Electronic Supplementary Material (ESI) for RSC Advances.

Isolation, Resolution and Biological Evaluation of Pestalachlorides E and F Containing Both Point and Axial Chirality

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[d]Laboratory for Marine Drugs and Bioproducts, Qingdao National Laboratory for Marine Science and Technology, Qingdao 266200, People's Republic of China

List of Supporting Information

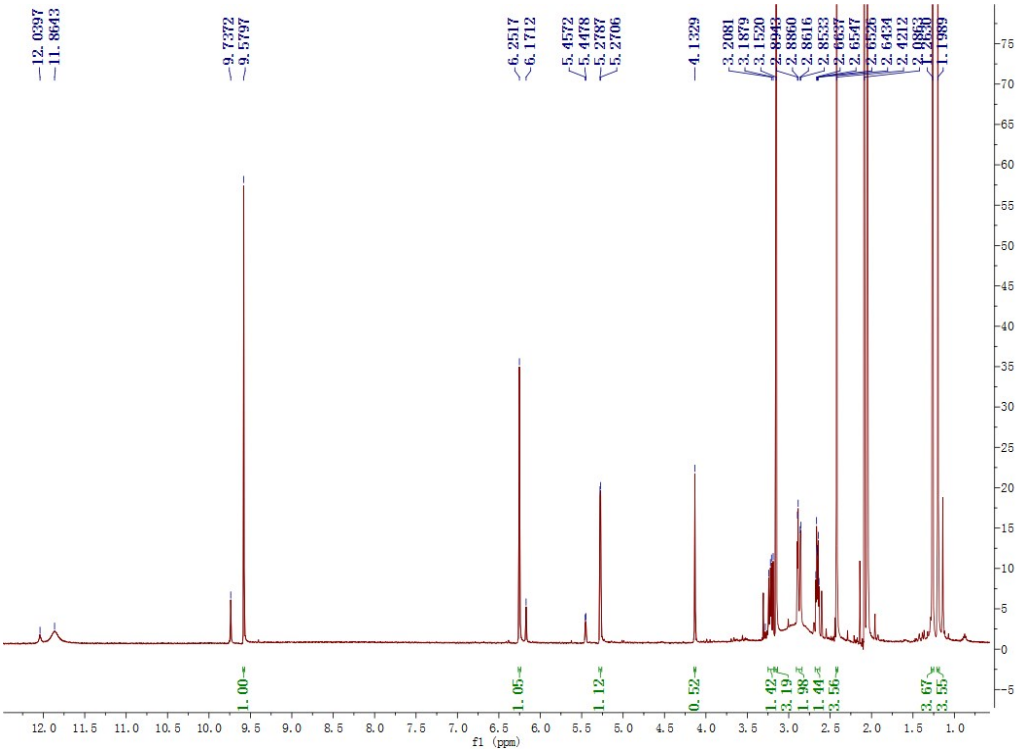

Figure S1. ^{1}H NMR (500 MHz) spectrum of compound **1** in acetone-d_6

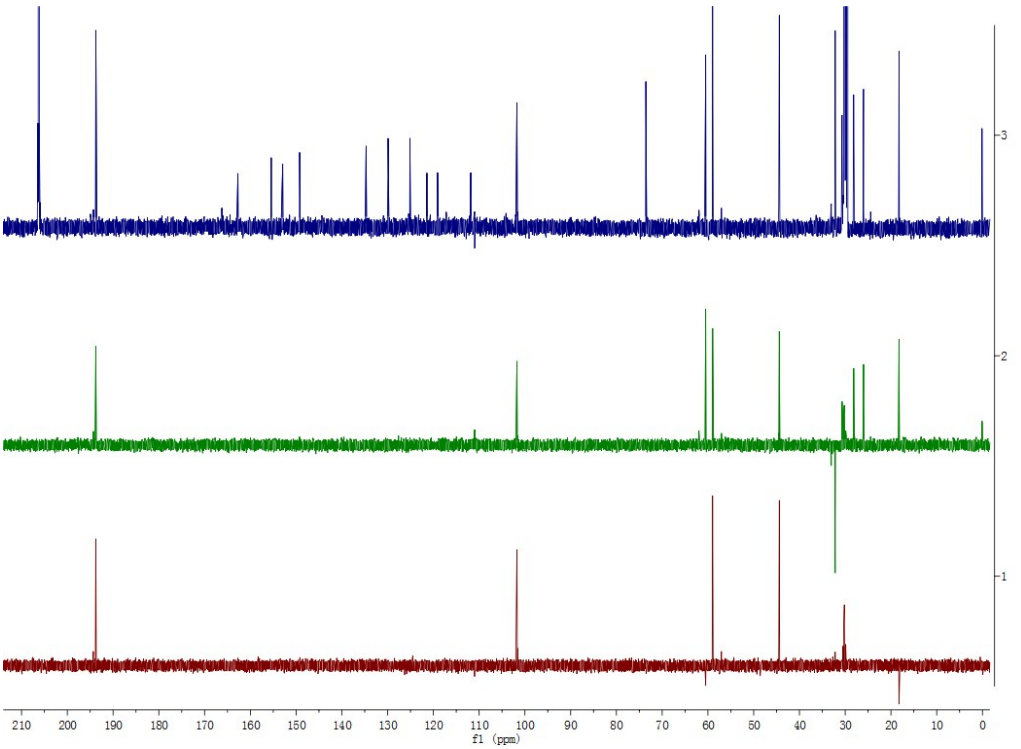

Figure S2. ^{13}C NMR and DEPT (125 MHz) spectra of compound **1** in acetone-d_6

