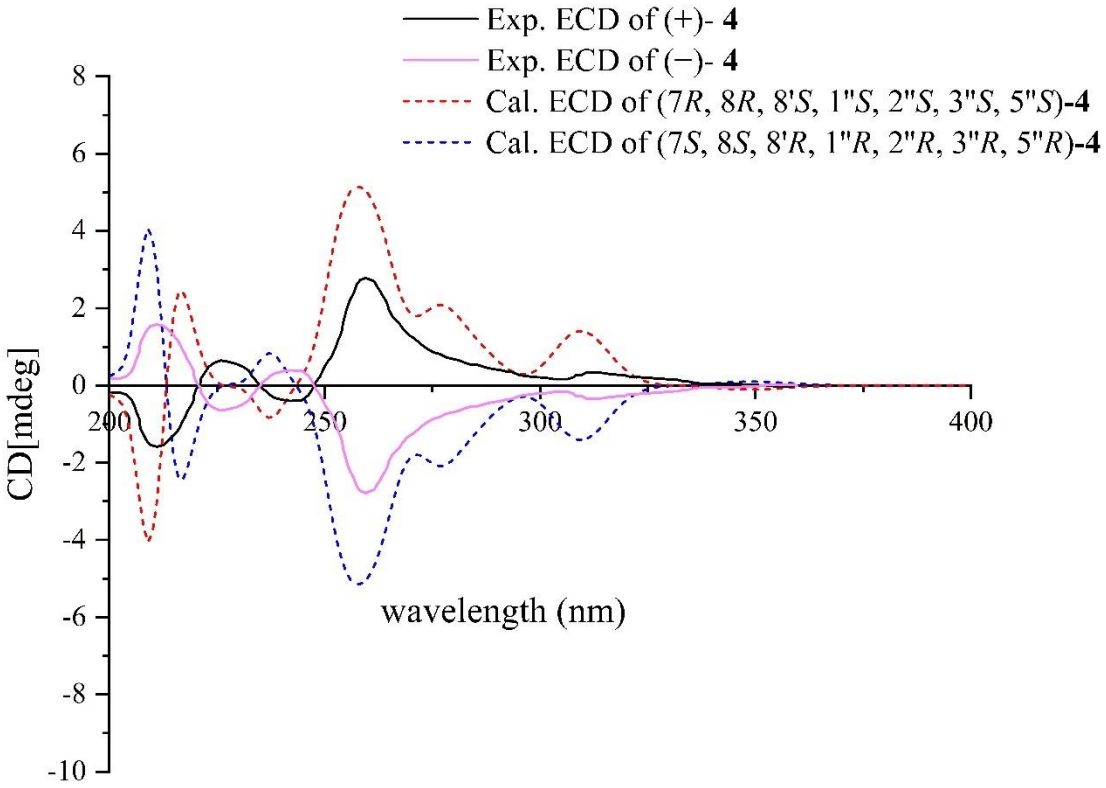


Figure S6. Computational methods for ECD of compound **4.**
b3lyp/6-31+g (d, p) scrf= (solvent= methanol)

2.5 ECD spectra calculation of **5**

Table S26. Energies of the optimized conformers of compound **5**

Boltzmann distributions of the optimized **5** at the B3LYP-D3/6-31+G(d) level in the gas phase.

conformer	Energy (Hartree)	Energy (kcal/mol)	Population (%)
1	-2296.742311	-1441227.548	14.58
2	-2296.742159	-1441227.453	12.41
3	-2296.742909	-1441227.923	27.45
4	-2296.743367	-1441228.211	44.59
5	-2296.739757	-1441225.945	0.97

Table S27. Standard orientation of conformation **5**A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.123005	-3.757900	1.588599
2	6	0	5.242099	-0.267810	1.253899
3	6	0	-3.355106	-4.204899	1.167899
4	6	0	-5.380007	-5.230196	0.934499
5	6	0	3.900599	-0.670308	1.072999
6	6	0	-1.479704	-2.819001	0.749399
7	6	0	6.131299	-0.671011	0.281699
8	6	0	0.640296	-2.846804	-1.752801
9	6	0	-3.956605	-3.740998	-0.044301
10	6	0	3.501498	-1.430207	-0.027801
11	6	0	-2.061403	-2.368900	-0.434501
12	6	0	7.964398	-1.068913	-1.016301
13	6	0	2.051297	-1.832906	-0.143101
14	6	0	5.722098	-1.448010	-0.845101
15	6	0	0.092798	-1.420503	-1.596401
16	6	0	-3.344004	-2.822099	-0.858301
17	6	0	4.417897	-1.842409	-1.028901
18	6	0	-1.409802	-1.349601	-1.304401
19	6	0	0.981699	-0.736404	-0.522401
20	6	0	1.554501	0.625795	-0.949801
21	6	0	0.333107	5.946197	2.053599
22	6	0	0.906102	1.691896	-0.032101
23	6	0	0.378501	0.844997	1.149499
24	6	0	1.902803	2.771095	0.434699
25	8	0	1.355901	0.771895	2.154699
26	6	0	0.965906	5.036996	1.043899
27	6	0	1.252005	3.761296	1.350499
28	6	0	-0.209697	2.393497	-0.849401
29	6	0	-0.984699	1.262998	1.770899

30	6	0	1.242907	5.655196	-0.288901
31	6	0	-1.629597	2.219199	-0.461901
32	6	0	-1.985398	1.697500	0.734299
33	6	0	-3.773596	3.410802	-1.029001
34	6	0	-2.625997	2.587601	-1.526401
35	6	0	-6.154895	4.046505	-0.771701
36	6	0	-5.067696	3.145204	-1.271801
37	6	0	-5.540198	1.954504	-2.044701
38	8	0	-4.188407	-5.119097	1.786499
39	8	0	7.491199	-0.417613	0.211499
40	8	0	1.962096	-2.852405	-1.152801
41	8	0	-5.194006	-4.352796	-0.222101
42	8	0	6.816298	-1.708212	-1.662701
43	8	0	1.590397	-2.422805	1.065899
44	8	0	0.169799	-0.492803	0.651999
45	8	0	-2.060101	-0.491400	-1.865301
46	8	0	0.116004	3.039297	-1.824101
47	8	0	-1.159799	1.235099	2.956899
48	8	0	-3.240698	1.466401	1.184299
49	1	0	-1.665406	-4.095701	2.514499
50	1	0	5.547300	0.324290	2.112499
51	1	0	-5.434908	-6.264596	0.570799
52	1	0	-6.238207	-4.857695	1.509499
53	1	0	3.149599	-0.364807	1.815399
54	1	0	-0.491003	-2.435802	1.063699
55	1	0	0.821596	-3.140204	-2.799701
56	1	0	0.043595	-3.617303	-1.234601
57	1	0	8.338799	-0.285514	-1.688301
58	1	0	8.672397	-1.856614	-0.726601
59	1	0	0.238499	-0.871903	-2.567701
60	1	0	-3.803303	-2.443198	-1.769801
61	1	0	4.093397	-2.443508	-1.879101
62	1	0	2.659301	0.659294	-0.859801
63	1	0	1.365301	0.845895	-2.019501
64	1	0	0.196407	5.469797	3.033199
65	1	0	0.943509	6.845296	2.213999
66	1	0	-0.658092	6.279598	1.715999
67	1	0	2.746903	2.282194	0.972399
68	1	0	2.346004	3.261494	-0.457501
69	1	0	1.042200	0.193096	2.901999
70	1	0	1.040504	3.361996	2.344299
71	1	0	2.319807	5.814094	-0.435501
72	1	0	0.896806	5.009896	-1.116701

73	1	0	0.750808	6.625596	-0.421501
74	1	0	-3.474395	4.295202	-0.465401
75	1	0	-2.113896	3.157800	-2.342301
76	1	0	-2.969298	1.639001	-2.015401
77	1	0	-5.769594	4.937405	-0.258901
78	1	0	-6.786295	4.400506	-1.598801
79	1	0	-6.812796	3.524506	-0.063501
80	1	0	-5.907897	2.254505	-3.036501
81	1	0	-4.738999	1.215403	-2.214301
82	1	0	-6.363298	1.434605	-1.538701
83	1	0	2.082696	-3.258706	1.243599
84	1	0	-3.939898	1.725202	0.501599

Table S28. Standard orientation of conformation **5**B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.382709	-3.606696	1.565499
2	6	0	5.488693	-2.244510	-1.627501
3	6	0	-3.694710	-3.887294	1.257999
4	6	0	-5.844411	-4.650090	1.203299
5	6	0	4.085293	-2.416008	-1.588801
6	6	0	-1.709308	-2.728197	0.685499
7	6	0	6.044094	-1.560711	-0.569701
8	6	0	0.153292	-2.931301	-2.003901
9	6	0	-4.345109	-3.316993	0.118599
10	6	0	3.312794	-1.919607	-0.540501
11	6	0	-2.339007	-2.174696	-0.428001
12	6	0	7.430596	-0.516014	0.910299
13	6	0	1.819093	-2.138904	-0.516001
14	6	0	5.250495	-1.049410	0.504699
15	6	0	-0.200405	-1.455300	-1.770301
16	6	0	-3.702207	-2.455294	-0.733701
17	6	0	3.887695	-1.210608	0.548299
18	6	0	-1.651205	-1.216698	-1.338601
19	6	0	0.857895	-0.913702	-0.770701
20	6	0	1.547898	0.385097	-1.221201
21	6	0	1.187407	5.738097	1.944199
22	6	0	1.104500	1.492597	-0.233201
23	6	0	0.591098	0.678698	0.977599
24	6	0	2.251902	2.443895	0.160199
25	8	0	1.639198	0.471796	1.887199
26	6	0	1.626806	4.785896	0.873099
27	6	0	1.794903	3.480596	1.139599

28	6	0	0.007601	2.333099	-0.936601
29	6	0	-0.655701	1.227901	1.727599
30	6	0	1.855607	5.397296	-0.472001
31	6	0	-1.380599	2.319402	-0.418001
32	6	0	-1.685800	1.808902	0.796899
33	6	0	-3.402996	3.779606	-0.756501
34	6	0	-2.419098	2.835804	-1.375401
35	6	0	-5.650994	4.697610	-0.261701
36	6	0	-4.737096	3.684008	-0.879701
37	6	0	-5.425498	2.585109	-1.625901
38	8	0	-4.573411	-4.711392	1.937399
39	8	0	7.377795	-1.253514	-0.358601
40	8	0	1.513692	-3.111303	-1.532301
41	8	0	-5.660110	-3.767790	0.050199
42	8	0	6.065196	-0.402412	1.426299
43	8	0	1.405092	-2.704603	0.719299
44	8	0	0.189296	-0.614301	0.478399
45	8	0	-2.242703	-0.273797	-1.823801
46	8	0	0.315102	2.954299	-1.933201
47	8	0	-0.729901	1.180501	2.923599
48	8	0	-2.913800	1.716605	1.358699
49	1	0	-1.885610	-4.025597	2.436399
50	1	0	6.086692	-2.634812	-2.446001
51	1	0	-6.062013	-5.658590	0.827899
52	1	0	-6.591410	-4.192789	1.865599
53	1	0	3.598692	-2.961207	-2.404401
54	1	0	-0.655707	-2.478199	0.910099
55	1	0	0.199891	-3.213301	-3.068301
56	1	0	-0.482109	-3.640300	-1.445101
57	1	0	8.013695	-1.115115	1.621999
58	1	0	7.796898	0.496285	0.694399
59	1	0	-0.077904	-0.898600	-2.740101
60	1	0	-4.194306	-1.995693	-1.589301
61	1	0	3.264196	-0.813806	1.357099
62	1	0	2.652798	0.290495	-1.222101
63	1	0	1.298998	0.654897	-2.267001
64	1	0	1.083407	5.259297	2.926599
65	1	0	1.905209	6.561396	2.060499
66	1	0	0.214008	6.184599	1.698099
67	1	0	3.077000	1.852594	0.619899
68	1	0	2.672702	2.900595	-0.760001
69	1	0	1.331297	-0.085503	2.653199
70	1	0	1.627203	3.086696	2.143899

71	1	0	2.926907	5.438694	-0.710901
72	1	0	1.369106	4.811697	-1.273101
73	1	0	1.465909	6.418897	-0.549801
74	1	0	-2.943995	4.602805	-0.207701
75	1	0	-1.918997	3.361103	-2.228201
76	1	0	-2.922199	1.950305	-1.843901
77	1	0	-5.110593	5.518009	0.228099
78	1	0	-6.306494	5.151711	-1.018101
79	1	0	-6.301095	4.240011	0.496499
80	1	0	-5.842698	2.958510	-2.572201
81	1	0	-4.743200	1.758208	-1.885201
82	1	0	-6.257199	2.156011	-1.053201
83	1	0	1.837691	-3.580104	0.855499
84	1	0	-3.635199	2.078606	0.750499

Table S29. Standard orientation of conformation **5**C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.097024	-3.568185	1.776600
2	6	0	5.597488	-1.994541	-1.656500
3	6	0	-3.375727	-3.993375	1.495500
4	6	0	-5.444434	-4.955760	1.506800
5	6	0	4.205686	-2.232731	-1.576600
6	6	0	-1.503818	-2.704289	0.827100
7	6	0	6.135393	-1.210245	-0.661200
8	6	0	0.322880	-2.998602	-1.890000
9	6	0	-4.070524	-3.579070	0.315700
10	6	0	3.426690	-1.702525	-0.549700
11	6	0	-2.177015	-2.303084	-0.325200
12	6	0	7.491802	0.006346	0.711400
13	6	0	1.946188	-1.994214	-0.479600
14	6	0	5.335397	-0.664239	0.390900
15	6	0	-0.119309	-1.533999	-1.761700
16	6	0	-3.506318	-2.732075	-0.604600
17	6	0	3.983696	-0.890229	0.474200
18	6	0	-1.574108	-1.359189	-1.309400
19	6	0	0.919296	-0.850607	-0.831500
20	6	0	1.539805	0.437389	-1.400800
21	6	0	0.583743	5.681696	1.837900
22	6	0	0.962214	1.605393	-0.563900
23	6	0	0.562908	0.888996	0.747000
24	6	0	1.969222	2.745986	-0.319300
25	8	0	1.665608	0.832788	1.618300

26	6	0	1.264434	4.399891	1.460400
27	6	0	1.300831	3.989391	0.182300
28	6	0	-0.244382	2.188202	-1.345900
29	6	0	-0.673587	1.445805	1.503900
30	6	0	1.859429	3.648186	2.605200
31	6	0	-1.583182	2.236512	-0.707500
32	6	0	-1.778884	1.886713	0.584300
33	6	0	-3.651972	3.624327	-1.068000
34	6	0	-2.707879	2.609520	-1.633700
35	6	0	-5.864665	4.604743	-0.535700
36	6	0	-4.990872	3.519936	-1.087600
37	6	0	-5.724781	2.343042	-1.648500
38	8	0	-4.177733	-4.838670	2.241100
39	8	0	7.455096	-0.822454	-0.500000
40	8	0	1.684780	-3.072812	-1.394500
41	8	0	-5.337528	-4.154361	0.286800
42	8	0	6.131603	0.087155	1.247600
43	8	0	1.580584	-2.461711	0.811300
44	8	0	0.239199	-0.471502	0.393500
45	8	0	-2.237202	-0.488784	-1.833500
46	8	0	-0.059179	2.568900	-2.482100
47	8	0	-0.681087	1.519505	2.701900
48	8	0	-2.959884	1.856722	1.248500
49	1	0	-1.567626	-3.868289	2.676800
50	1	0	6.200384	-2.411545	-2.458100
51	1	0	-5.564342	-6.006760	1.213300
52	1	0	-6.235031	-4.519655	2.131900
53	1	0	3.733681	-2.858527	-2.341400
54	1	0	-0.478715	-2.340697	1.025700
55	1	0	0.398278	-3.348303	-2.932700
56	1	0	-0.277425	-3.704898	-1.290200
57	1	0	8.117998	-0.509259	1.451400
58	1	0	7.800409	1.017843	0.416200
59	1	0	-0.056206	-1.044900	-2.772800
60	1	0	-4.035215	-2.389871	-1.492500
61	1	0	3.354799	-0.468224	1.263800
62	1	0	2.646405	0.431181	-1.334900
63	1	0	1.327706	0.572890	-2.480600
64	1	0	0.053247	6.148800	0.998600
65	1	0	-0.152358	5.520501	2.637800
66	1	0	1.310749	6.416690	2.210000
67	1	0	2.754019	2.396480	0.390800
68	1	0	2.496124	2.974782	-1.271100

69	1	0	1.433104	0.308790	2.432700
70	1	0	0.838935	4.588794	-0.604400
71	1	0	1.070725	3.185292	3.220800
72	1	0	2.512923	2.823082	2.274000
73	1	0	2.451033	4.296182	3.262100
74	1	0	-3.161065	4.506923	-0.656300
75	1	0	-2.290576	3.012717	-2.591700
76	1	0	-3.230486	1.665323	-1.935000
77	1	0	-5.294858	5.472038	-0.177800
78	1	0	-6.564762	4.973848	-1.298400
79	1	0	-6.467567	4.242447	0.308100
80	1	0	-6.209179	2.604045	-2.600600
81	1	0	-5.058787	1.489337	-1.856300
82	1	0	-6.512184	1.987747	-0.972000
83	1	0	2.040978	-3.311415	1.008100
84	1	0	-3.730882	2.137727	0.659800

Table S30. Standard orientation of conformation **5**D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.032295	-3.953406	-0.354104
2	6	0	5.648605	-1.216905	-1.771604
3	6	0	-3.316595	-4.481006	0.700096
4	6	0	-2.584694	-5.652705	2.514496
5	6	0	4.290805	-1.612805	-1.770304
6	6	0	-3.398095	-2.919006	-1.073604
7	6	0	6.080705	-0.533804	-0.657304
8	6	0	0.503405	-2.722605	-2.297904
9	6	0	-2.009995	-4.013005	1.037396
10	6	0	3.442405	-1.325705	-0.702604
11	6	0	-2.111695	-2.468305	-0.752404
12	6	0	7.272805	0.605296	0.919196
13	6	0	2.002805	-1.781205	-0.721104
14	6	0	5.209105	-0.237605	0.437196
15	6	0	-0.080895	-1.338405	-1.979904
16	6	0	-1.382295	-3.012105	0.334596
17	6	0	3.889605	-0.617405	0.444896
18	6	0	-1.557795	-1.355405	-1.575004
19	6	0	0.860305	-0.709905	-0.915804
20	6	0	1.338405	0.713095	-1.250804
21	6	0	0.135004	5.662895	2.336396
22	6	0	0.720505	1.655195	-0.187304
23	6	0	0.320705	0.675495	0.941096

24	6	0	1.705905	2.731095	0.310396
25	8	0	1.374405	0.555095	1.859596
26	6	0	0.725504	4.882995	1.200596
27	6	0	1.086004	3.599595	1.361296
28	6	0	-0.481195	2.377295	-0.849404
29	6	0	-1.006295	0.966595	1.698396
30	6	0	0.874604	5.635395	-0.082904
31	6	0	-1.858595	2.104195	-0.376104
32	6	0	-2.099795	1.454595	0.785496
33	6	0	-4.074595	3.263094	-0.657304
34	6	0	-2.949295	2.530394	-1.319804
35	6	0	-6.442996	3.795694	-0.159204
36	6	0	-5.377095	2.984094	-0.829704
37	6	0	-5.880395	1.865294	-1.686204
38	8	0	-3.697794	-5.487606	1.567496
39	8	0	7.346505	-0.033904	-0.400904
40	8	0	1.867405	-2.720405	-1.803704
41	8	0	-1.525195	-4.718805	2.134696
42	8	0	5.903805	0.461096	1.417596
43	8	0	1.672505	-2.482605	0.467496
44	8	0	0.128705	-0.617205	0.330296
45	8	0	-2.280295	-0.482805	-2.013904
46	8	0	-0.257995	3.123595	-1.780404
47	8	0	-1.092595	0.817895	2.884796
48	8	0	-3.307795	1.127994	1.301496
49	1	0	-5.027495	-4.302806	-0.612104
50	1	0	6.306305	-1.444804	-2.605404
51	1	0	-2.949694	-5.369006	3.510796
52	1	0	-2.196794	-6.672805	2.397696
53	1	0	3.903005	-2.166905	-2.631504
54	1	0	-3.936195	-2.452906	-1.904004
55	1	0	0.610305	-2.921405	-3.376704
56	1	0	-0.021395	-3.557905	-1.802504
57	1	0	7.940005	0.055096	1.595696
58	1	0	7.473605	1.676296	0.784496
59	1	0	-0.027495	-0.704005	-2.907204
60	1	0	-0.380095	-2.643905	0.609996
61	1	0	3.206005	-0.388105	1.269796
62	1	0	2.444305	0.793795	-1.240104
63	1	0	1.055105	1.022795	-2.276504
64	1	0	0.092604	5.090595	3.272396
65	1	0	0.719704	6.570495	2.539096
66	1	0	-0.891396	5.979295	2.104696

67	1	0	2.606105	2.233495	0.739296
68	1	0	2.062504	3.322795	-0.558504
69	1	0	1.160005	-0.136105	2.544696
70	1	0	0.968205	3.099595	2.324896
71	1	0	1.929804	5.858395	-0.290504
72	1	0	0.493004	5.053895	-0.941704
73	1	0	0.334504	6.589095	-0.085204
74	1	0	-3.753596	4.094594	-0.028704
75	1	0	-2.522495	3.191295	-2.116304
76	1	0	-3.303595	1.618994	-1.867204
77	1	0	-6.039496	4.639294	0.415796
78	1	0	-7.142296	4.215294	-0.896004
79	1	0	-7.033995	3.183694	0.535696
80	1	0	-6.326895	2.255094	-2.612404
81	1	0	-5.078295	1.171494	-1.988804
82	1	0	-6.652695	1.273694	-1.179004
83	1	0	2.216505	-3.301505	0.546296
84	1	0	-4.066395	1.428294	0.705696

Table S31. Standard orientation of conformation **5**E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.558551	5.822603	-1.073205
2	6	0	-3.423426	-3.454973	1.457895
3	6	0	-1.358251	5.779610	0.049095
4	6	0	-2.636948	6.253720	1.876995
5	6	0	-2.918216	-2.176877	1.132695
6	6	0	-0.167661	4.573500	-1.601105
7	6	0	-4.222331	-4.049967	0.505995
8	6	0	-2.496888	1.313219	-2.184205
9	6	0	-1.771561	4.545613	0.638295
10	6	0	-3.211111	-1.556475	-0.083105
11	6	0	-0.584871	3.364804	-1.033005
12	6	0	-5.570042	-5.439556	-0.700605
13	6	0	-2.644300	-0.182780	-0.350605
14	6	0	-4.520926	-3.414965	-0.738205
15	6	0	-1.043891	0.923807	-1.879205
16	6	0	-1.402971	3.325410	0.123995
17	6	0	-4.031816	-2.171668	-1.062505
18	6	0	-0.091981	2.104800	-1.660605
19	6	0	-1.105099	-0.040992	-0.664105
20	6	0	-0.342609	-1.361698	-0.859905
21	6	0	4.480078	-2.887837	2.754595

22	6	0	0.857991	-1.331308	0.118295
23	6	0	0.427500	-0.253905	1.141295
24	6	0	1.118680	-2.692110	0.794695
25	8	0	-0.279405	-0.858699	2.194795
26	6	0	3.474377	-3.016829	1.649795
27	6	0	2.209481	-2.600219	1.816695
28	6	0	2.122794	-0.962318	-0.699505
29	6	0	1.529107	0.673186	1.730495
30	6	0	4.006472	-3.617634	0.388895
31	6	0	2.904504	0.241575	-0.340305
32	6	0	2.626810	0.986478	0.752895
33	6	0	5.350303	0.149355	-0.747105
34	6	0	4.024307	0.606466	-1.279105
35	6	0	7.379991	-1.264061	-0.647105
36	6	0	6.052995	-0.886050	-1.235005
37	6	0	5.600488	-1.727547	-2.384605
38	8	0	-1.874143	6.843114	0.766895
39	8	0	-4.841441	-5.287862	0.564795
40	8	0	-3.341095	0.361626	-1.483905
41	8	0	-2.567659	4.798020	1.751595
42	8	0	-5.340233	-4.237058	-1.504105
43	8	0	-2.898293	0.690622	0.740895
44	8	0	-0.487493	0.629503	0.463495
45	8	0	1.044618	2.010390	-2.074305
46	8	0	2.419888	-1.673021	-1.638405
47	8	0	1.474610	1.052187	2.867095
48	8	0	3.285419	2.113672	1.129095
49	1	0	-0.237243	6.758201	-1.521505
50	1	0	-3.192130	-3.933475	2.405595
51	1	0	-2.139145	6.540016	2.813095
52	1	0	-3.685645	6.555429	1.757795
53	1	0	-2.267012	-1.663683	1.853995
54	1	0	0.487739	4.557295	-2.476305
55	1	0	-2.776489	1.187721	-3.243005
56	1	0	-2.779179	2.319421	-1.828605
57	1	0	-5.135949	-6.293460	-1.237005
58	1	0	-6.641543	-5.491247	-0.466605
59	1	0	-0.629895	0.357004	-2.757505
60	1	0	-1.710079	2.373813	0.588295
61	1	0	-4.259912	-1.670567	-2.004005
62	1	0	-0.982016	-2.245193	-0.659505
63	1	0	-0.005110	-1.504501	-1.906405
64	1	0	4.039081	-2.530534	3.694295