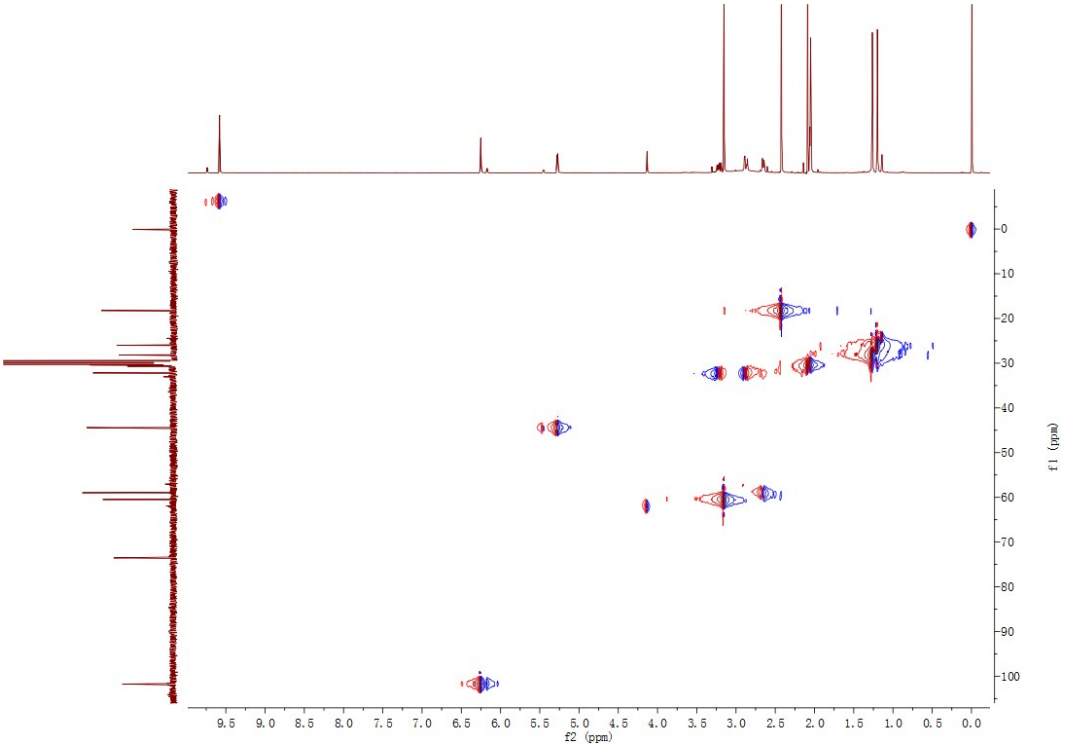

Figure S3. HSQC spectrum of compound **1** in acetone-d_6

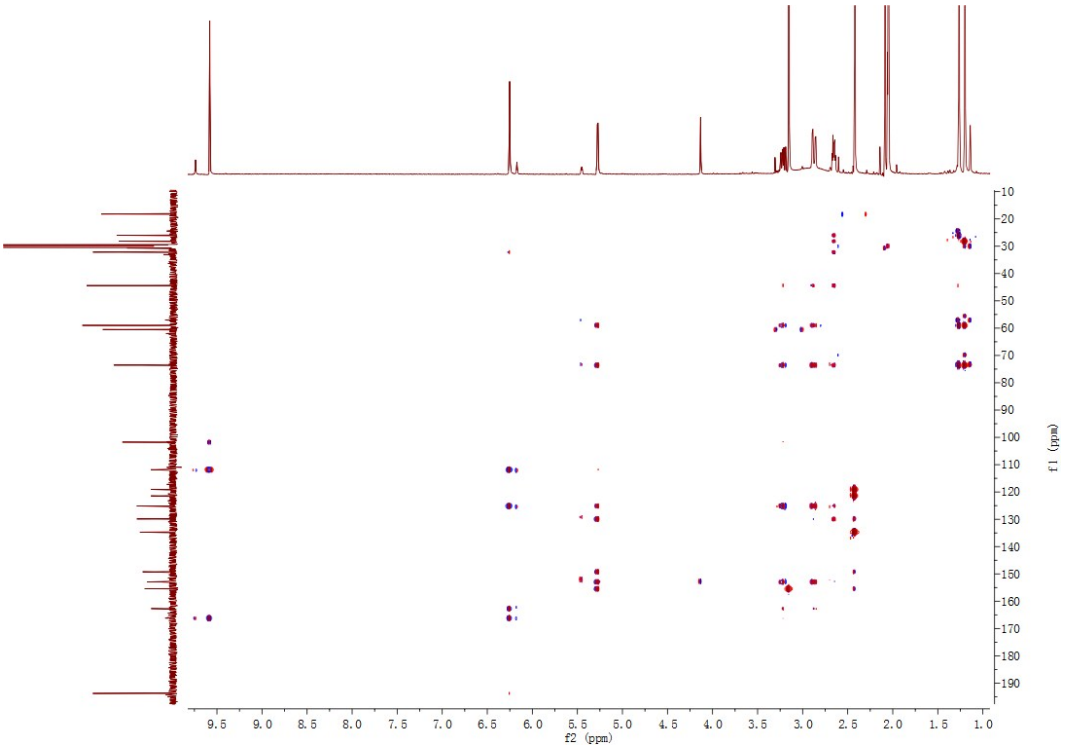

Figure S4. HMBC spectrum of compound **1** in acetone-d_6

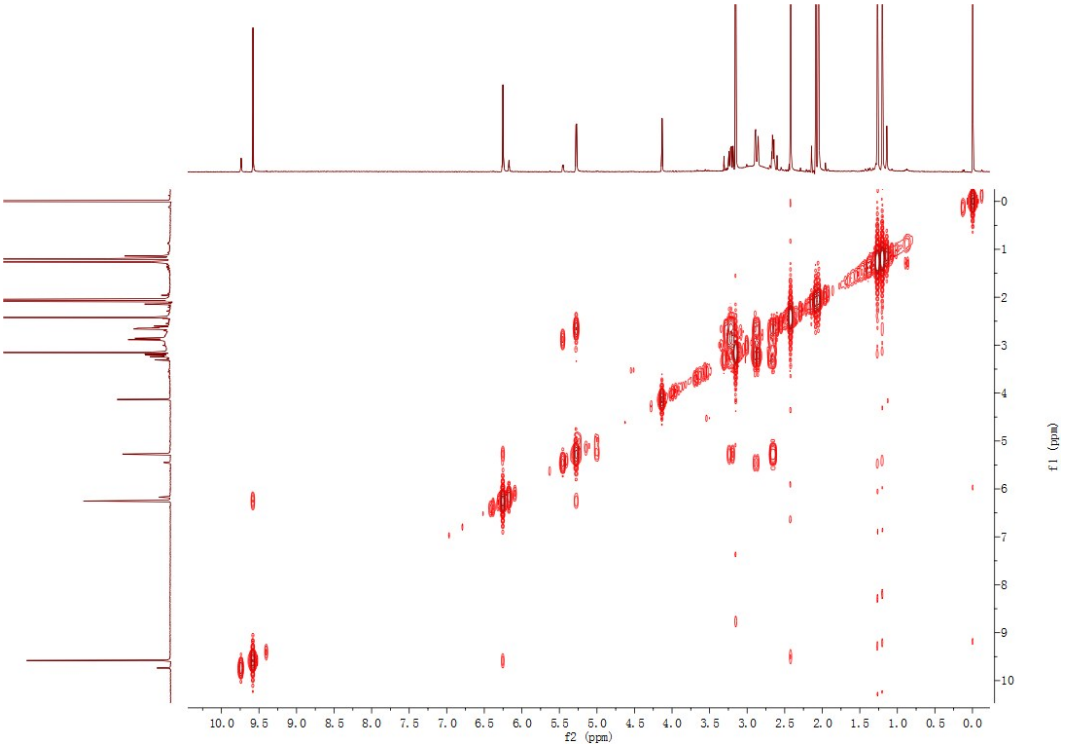

Figure S5. ^{1}H-^{1}H COSY spectrum of compound **1** in acetone-d_6

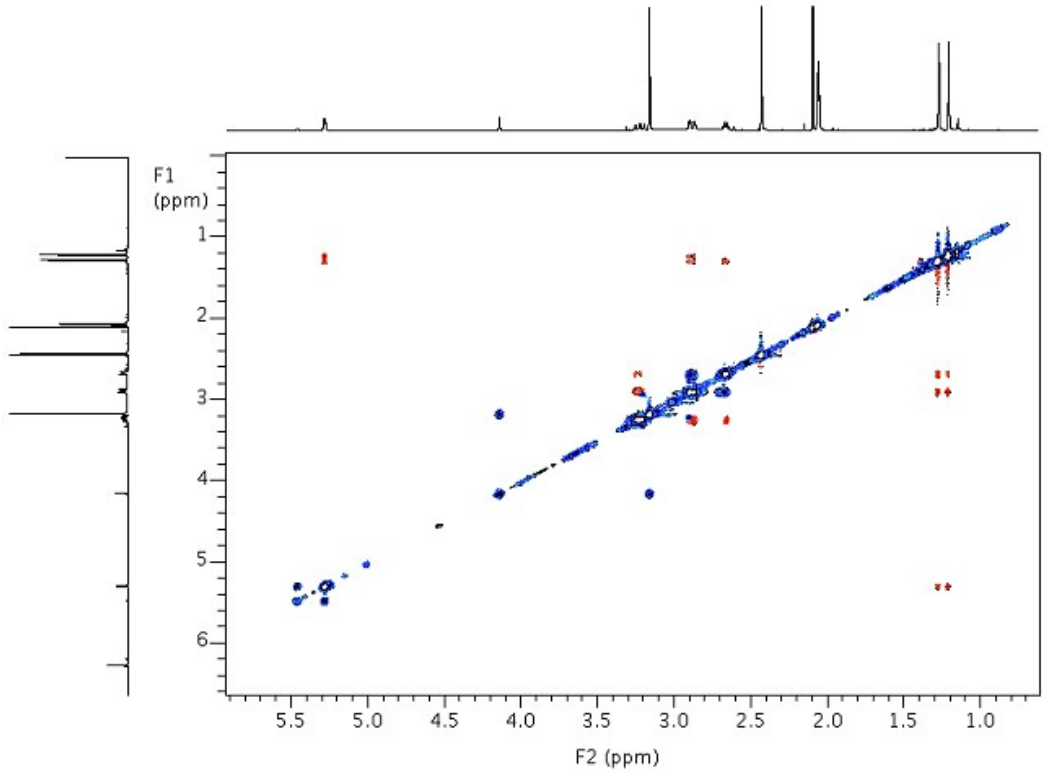

Figure S6. NOESY spectrum of compound **1** in acetone-d_6

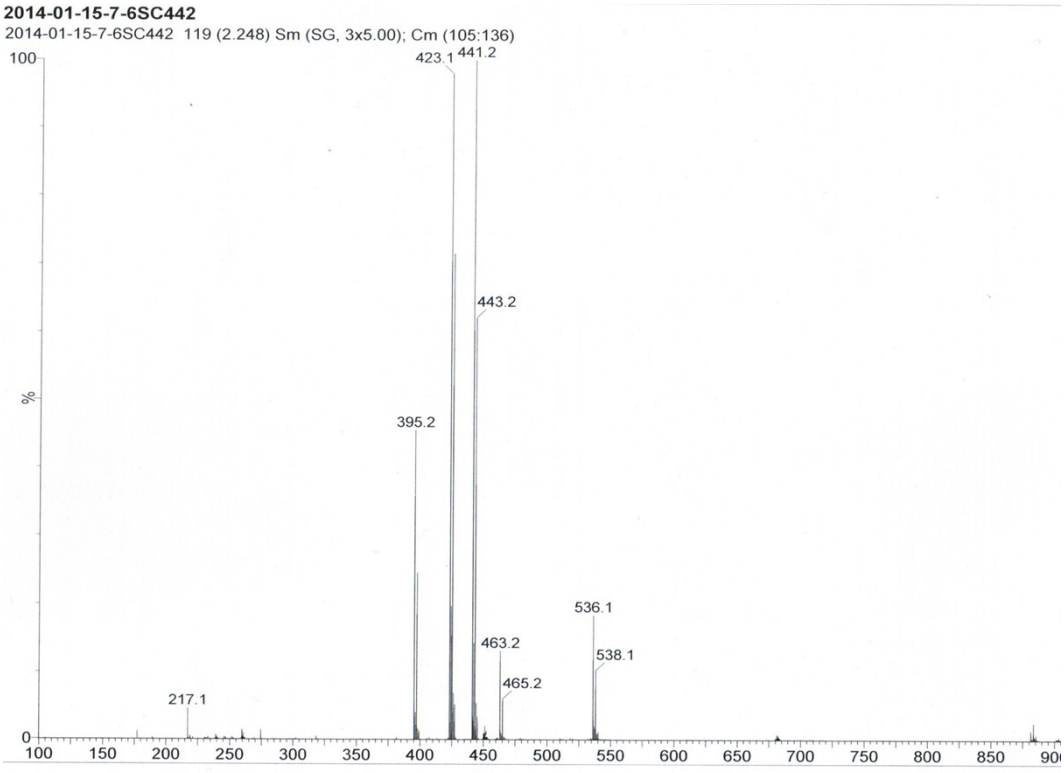

Figure S7. ESIMS spectrum of compound **1**

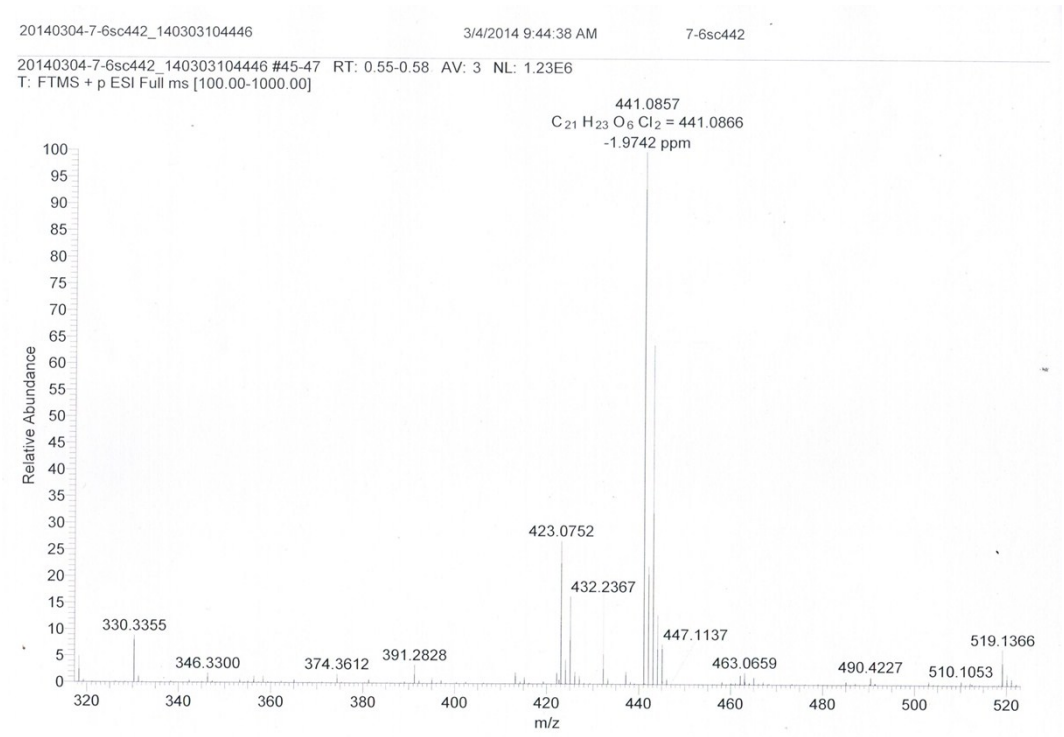

Figure S8. HRESIMS spectrum of compound **1**

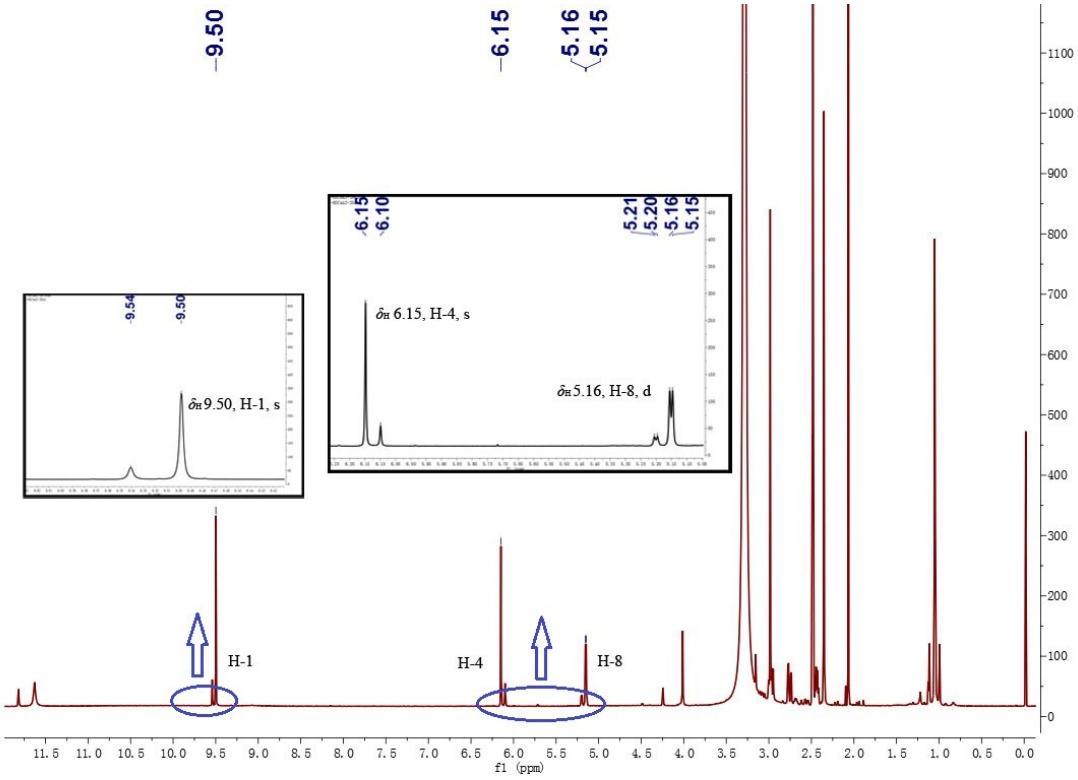

Figure S9. [1]H NMR (500 MHz) spectrum of compound **1** in DMSO-d_6 at 35℃

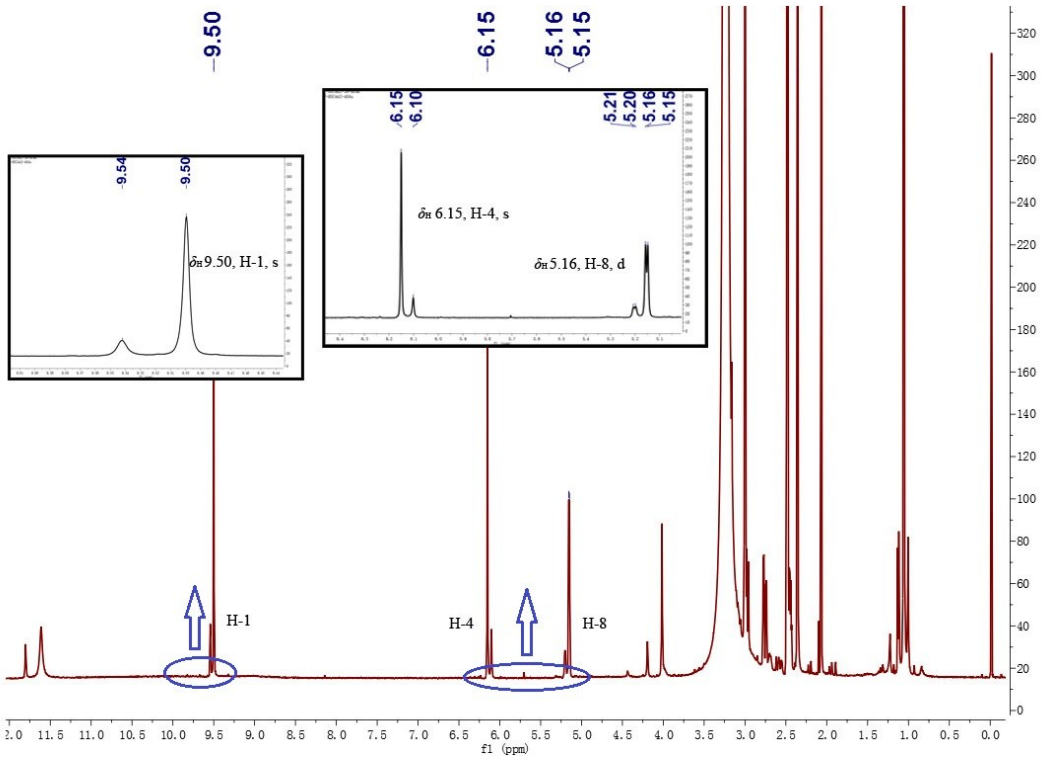