65	1	0	4.963871	-3.849441	2.969895
66	1	0	5.272384	-2.177144	2.479995
67	1	0	0.184277	-3.037603	1.291795
68	1	0	1.352774	-3.446612	0.012395
69	1	0	-0.647500	-0.161296	2.805295
70	1	0	1.881484	-2.165616	2.763295
71	1	0	4.304264	-4.662736	0.538295
72	1	0	3.276973	-3.596628	-0.436805
73	1	0	4.889677	-3.067741	0.029795
74	1	0	5.718508	0.720753	0.102295
75	1	0	3.817303	0.171968	-2.286005
76	1	0	4.035316	1.705266	-1.454105
77	1	0	7.716897	-0.569964	0.132795
78	1	0	7.340583	-2.264561	-0.195005
79	1	0	8.161391	-1.286667	-1.419305
80	1	0	6.097380	-2.702851	-2.423605
81	1	0	4.510786	-1.921238	-2.340405
82	1	0	5.794092	-1.224348	-3.341805
83	1	0	-3.867091	0.856230	0.827295
84	1	0	3.978421	2.377767	0.450795

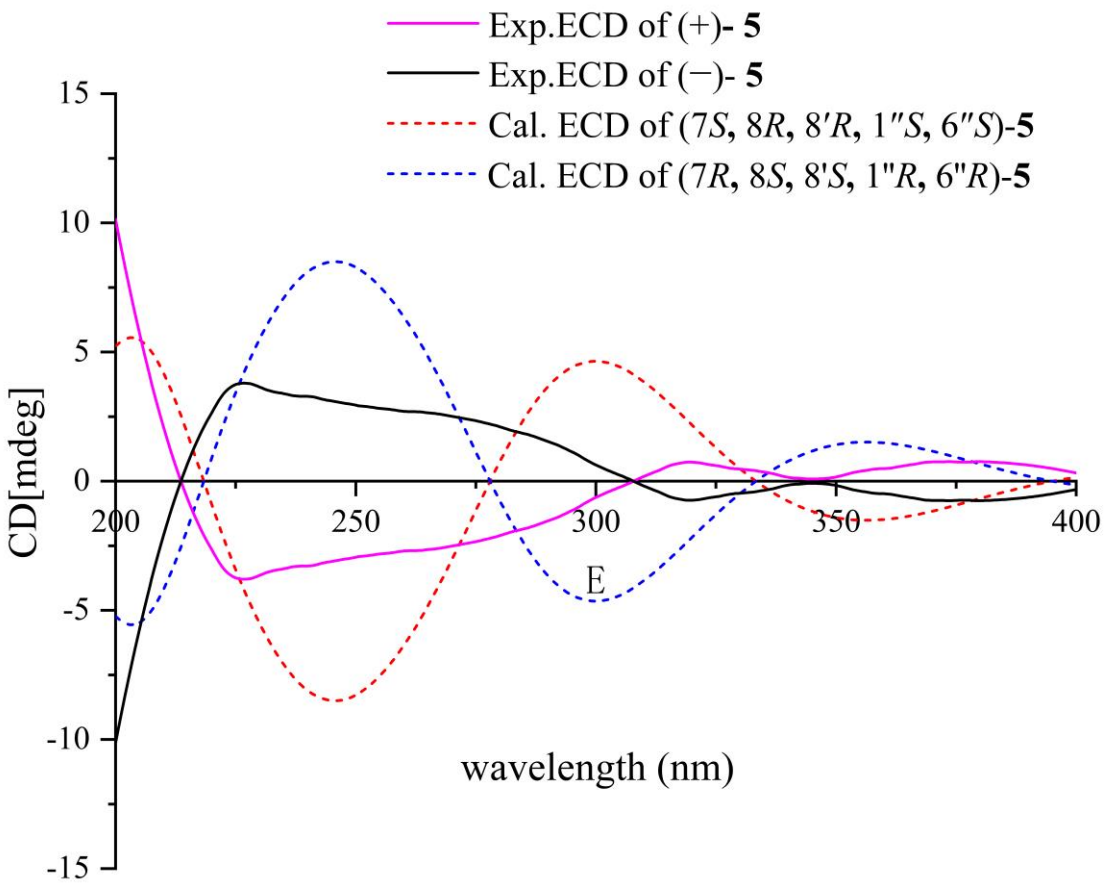


Figure S7. Computational methods for ECD of compound **5.**
b3lyp/6-31+g(d, p) scrf=(solvent= methanol)

2.6 ECD spectra calculation of **6**

Table S32. Energies of the optimized conformers of compound **6**

Boltzmann distributions of the optimized **6** at the B3LYP-D3/6-31+G(d) level in the gas phase

conformer	Energy (Hartree)	Energy (kcal/mol)	Population (%)
1	-2336.059338	-1465899.355	19.31
2	-2336.060059	-1465899.807	41.45
3	-2336.059357	-1465899.367	19.71
4	-2336.059348	-1465899.361	19.52
5	-2335.924454	-1465814.714	0.01

Table S33. Standard orientation of conformation **6**A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.761074	1.702256	0.418779
2	6	0	-3.417570	-2.786084	1.236396
3	6	0	5.797037	1.541384	-0.480963
4	6	0	7.429503	1.832305	-1.982016
5	6	0	-2.018890	-2.857617	1.334736
6	6	0	4.011704	0.557252	0.735548
7	6	0	-3.948448	-2.688057	-0.035989
8	6	0	1.912068	-3.165893	2.026903
9	6	0	6.094198	0.298223	-1.047848
10	6	0	-1.197595	-2.821099	0.201692
11	6	0	4.300719	-0.694420	0.168068
12	6	0	-5.264749	-2.728741	-1.836989
13	6	0	0.313528	-2.814803	0.354238
14	6	0	-3.136652	-2.665791	-1.165678
15	6	0	2.275904	-1.821555	1.371217
16	6	0	5.376017	-0.832619	-0.745832
17	6	0	-1.760336	-2.721602	-1.085540
18	6	0	3.519171	-1.929247	0.478076
19	6	0	0.945184	-1.420231	0.651346
20	6	0	1.000372	-0.437971	-0.530269
21	6	0	-1.389495	5.215345	0.763871
22	6	0	0.039246	0.711474	-0.155373
23	6	0	-0.024965	0.588135	1.375942
24	6	0	0.545015	2.103061	-0.635667
25	8	0	1.008994	1.320113	1.983904
26	6	0	-0.271657	4.221823	0.555796
27	6	0	-0.420466	3.211639	-0.317085
28	6	0	-1.325350	0.497096	-0.837644
29	6	0	-1.352063	0.971829	2.014525

30	6	0	0.958592	4.478020	1.386898
31	6	0	-2.597454	0.660556	-0.108924
32	6	0	-2.588442	0.866026	1.232759
33	6	0	-3.932706	2.034022	-1.670505
34	6	0	-3.862154	0.713646	-0.926837
35	6	0	-4.532523	4.388618	-2.152630
36	6	0	-4.585159	3.146281	-1.296464
37	6	0	-5.402577	3.284807	-0.037897
38	8	0	6.683640	2.479622	-0.934012
39	8	0	-5.267829	-2.554703	-0.412213
40	8	0	0.655384	-3.595203	1.472702
41	8	0	7.191930	0.425374	-1.870104
42	8	0	-3.922343	-2.517570	-2.291954
43	8	0	0.969737	-3.238021	-0.827438
44	8	0	0.104973	-0.792134	1.647573
45	8	0	3.891134	-3.014734	0.051776
46	8	0	-1.339622	0.286473	-2.045346
47	8	0	-1.398838	1.323666	3.191825
48	8	0	-3.719127	1.058592	1.942671
49	6	0	0.976680	-4.645810	-1.053748
50	1	0	4.535441	2.668035	0.857940
51	1	0	-4.052716	-2.799979	2.115655
52	1	0	7.065122	2.191921	-2.953108
53	1	0	8.492550	2.035119	-1.844167
54	1	0	-1.555499	-2.940026	2.309720
55	1	0	3.176021	0.677166	1.413591
56	1	0	1.763774	-3.064506	3.105528
57	1	0	2.672377	-3.923088	1.822977
58	1	0	-5.573041	-3.756284	-2.076264
59	1	0	-5.922720	-1.987871	-2.293139
60	1	0	2.457796	-1.064991	2.133966
61	1	0	5.601804	-1.801980	-1.174102
62	1	0	-1.138034	-2.673238	-1.970068
63	1	0	2.003986	-0.042924	-0.676715
64	1	0	0.700620	-0.915346	-1.461936
65	1	0	-2.265150	4.973692	0.153346
66	1	0	-1.700701	5.234619	1.818004
67	1	0	-1.064998	6.235340	0.514255
68	1	0	1.529967	2.274645	-0.200185
69	1	0	0.670391	2.022760	-1.722553
70	1	0	0.753090	1.432140	2.919081
71	1	0	-1.367336	3.162983	-0.854911
72	1	0	0.710137	4.445100	2.456912

73	1	0	1.754704	3.754076	1.209567
74	1	0	1.349126	5.485490	1.186128
75	1	0	-3.349635	2.060132	-2.589192
76	1	0	-3.832604	-0.094221	-1.662354
77	1	0	-4.726512	0.558646	-0.279307
78	1	0	-4.117372	5.236048	-1.588286
79	1	0	-3.919711	4.242231	-3.047661
80	1	0	-5.540451	4.689800	-2.470808
81	1	0	-6.432101	3.584304	-0.279348
82	1	0	-5.435993	2.373032	0.560051
83	1	0	-4.987721	4.080681	0.597151
84	1	0	-3.443864	1.238681	2.865560
85	1	0	-0.040630	-5.056610	-1.036249
86	1	0	1.414318	-4.783246	-2.044458
87	1	0	1.590738	-5.157648	-0.307045

Table S34. Standard orientation of conformation **6**B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.850401	1.720324	-0.771423
2	6	0	3.227710	-3.093355	-0.978952
3	6	0	-5.817923	1.790666	0.212296
4	6	0	-7.328782	2.451776	1.722949
5	6	0	1.823953	-3.126658	-1.013672
6	6	0	-4.136812	0.514883	-0.874349
7	6	0	3.813234	-2.709320	0.212497
8	6	0	-2.160746	-3.449129	-1.438928
9	6	0	-6.083037	0.713492	1.063703
10	6	0	1.052720	-2.779479	0.100976
11	6	0	-4.394885	-0.571050	-0.022371
12	6	0	5.204219	-2.328394	1.918872
13	6	0	-0.462619	-2.768798	0.013799
14	6	0	3.050264	-2.367390	1.324463
15	6	0	-2.472284	-1.984527	-1.078913
16	6	0	-5.400294	-0.474428	0.972916
17	6	0	1.671223	-2.383674	1.303482
18	6	0	-3.654246	-1.864898	-0.106773
19	6	0	-1.092006	-1.463174	-0.557657
20	6	0	-1.045012	-0.240556	0.370623
21	6	0	1.949235	5.050433	-1.066612
22	6	0	-0.115193	0.780953	-0.325761
23	6	0	-0.151622	0.301157	-1.788629
24	6	0	-0.617370	2.238533	-0.137955

25	8	0	-1.208080	0.912071	-2.487910
26	6	0	1.092511	4.131550	-0.231585
27	6	0	0.259386	3.254365	-0.814901
28	6	0	1.295479	0.721312	0.297639
29	6	0	1.136753	0.474373	-2.583144
30	6	0	1.276267	4.289002	1.255252
31	6	0	2.514916	0.600824	-0.524548
32	6	0	2.418440	0.498742	-1.874225
33	6	0	4.399844	2.083483	0.169326
34	6	0	3.853584	0.673798	0.161112
35	6	0	5.276280	4.213032	1.085505
36	6	0	4.675085	2.837262	1.245354
37	6	0	4.448809	2.412690	2.674892
38	8	0	-6.659941	2.828625	0.505057
39	8	0	5.150549	-2.543907	0.500512
40	8	0	-0.874010	-3.772181	-0.879798
41	8	0	-7.114323	1.049443	1.912830
42	8	0	3.884702	-1.972233	2.350942
43	8	0	-1.065436	-2.896197	1.290243
44	8	0	-0.318927	-1.101664	-1.725435
45	8	0	-4.013586	-2.823670	0.564003
46	8	0	1.390863	0.845486	1.513128
47	8	0	1.108815	0.535331	-3.810551
48	8	0	3.510193	0.460568	-2.665774
49	6	0	-1.068227	-4.212291	1.839075
50	1	0	-4.648071	2.557395	-1.430634
51	1	0	3.826022	-3.350595	-1.846427
52	1	0	-6.886937	3.008983	2.559318
53	1	0	-8.397268	2.647130	1.621239
54	1	0	1.318461	-3.428143	-1.922492
55	1	0	-3.354358	0.458669	-1.621032
56	1	0	-2.081003	-3.593744	-2.519720
57	1	0	-2.911818	-4.124781	-1.024070
58	1	0	5.510722	-3.259877	2.414600
59	1	0	5.889400	-1.506872	2.133449
60	1	0	-2.703724	-1.414154	-1.978143
61	1	0	-5.602878	-1.318095	1.621905
62	1	0	1.087234	-2.095712	2.168350
63	1	0	-2.031853	0.198925	0.506612
64	1	0	-0.671861	-0.503661	1.359165
65	1	0	1.780244	4.906345	-2.138819
66	1	0	1.750977	6.104162	-0.825490
67	1	0	3.012838	4.873620	-0.859098

68	1	0	-1.633929	2.288710	-0.538971
69	1	0	-0.679966	2.411917	0.938561
70	1	0	-1.028176	0.768173	-3.436549
71	1	0	0.218356	3.242145	-1.904654
72	1	0	1.069271	5.325206	1.557298
73	1	0	0.644938	3.623772	1.846107
74	1	0	2.316485	4.075918	1.525021
75	1	0	4.599179	2.498992	-0.818326
76	1	0	3.741923	0.291088	1.174072
77	1	0	4.554361	0.023095	-0.374136
78	1	0	6.238563	4.281583	1.612049
79	1	0	5.445398	4.467501	0.034094
80	1	0	4.624913	4.982217	1.524296
81	1	0	3.900860	3.192672	3.220651
82	1	0	3.878339	1.487063	2.766711
83	1	0	5.409342	2.286128	3.195013
84	1	0	3.190481	0.422485	-3.590664
85	1	0	-0.052529	-4.624610	1.888697
86	1	0	-1.475883	-4.110604	2.846694
87	1	0	-1.705324	-4.879580	1.251341

Table S35. Standard orientation of conformation **6**C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.805252	1.440782	-0.490812
2	6	0	3.574578	-2.622564	-1.327774
3	6	0	-5.813143	1.316906	0.445861
4	6	0	-7.640455	1.569256	1.710092
5	6	0	2.180101	-2.786491	-1.351765
6	6	0	-4.007818	0.307158	-0.718506
7	6	0	4.155570	-2.404316	-0.092947
8	6	0	-1.790701	-3.431655	-1.738656
9	6	0	-6.029366	0.123613	1.142129
10	6	0	1.412175	-2.724292	-0.183134
11	6	0	-4.217722	-0.895006	-0.024257
12	6	0	5.554324	-2.213643	1.638235
13	6	0	-0.100614	-2.829506	-0.253741
14	6	0	3.397439	-2.352131	1.072297
15	6	0	-2.188526	-2.042574	-1.201987
16	6	0	-5.257190	-0.992940	0.935434
17	6	0	2.026135	-2.503470	1.064906
18	6	0	-3.383212	-2.114836	-0.240377
19	6	0	-0.848644	-1.502942	-0.596722

20	6	0	-0.904262	-0.448702	0.520819
21	6	0	1.147470	5.248619	-1.137507
22	6	0	-0.018426	0.718057	0.031681
23	6	0	-0.030044	0.509156	-1.492348
24	6	0	-0.568933	2.107759	0.467043
25	8	0	-1.124284	1.164195	-2.083306
26	6	0	0.094568	4.205684	-0.848938
27	6	0	0.326953	3.245534	0.061363
28	6	0	1.387824	0.607779	0.651541
29	6	0	1.242356	0.911458	-2.224502
30	6	0	-1.175309	4.358272	-1.645127
31	6	0	2.609220	0.789896	-0.154997
32	6	0	2.517697	0.919335	-1.503258
33	6	0	4.193646	2.454513	0.708210
34	6	0	3.922242	0.970676	0.563122
35	6	0	4.299619	4.697025	1.753307
36	6	0	4.018478	3.214465	1.801851
37	6	0	3.537417	2.709395	3.137554
38	8	0	-6.702020	2.266692	0.869911
39	8	0	5.479053	-2.161622	0.205335
40	8	0	-0.443903	-3.694817	-1.307375
41	8	0	-7.063080	0.300810	2.035470
42	8	0	4.220981	-2.075463	2.144936
43	8	0	-0.667713	-3.227582	0.981355
44	8	0	-0.115474	-0.889102	-1.682096
45	8	0	-3.674103	-3.164006	0.319222
46	8	0	1.467778	0.462892	1.866186
47	8	0	1.211492	1.192523	-3.421287
48	8	0	3.604080	1.141924	-2.270767
49	6	0	-0.532602	-4.610938	1.299769
50	1	0	-4.635316	2.370464	-1.023075
51	1	0	4.168752	-2.657555	-2.234663
52	1	0	-7.799591	2.143285	2.624014
53	1	0	-8.573782	1.417360	1.152336
54	1	0	1.678043	-2.962789	-2.294592
55	1	0	-3.199382	0.398722	-1.432477
56	1	0	-1.782554	-3.464413	-2.831060
57	1	0	-2.456044	-4.204149	-1.345885
58	1	0	5.961333	-3.187746	1.943396
59	1	0	6.166184	-1.384928	1.997839
60	1	0	-2.444504	-1.377352	-2.026254
61	1	0	-5.412060	-1.920314	1.474027
62	1	0	1.442882	-2.434449	1.974209

63	1	0	-1.919448	-0.090083	0.683569
64	1	0	-0.544638	-0.848305	1.467919
65	1	0	2.053489	5.085855	-0.545428
66	1	0	1.425637	5.236981	-2.200952
67	1	0	0.771655	6.259103	-0.923567
68	1	0	-1.578316	2.212168	0.067617
69	1	0	-0.645941	2.072583	1.560798
70	1	0	-0.918898	1.236093	-3.034855
71	1	0	1.292410	3.270255	0.566817
72	1	0	-0.960481	4.297651	-2.721186
73	1	0	-1.921578	3.597773	-1.412711
74	1	0	-1.617039	5.349140	-1.469070
75	1	0	4.521515	2.942129	-0.209353
76	1	0	3.866669	0.471568	1.530079
77	1	0	4.722759	0.506048	-0.021198
78	1	0	5.059495	4.977630	2.495956
79	1	0	4.651763	5.016160	0.766893
80	1	0	3.395771	5.272981	1.998469
81	1	0	2.618606	3.236708	3.430398
82	1	0	3.313913	1.642365	3.142679
83	1	0	4.281984	2.922306	3.917669
84	1	0	3.283923	1.244810	-3.190792
85	1	0	0.520017	-4.920364	1.290200
86	1	0	-0.943280	-4.723888	2.304892
87	1	0	-1.099969	-5.231366	0.599553

Table S36. Standard orientation of conformation **6**D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.815091	1.416308	-0.527416
2	6	0	3.582216	-2.612726	-1.322718
3	6	0	-5.820121	1.300581	0.413315
4	6	0	-7.431585	1.667862	1.920275
5	6	0	2.188497	-2.783307	-1.344991
6	6	0	-4.012970	0.283290	-0.741489
7	6	0	4.163179	-2.387390	-0.089150
8	6	0	-1.781164	-3.456531	-1.719770
9	6	0	-6.036188	0.112445	1.118445
10	6	0	1.421216	-2.720375	-0.175955
11	6	0	-4.220965	-0.912771	-0.036312
12	6	0	5.562491	-2.184706	1.640224
13	6	0	-0.091054	-2.833849	-0.244759
14	6	0	3.405765	-2.334808	1.076535

15	6	0	-2.183836	-2.063405	-1.196942
16	6	0	-5.265241	-1.006181	0.918579
17	6	0	2.035140	-2.492151	1.070766
18	6	0	-3.378688	-2.130158	-0.235154
19	6	0	-0.846896	-1.513194	-0.594448
20	6	0	-0.909294	-0.453913	0.518034
21	6	0	1.121683	5.245837	-1.158869
22	6	0	-0.026825	0.714034	0.025671
23	6	0	-0.034979	0.498951	-1.497606
24	6	0	-0.583541	2.103356	0.454379
25	8	0	-1.129339	1.149474	-2.093246
26	6	0	0.072874	4.199363	-0.868186
27	6	0	0.308188	3.243345	0.045707
28	6	0	1.378515	0.611789	0.648894
29	6	0	1.237940	0.901422	-2.228884
30	6	0	-1.196654	4.343921	-1.666406
31	6	0	2.600803	0.795301	-0.155807
32	6	0	2.511733	0.917724	-1.504900
33	6	0	4.171436	2.471314	0.709442
34	6	0	3.911276	0.985520	0.564484
35	6	0	4.263148	4.714185	1.755102
36	6	0	3.994045	3.229396	1.804010
37	6	0	3.522154	2.719966	3.141335
38	8	0	-6.746307	2.235165	0.788075
39	8	0	5.485756	-2.137621	0.207262
40	8	0	-0.430323	-3.706473	-1.293610
41	8	0	-7.120433	0.271302	1.953227
42	8	0	4.228914	-2.051038	2.147633
43	8	0	-0.654999	-3.228754	0.992768
44	8	0	-0.117018	-0.900181	-1.682420
45	8	0	-3.662836	-3.173353	0.338863
46	8	0	1.456400	0.472497	1.864362
47	8	0	1.208878	1.176418	-3.427107
48	8	0	3.598833	1.141130	-2.271087
49	6	0	-0.512094	-4.609708	1.318140
50	1	0	-4.651035	2.339210	-1.073141
51	1	0	4.175824	-2.648165	-2.229955
52	1	0	-7.065175	2.149145	2.836386
53	1	0	-8.506978	1.799393	1.792023
54	1	0	1.686563	-2.965536	-2.286758
55	1	0	-3.199251	0.372475	-1.449712
56	1	0	-1.779302	-3.502640	-2.811674
57	1	0	-2.439950	-4.227884	-1.313801

58	1	0	5.974212	-3.155930	1.948197
59	1	0	6.170820	-1.352028	1.996655
60	1	0	-2.440805	-1.406938	-2.027873
61	1	0	-5.428048	-1.933536	1.454839
62	1	0	1.452244	-2.422445	1.980237
63	1	0	-1.926350	-0.098314	0.676312
64	1	0	-0.550589	-0.847621	1.467986
65	1	0	2.027407	5.089250	-0.564670
66	1	0	1.401664	5.231532	-2.221795
67	1	0	0.741081	6.255437	-0.949266
68	1	0	-1.592765	2.201911	0.053000
69	1	0	-0.661940	2.072166	1.548187
70	1	0	-0.922990	1.216589	-3.044940
71	1	0	1.272930	3.273801	0.552218
72	1	0	-0.980087	4.282126	-2.742031
73	1	0	-1.939405	3.580171	-1.433416
74	1	0	-1.643576	5.332968	-1.493139
75	1	0	4.492474	2.961947	-0.208961
76	1	0	3.857729	0.486546	1.531601
77	1	0	4.716021	0.526339	-0.018347
78	1	0	5.021733	5.000988	2.496693
79	1	0	4.611326	5.036188	0.768213
80	1	0	3.354937	5.282721	2.001493
81	1	0	2.601682	3.241516	3.439156
82	1	0	3.305027	1.651627	3.146227
83	1	0	4.269224	2.936336	3.918115
84	1	0	3.280324	1.237875	-3.192365
85	1	0	0.542104	-4.913670	1.308822
86	1	0	-0.920954	-4.719637	2.324338
87	1	0	-1.077021	-5.236854	0.621935

Table S37. Standard orientation of conformation **6**E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.029896	-2.822611	-0.487882
2	6	0	-2.748695	3.464602	-0.294114
3	6	0	5.988898	-1.966414	-0.979583
4	6	0	7.760401	-0.998520	-2.042983
5	6	0	-1.875497	2.861903	0.637990
6	6	0	4.076595	-2.250007	0.386615
7	6	0	-2.154192	4.240798	-1.264915
8	6	0	2.689200	2.121400	1.991999
9	6	0	6.017800	-0.578213	-0.632687

10	6	0	-0.492397	3.041201	0.572091
11	6	0	4.100297	-0.895206	0.715011
12	6	0	-1.691687	5.603992	-3.034518
13	6	0	0.380901	2.332103	1.576395
14	6	0	-0.740991	4.429995	-1.325813
15	6	0	2.320399	0.868298	1.181003
16	6	0	5.088099	-0.012309	0.206010
17	6	0	0.117006	3.844997	-0.423710
18	6	0	3.051996	-0.375102	1.651808
19	6	0	0.766999	0.836001	1.229700
20	6	0	0.046796	-0.220895	2.070002
21	6	0	-2.514507	-4.965401	-1.127288
22	6	0	-0.859004	-1.024797	1.107803
23	6	0	-0.227501	-0.704002	-0.270497
24	6	0	-0.869107	-2.531796	1.428008
25	8	0	0.821798	-1.612205	-0.533992
26	6	0	-1.470607	-4.241100	-0.331488
27	6	0	-1.817307	-3.302897	0.564109
28	6	0	-2.310003	-0.493194	1.221299
29	6	0	-1.148799	-0.630004	-1.506199
30	6	0	-0.058007	-4.645203	-0.611185
31	6	0	-3.162701	-0.478797	-0.005202
32	6	0	-2.615799	-0.528901	-1.236901
33	6	0	-5.165505	-1.713191	0.747698
34	6	0	-4.646802	-0.405994	0.222195
35	6	0	-6.090108	-4.003790	0.601904
36	6	0	-5.606005	-2.726493	-0.015199
37	6	0	-5.654202	-2.669997	-1.509100
38	8	0	7.032799	-2.257919	-1.839680
39	8	0	-2.769589	4.939896	-2.293818
40	8	0	1.620602	3.059801	1.704895
41	8	0	7.086302	0.044183	-1.264487
42	8	0	-0.420088	5.259192	-2.395615
43	8	0	-0.199502	2.260907	2.876094
44	8	0	0.360301	0.600297	-0.157100
45	8	0	2.814194	-0.926798	2.702109
46	8	0	-2.734004	-0.112090	2.286797
47	8	0	-0.730797	-0.687609	-2.622698
48	8	0	-3.421398	-0.506803	-2.342903
49	6	0	-0.391901	3.527410	3.548990
50	1	0	5.004694	-3.878112	-0.745279
51	1	0	-3.823895	3.320504	-0.242515
52	1	0	8.771900	-1.125721	-1.634681

53	1	0	7.680503	-0.732723	-3.105484
54	1	0	-2.299899	2.244306	1.437891
55	1	0	3.302294	-2.894604	0.813416
56	1	0	3.602201	2.635898	1.659799
57	1	0	2.705297	1.936203	3.081300
58	1	0	-1.681086	5.192989	-4.052417
59	1	0	-1.835885	6.687892	-2.937622
60	1	0	2.568201	1.053995	0.095702
61	1	0	5.114000	1.041092	0.470107
62	1	0	1.196907	3.983695	-0.452709
63	1	0	0.755094	-0.879495	2.616205
64	1	0	-0.555305	0.241908	2.893500
65	1	0	-3.535806	-4.635099	-0.890290
66	1	0	-2.369105	-4.809405	-2.204888
67	1	0	-2.469209	-6.047401	-0.944684
68	1	0	0.170893	-2.916998	1.341211
69	1	0	-1.151909	-2.673592	2.495108
70	1	0	1.345900	-1.307408	-1.321292
71	1	0	-2.871807	-3.065395	0.730106
72	1	0	0.048394	-5.205306	-1.546983
73	1	0	0.600395	-3.761605	-0.685386
74	1	0	0.335991	-5.278602	0.195118
75	1	0	-5.152906	-1.787688	1.835098
76	1	0	-4.861101	0.402909	0.958892
77	1	0	-5.168100	-0.111696	-0.715507
78	1	0	-5.394909	-4.828692	0.392607
79	1	0	-6.191010	-3.937487	1.693303
80	1	0	-7.072908	-4.293090	0.206103
81	1	0	-6.388401	-1.925297	-1.849803
82	1	0	-4.682501	-2.359700	-1.929699
83	1	0	-5.924503	-3.626098	-1.968997
84	1	0	-2.865396	-0.469207	-3.183102
85	1	0	-0.984699	4.208309	2.931987
86	1	0	-0.936303	3.227313	4.451790
87	1	0	0.585300	3.959409	3.787090

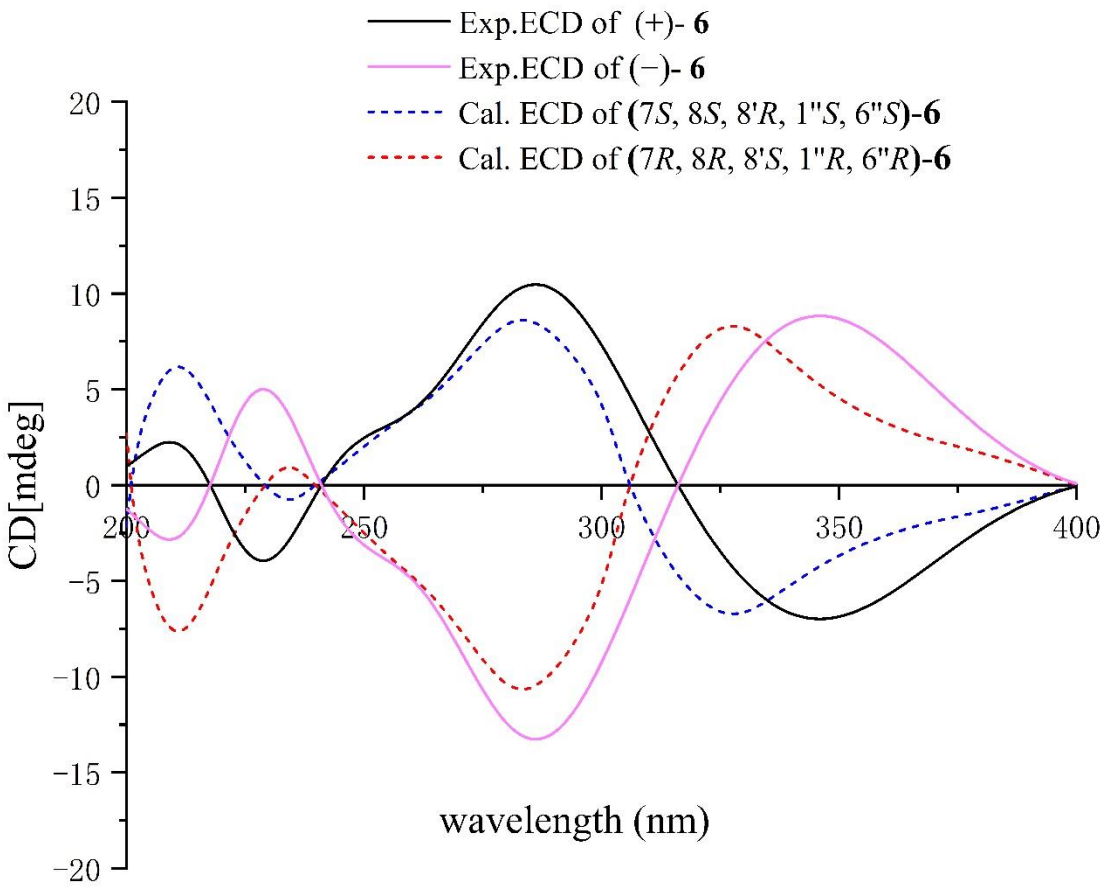
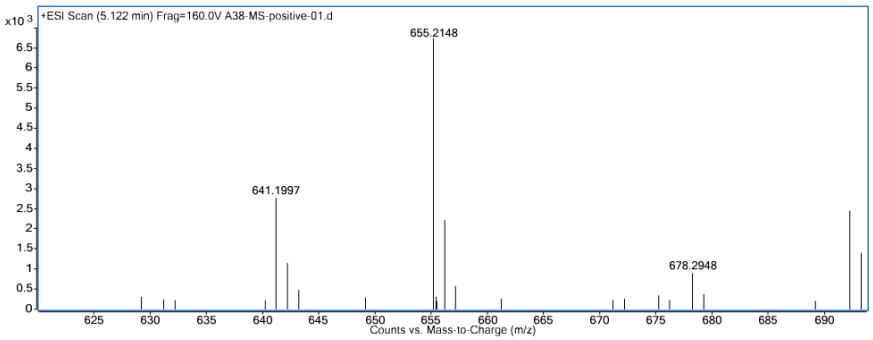


Figure S8. Computational methods for ECD of compound **6.**

b3lyp/6-31+g(d, p) scrf=(solvent= methanol)

3 Select Spectra for Compounds 1–6



Elemental Composition Calculator

Target m/z:	655.2148	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C35H36NaO11		655.2150		0.21	

Figure S9. HRESIMS spectrum of **1.**

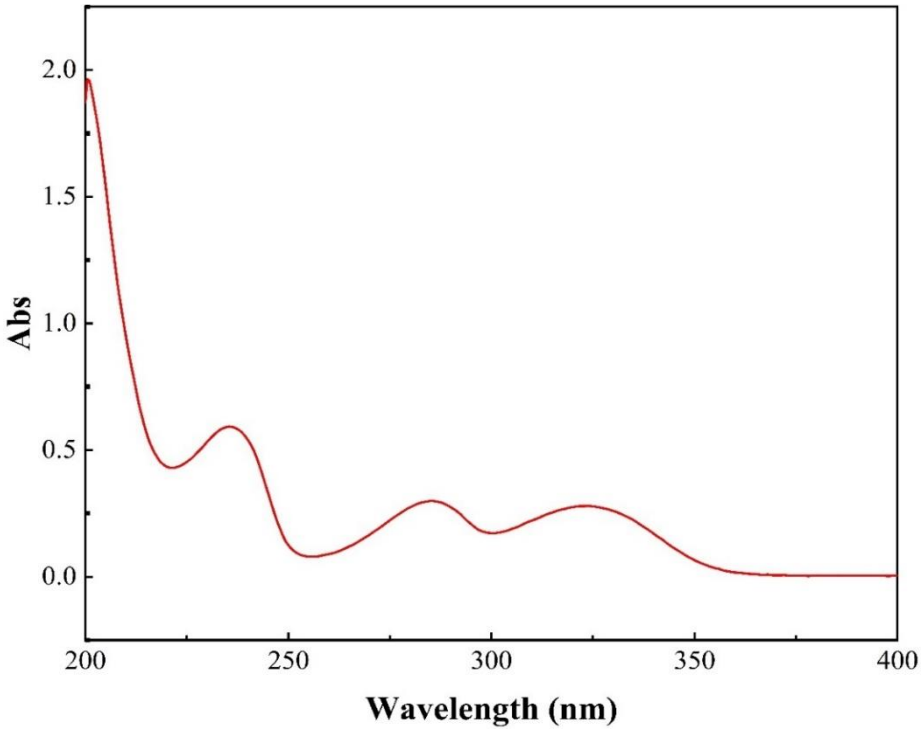


Figure S10. UV spectrum of **1.**

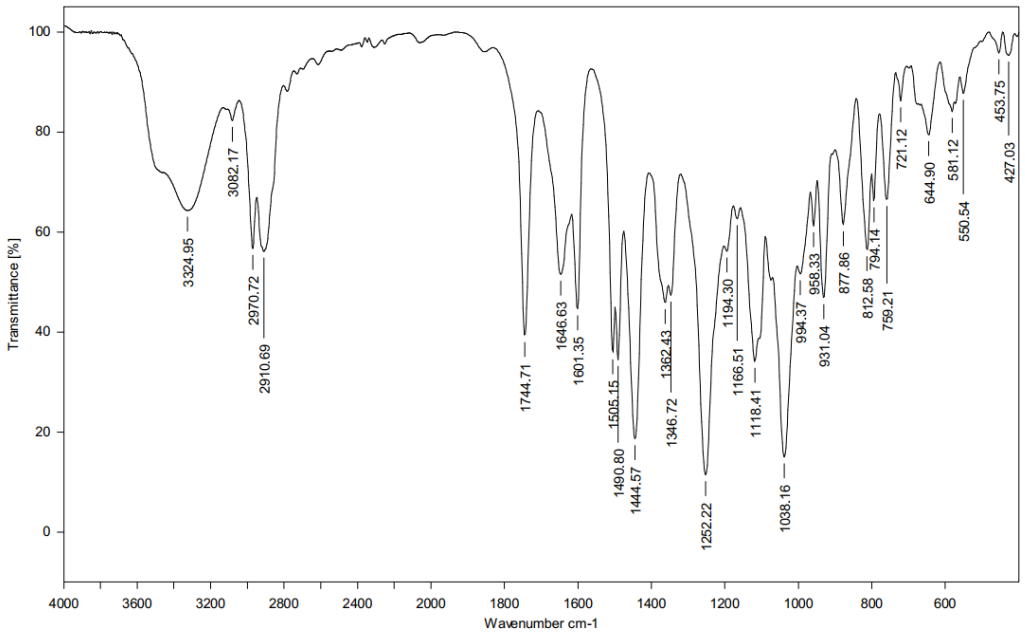


Figure S11. IR spectrum of **1.**

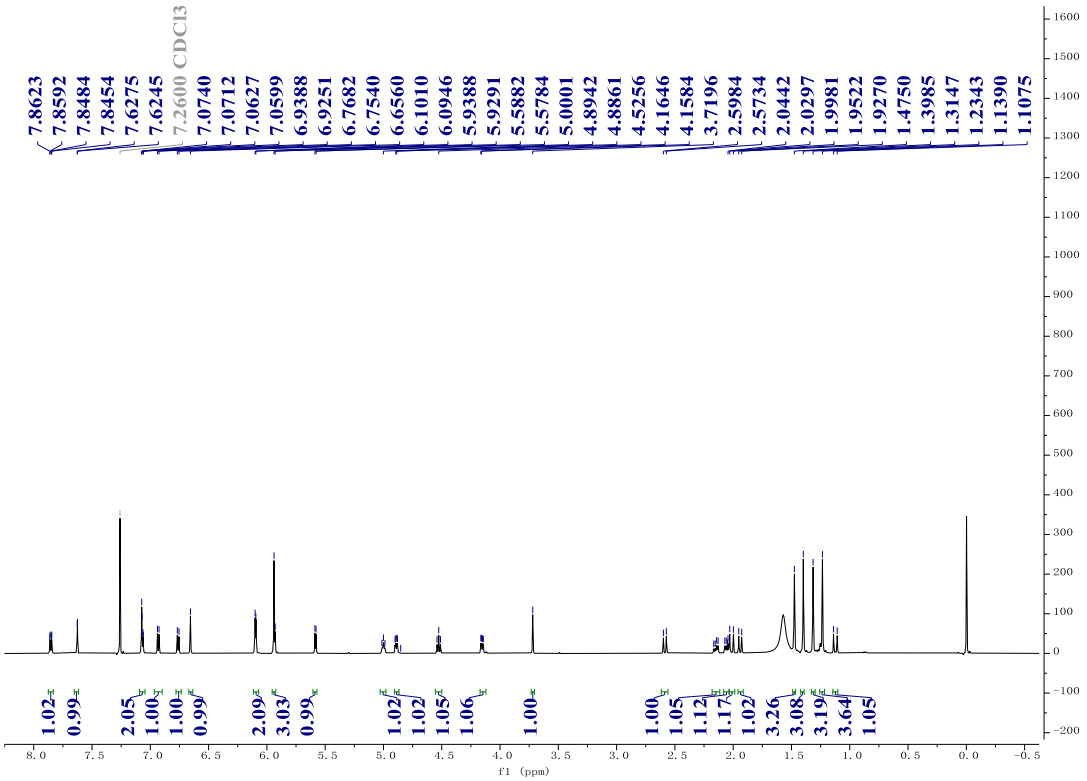


Figure S12. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **1**.

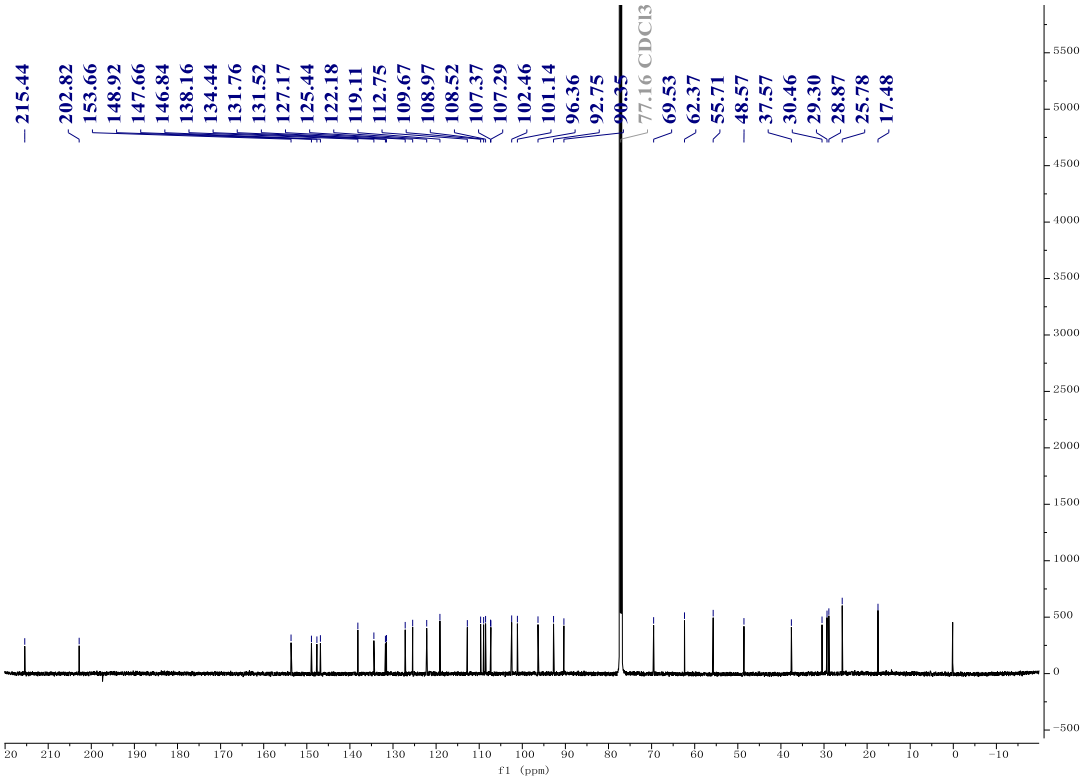


Figure S13. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **1**.

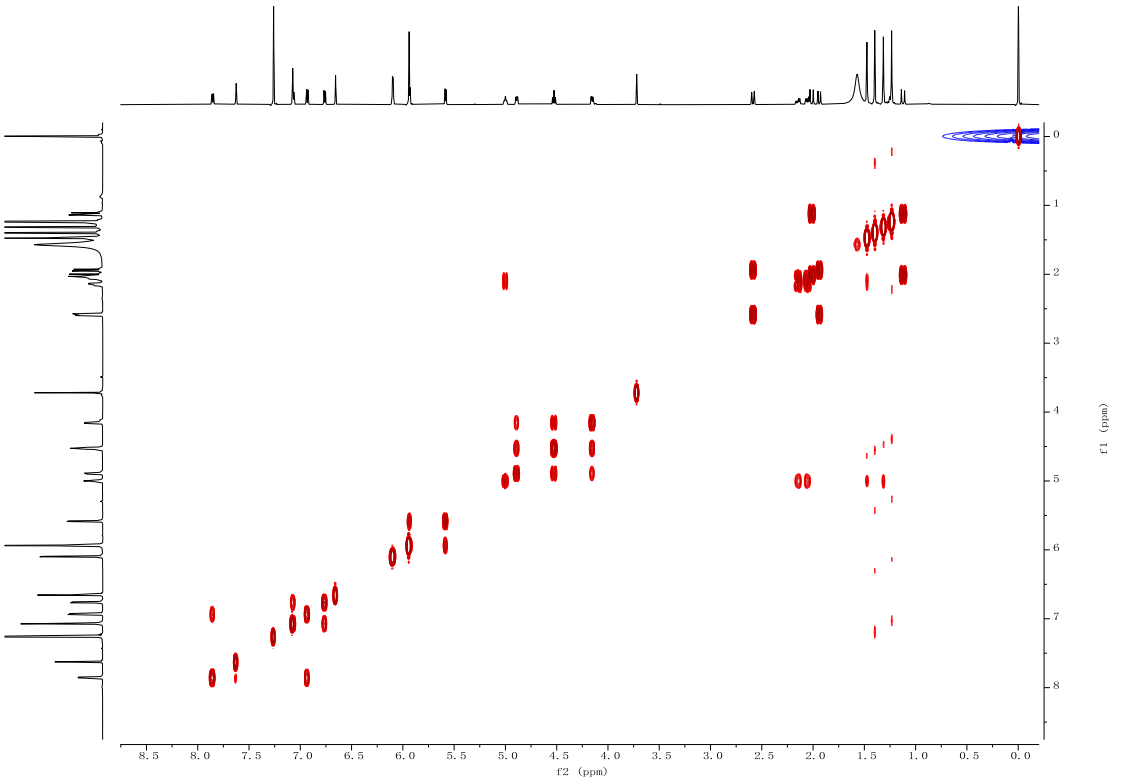


Figure S14. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **1**.

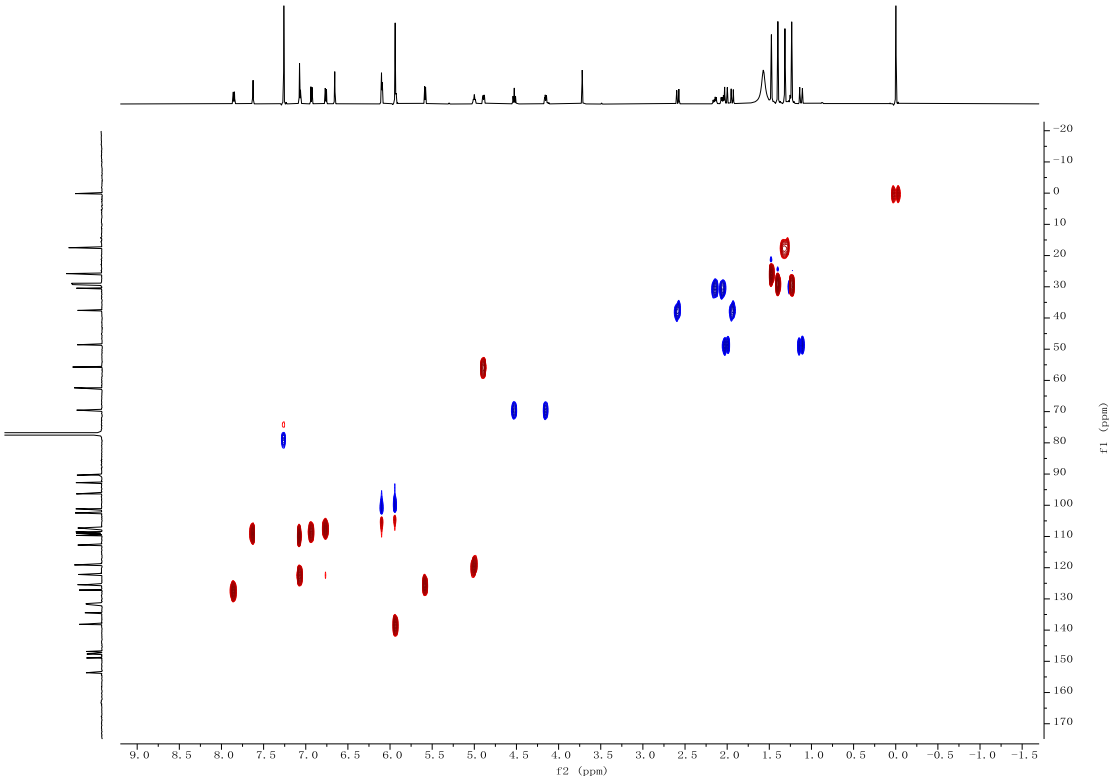


Figure S15. HSQC (600 MHz, $CDCl_3$) spectrum of **1**.

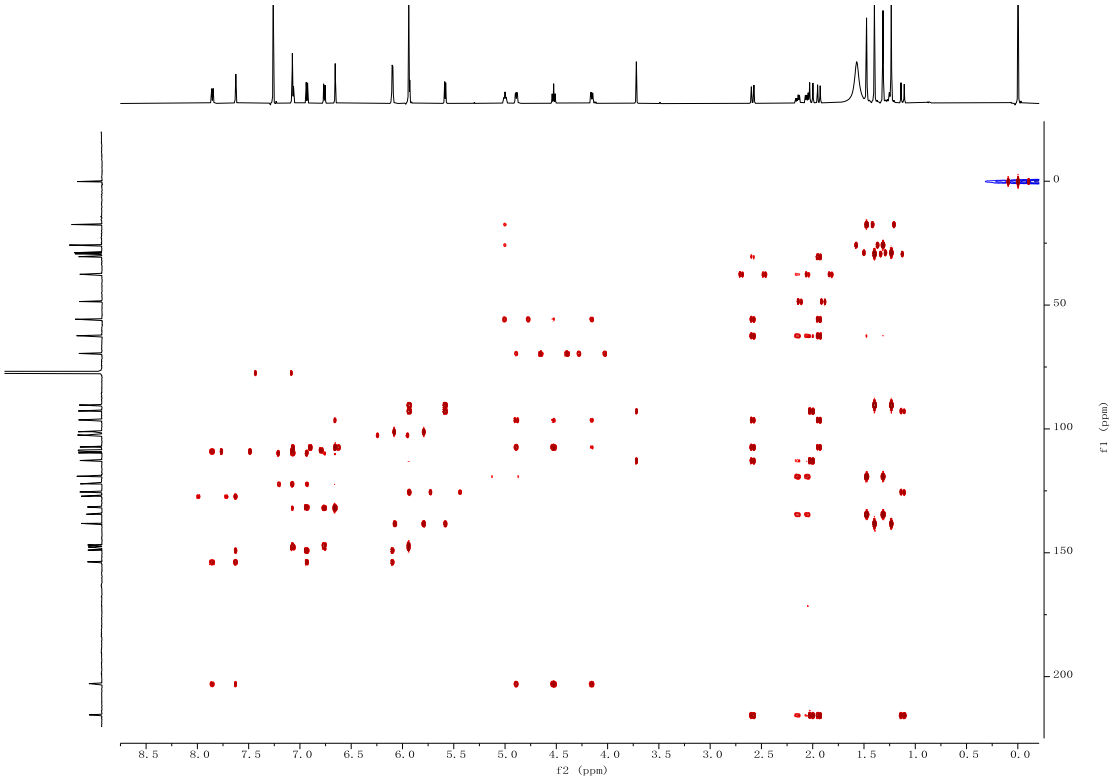


Figure S16. HMBC (600 MHz, $CDCl_3$) spectrum of **1**.