Figure S10. [1]H NMR (500 MHz) spectrum of compound **1** in DMSO-d_6 at 45℃

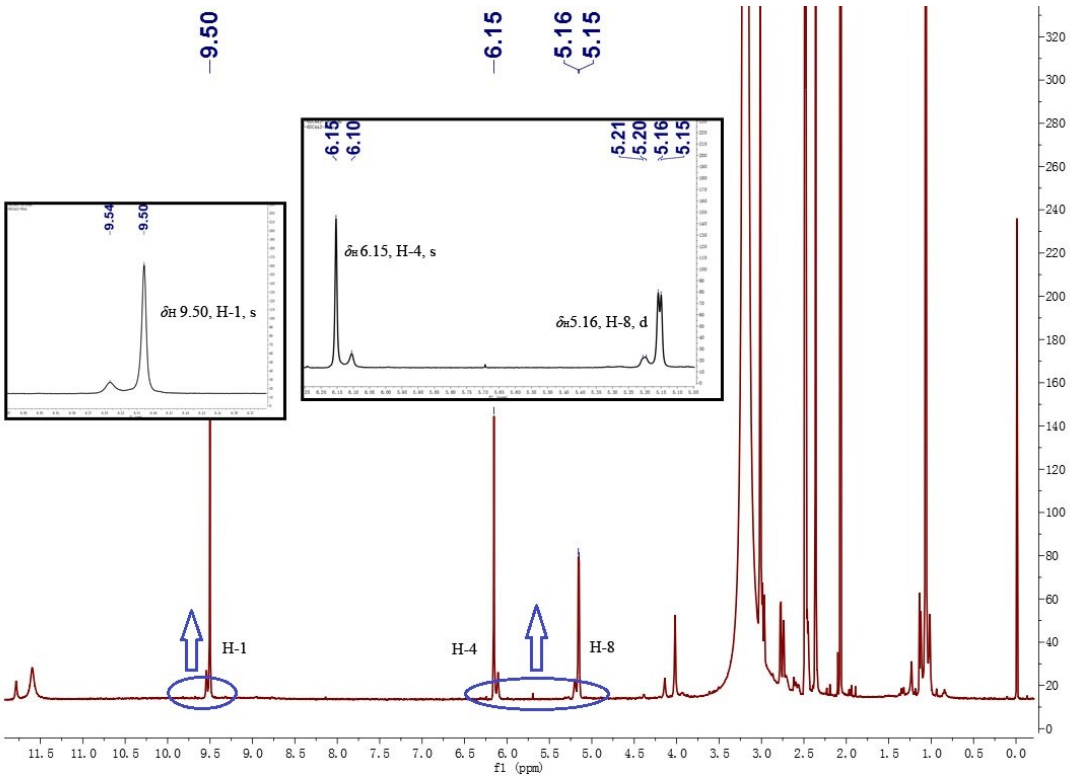

Figure S11. [1]H NMR (500 MHz) spectrum of compound **1** in DMSO-d_6 at 55℃

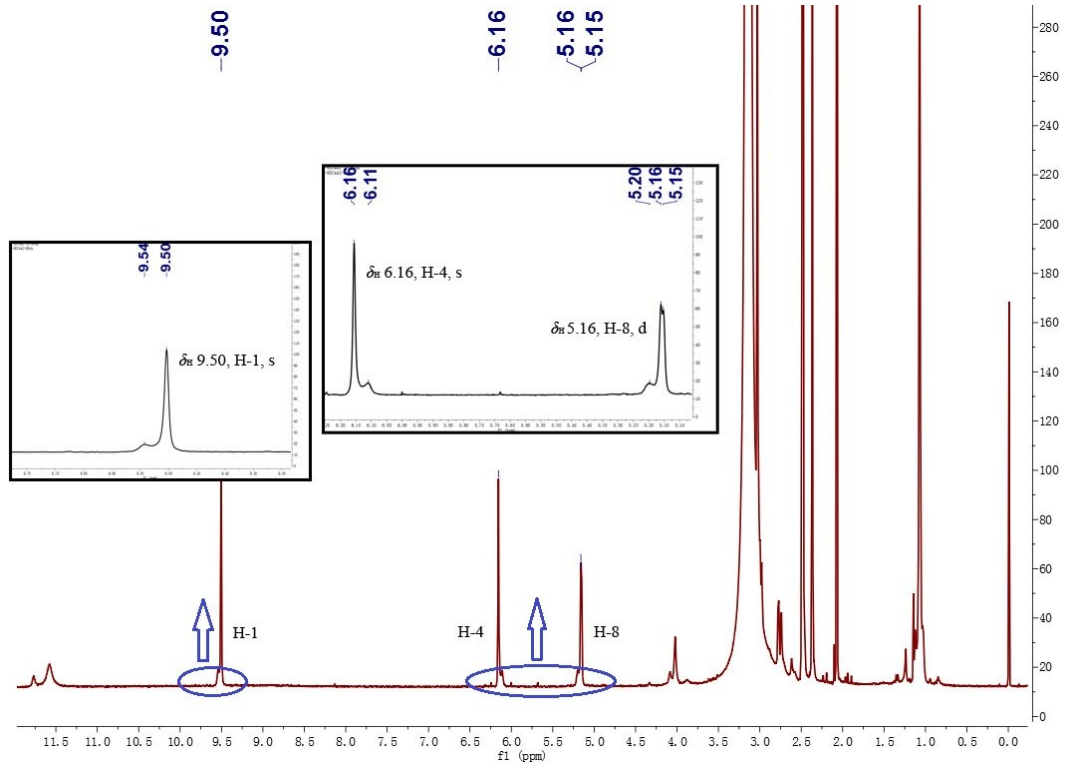

Figure S12. [1]H NMR (500 MHz) spectrum of compound **1** in DMSO-d_6 at 65℃

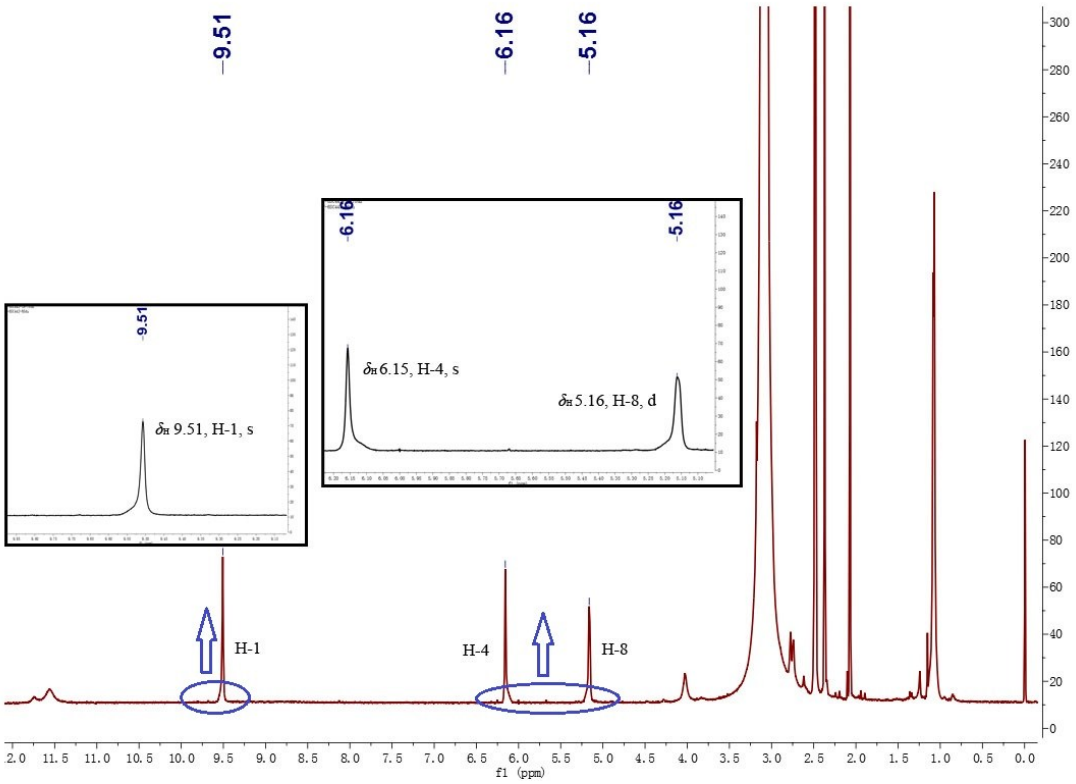

Figure S13. [1]H NMR (500 MHz) spectrum of compound **1** in DMSO-d_6 at 75℃

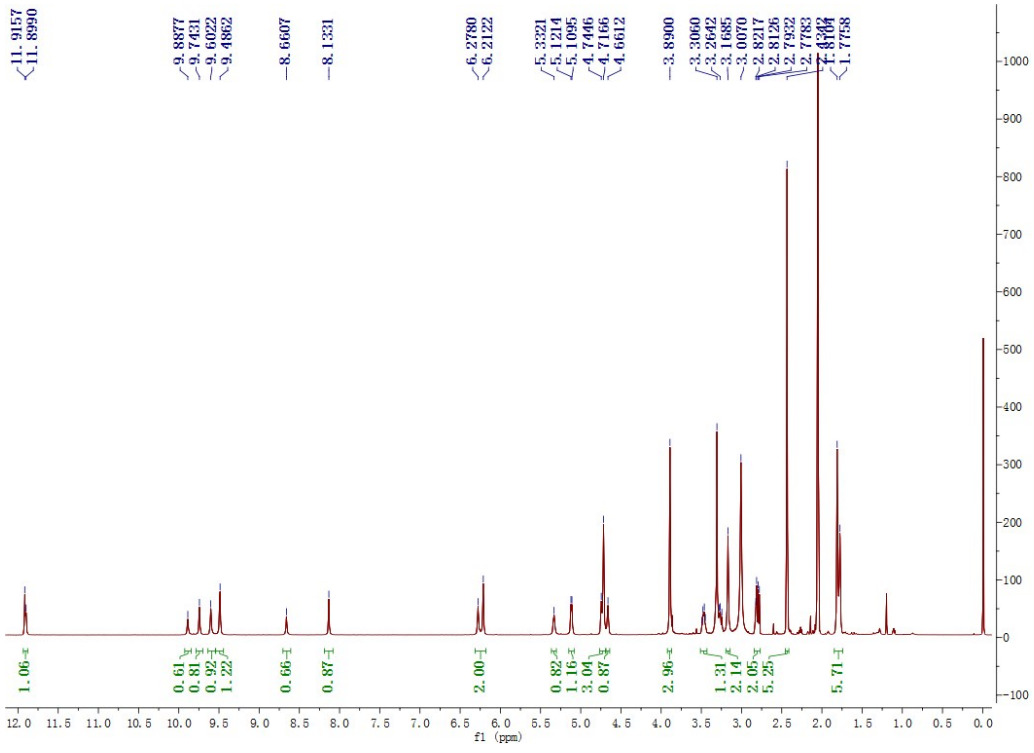

Figure S14. [1]H NMR (500 MHz) spectrum of compound **2** in acetone-d_6

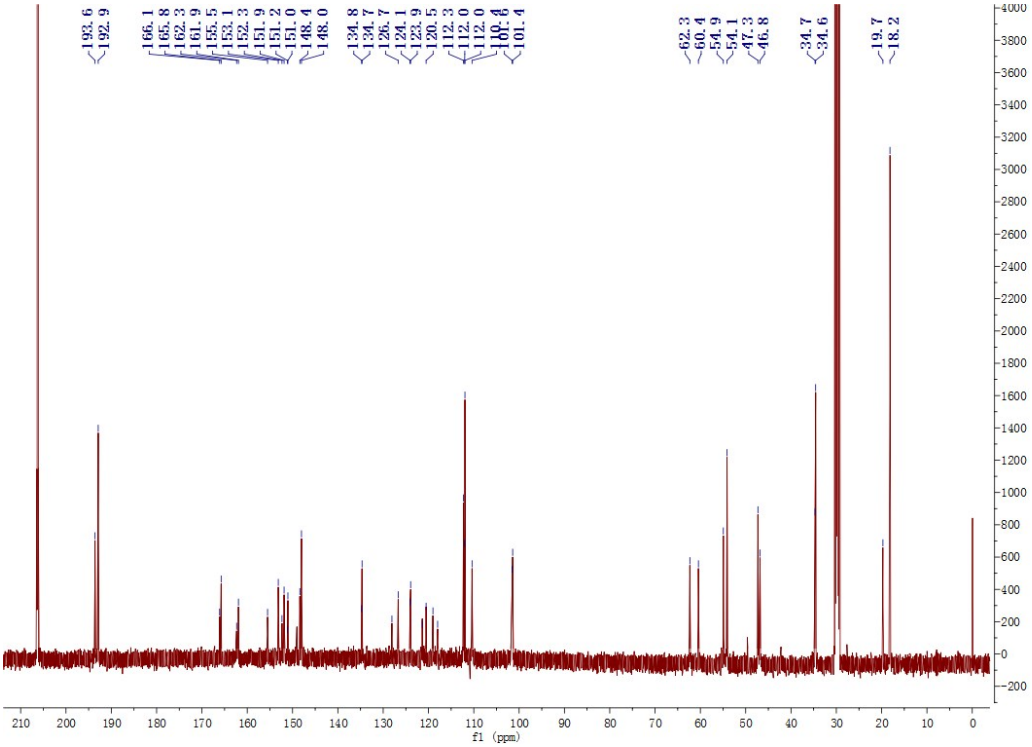

Figure S15. ^{13}C NMR (125 MHz) spectrum of compound **2** in acetone-d_6

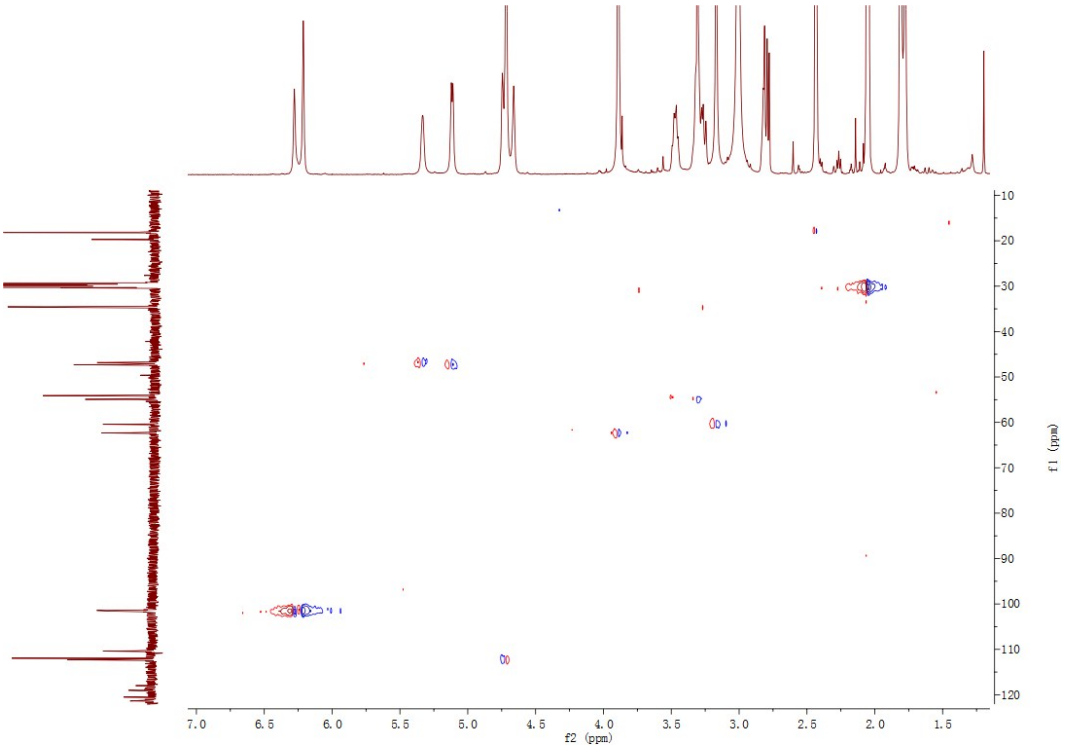

Figure S16. HSQC spectrum of compound **2** in acetone-d_6

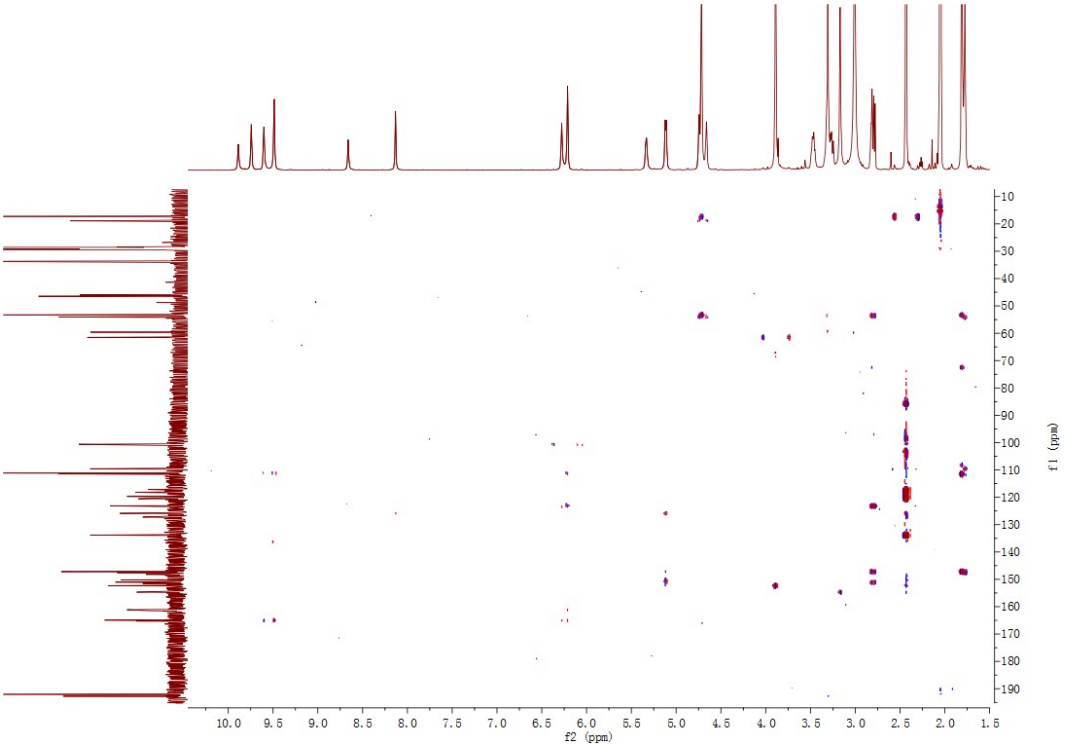

Figure S17. HMBC spectrum of compound **2** in acetone-d_6

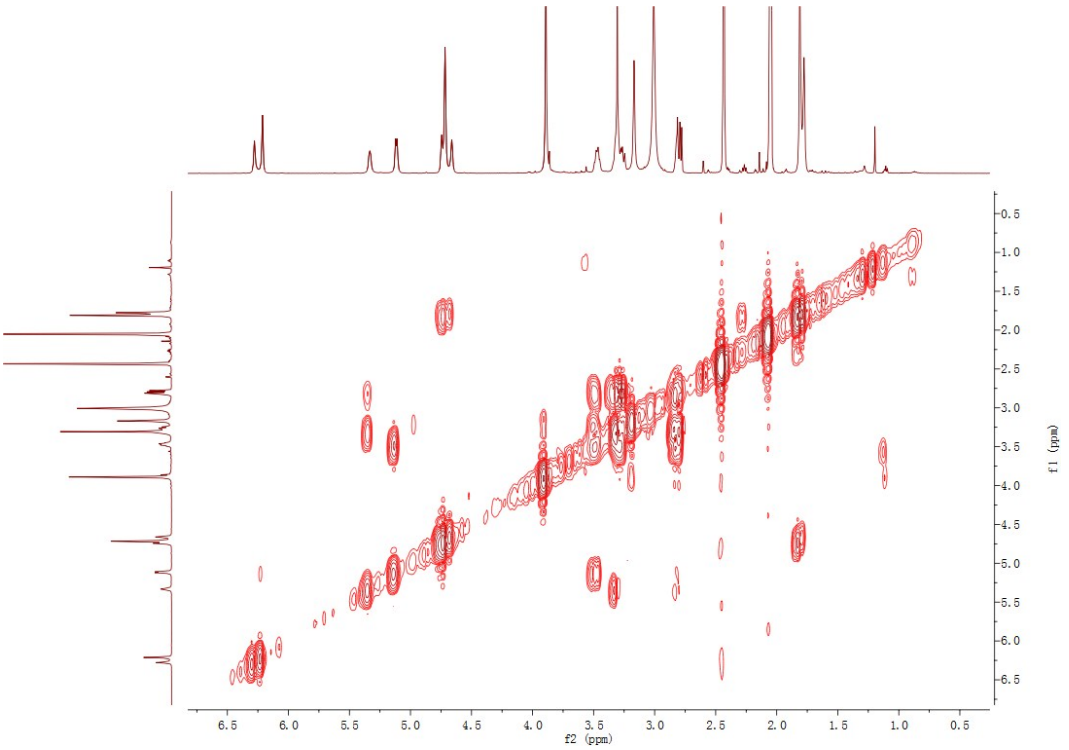

Figure S18. ^{1}H-^{1}H COSY spectrum of compound **2** in acetone-d_6

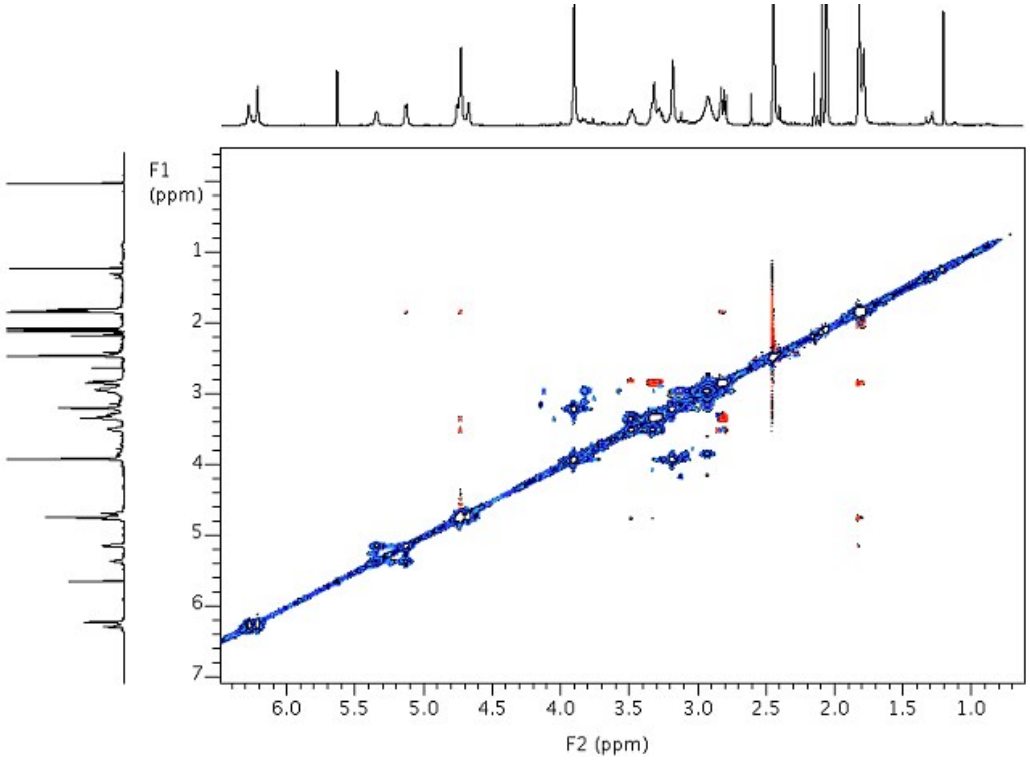

Figure S19. NOESY spectrum of compound **2** in acetone-d_6

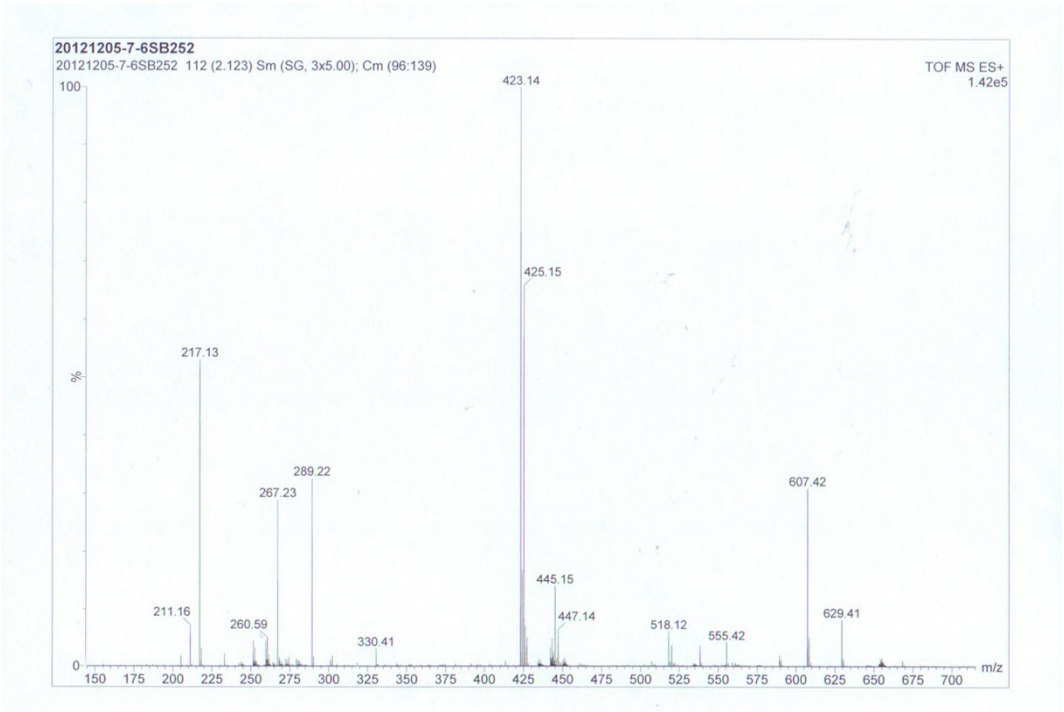

Figure S20. ESIMS spectrum of compound **2**

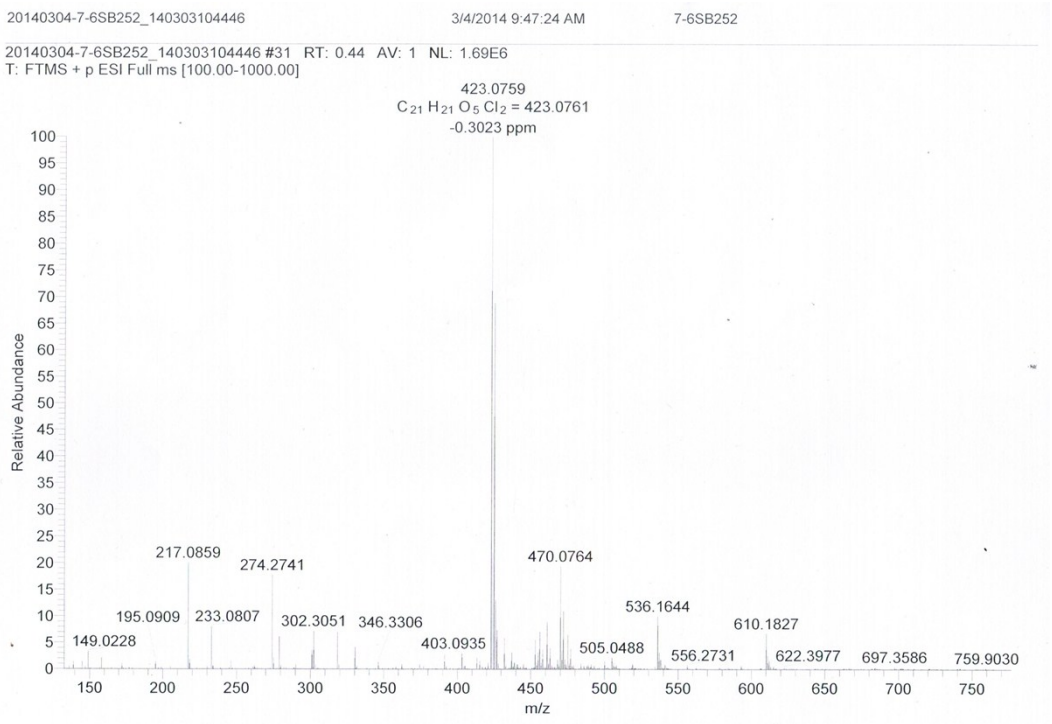

Figure S21. HRESIMS spectrum of compound

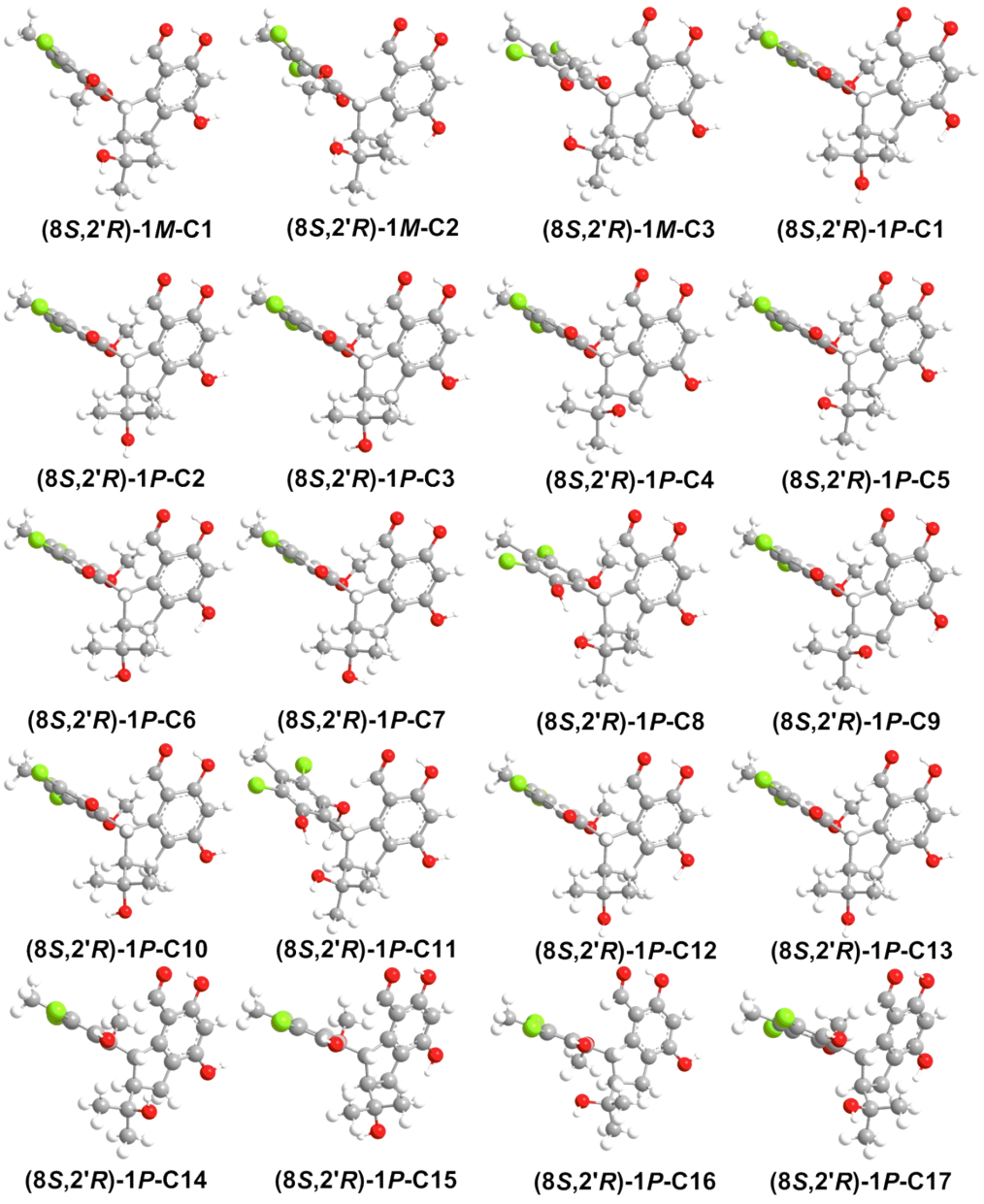

Figure S22. B3LYP/6-31+G(d) optimized lowest energy 3D conformers of compound (8*S*,2′*R)*-**1** (in *M* and *P* types of atrop-isomers)

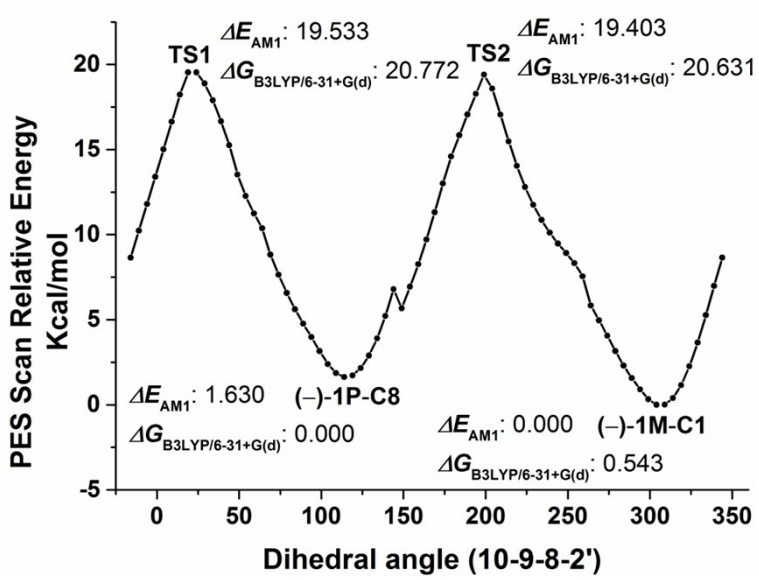