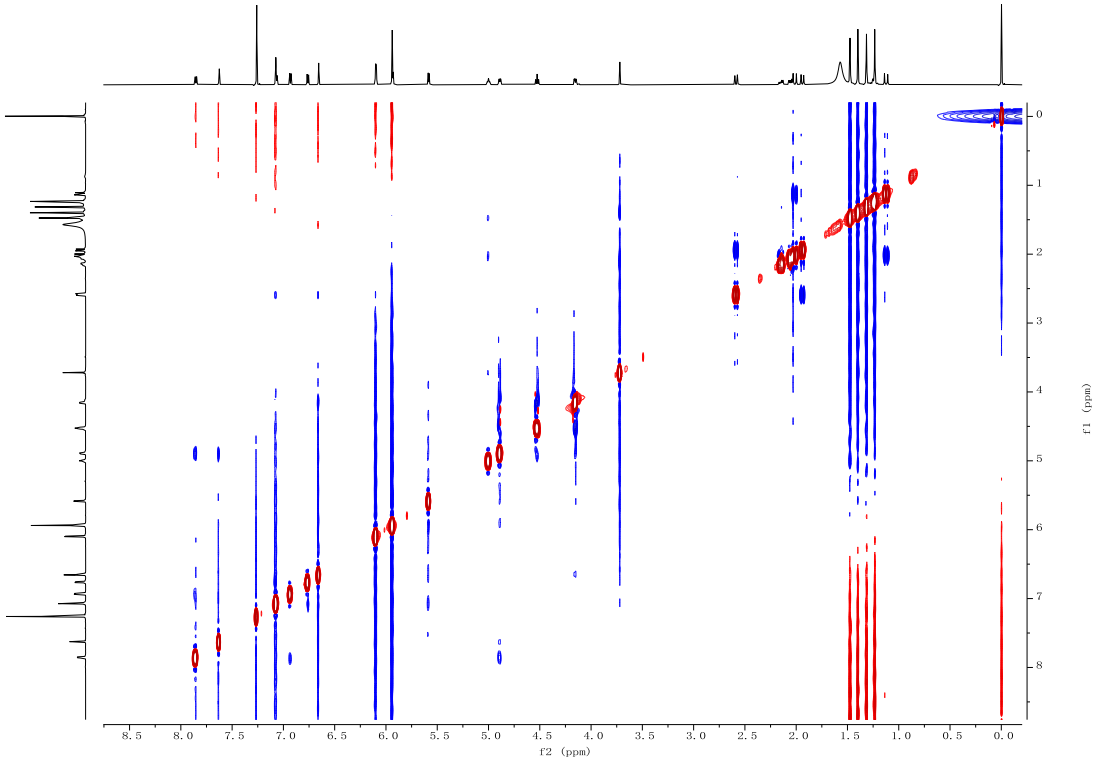


Figure S17. ^{1}H-^{1}H ROESY (600 MHz, $CDCl_3$) spectrum of **1**.

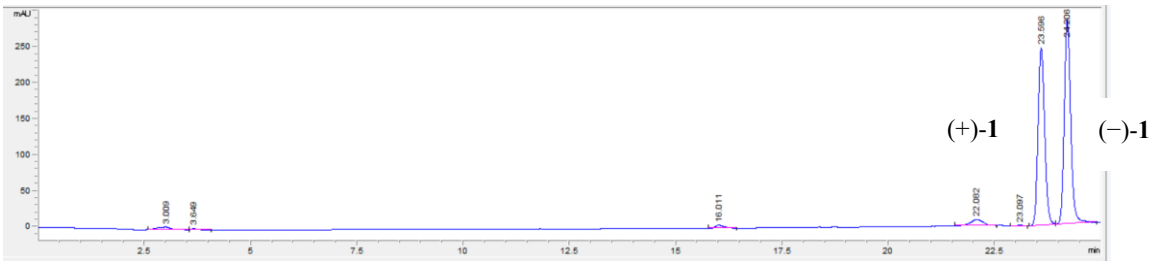
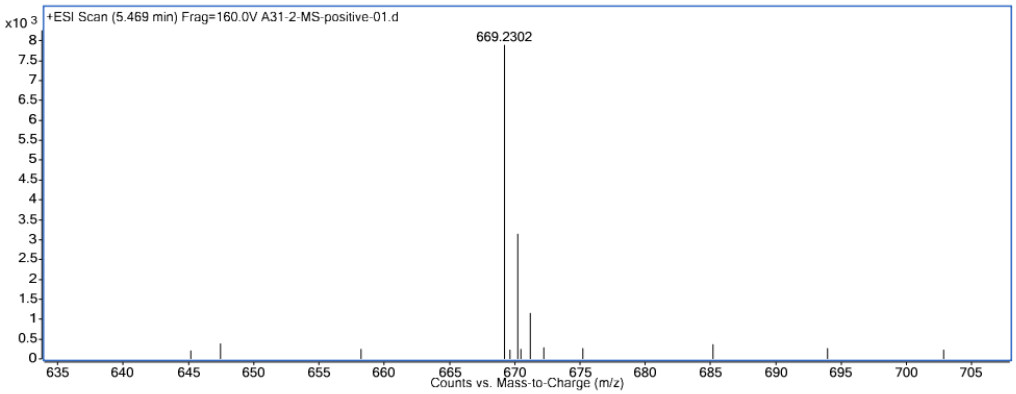


Figure S18. Chiral HPLC chromatogram of **1**.



Elemental Composition Calculator

Target m/z:	669.2302	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C36H38NaO11		669.2306		0.58	

Figure S19. HRESIMS spectrum of **2**.

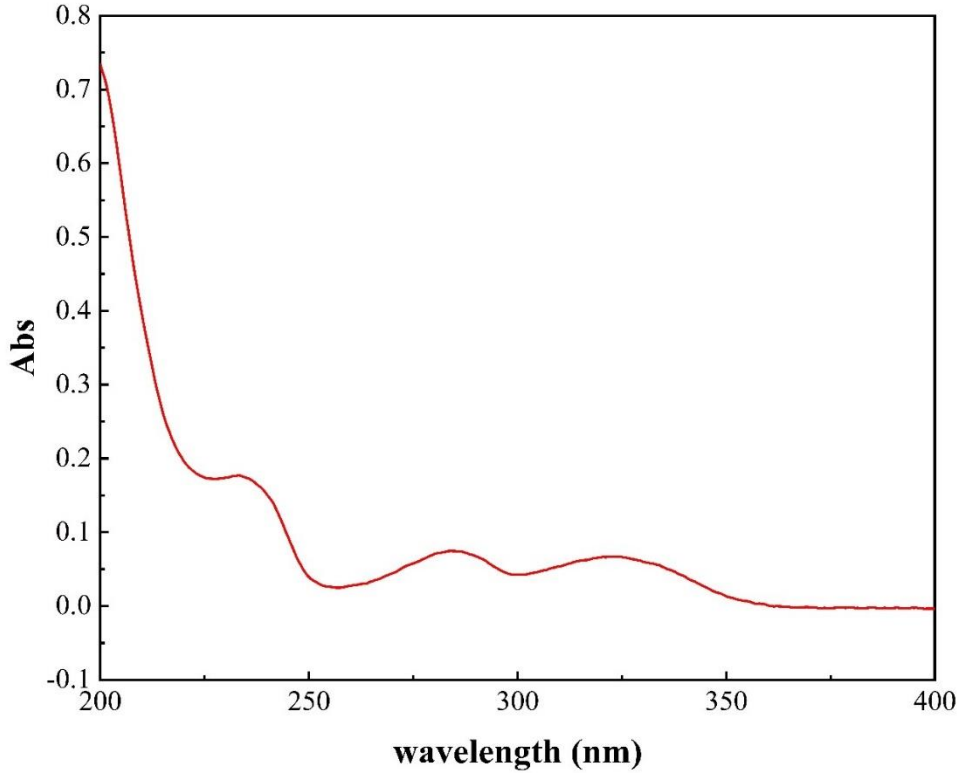


Figure S20. UV spectrum of **2**.

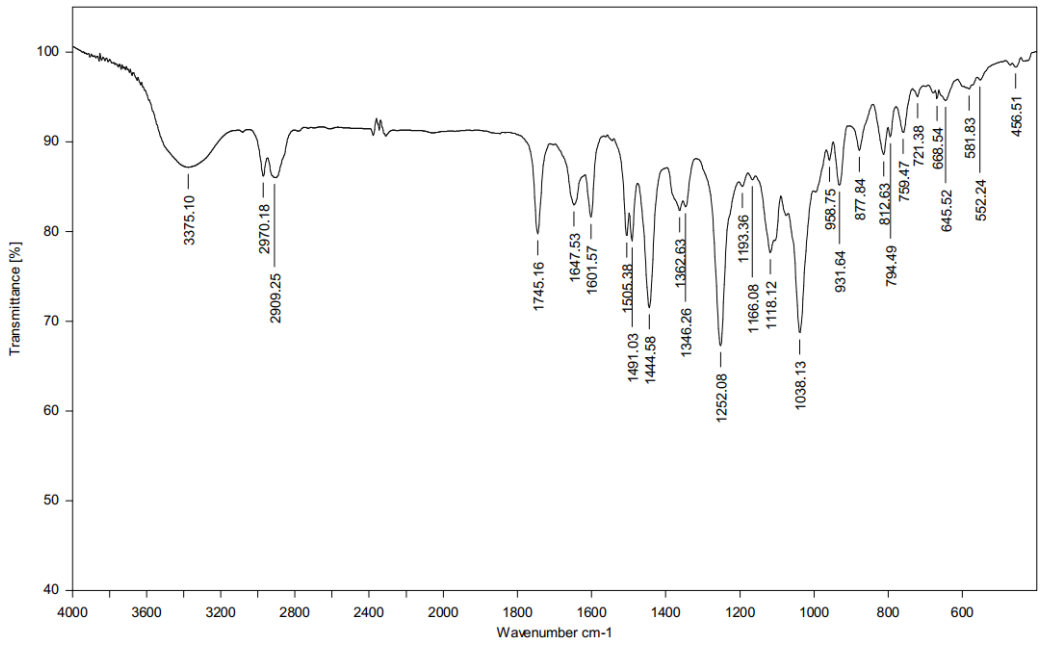


Figure S21. IR spectrum of **2**.

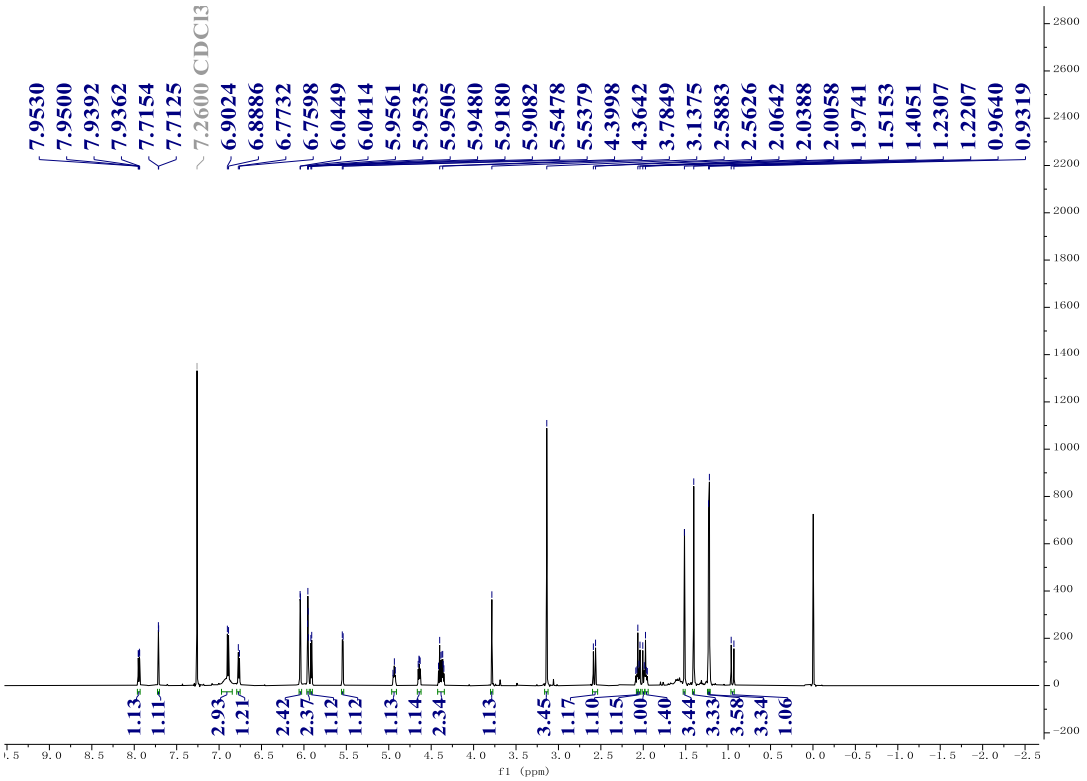


Figure S22. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **2**.

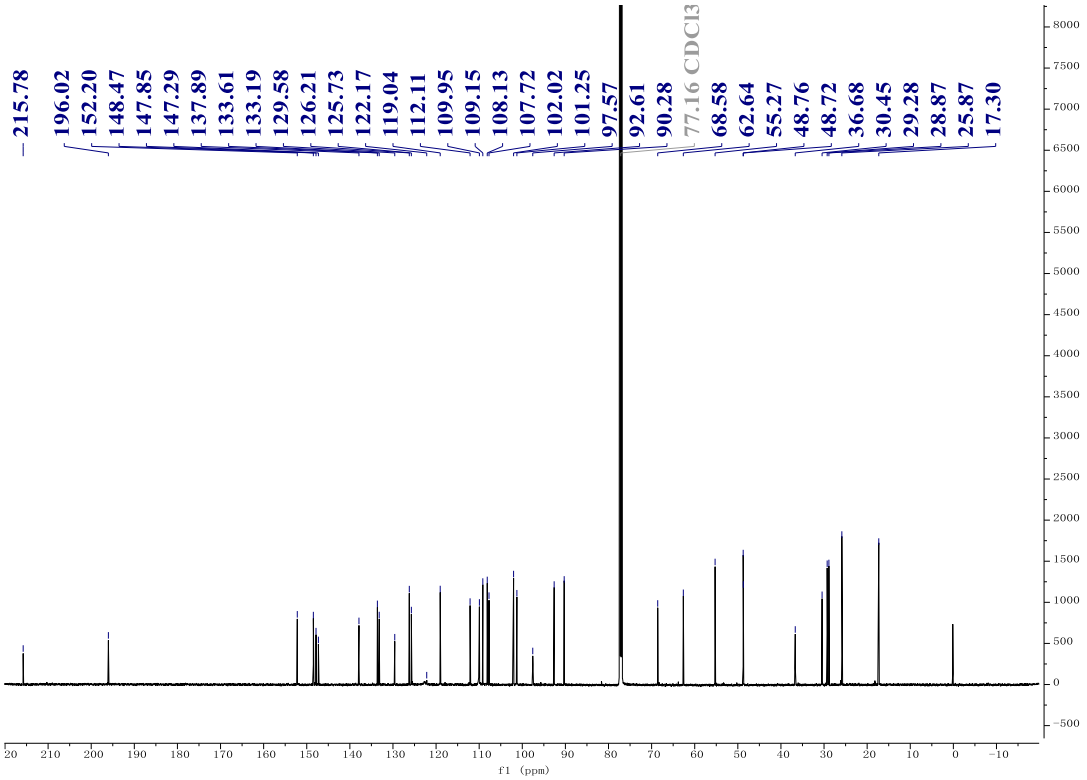


Figure S23. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **2**.

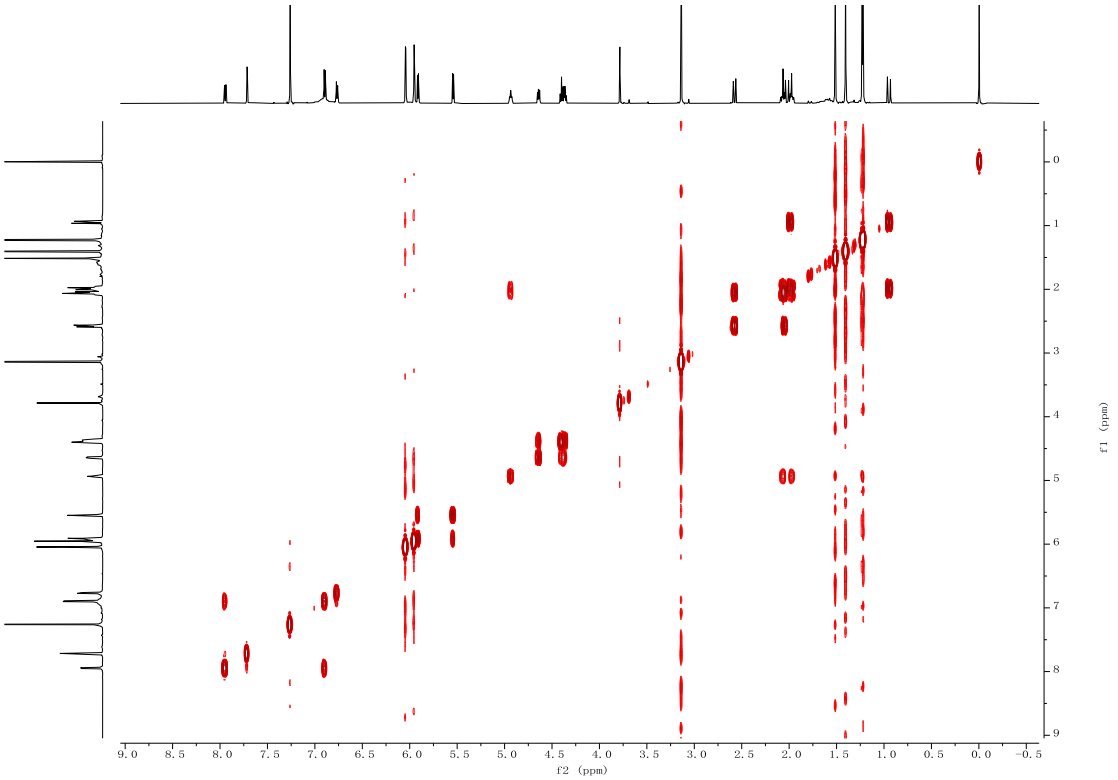


Figure S24. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **2**.

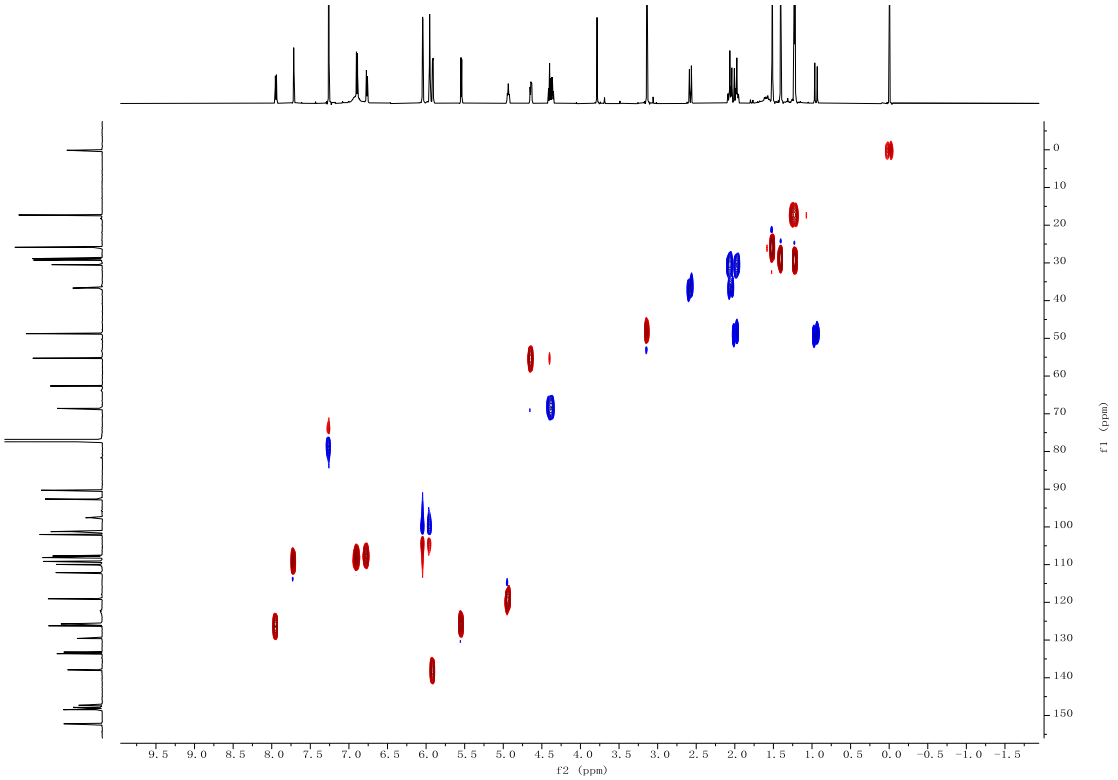


Figure S25. HSQC (600 MHz, $CDCl_3$) spectrum of **2**.

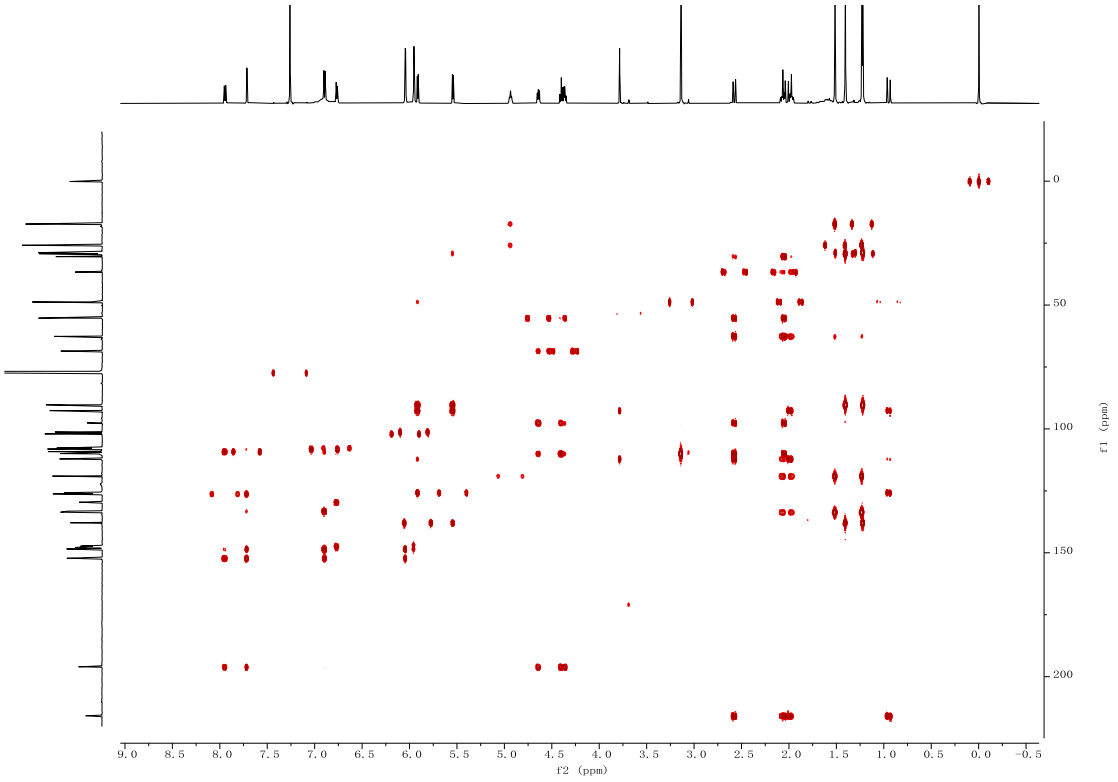


Figure S26. HMBC (600 MHz, $CDCl_3$) spectrum of **2**.

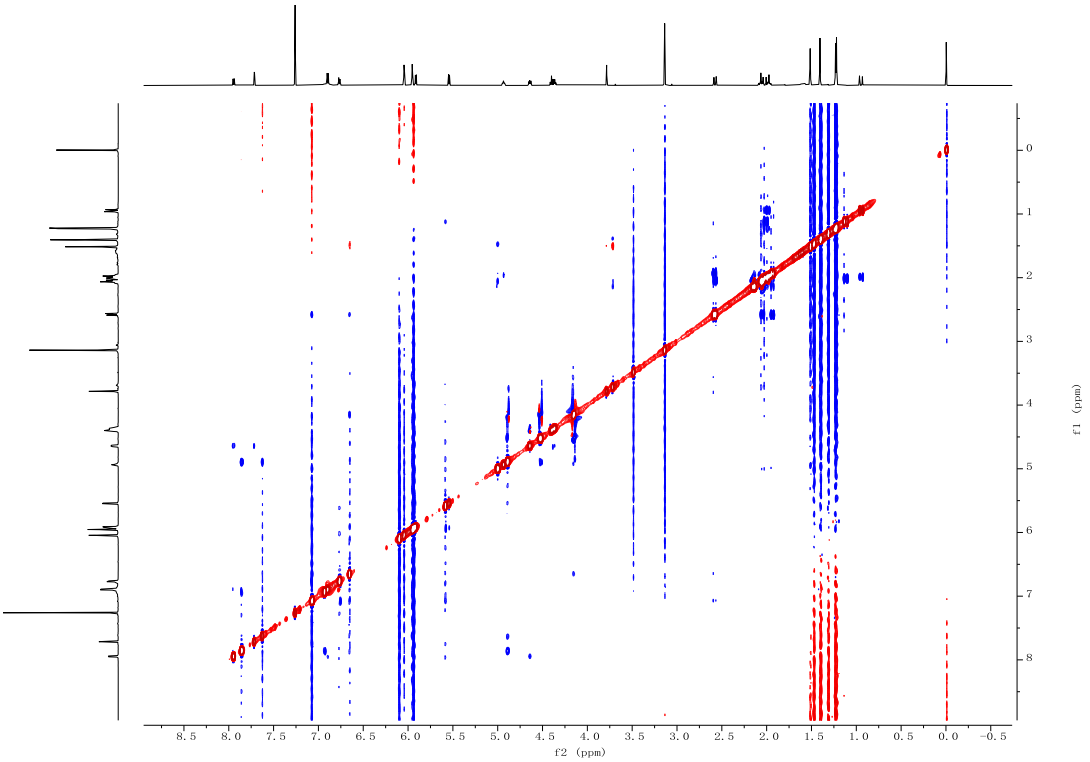


Figure S27. ^{1}H-^{1}H ROESY (600 MHz, $CDCl_3$) spectrum of **2**.

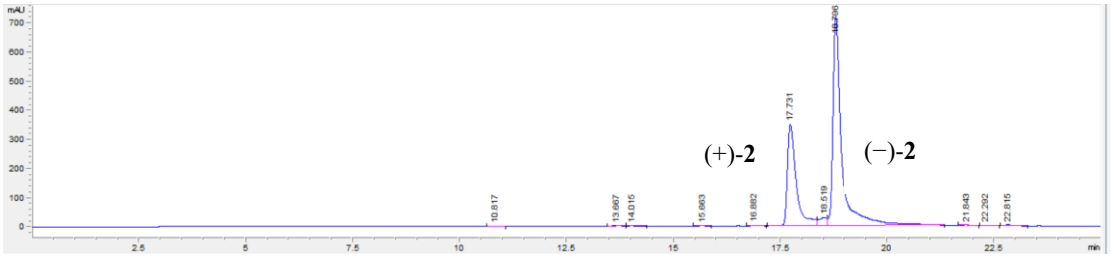
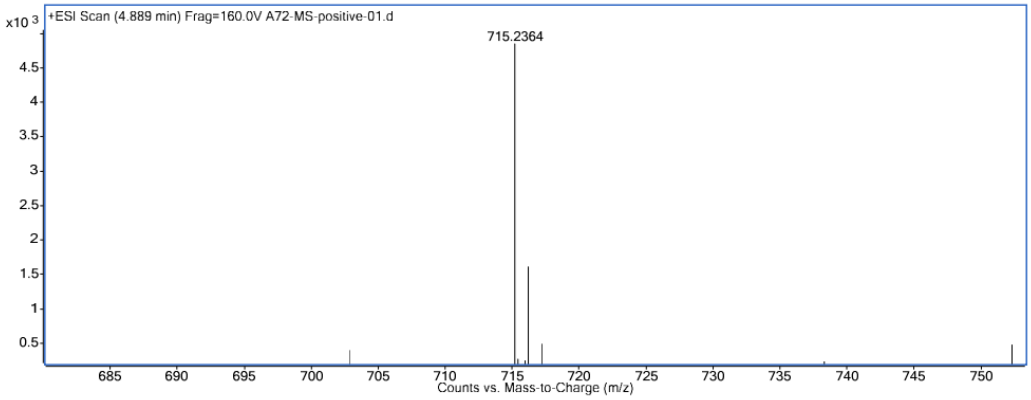


Figure S28. Chiral HPLC chromatogram of **2**.



Elemental Composition Calculator

Target m/z:	715.2364	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C37H40NaO13		715.2361		-0.35	

Figure S29. HRESIMS spectrum of **3**.

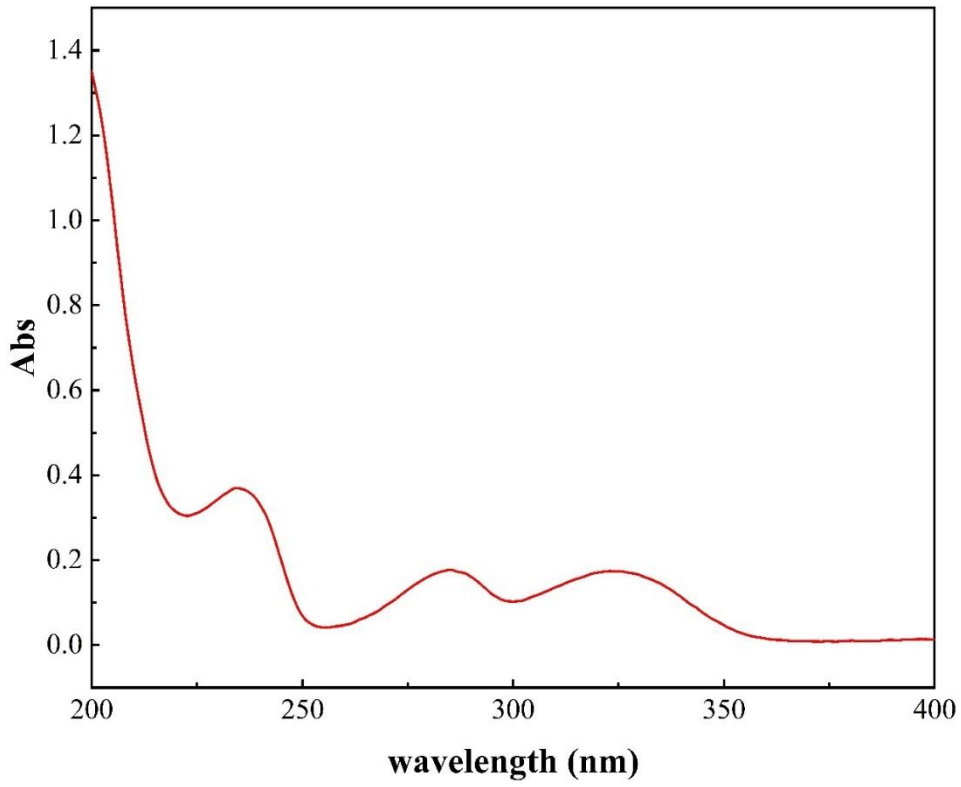


Figure S30. UV spectrum of **3.**

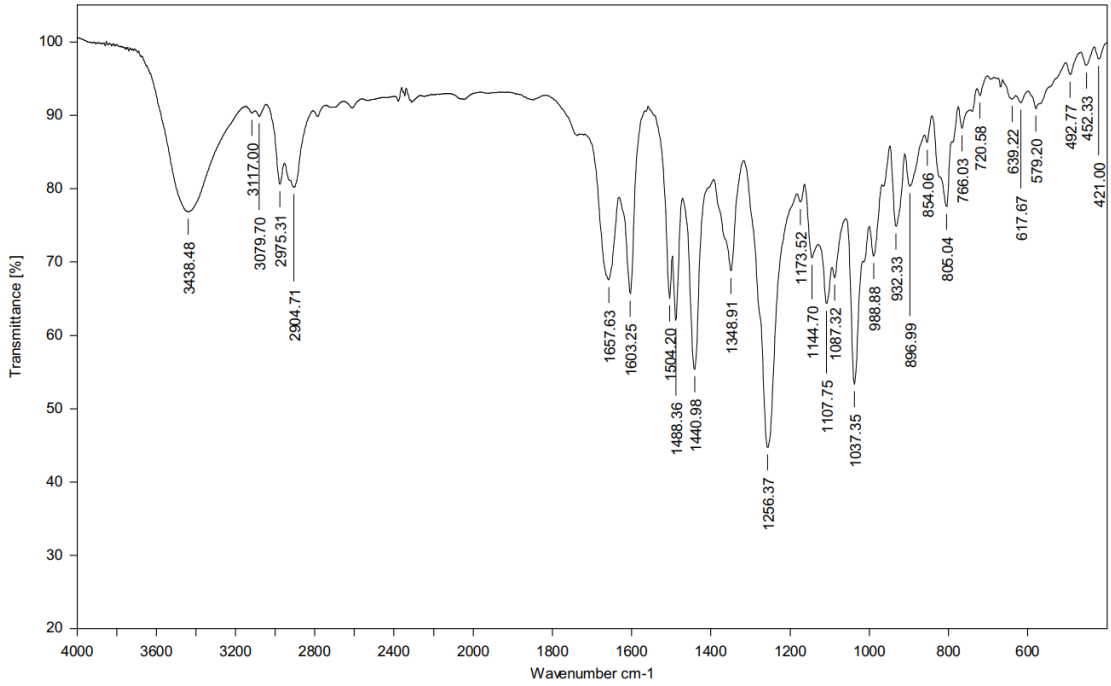


Figure S31. IR spectrum of **3.**

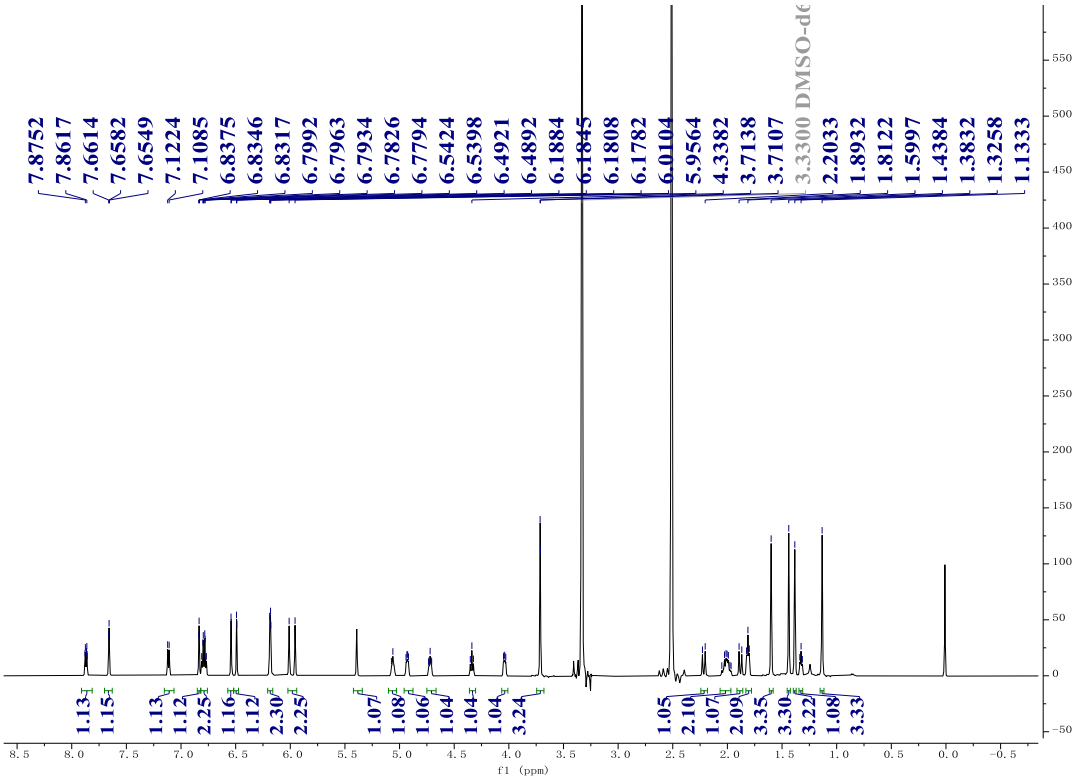


Figure S32. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **3**.

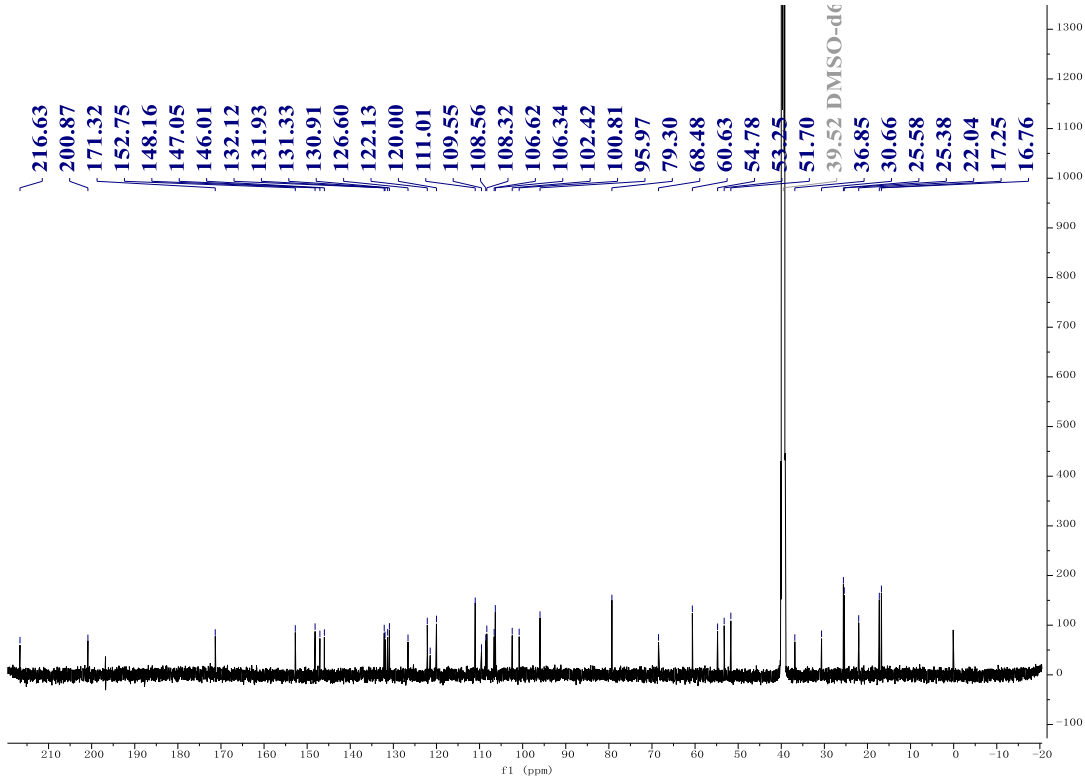


Figure S33. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **3**.

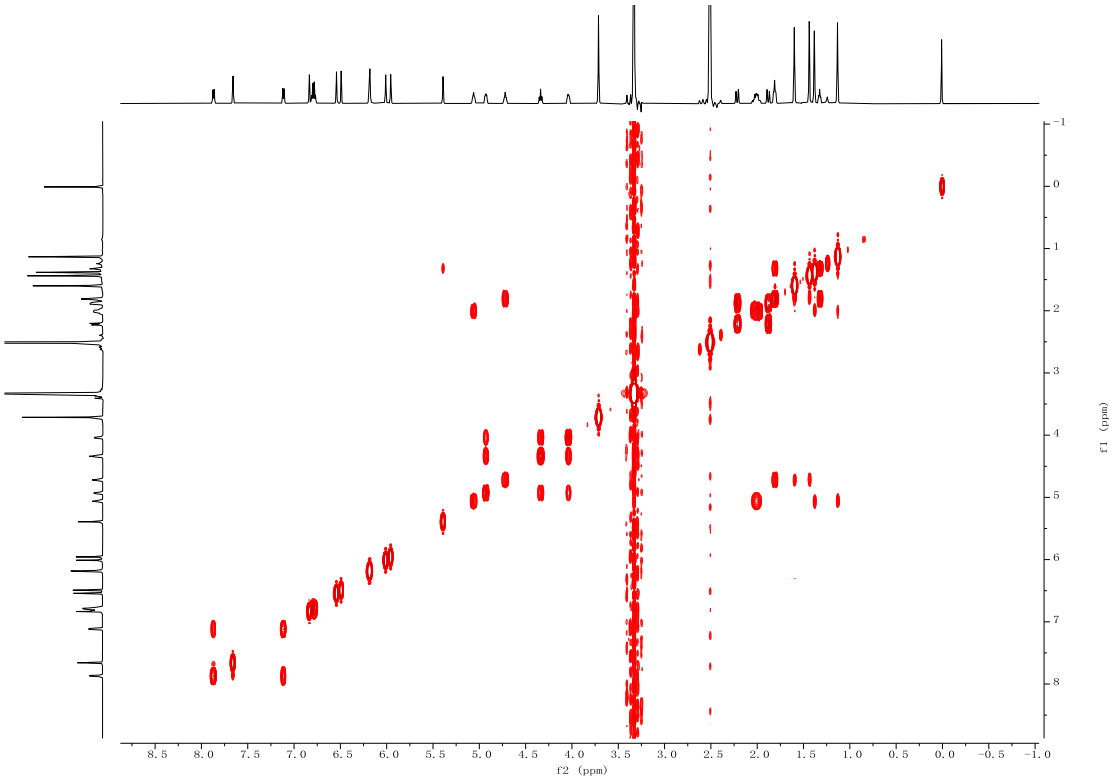


Figure S34. ^{1}H-^{1}H COSY spectrum (600 MHz, DMSO-d_6) of **3**.

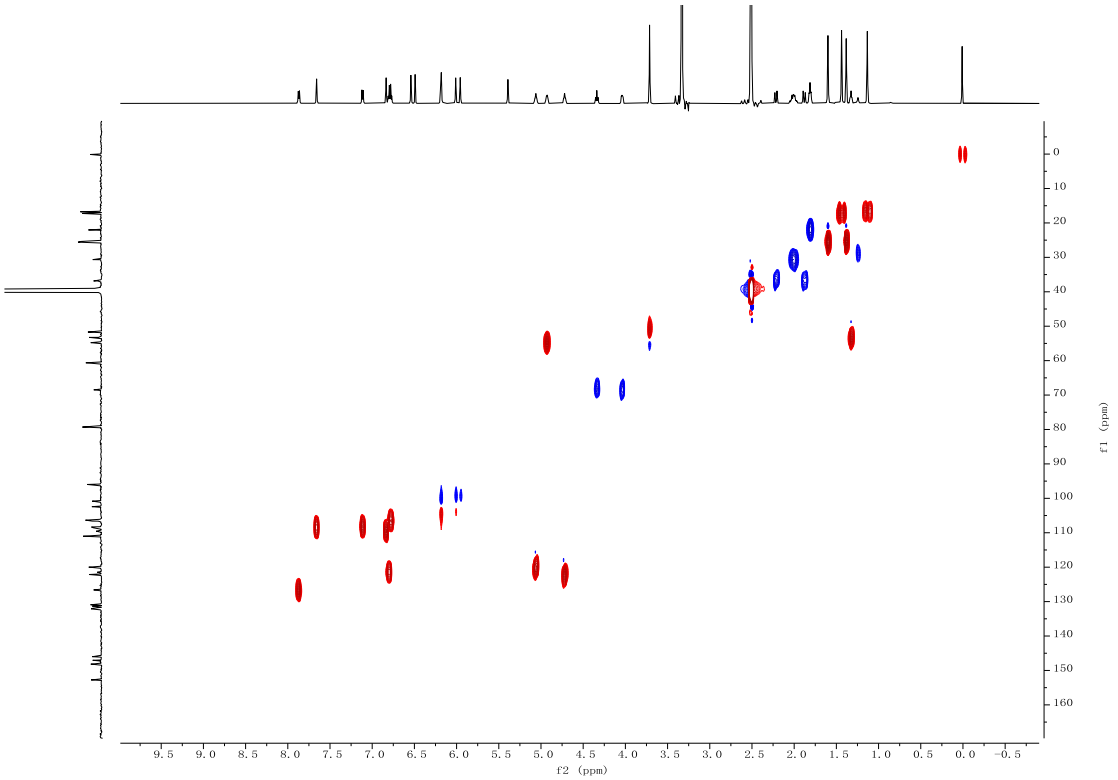


Figure S35. HSQC (600 MHz, DMSO-d_6) spectrum of **3**.

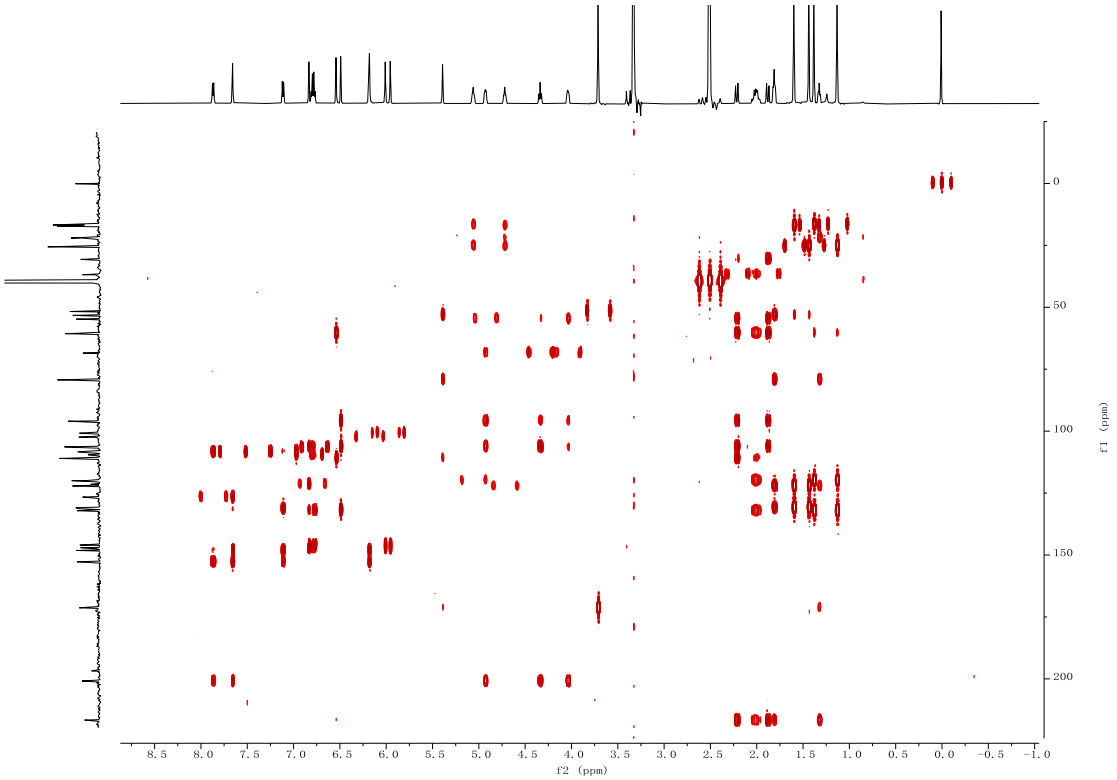


Figure S36. HMBC (600 MHz, DMSO-d_6) spectrum of **3**.