Figure S23. 1D PES scan on the dihedral angle of 10-9-8-2′ in (8*S*,2′*R*)-**1M-C1** and the relative energy profiles of the related transitional state and lowest energy conformers

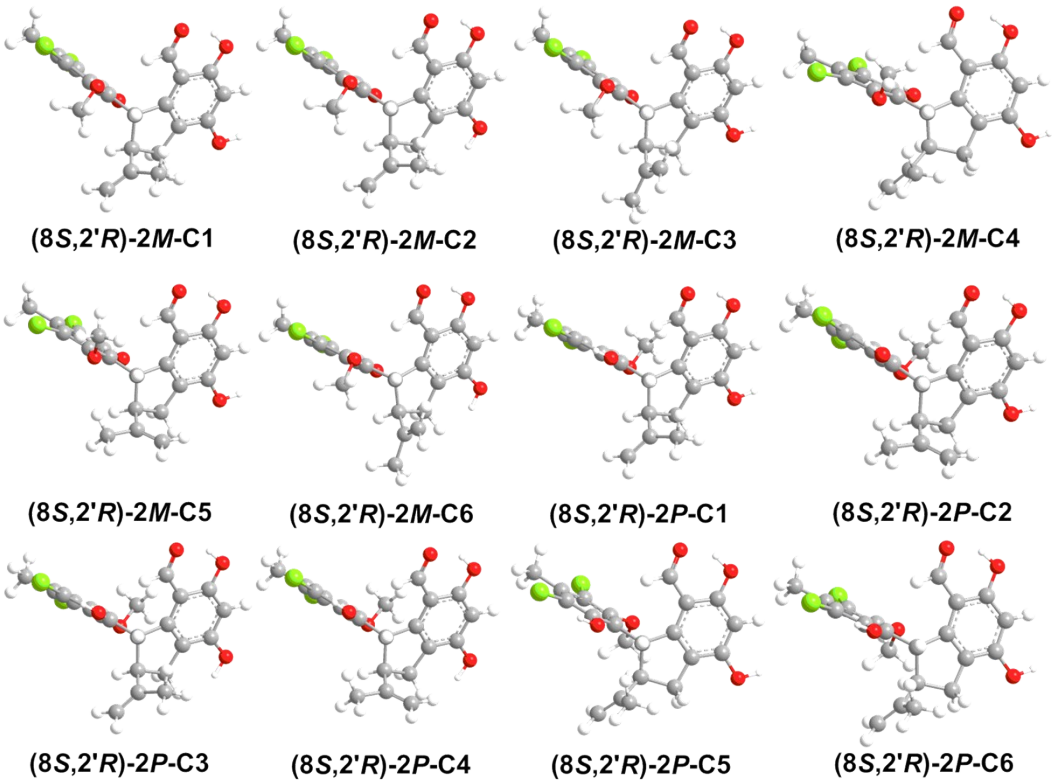

Figure S24. B3LYP/6-31+G(d) optimized lowest energy 3D conformers of compound (8*S*,2′*R*)-**2** (in *M* and *P* types of atrop-isomers)

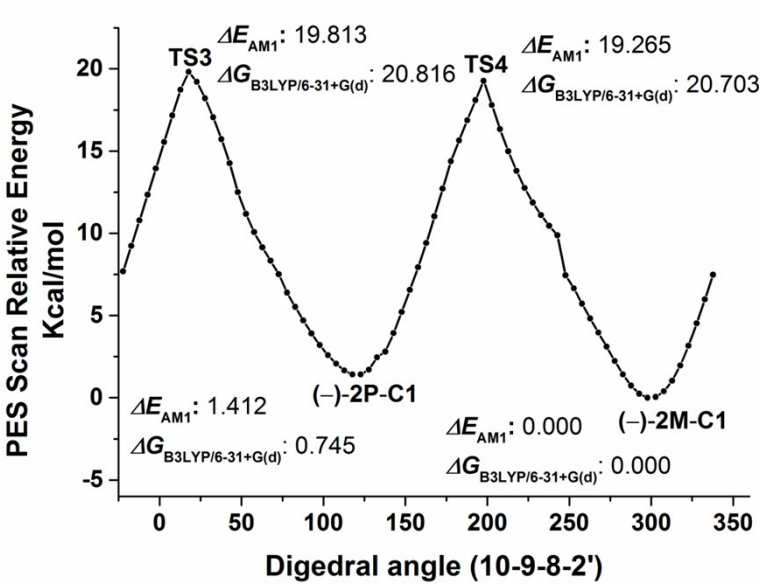

Figure S25. 1D PES scan on the dihedral angle of 10-9-8-2′ in (8*S*,2′*R*)-**2M-C1** and the relative energy profiles of the related transitional state and lowest energy conformers

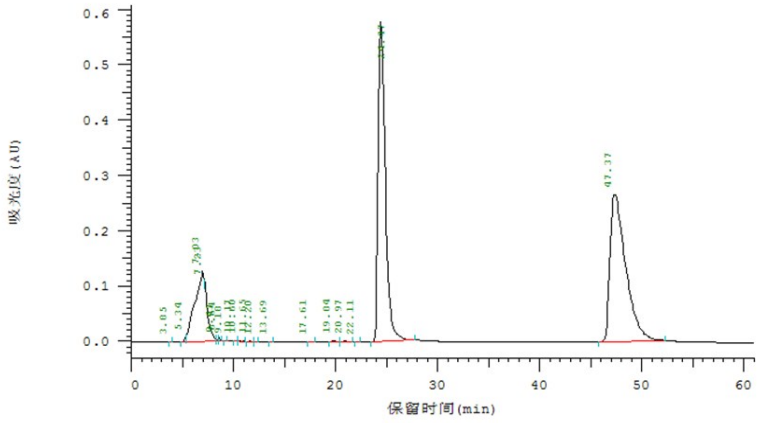

Figure S26. Chiral HPLC spectrum for compound **1** (85% n-hexane/isopropanol, 2.0 mL/min)

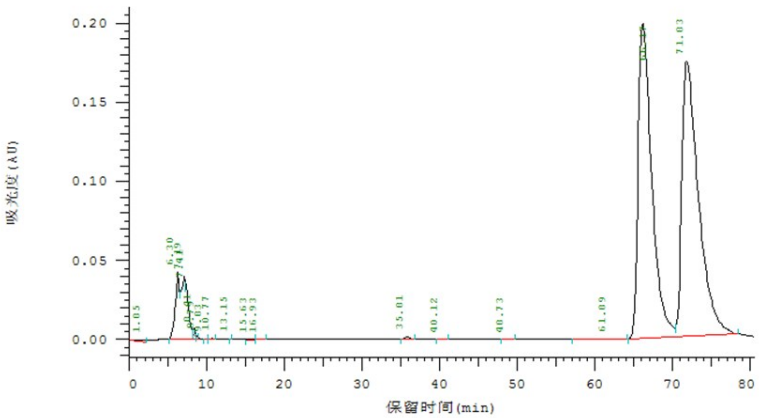

Figure S27. Chiral HPLC spectrum for compound **2** (95% n-hexane/isopropanol, 2.0 mL/min)

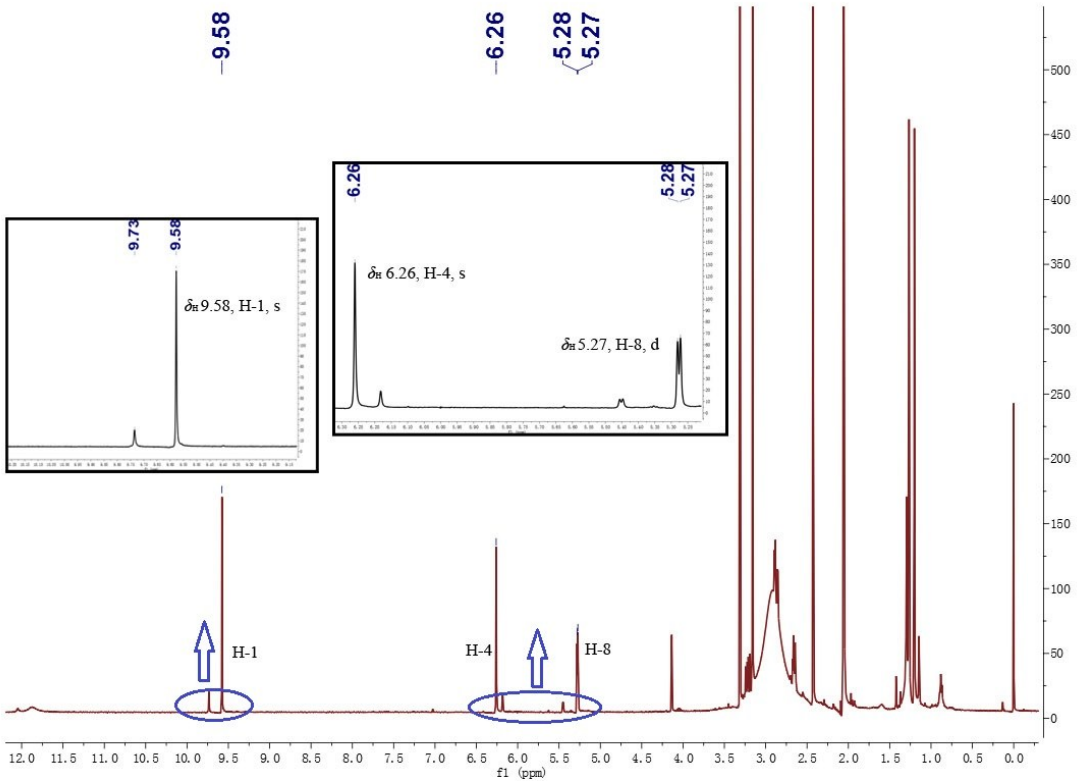

Figure S28. [1]H NMR (500 MHz) spectrum of compound (+)-**1** in acetone-d_6

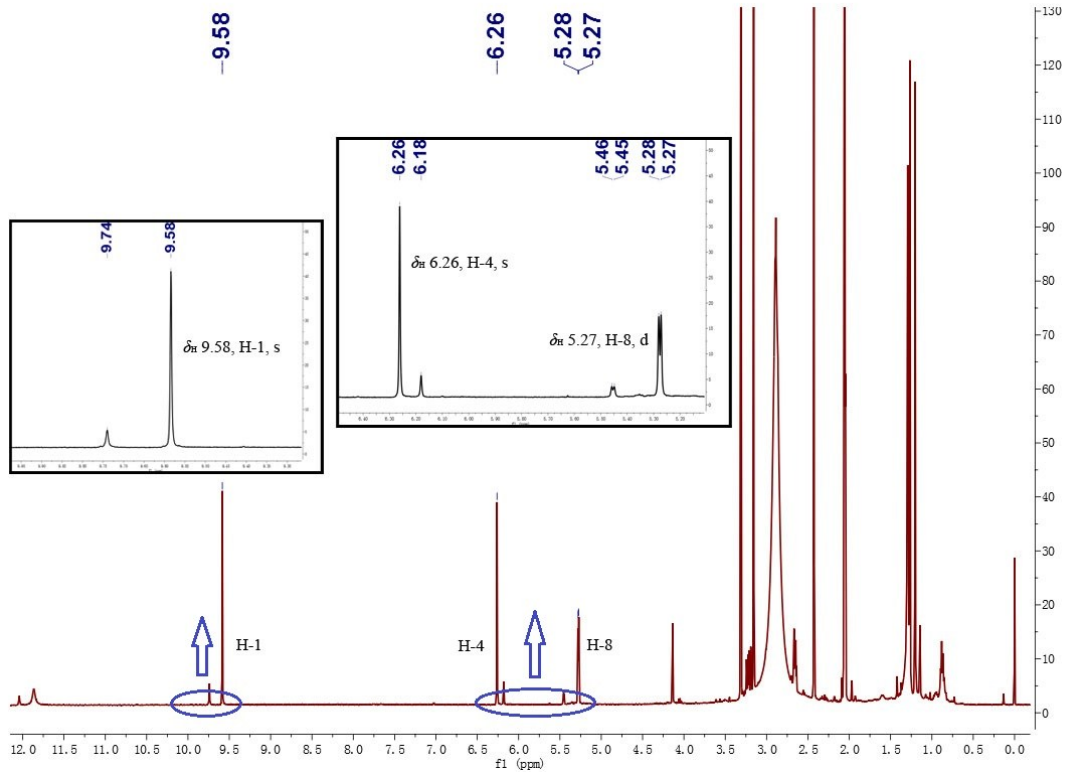

Figure S29. [1]H NMR (500 MHz) spectrum of compound (−)-**1** in acetone-d_6

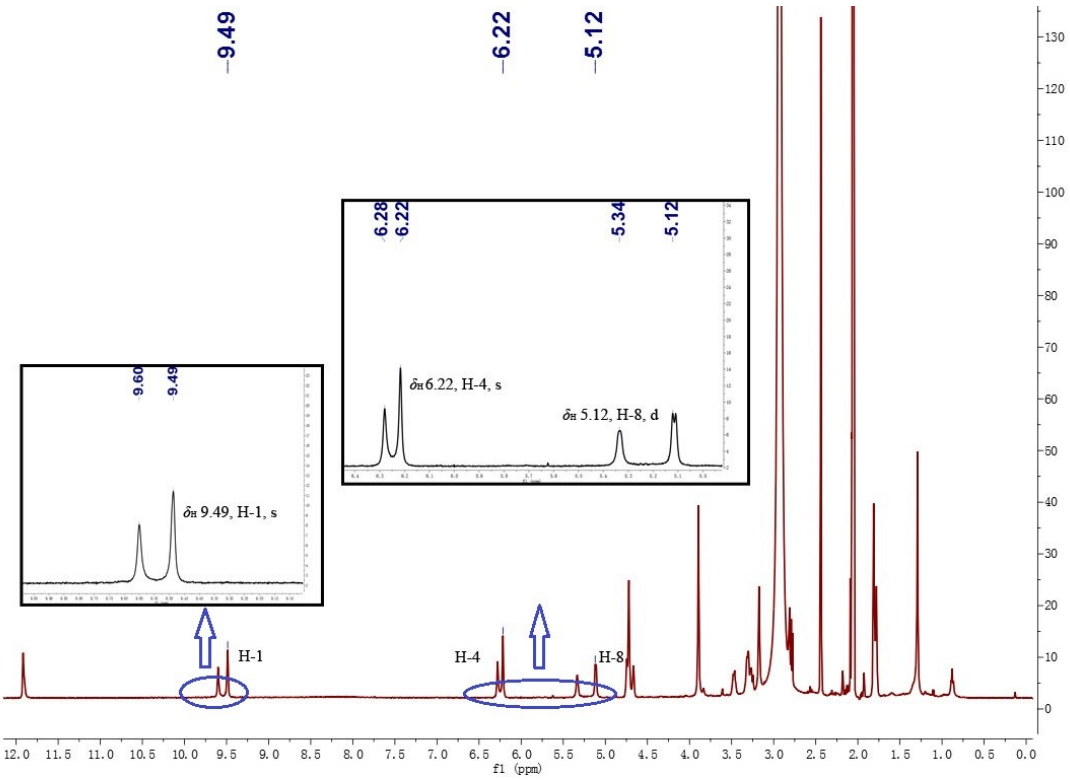

Figure S30. ^{1}H NMR (500 MHz) spectrum of compound (+)-**2** in acetone-d_6

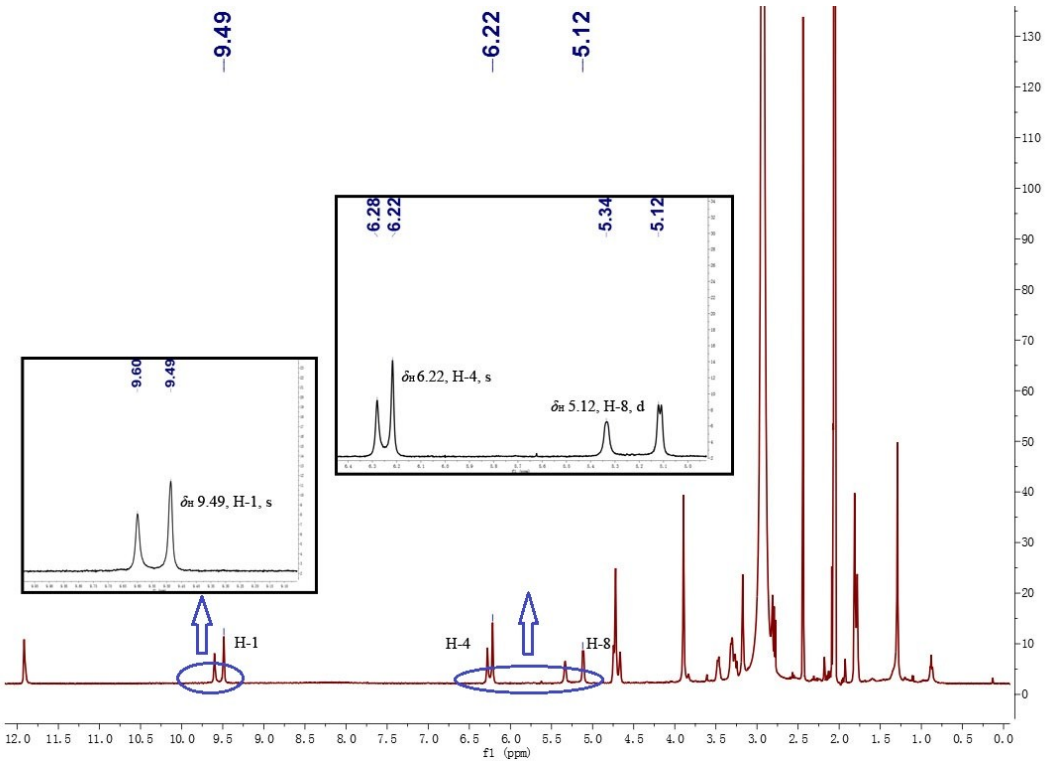

Figure S31. ^{1}H NMR (500 MHz) spectrum of compound (–)-**2** in acetone-d_6

Conformers	Experimental	Calculated	Occupation
(8*S*,2′*R*)-**1*M*-C3**	4.13	4.133917	**1b** minor
(8*S*,2′*R*)-**1*P*-C8**	3.15	3.211117	**1a** major
(8*S*,2′*R*)-**2*M*-C1**	3.89	3.919817	**2b** major
(8*S*,2′*R*)-**2*P*-C1**	3.17	3.133250	**2a** minor

Table S1. Calculated ^{1}H NMR chemical shifts at CH_3-16 for four lowest energy conformers representing atrop-isomers in the inseparable mixtures of (−)-**1** or (+)-**1** and (−)-**2** or (+)-**2**

Conf.	MMFF energy		Gibbs free energy (298.15 K)		
	rel. E (Kcal/mol)	Boltzmann Distribution	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
(8*S*,2′R)-1					
1M-C1	0.00	0.285	-2184.910692	0.585	0.255
1M-C2	1.50	0.023	-2184.909313	1.451	0.059
1M-C3	1.66	0.017	-2184.911625	0.000	0.686
1P-C1	0.42	0.14	-2184.909976	0.992	0.044
1P-C2	0.69	0.089	-2184.90972	1.153	0.033
1P-C3	0.87	0.066	-2184.910006	0.973	0.045
1P-C4	0.93	0.06	-2184.910796	0.478	0.104
1P-C5	0.94	0.058	-2184.909991	0.983	0.044
1P-C6	1.03	0.051	-2184.910004	0.975	0.045
1P-C7	1.30	0.032	-2184.909209	1.473	0.019
1P-C8	1.42	0.026	-2184.911557	0.000	0.233
1P-C9	1.56	0.02	-2184.91023	0.833	0.057
1P-C10	1.60	0.019	-2184.910003	0.975	0.045
1P-C11	1.74	0.015	-2184.91014	0.889	0.052
1P-C12	1.83	0.013	-2184.91025	0.820	0.058
1P-C13	1.99	0.01	-2184.909717	1.155	0.033
1P-C14	2.06	0.009	-2184.910708	0.533	0.095
1P-C15	2.07	0.009	-2184.910428	0.708	0.071
1P-C16	2.09	0.008	-2184.908013	2.224	0.005
1P-C17	2.15	0.008	-2184.908951	1.635	0.015
(8*S*,2′*R*)-**2**					
2M-C1	0.00	0.371	-2108.489953	0	0.508
2M-C2	1.00	0.069	-2108.488835	0.702	0.155
2M-C3	1.40	0.035	-2108.487968	1.246	0.062
2M-C4	1.91	0.015	-2108.489282	0.421	0.249
2M-C5	2.29	0.008	-2108.485811	2.599	0.006
2M-C6	2.32	0.007	-2108.48688	1.928	0.020

2P-C1	0.37	0.199	-2108.488765	0	0.380
2P-C2	0.62	0.13	-2108.486934	1.149	0.055
2P-C3	1.00	0.068	-2108.488132	0.702	0.194
2P-C4	1.28	0.043	-2108.486359	0.397	0.030
2P-C5	1.53	0.028	-2108.488012	1.510	0.171
2P-C6	2.03	0.012	-2108.488008	1.246	0.170

Table S2. Energy analysis for compound **1**–**2**

NO	(8*S*,2′*R*)-**1M-C1**		NO	(8*S*,2′*R*)-**1M-C2**		NO	(8*S*,2′*R*)-**1M-C3**	
	Excitation energies(eV)	Rotatory Strengths*		Excitation energies(eV)	Rotatory Strengths*		Excitation energies(eV)	Rotatory Strengths*
1	3.7913	13.4177	1	3.8076	15.3733	1	3.7326	5.1453
2	3.8658	-11.6103	2	3.866	-11.1989	2	3.8168	0.3977
3	3.9806	13.8806	3	4.0471	16.2736	3	3.975	1.0321
4	4.3628	14.182	4	4.4029	14.8784	4	4.4065	39.9549
5	4.6165	-52.2191	5	4.61	-36.7235	5	4.5553	-3.1671
6	4.6794	97.7391	6	4.6811	76.6426	6	4.6348	63.4603
7	4.7401	-61.091	7	4.7164	-61.8246	7	4.6697	-89.4813
8	4.793	-0.7346	8	4.783	-4.9106	8	4.8347	-7.0799
9	4.9102	1.2003	9	4.8448	2.3238	9	4.8828	-2.8306
10	4.9563	-7.761	10	4.9227	-7.1784	10	4.9108	0.0005
11	5.0863	-0.2453	11	5.0949	-0.0275	11	5.0067	-0.7445
12	5.2251	-3.8344	12	5.1454	-22.6015	12	5.1461	-0.761
13	5.242	-1.7406	13	5.2244	-1.4707	13	5.1874	-6.6205
14	5.2716	-3.4529	14	5.2399	0.7596	14	5.2823	-6.2743
15	5.2946	-30.8501	15	5.276	-13.8489	15	5.3234	-3.7768
16	5.3854	-25.0334	16	5.3459	0.1509	16	5.381	-0.1365
17	5.4123	14.5478	17	5.367	-0.8002	17	5.5037	-22.4038
18	5.4441	5.1223	18	5.4123	-44.6004	18	5.52	-31.6565
19	5.4551	-33.7041	19	5.4808	59.0292	19	5.5285	-4.2861
20	5.5199	-29.6712	20	5.5128	2.3962	20	5.5468	-7.5969
21	5.5444	3.2182	21	5.5163	1.5576	21	5.5554	-0.3905
22	5.5904	26.3733	22	5.5498	-11.2027	22	5.6086	11.4483
23	5.606	35.1831	23	5.5908	-8.3803	23	5.6534	-0.5234
24	5.6135	0.1344	24	5.6237	-22.3228	24	5.6978	28.0457
25	5.6192	0.3191	25	5.6367	-1.9183	25	5.715	2.3328
26	5.6768	-1.2427	26	5.7019	1.2964	26	5.718	0.4017
27	5.6897	-1.3279	27	5.7121	-2.8957	27	5.7286	2.794
28	5.7146	3.7226	28	5.7348	8.7494	28	5.7517	2.3789
29	5.7582	-5.2154	29	5.7388	10.3284	29	5.7724	-31.1767
30	5.7715	3.1033	30	5.7715	-8.1357	30	5.8253	-0.9228
31	5.8207	-59.904	31	5.7924	10.6129	31	5.8547	3.2173
32	5.8341	10.525	32	5.8189	-42.7748	32	5.8999	10.4457
33	5.851	-33.6443	33	5.8495	-5.091	33	5.9142	-41.2628
34	5.8805	-48.7963	34	5.8708	-99.6803	34	5.9218	-5.4534
35	5.9251	-3.5516	35	5.8732	47.3333	35	5.9305	-6.8802