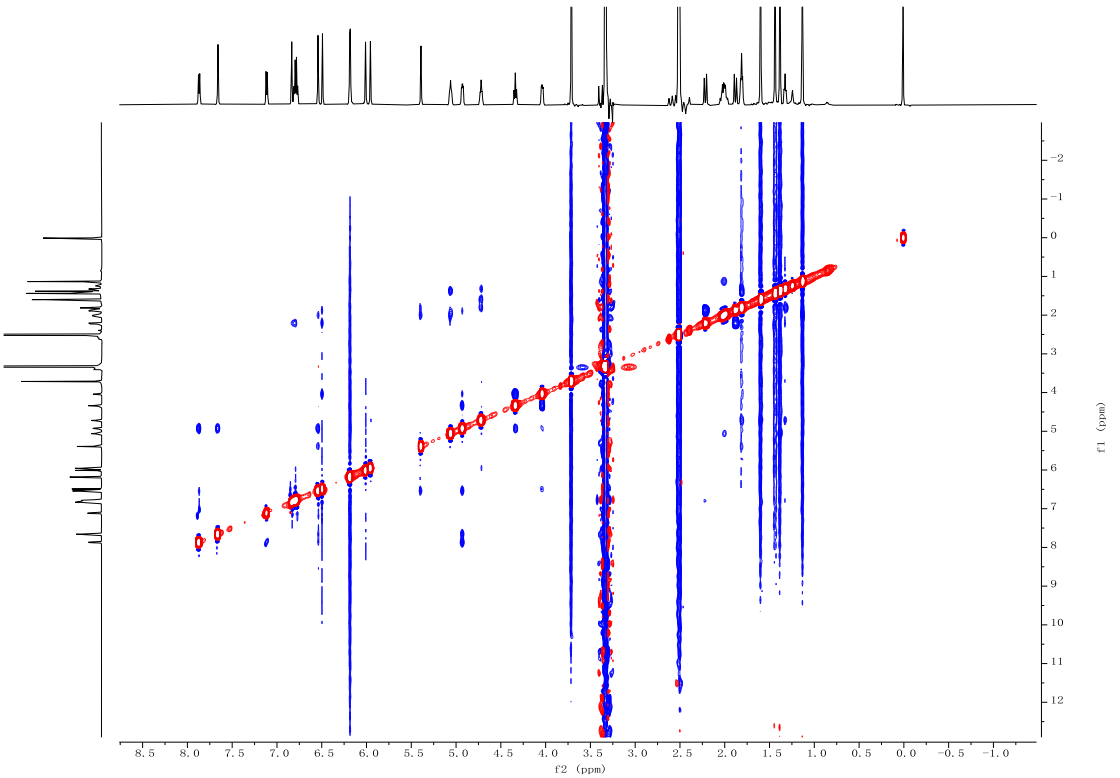


Figure S37. ^{1}H-^{1}H ROESY (600 MHz, DMSO-d_6) spectrum of **3**.

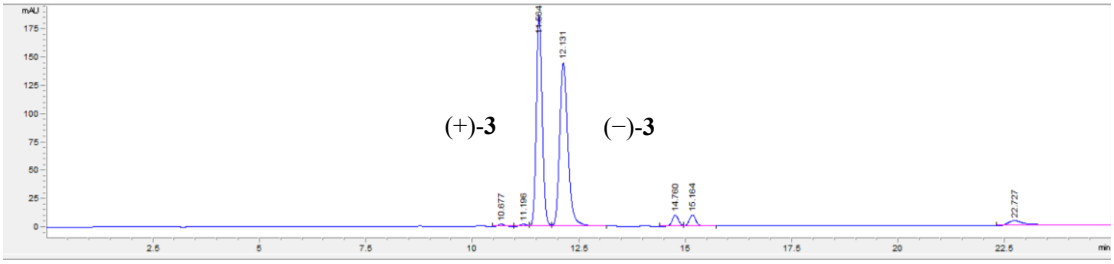
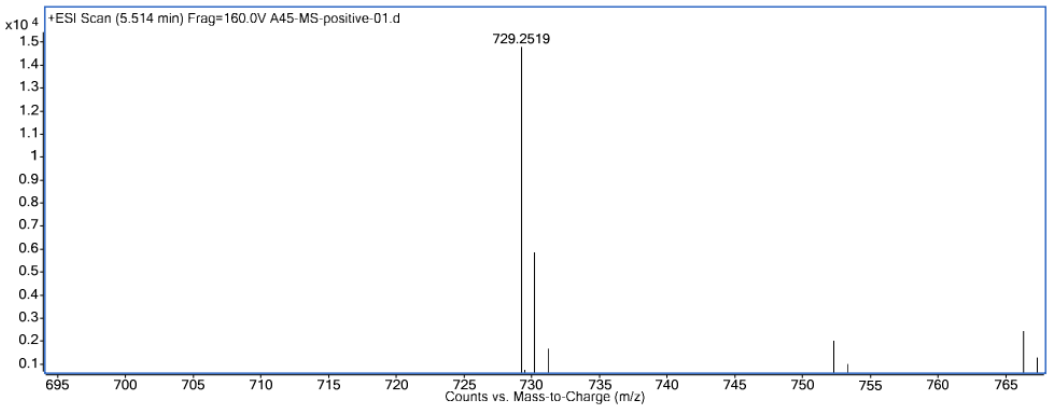


Figure S38. Chiral HPLC chromatogram of **3**.



Elemental Composition Calculator

Target m/z:	729.2519	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C38H42NaO13		729.2518		-0.13	

Figure S39. HRESIMS spectrum of **4**.

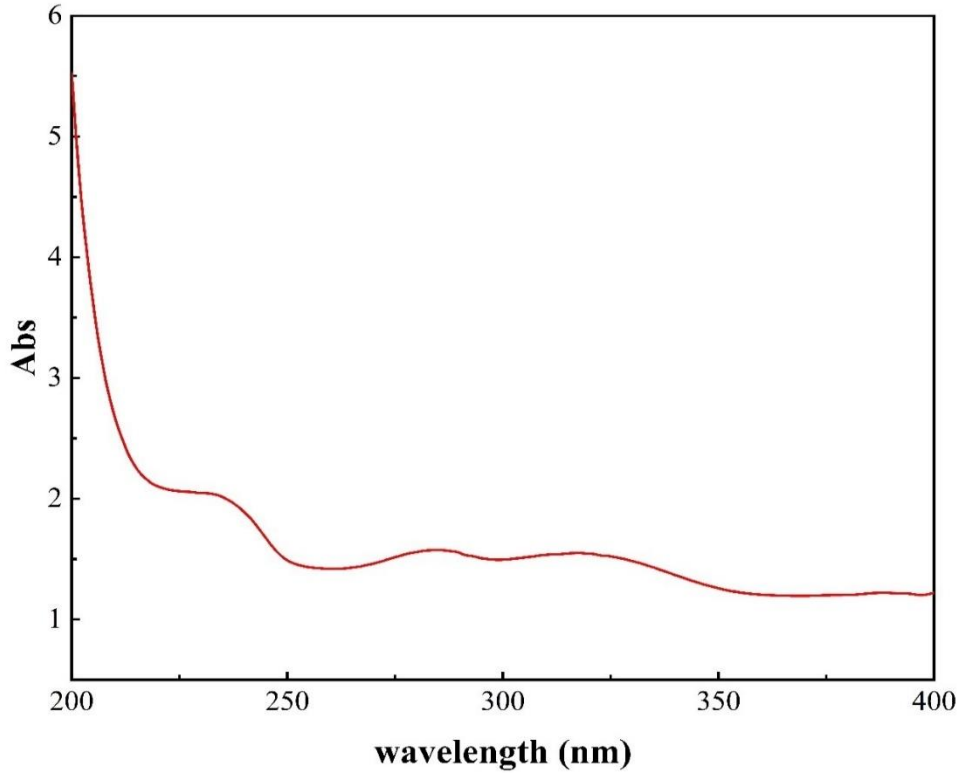


Figure S40. UV spectrum of **4**.

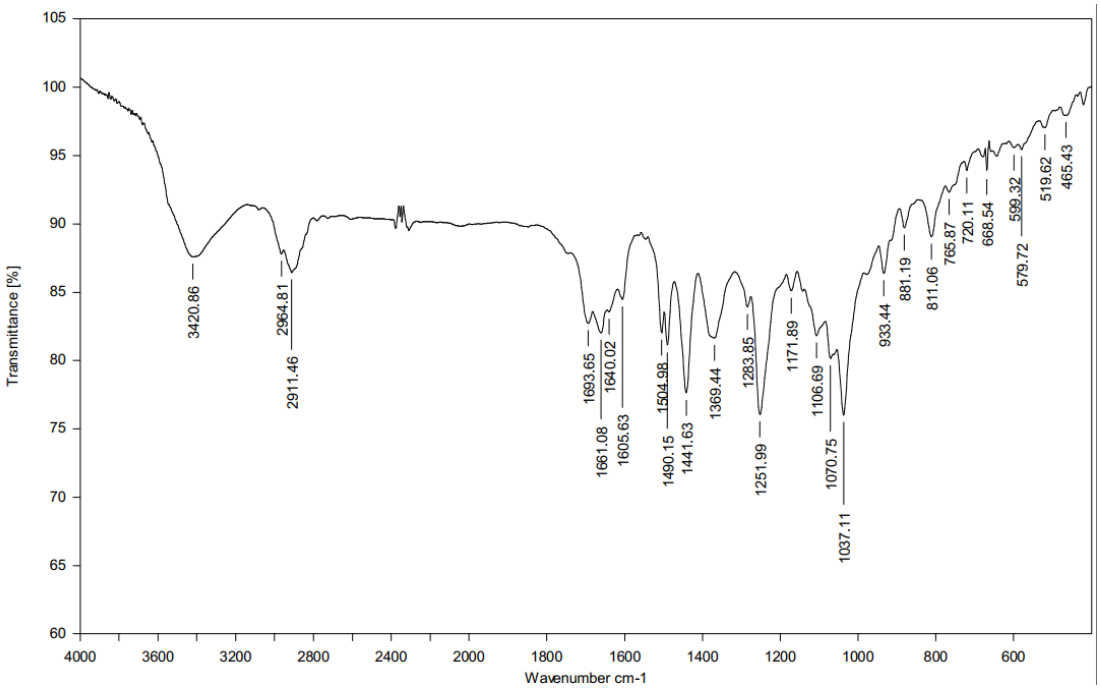


Figure S41. IR spectrum of **4**.

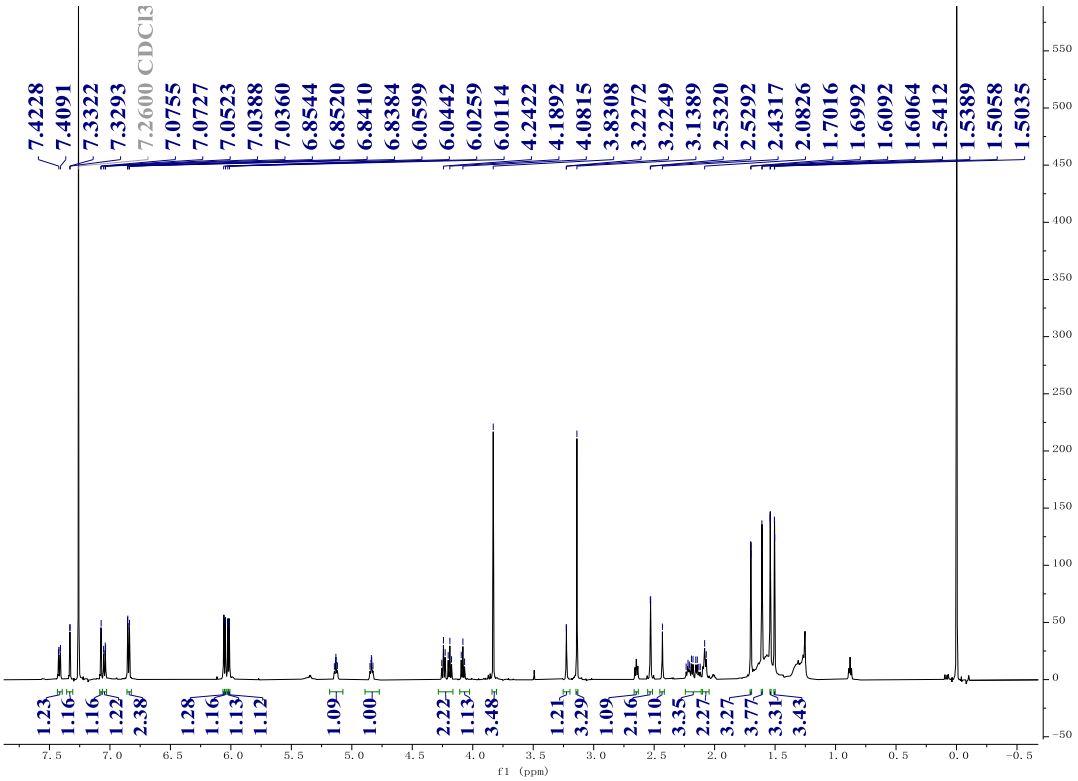


Figure S42. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **4.**

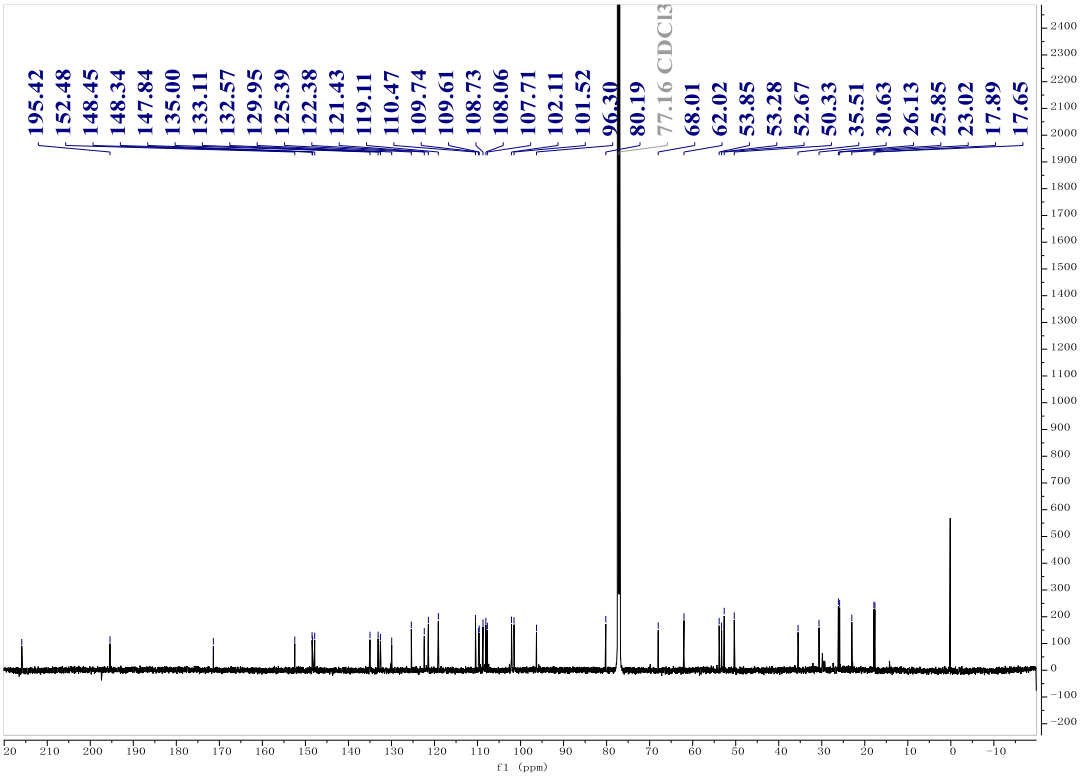


Figure S43. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **4**.

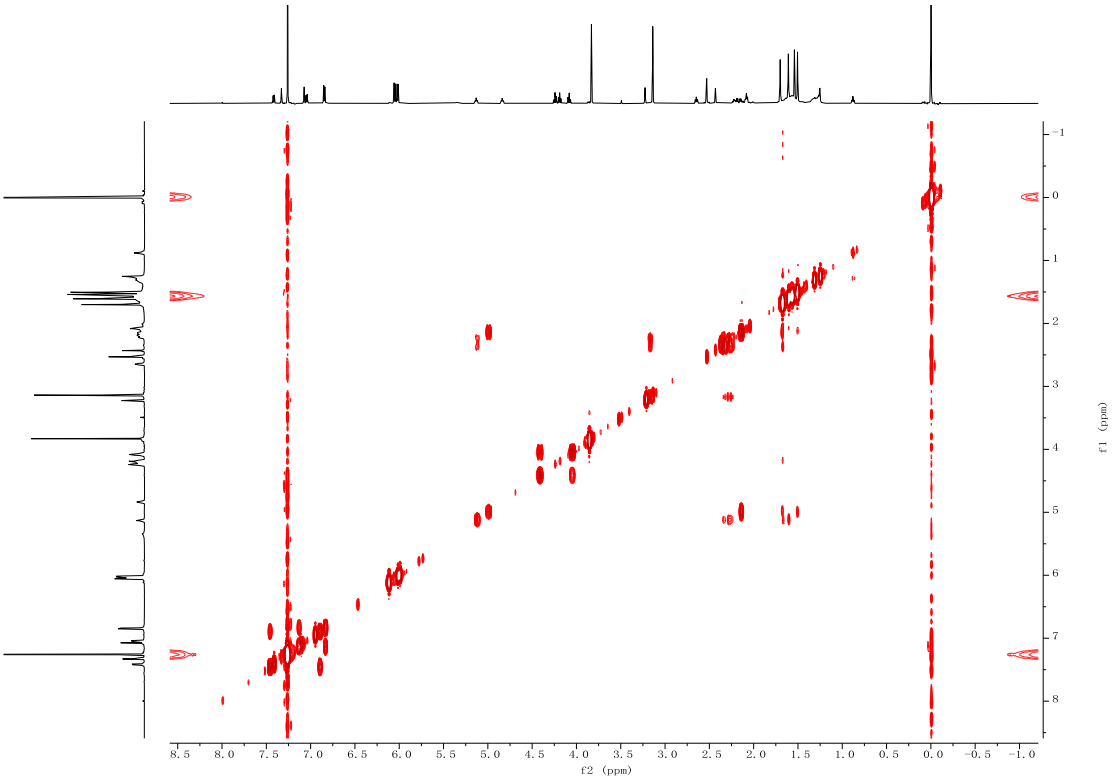


Figure S44. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **4**.

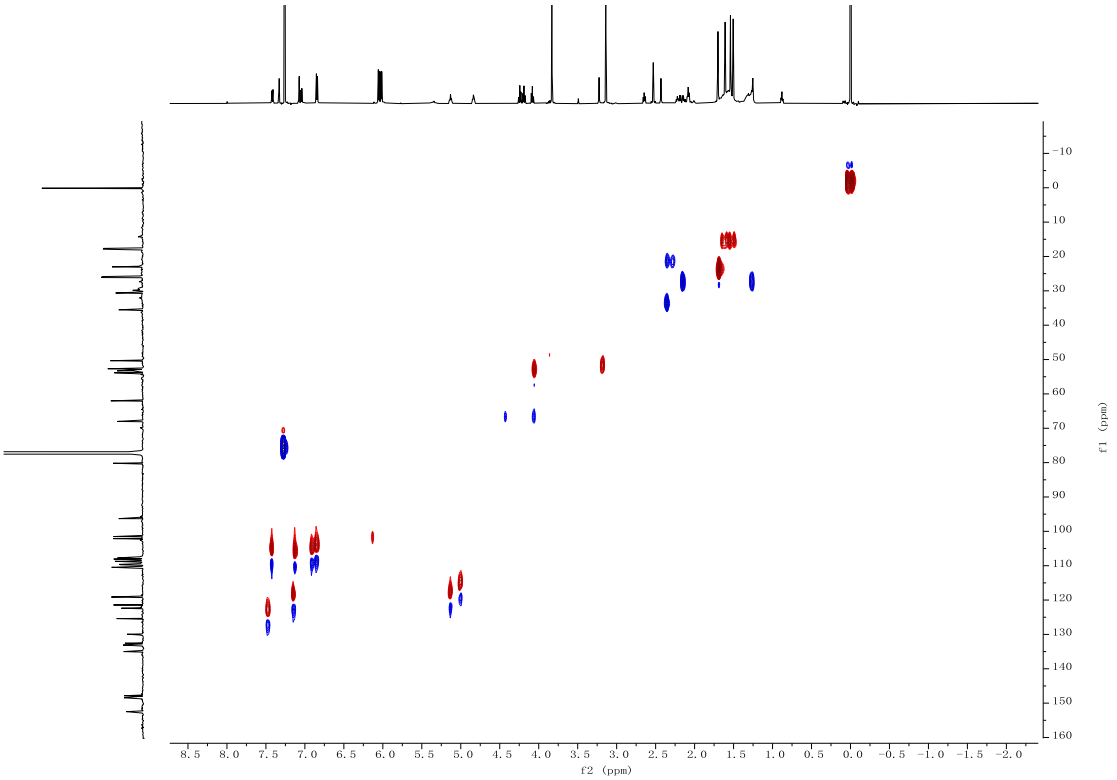


Figure S45. HSQC (600 MHz, $CDCl_3$) spectrum of **4**.

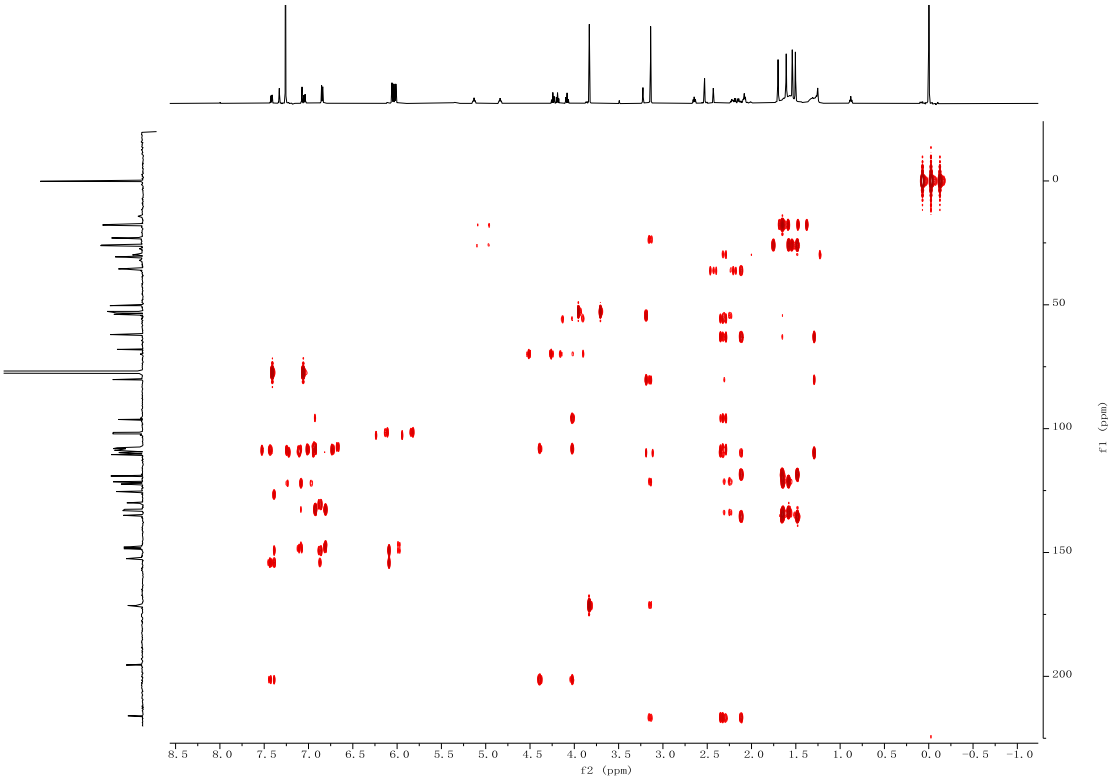


Figure S46. HMBC (600 MHz, $CDCl_3$) spectrum of **4**.

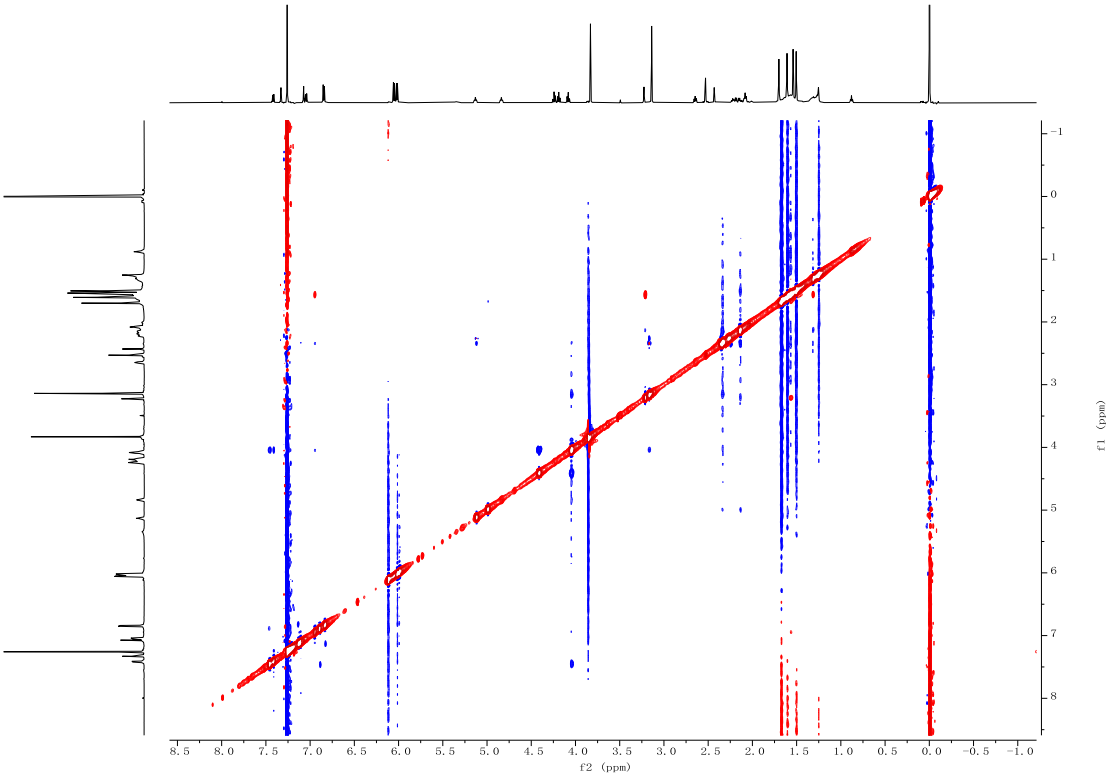


Figure S47. ^{1}H-^{1}H ROESY (600 MHz, $CDCl_3$) spectrum of **4**.