36	5.9396	-11.3839	36	5.9005	-6.6362	36	5.9975	18.1991
37	5.9692	-6.0099	37	5.9576	-4.6275	37	6.0078	-41.7405
38	5.9939	-65.6035	38	5.9731	-65.0512	38	6.0246	-25.0473
39	6.0008	-3.575	39	6.0032	-6.5778	39	6.0711	3.8122
40	6.028	-4.8961	40	6.0228	-15.0344	40	6.0937	-3.9755
41	6.0519	-49.9193	41	6.0464	-30.0574	41	6.101	5.5879
42	6.0623	55.3544	42	6.0752	-13.5747	42	6.1234	-36.5541
43	6.0891	-5.674	43	6.0842	5.3196	43	6.1281	-3.181
44	6.1121	2.7981	44	6.1184	10.8089	44	6.1651	66.8695
45	6.1278	7.4343	45	6.1325	4.7784	45	6.1753	19.9561
46	6.133	9.5111	46	6.1442	3.876	46	6.1953	-21.8823
47	6.1487	-0.0887	47	6.1565	19.2225	47	6.2103	3.0898
48	6.1588	15.3067	48	6.1775	2.6117	48	6.2219	16.0015
49	6.1819	28.3492	49	6.1859	30.0941	49	6.2288	12.1289
50	6.1856	-2.4348	50	6.2211	-29.5814	50	6.2356	7.786
51	6.2299	-1.3267	51	6.228	24.5542	51	6.2982	1.7274
52	6.249	-10.3728	52	6.236	-18.1463	52	6.3019	4.3693
53	6.3042	4.4166	53	6.2556	-8.1762	53	6.3174	12.3158
54	6.3137	48.9236	54	6.2876	7.9981	54	6.3336	-29.9019
55	6.333	-6.3584	55	6.3249	5.5781	55	6.3518	18.6024
56	6.3393	-3.3718	56	6.3289	-0.6158	56	6.3668	4.1607
57	6.3456	23.233	57	6.3451	47.4258	57	6.368	7.1213
58	6.35	-13.9528	58	6.3622	31.0983	58	6.4023	-0.3921
59	6.3764	-14.4396	59	6.3751	3.9304	59	6.42	-25.5615
60	6.383	29.8672	60	6.3879	6.4341	60	6.4266	-9.4962
	(8*S*,2′*R*)-**1P-C1**			(8*S*,2′*R*)-**1P-C2**			(8*S*,2′*R*)-**1P-C3**	
1	3.7722	11.737	1	3.7516	9.8124	1	3.7616	10.1463
2	3.8917	-6.7188	2	3.8872	-6.2074	2	3.8902	-5.8728
3	4.057	-0.5203	3	3.9951	-0.2588	3	4.0125	-0.1984
4	4.3523	29.123	4	4.3039	24.927	4	4.3151	23.4026
5	4.5779	-25.8913	5	4.5868	-29.3427	5	4.5764	-25.3881
6	4.6462	-23.8265	6	4.6624	-14.2701	6	4.6514	-16.3356
7	4.6713	11.4057	7	4.6742	13.5359	7	4.6664	12.9748
8	4.8745	1.4541	8	4.864	0.8378	8	4.8719	1.1009
9	4.9164	-8.7813	9	4.9315	-10.5429	9	4.9183	-9.5897
10	5.0238	-0.5964	10	5.0313	-0.5825	10	5.0334	-0.6392
11	5.1233	-8.1549	11	5.1214	0.4072	11	5.109	-1.2204
12	5.2189	0.7115	12	5.1615	-0.1153	12	5.1342	0.1432
13	5.2836	-6.3277	13	5.2124	-4.1423	13	5.2015	-5.0558
14	5.3008	1.7751	14	5.2771	-6.4768	14	5.2778	-6.3399
15	5.3486	-1.2236	15	5.3312	11.8322	15	5.313	4.8615
16	5.3839	-32.944	16	5.356	-52.0463	16	5.363	-44.9927
17	5.4735	-0.7633	17	5.4747	-2.4988	17	5.5065	-2.8728
18	5.5149	-55.3503	18	5.4971	10.9529	18	5.5357	-26.6149
19	5.5289	32.2127	19	5.5189	-12.3961	19	5.5421	-24.3034
20	5.5734	-2.1876	20	5.5391	-37.0018	20	5.5565	0.0127
21	5.5785	22.5053	21	5.5912	15.197	21	5.5941	22.113
22	5.6156	0.843	22	5.6514	23.5292	22	5.6424	11.5264
23	5.6793	6.28	23	5.6542	-20.6391	23	5.6693	-15.3602

24	5.7096	-4.9152	24	5.678	-4.5021	24	5.6808	7.5434
25	5.7345	-1.8884	25	5.7311	-1.9817	25	5.7176	-8.4366
26	5.7469	0.059	26	5.7523	7.3582	26	5.7339	2.0196
27	5.7863	-76.2102	27	5.7629	-1.7247	27	5.7386	-2.5912
28	5.792	-7.2479	28	5.7678	-6.2359	28	5.7752	-17.1082
29	5.8003	13.6794	29	5.7864	-8.4484	29	5.7857	-1.2372
30	5.8223	-18.6068	30	5.7881	-20.9512	30	5.8067	-7.9832
31	5.8605	-22.1821	31	5.849	-68.2969	31	5.8334	-33.4672
32	5.8977	-0.4562	32	5.8889	4.0428	32	5.906	13.6525
33	5.9129	28.9079	33	5.9145	-5.8864	33	5.9225	-20.3484
34	5.9382	-29.5514	34	5.9309	42.3028	34	5.9326	-25.1835
35	5.9692	-94.5389	35	5.9618	-80.3073	35	5.9463	-10.1227
36	6.0375	20.7742	36	6.0193	38.0782	36	5.9954	-56.3912
37	6.04	19.6666	37	6.04	22.772	37	6.0279	-8.3056
38	6.0446	-29.8546	38	6.0473	-6.7756	38	6.0659	34.9392
39	6.0916	31.3386	39	6.0697	-20.3844	39	6.0755	-8.0751
40	6.113	17.7062	40	6.098	-23.4716	40	6.0827	-7.0585
41	6.128	-2.7598	41	6.1061	4.5728	41	6.0966	11.6275
42	6.136	76.5626	42	6.1112	11.6765	42	6.1136	7.0936
43	6.1455	-1.4863	43	6.1274	19.5869	43	6.1251	-29.41
44	6.1515	13.4122	44	6.1401	-27.162	44	6.1483	172.2585
45	6.1719	-3.7347	45	6.1509	31.0187	45	6.1755	-2.2996
46	6.1823	8.1685	46	6.1718	65.0889	46	6.1803	-1.3996
47	6.2037	32.9275	47	6.1896	2.8422	47	6.209	-5.7442
48	6.2609	-5.651	48	6.2413	12.5964	48	6.2308	5.5002
49	6.2893	-32.9364	49	6.2477	7.5895	49	6.2539	-4.8019
50	6.2939	1.2903	50	6.2758	12.8458	50	6.2723	17.8835
51	6.3097	21.0602	51	6.2869	-4.2111	51	6.2797	-20.4975
52	6.3359	8.4605	52	6.3018	-27.2736	52	6.2902	-16.6167
53	6.3577	-3.8836	53	6.3199	-1.6928	53	6.3108	26.1878
54	6.3708	-3.0644	54	6.3437	2.5087	54	6.3377	2.2578
55	6.3847	18.6252	55	6.352	21.9755	55	6.3527	-9.7991
56	6.4079	3.0937	56	6.3527	-22.0197	56	6.4062	3.9832
57	6.4136	-2.4418	57	6.3645	-1.6762	57	6.4104	-5.9976
58	6.4154	-20.4478	58	6.4031	-4.8945	58	6.4156	6.4869
59	6.439	-1.4499	59	6.4127	9.4908	59	6.4275	3.7727
60	6.4417	6.6961	60	6.4149	3.5025	60	6.4317	-2.0066
	(8*S*,2′*R*)-**1P-C4**			(8*S*,2′*R*)-**1P-C5**			(8*S*,2′*R*)-**1P-C6**	
1	3.7563	7.886	1	3.7842	4.4935	1	3.7802	12.0042
2	3.8873	-5.3296	2	3.8364	4.2637	2	3.8925	-6.4893
3	4.0574	0.0315	3	3.9025	-3.747	3	4.0758	-0.6338
4	4.3375	27.4689	4	4.2316	19.7872	4	4.3644	28.2492
5	4.5545	-5.5791	5	4.6182	-44.2564	5	4.567	-21.2653
6	4.6449	-25.693	6	4.6663	14.0071	6	4.6345	-24.761
7	4.6853	0.7223	7	4.795	4.9119	7	4.667	8.6526
8	4.8563	0.2627	8	4.8302	-3.2602	8	4.8797	2.0439
9	4.8792	-10.2035	9	5.0219	-3.5635	9	4.9032	-8.9826
10	4.9716	-1.4948	10	5.1122	-7.8157	10	5.0139	-0.3635
11	5.0742	0.5801	11	5.2001	0.17	11	5.105	-7.3429

12	5.158	-4.8477	12	5.2205	-0.8848	12	5.2262	-0.7777
13	5.2474	0.0357	13	5.2245	2.2854	13	5.2773	-3.9096
14	5.2514	-7.298	14	5.2822	-7.7416	14	5.2872	1.4214
15	5.3093	1.9763	15	5.367	15.4437	15	5.2967	-3.0008
16	5.3433	-23.3568	16	5.3941	-52.3181	16	5.3758	-32.8195
17	5.3883	-16.6772	17	5.447	3.2642	17	5.4891	29.998
18	5.4849	0.8678	18	5.4528	3.7278	18	5.5057	-68.2065
19	5.4996	-44.14	19	5.4672	2.8051	19	5.5583	-1.3007
20	5.5416	29.5618	20	5.4818	-0.3584	20	5.5836	4.4901
21	5.5634	16.3141	21	5.5162	-41.098	21	5.5943	32.4897
22	5.6108	7.4019	22	5.5504	0.1193	22	5.6186	-3.7624
23	5.6455	-10.6416	23	5.6526	-90.8538	23	5.6767	4.9436
24	5.6731	5.5662	24	5.6742	0.442	24	5.6941	9.2612
25	5.688	-8.2179	25	5.7171	62.5276	25	5.7186	-13.2045
26	5.6939	-8.1101	26	5.7379	17.4299	26	5.7385	-11.0152
27	5.7118	1.1504	27	5.7748	1.9346	27	5.7577	-52.7521
28	5.7443	-0.2541	28	5.8016	-10.7389	28	5.7782	14.0132
29	5.7725	-42.7238	29	5.8144	-25.3587	29	5.8135	-58.0192
30	5.8019	-16.9275	30	5.8216	3.8595	30	5.8223	21.6707
31	5.8265	8.0393	31	5.8333	-20.9887	31	5.868	3.2923
32	5.839	-16.5584	32	5.8493	9.2793	32	5.8974	-6.4158
33	5.8703	-4.0839	33	5.9025	-82.6916	33	5.9363	-40.1954
34	5.8737	-6.3551	34	5.9483	44.4551	34	5.943	-21.9805
35	5.9423	-65.4099	35	5.98	2.4567	35	5.985	-7.6093
36	5.9639	-4.8645	36	5.9923	-3.6141	36	6.0209	-0.3027
37	6.0217	44.0385	37	5.9992	-33.6412	37	6.0399	-77.037
38	6.0367	-24.5026	38	6.0163	22.5777	38	6.0678	-2.2939
39	6.0485	-4.0713	39	6.0492	4.0557	39	6.0738	26.0568
40	6.058	-20.4945	40	6.0633	-13.5114	40	6.0982	-6.4121
41	6.0768	-15.4209	41	6.0702	-20.9024	41	6.1038	-20.6412
42	6.0945	-0.9094	42	6.1093	-6.1296	42	6.1376	22.8582
43	6.1003	-5.7425	43	6.1413	-0.1424	43	6.1486	10.7916
44	6.1318	-10.4946	44	6.1469	7.0315	44	6.1635	177.5129
45	6.1453	6.8438	45	6.1539	9.239	45	6.1897	15.6537
46	6.1562	57.6089	46	6.157	18.8212	46	6.1973	-1.8958
47	6.1648	19.4744	47	6.176	-15.8497	47	6.2127	-2.2426
48	6.1763	14.5854	48	6.195	61.3411	48	6.2445	9.5555
49	6.2036	32.1607	49	6.1991	9.4432	49	6.2673	1.6317
50	6.2106	26.2521	50	6.2127	7.5375	50	6.2916	-19.9711
51	6.2598	32.2607	51	6.2565	13.4974	51	6.3369	-7.4889
52	6.267	4.3154	52	6.2628	6.8562	52	6.3477	24.8413
53	6.2827	-14.3363	53	6.289	-2.8563	53	6.3657	-13.0912
54	6.297	11.6957	54	6.2956	0.8967	54	6.3786	-5.6369
55	6.3275	-10.7866	55	6.3035	-3.6838	55	6.3963	23.3097
56	6.3487	0.2582	56	6.3203	-14.0243	56	6.4043	1.2711
57	6.3666	22.5132	57	6.3276	15.0164	57	6.4191	-2.0096
58	6.3729	-25.7353	58	6.3966	-7.1232	58	6.4231	-4.2405
59	6.381	6.0881	59	6.4134	-3.0344	59	6.4433	-13.8864
60	6.3883	-4.1119	60	6.4254	-2.6042	60	6.4483	-22.1985