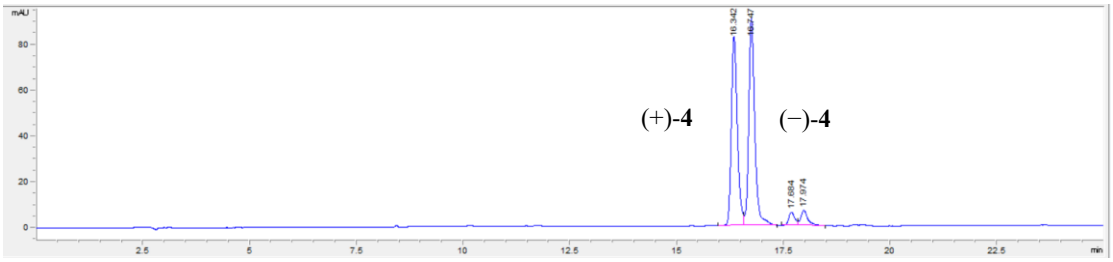
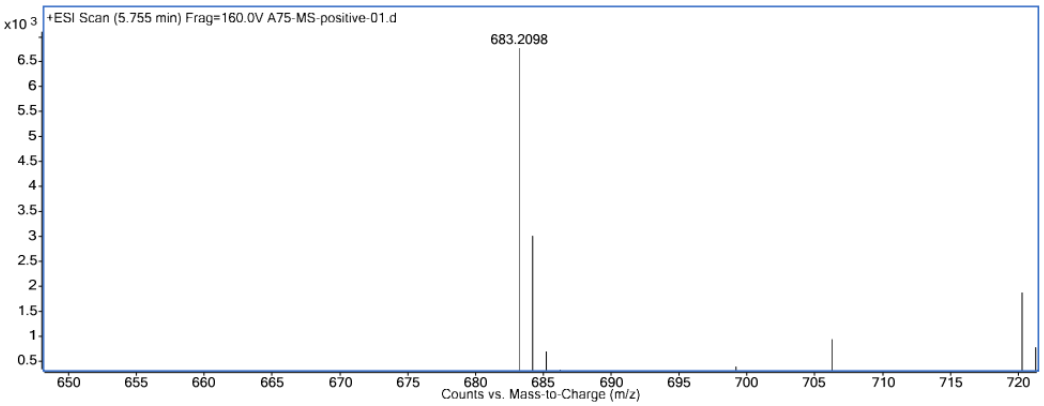


Figure S48. Chiral HPLC chromatogram of **4**.



Elemental Composition Calculator

Target m/z:	683.2098	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C36H36NaO12		683.2099		0.13	

Figure S49. HRESIMS spectrum of **5**.

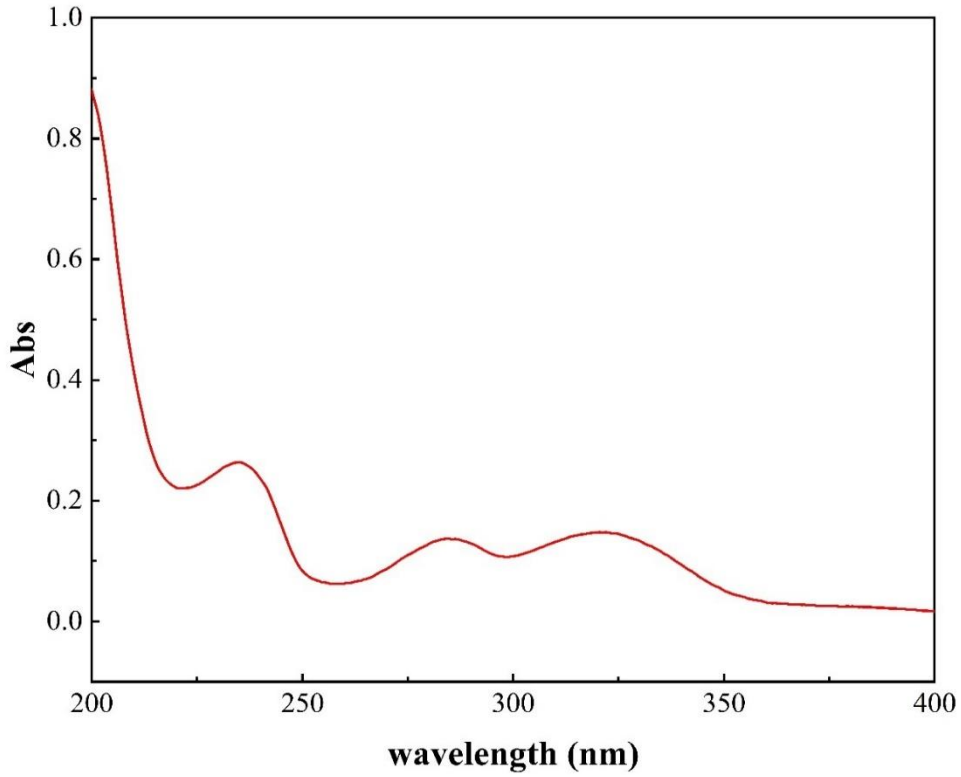


Figure S50. UV spectrum of **5**.

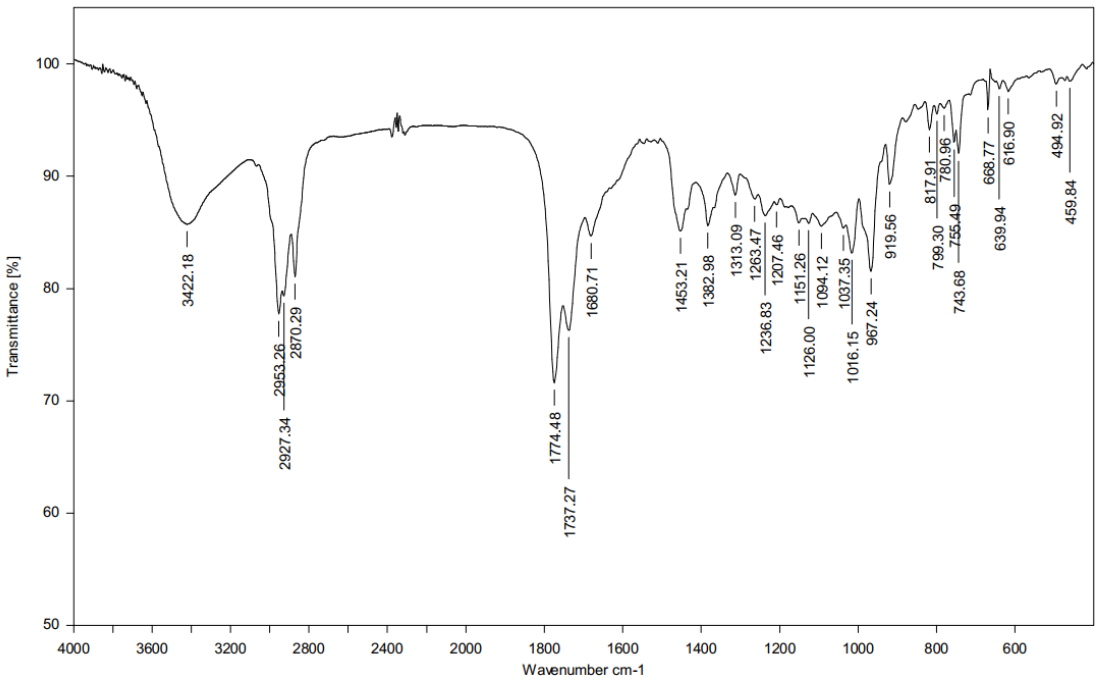


Figure S51. IR spectrum of **5**.

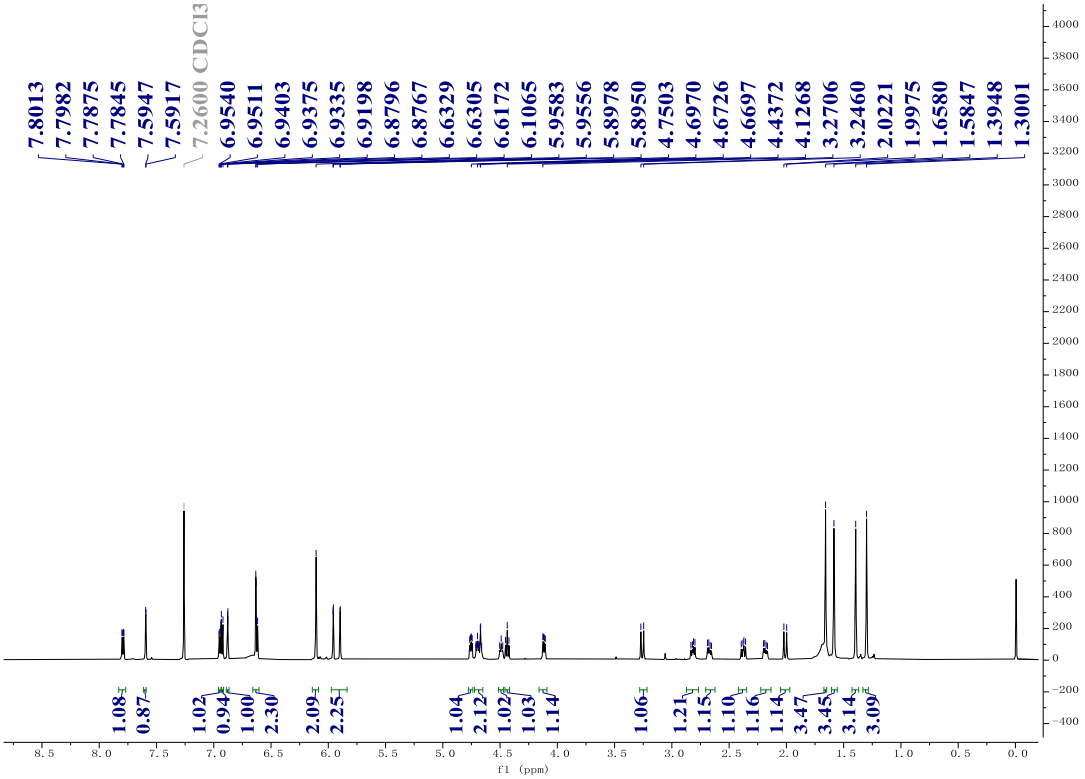


Figure S52. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **5**.

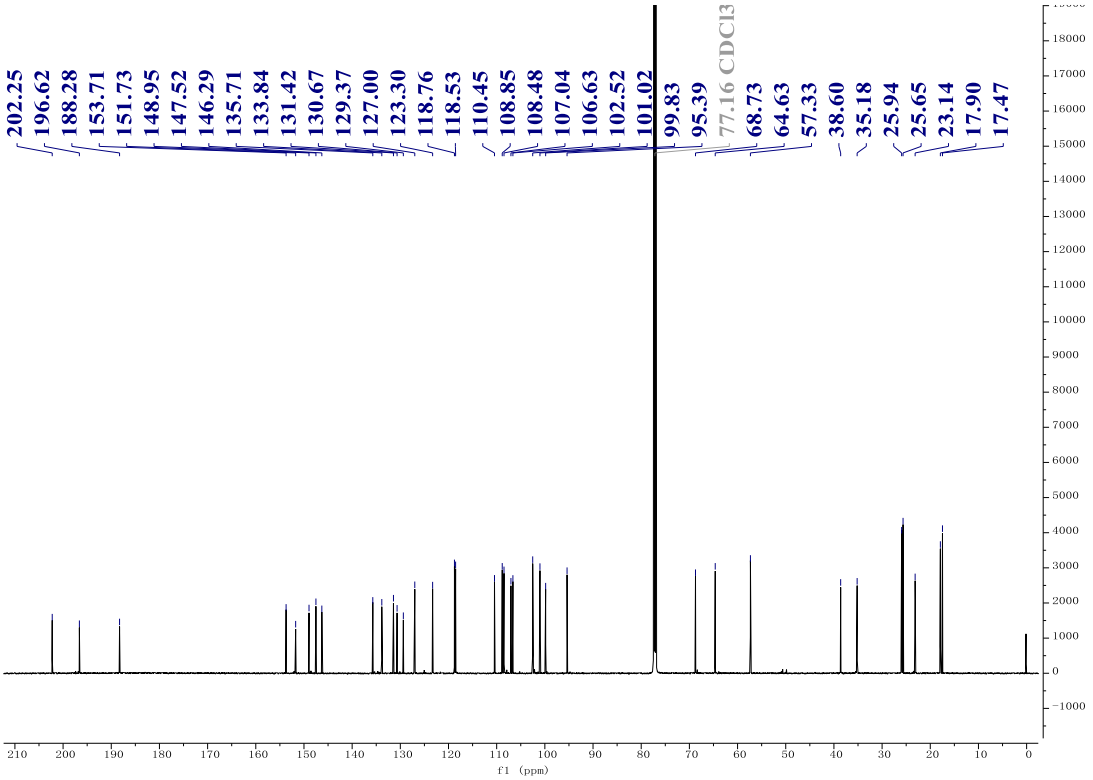


Figure S53. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **5**.

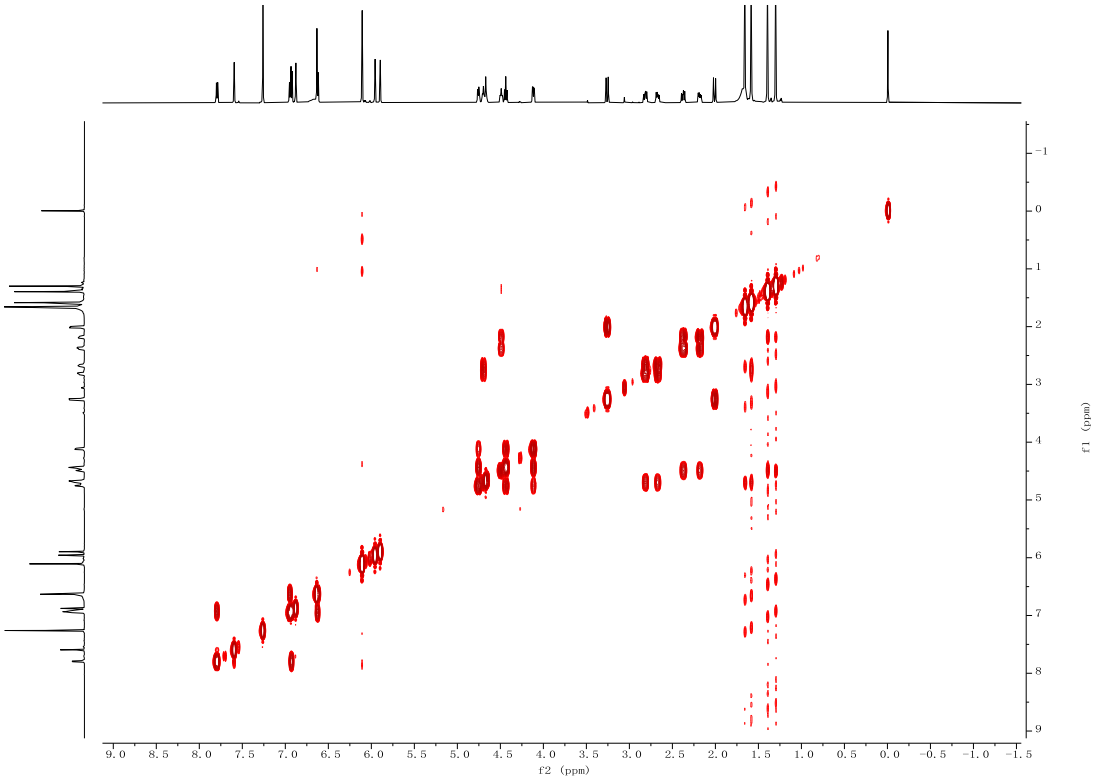


Figure S54. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **5**.

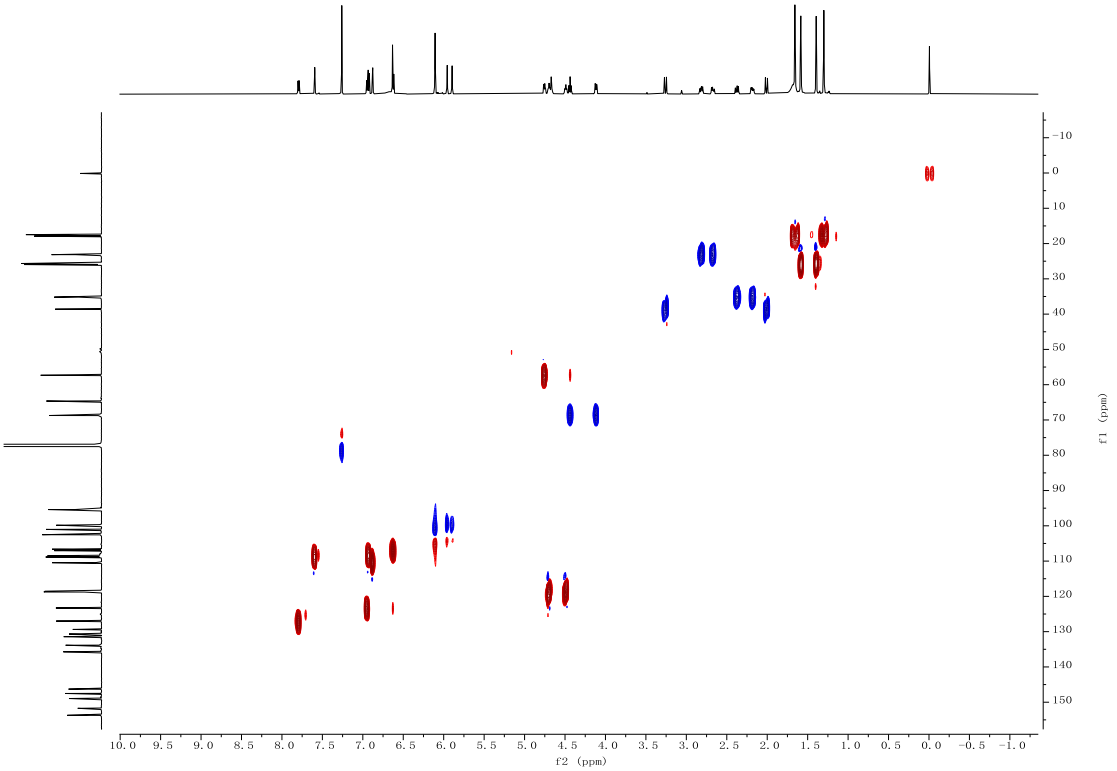


Figure S55. HSQC (600 MHz, $CDCl_3$) spectrum of **5**.

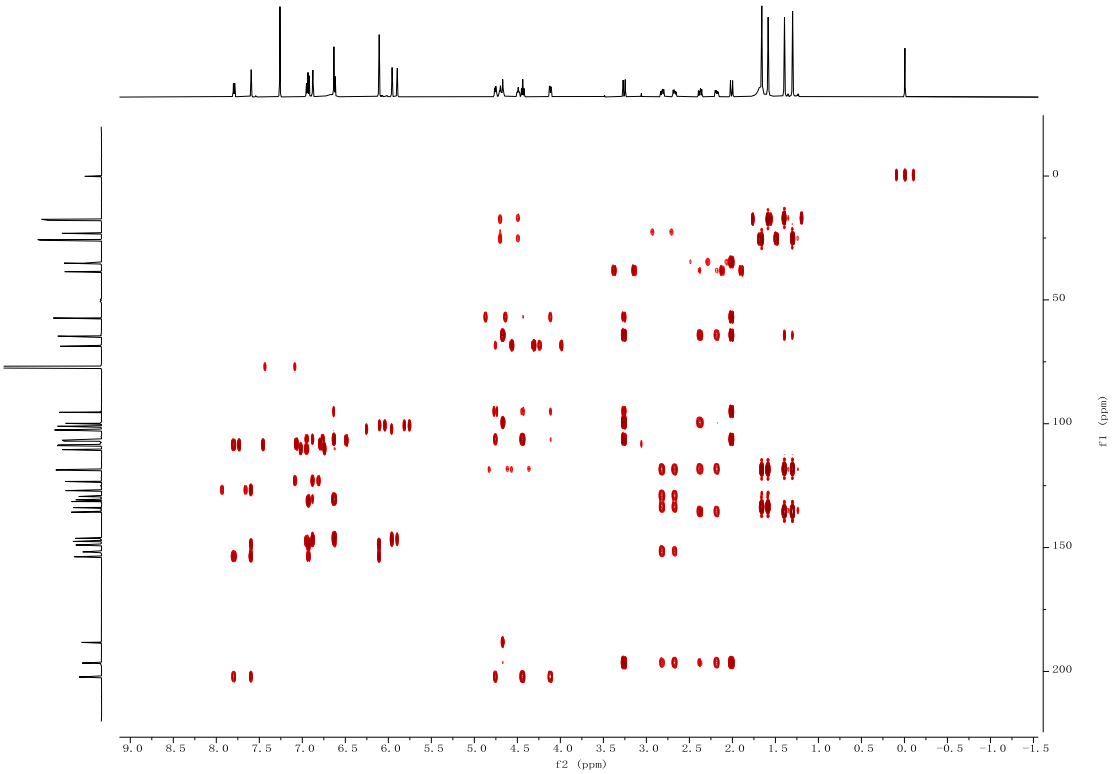


Figure S56. HMBC (600 MHz, $CDCl_3$) spectrum of **5**.

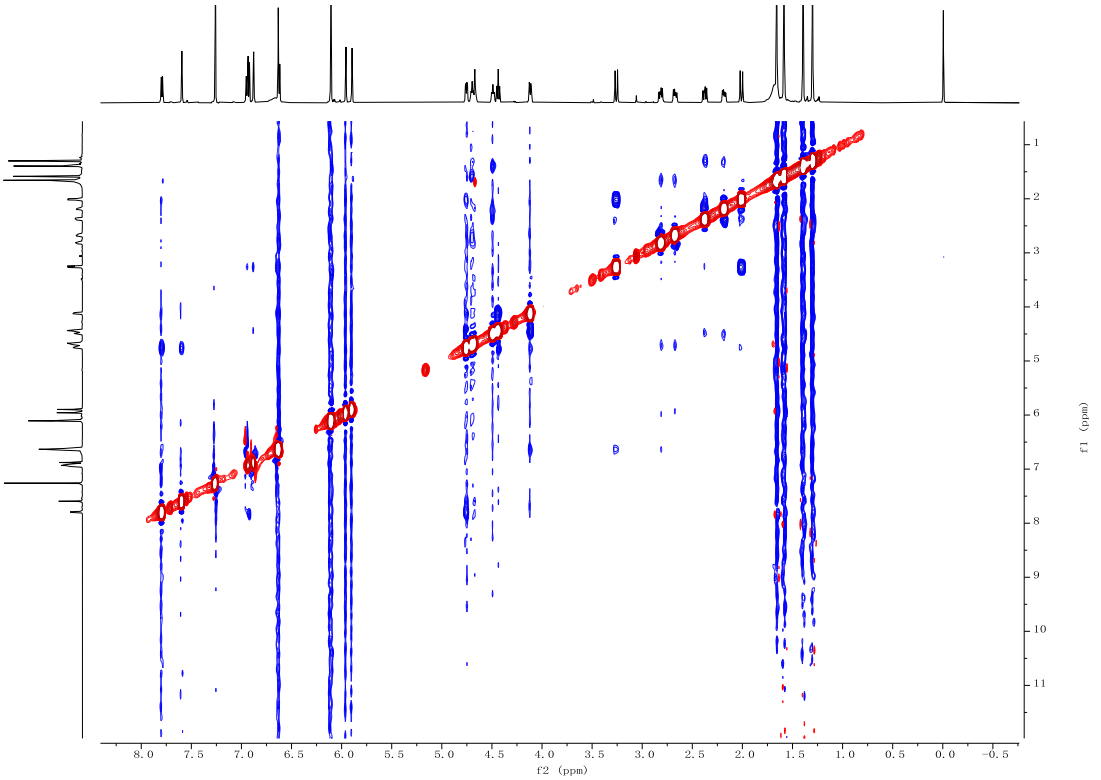


Figure S57. ^{1}H-^{1}H ROESY (600 MHz, $CDCl_3$) spectrum of **5**.

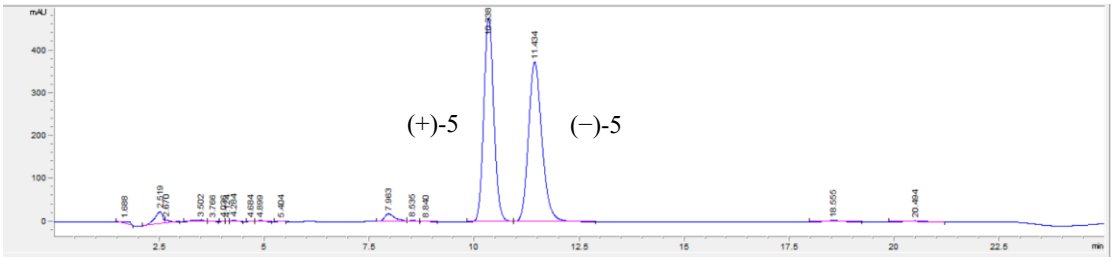
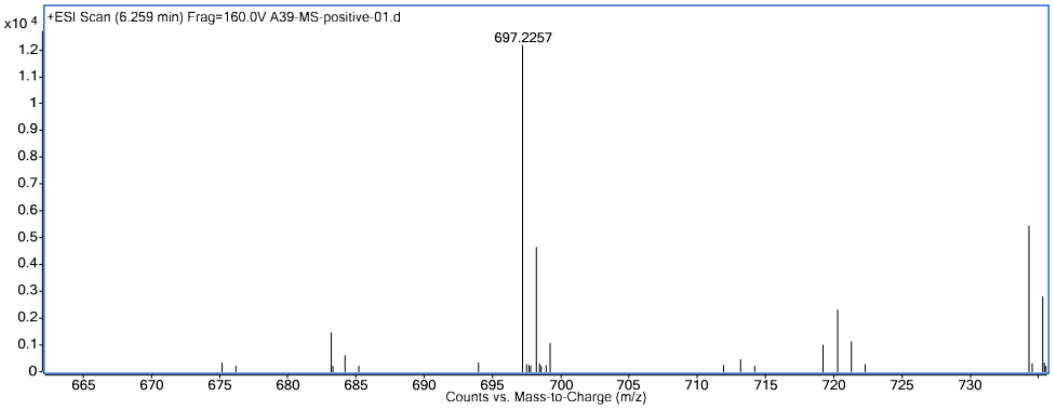


Figure S58. Chiral HPLC chromatogram of **5**.



Elemental Composition Calculator

Target m/z:	697.2257	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C37H38NaO12		697.2255		-0.17	

Figure S59. HRESIMS spectrum of **6**.

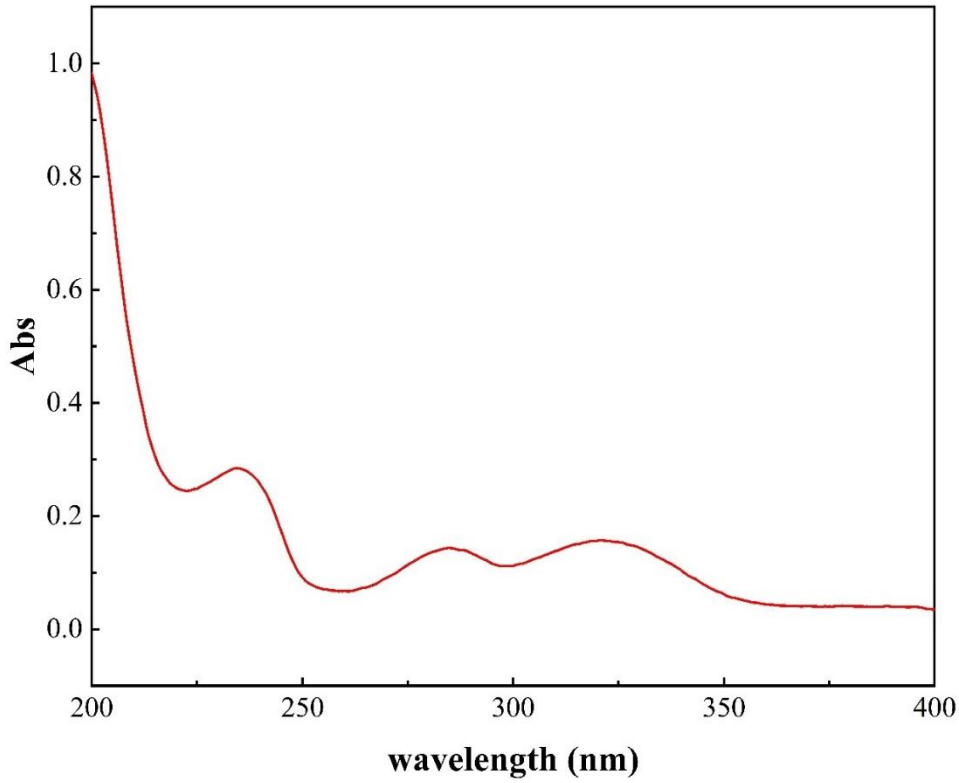


Figure S60. UV spectrum of **6**.

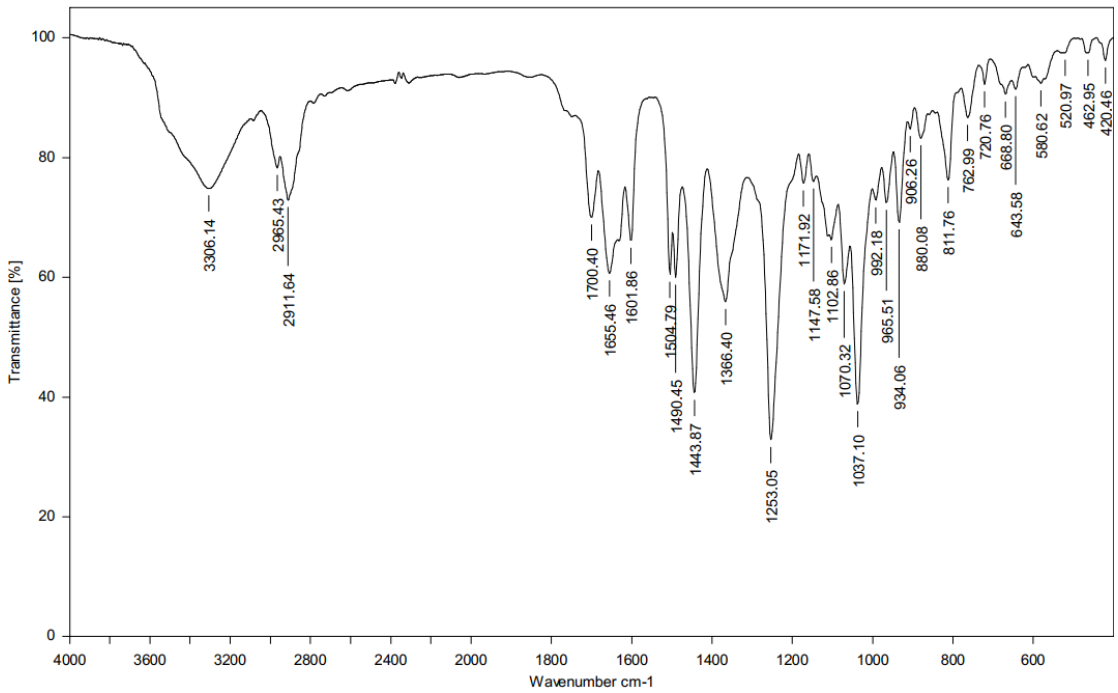


Figure S61. IR spectrum of **6**.

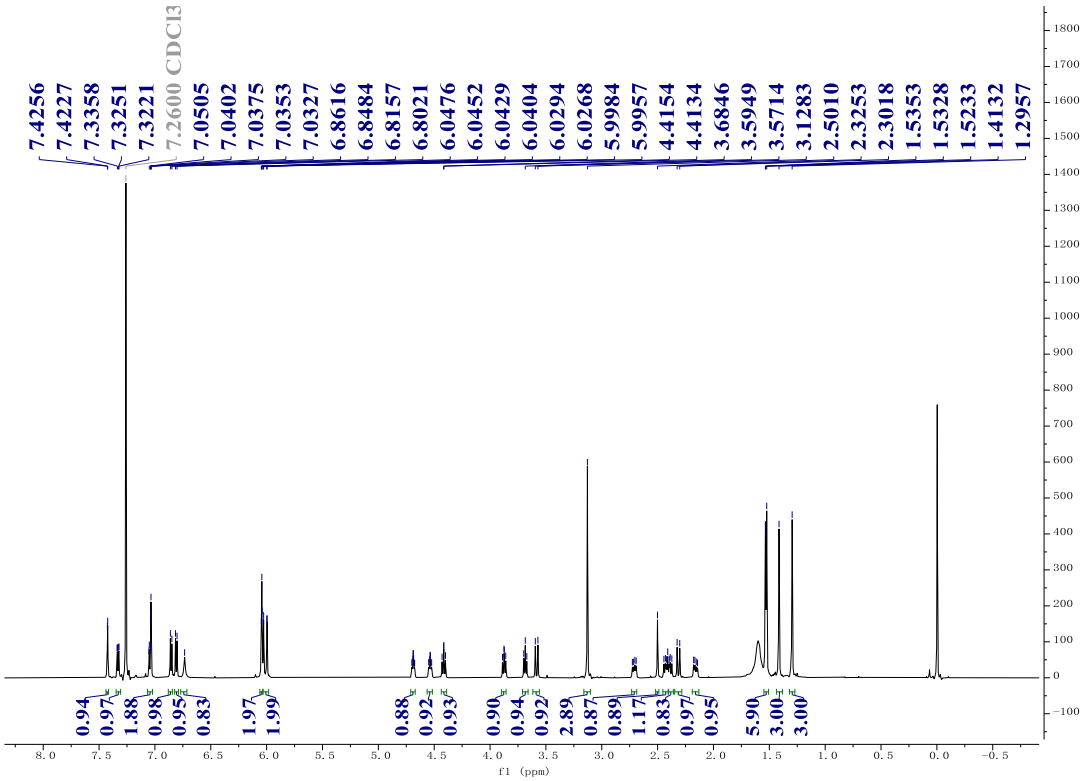


Figure S62. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **6**.

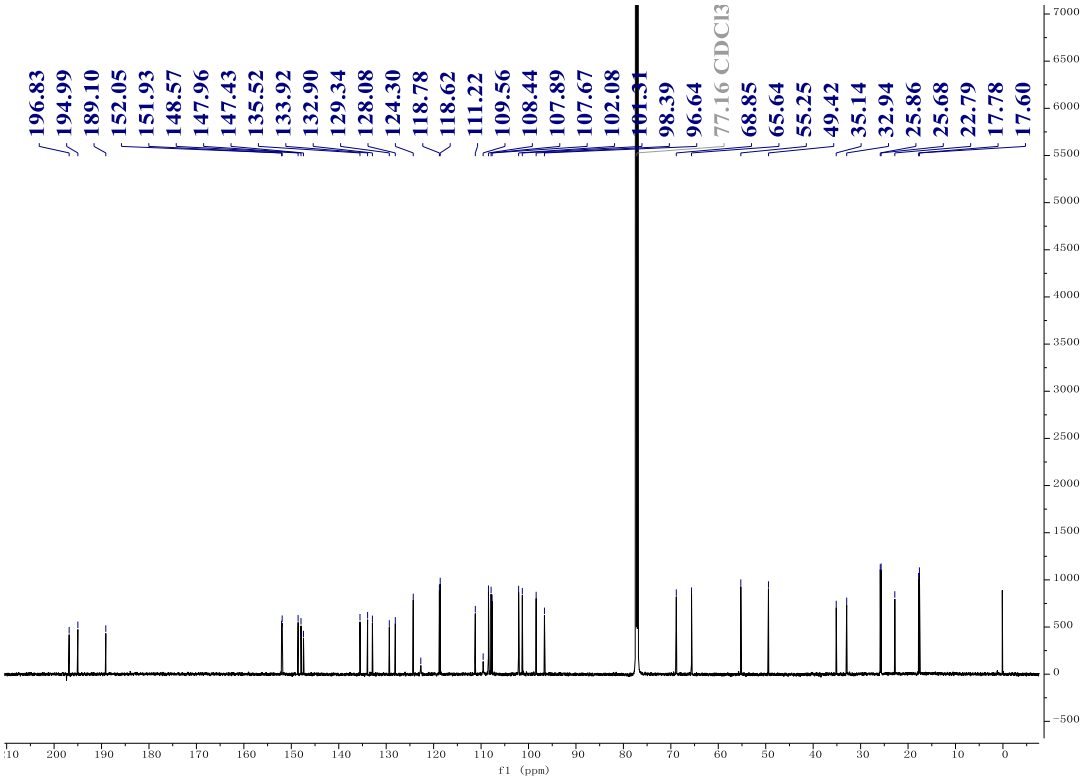


Figure S63. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **6**.

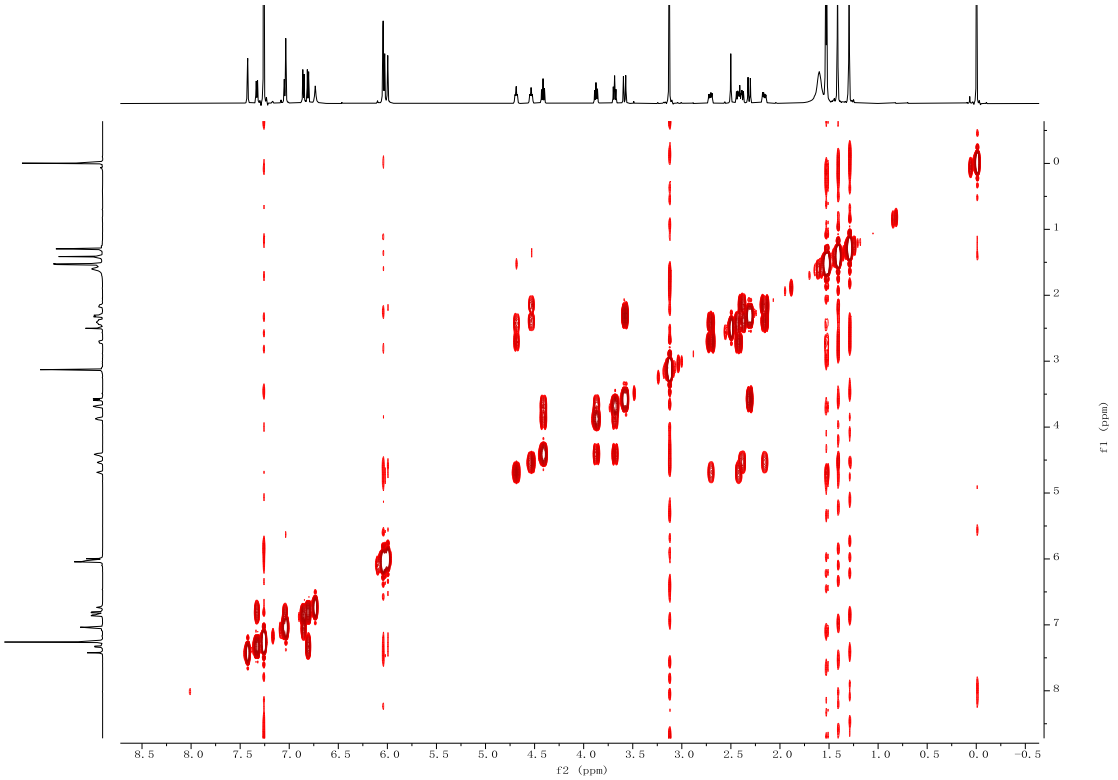


Figure S64. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **6**.

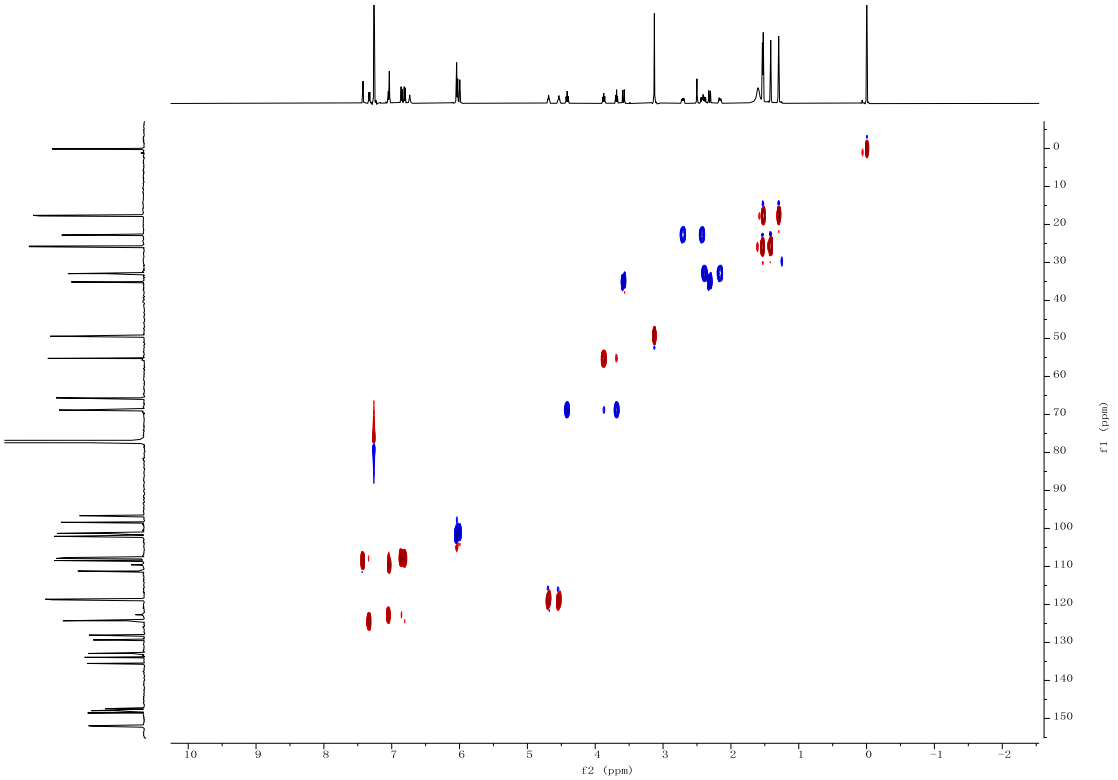


Figure S65. HSQC (600 MHz, $CDCl_3$) spectrum of **6**.

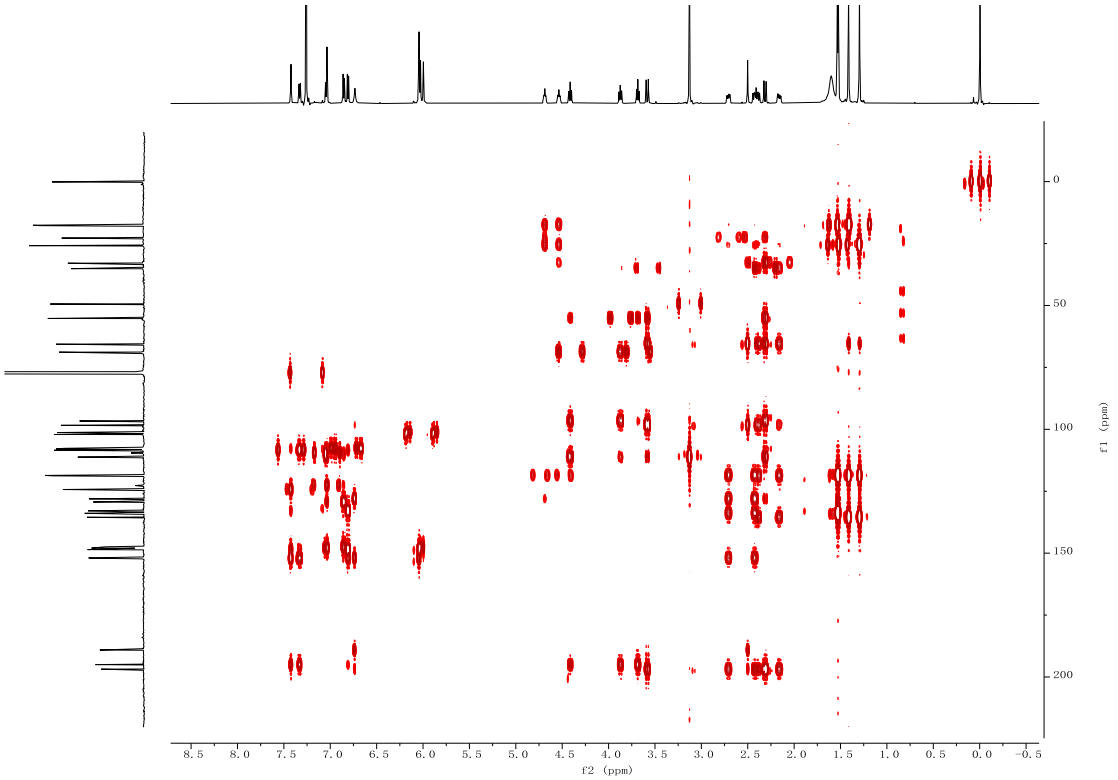


Figure S66. HMBC (600 MHz, $CDCl_3$) spectrum of **6**.

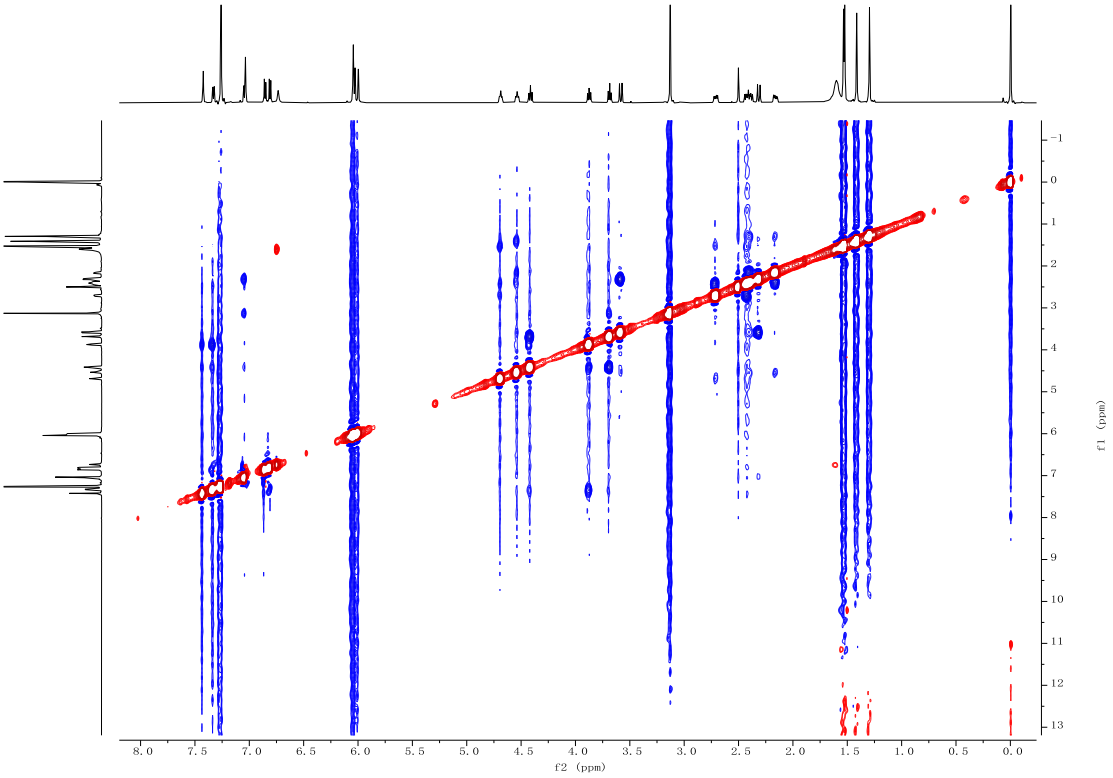


Figure S67. ^{1}H-^{1}H ROESY (600 MHz, $CDCl_3$) spectrum of **6**.

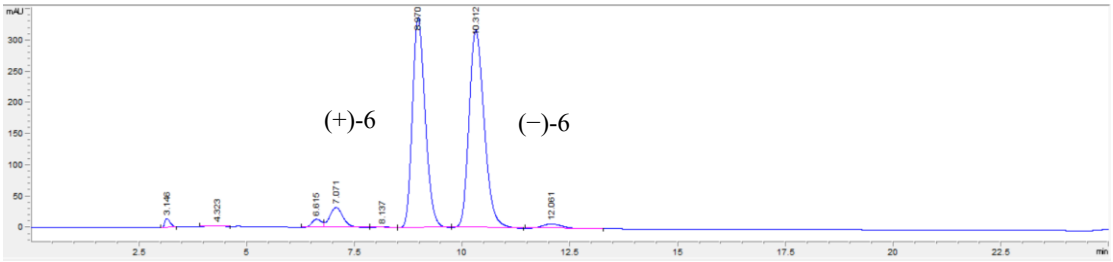


Figure S68. Chiral HPLC chromatogram of **6**.