	(8*S*,2′*R*)-**1P-C7**			(8*S*,2′*R*)-**1P-C8**			(8*S*,2′*R*)-**1P-C9**	
1	3.7829	9.8449	1	3.496	0.2019	1	3.7777	9.2008
2	3.8651	-5.2214	2	3.7406	22.0152	2	3.8904	-5.5224
3	3.9457	-0.7701	3	3.8083	-16.6771	3	4.1166	-0.3747
4	4.246	20.5264	4	4.0309	14.0015	4	4.3757	30.0193
5	4.6055	-43.0003	5	4.5371	-30.1328	5	4.5411	-1.4418
6	4.6607	14.4069	6	4.6071	31.804	6	4.6381	-31.7605
7	4.7336	5.2642	7	4.8816	2.229	7	4.686	-3.4673
8	4.8751	0.2679	8	4.9765	3.191	8	4.8549	-2.7668
9	5.0108	-5.8889	9	5.0037	10.702	9	4.8747	-5.881
10	5.0391	-4.1445	10	5.0842	-3.2746	10	4.9336	-1.472
11	5.0823	-1.4106	11	5.1183	2.5043	11	5.0563	-6.5189
12	5.196	-0.2783	12	5.1621	1.5884	12	5.1198	1.2561
13	5.2247	-3.1723	13	5.2014	-16.9848	13	5.2471	-6.279
14	5.2934	-9.3436	14	5.2577	-1.1215	14	5.2833	1.6037
15	5.3581	16.6904	15	5.2619	-30.4229	15	5.3507	-27.7536
16	5.3985	-58.6615	16	5.3328	-7.2751	16	5.383	-5.3469
17	5.4748	16.8905	17	5.3461	5.4512	17	5.422	-0.286
18	5.5127	-16.3807	18	5.3988	-28.4559	18	5.4524	1.4366
19	5.5317	1.991	19	5.4694	30.8298	19	5.4773	-25.1798
20	5.5694	-71.4568	20	5.504	-0.8128	20	5.5117	-5.7278
21	5.6366	-8.574	21	5.5318	-9.3778	21	5.5569	44.5272
22	5.6486	-2.9965	22	5.6053	18.3226	22	5.6145	4.8931
23	5.6517	-38.498	23	5.609	-5.6269	23	5.6307	-2.5094
24	5.6673	74.3275	24	5.6504	-66.0822	24	5.6641	-1.1261
25	5.7469	10.1179	25	5.664	-32.4769	25	5.6914	-1.7733
26	5.7538	0.47	26	5.6808	10.4789	26	5.7062	9.7184
27	5.7982	-77.8592	27	5.6995	-2.251	27	5.7245	-11.9349
28	5.8321	25.3509	28	5.7607	7.5024	28	5.7571	-17.7051
29	5.8421	-5.0984	29	5.7701	-0.5961	29	5.7786	-80.8073
30	5.8538	14.9192	30	5.8023	73.3201	30	5.7889	52.5477
31	5.8643	-0.9509	31	5.8216	-28.5312	31	5.8282	-46.207
32	5.9237	15.0506	32	5.8404	-52.704	32	5.8404	-11.4507
33	5.9519	-9.5431	33	5.8676	18.8229	33	5.8666	-6.5969
34	5.9592	-59.8234	34	5.8712	-50.8749	34	5.8895	13.7567
35	5.9898	-0.9109	35	5.8904	-34.3994	35	5.9348	-45.2027
36	6.0022	-20.6523	36	5.898	3.8777	36	5.9684	-47.7039
37	6.0375	-43.8106	37	5.9112	20.8168	37	5.9908	-27.0599
38	6.0531	-15.5204	38	5.9224	33.417	38	5.9936	29.122
39	6.0619	16.6002	39	5.9441	1.5249	39	6.0376	17.5285
40	6.0902	20.7605	40	5.9787	-8.1778	40	6.0829	-19.3831
41	6.1348	-3.3139	41	6.0255	-3.9508	41	6.0965	-22.5427
42	6.1459	64.5513	42	6.0515	37.5428	42	6.1068	-7.3453
43	6.1581	13.3192	43	6.0817	17.4907	43	6.1196	64.5971
44	6.1654	57.1486	44	6.1107	18.2087	44	6.1263	-26.8314
45	6.1843	63.2627	45	6.1459	-39.2648	45	6.1493	41.1019
46	6.2054	-1.7334	46	6.175	-5.4466	46	6.2081	-1.862
47	6.2307	-9.7837	47	6.1789	20.173	47	6.2187	45.6681
48	6.2493	-3.602	48	6.1827	-18.8715	48	6.2302	4.3156

49	6.2536	-18.6277	49	6.194	-24.8657	49	6.2353	60.207
50	6.2808	0.222	50	6.2208	5.5611	50	6.2499	1.5436
51	6.2834	23.0238	51	6.2403	9.2643	51	6.2594	-12.7842
52	6.3055	-2.8369	52	6.2593	1.1846	52	6.2779	-12.105
53	6.3111	1.9628	53	6.2803	40.673	53	6.2961	7.1664
54	6.3509	9.9106	54	6.313	5.0696	54	6.3036	3.1256
55	6.3739	2.8013	55	6.3287	2.2959	55	6.3176	4.9994
56	6.3798	-20.9791	56	6.3324	-4.6944	56	6.3296	1.019
57	6.3953	-20.5554	57	6.3545	5.0281	57	6.343	3.0266
58	6.4049	-15.0269	58	6.37	4.7819	58	6.3552	0.9019
59	6.4314	-6.792	59	6.385	-19.5614	59	6.3808	-8.9521
60	6.4555	0.4149	60	6.4029	26.6076	60	6.4222	-5.584
	(8*S*,2′*R*)-**1P-C10**			(8*S*,2′*R*)-**1P-C11**			(8*S*,2′*R*)-**1P-C12**	
1	3.7613	10.1312	1	3.6402	0.885	1	3.7641	12.2251
2	3.8901	-5.8746	2	3.7997	12.4583	2	3.8911	-7.2215
3	4.0123	-0.1955	3	3.8741	-1.5775	3	4.0478	0.218
4	4.3149	23.4326	4	4.1385	23.5837	4	4.3176	33.436
5	4.5763	-25.3869	5	4.5695	-15.4567	5	4.567	-46.4814
6	4.6513	-16.3185	6	4.6266	10.719	6	4.6389	1.3971
7	4.6663	12.9597	7	4.8831	3.2311	7	4.6563	0.964
8	4.8716	1.0881	8	4.9122	-5.6698	8	4.8483	2.2994
9	4.9182	-9.5768	9	4.9525	-1.0458	9	4.9146	-9.9744
10	5.0331	-0.6327	10	5.0724	-0.7346	10	5.0056	-0.158
11	5.1089	-1.2235	11	5.1316	-3.4802	11	5.1305	-14.2902
12	5.134	0.1477	12	5.1651	0.3855	12	5.2053	2.1562
13	5.2015	-5.0647	13	5.2122	-5.5376	13	5.2467	-4.5698
14	5.2776	-6.3285	14	5.2477	-6.5101	14	5.2644	-1.2055
15	5.313	4.9012	15	5.2715	-1.5204	15	5.3558	-1.8732
16	5.363	-45.0345	16	5.3121	-0.9394	16	5.3865	-38.4999
17	5.5064	-2.8425	17	5.3381	-16.0437	17	5.4589	6.0727
18	5.5357	-26.0321	18	5.4011	17.63	18	5.4974	-41.4712
19	5.5419	-24.7889	19	5.4465	11.177	19	5.5204	23.5203
20	5.5563	-0.0483	20	5.485	-52.6807	20	5.5468	-2.9405
21	5.5941	22.1221	21	5.51	1.0475	21	5.6049	16.4214
22	5.6426	11.3849	22	5.5259	-14.7512	22	5.6493	14.6799
23	5.6694	-15.2966	23	5.5503	-19.8555	23	5.6695	-4.5592
24	5.6808	7.4752	24	5.5997	-0.7155	24	5.6817	-3.5002
25	5.7176	-8.2643	25	5.6635	8.6555	25	5.7156	-5.8942
26	5.7339	1.8621	26	5.6729	16.9882	26	5.7208	1.6679
27	5.7385	-2.51	27	5.7054	-15.5699	27	5.7532	-34.7049
28	5.7752	-17.079	28	5.7202	-1.8298	28	5.7629	3.0823
29	5.7856	-1.2899	29	5.7269	16.7388	29	5.7861	16.6437
30	5.8066	-7.9494	30	5.7736	-20.3401	30	5.8292	-137.127
31	5.8335	-33.6042	31	5.7986	-3.8542	31	5.8566	43.6131
32	5.906	13.4847	32	5.8127	-0.564	32	5.8861	-2.7472
33	5.9225	-19.2132	33	5.8284	39.762	33	5.8981	1.1279
34	5.9326	-26.1743	34	5.8416	-22.4499	34	5.9308	-10.1395
35	5.9462	-10.0978	35	5.876	48.6095	35	5.9638	-93.7299
36	5.9955	-56.4262	36	5.8938	-3.8491	36	6.0139	-12.7417

37	6.0279	-8.1489	37	5.9026	-0.2112	37	6.031	-21.5909
38	6.066	34.8641	38	5.9419	-55.7671	38	6.0455	104.7444
39	6.0755	-8.1001	39	5.9509	-21.4525	39	6.0558	38.5968
40	6.0827	-7.0587	40	5.9792	1.3895	40	6.0784	19.6717
41	6.0966	11.5027	41	6.0267	23.4725	41	6.0998	11.3247
42	6.1135	7.2159	42	6.085	18.3565	42	6.1077	-7.9054
43	6.125	-29.5362	43	6.1149	-23.3452	43	6.1285	-0.4057
44	6.1483	172.386	44	6.1368	-2.9848	44	6.1488	8.3467
45	6.1755	-2.2805	45	6.1409	-8.1697	45	6.1848	-8.2716
46	6.1802	-1.4058	46	6.1537	1.1621	46	6.2044	-3.1383
47	6.2091	-5.642	47	6.173	6.5906	47	6.2439	-5.9476
48	6.2308	5.3582	48	6.1839	-3.4832	48	6.2545	-1.8028
49	6.2538	-4.7262	49	6.1941	-0.2053	49	6.2672	3.224
50	6.2721	17.2269	50	6.2128	41.9944	50	6.2745	-9.7976
51	6.2798	-19.5457	51	6.225	-21.4631	51	6.2913	-3.9647
52	6.2901	-16.8521	52	6.2293	18.189	52	6.3146	59.7383
53	6.3107	26.1584	53	6.2349	0.1308	53	6.3218	-0.2611
54	6.3375	2.2736	54	6.2531	8.6624	54	6.3361	-7.8656
55	6.3527	-9.7909	55	6.273	15.6682	55	6.3677	15.6911
56	6.4062	4.2314	56	6.2942	-29.2269	56	6.3904	-6.2012
57	6.4106	-6.3383	57	6.3006	-2.2156	57	6.4109	-22.4807
58	6.4156	6.5999	58	6.3136	0.0946	58	6.4195	5.2797
59	6.4273	4.0118	59	6.3218	-1.7243	59	6.4436	-2.8168
60	6.4317	-2.2316	60	6.3368	23.246	60	6.4544	-0.195
	(8*S*,2′*R*)-**1P-C13**			(8*S*,2′*R*)-**1P-C14**			(8*S*,2′*R*)-**1P-C15**	
1	3.7516	9.8253	1	3.7355	5.7196	1	3.7717	12.6738
2	3.8871	-6.2144	2	3.8558	-4.585	2	3.8924	-6.9023
3	3.9952	-0.2629	3	4.045	0.2648	3	4.0675	0.1677
4	4.3038	24.9412	4	4.2884	33.7804	4	4.3278	32.4618
5	4.5868	-29.3319	5	4.5607	-16.0348	5	4.5587	-40.0248
6	4.6624	-14.3244	6	4.6409	-47.9298	6	4.6262	-7.862
7	4.6742	13.5741	7	4.6417	36.9595	7	4.653	4.8502
8	4.8638	0.8537	8	4.845	1.9214	8	4.8558	2.2787
9	4.9313	-10.5599	9	4.877	-10.6262	9	4.9007	-9.4536
10	5.0313	-0.5815	10	4.9879	-0.7314	10	4.9951	0.2375
11	5.1213	0.4122	11	5.0956	-1.1361	11	5.1134	-13.275
12	5.1615	-0.1192	12	5.1098	0.9839	12	5.2127	0.4058
13	5.2123	-4.1392	13	5.1644	-7.4865	13	5.2452	-4.2601
14	5.2769	-6.4975	14	5.2118	-4.7996	14	5.252	-1.6782
15	5.3311	11.8047	15	5.2769	-1.2468	15	5.3003	-0.5157
16	5.3559	-52.0638	16	5.359	-45.3572	16	5.3775	-38.6375
17	5.4747	-2.5195	17	5.4846	6.0152	17	5.4734	41.5176
18	5.4974	10.9654	18	5.5142	-38.6596	18	5.4942	-73.3214
19	5.5189	-12.4077	19	5.5231	11.3504	19	5.5307	-6.2255
20	5.5391	-37.0567	20	5.5586	27.0792	20	5.568	17.6676
21	5.5912	15.2901	21	5.5837	22.4382	21	5.5933	2.9729
22	5.6513	23.7246	22	5.6214	-3.2891	22	5.6419	3.7827
23	5.6541	-20.9712	23	5.6526	2.3565	23	5.6752	14.973
24	5.678	-4.4728	24	5.6549	-40.8599	24	5.6914	-19.6037

25	5.731	-1.943	25	5.6824	-0.2161	25	5.6993	20.8881
26	5.7521	7.355	26	5.7087	-1.5807	26	5.7179	-8.331
27	5.7629	-1.5987	27	5.75	2.4779	27	5.7343	-10.729
28	5.7678	-6.2147	28	5.7616	5.6963	28	5.7436	3.268
29	5.7863	-8.5064	29	5.781	-5.8532	29	5.7978	-9.0777
30	5.788	-20.8585	30	5.7958	-113.578	30	5.8286	-90.1266
31	5.8488	-68.3237	31	5.835	38.1898	31	5.8519	1.6937
32	5.889	4.1687	32	5.8758	-3.5547	32	5.8918	-5.7265
33	5.9144	-5.9031	33	5.8863	13.1142	33	5.9267	-23.197
34	5.9308	42.3414	34	5.936	-11.4896	34	5.9359	-17.7262
35	5.9617	-80.4523	35	5.9526	-26.2047	35	5.9611	-6.2193
36	6.0193	38.4093	36	5.9611	-0.0923	36	6.0174	-1.319
37	6.04	22.8191	37	6.009	-1.5382	37	6.0291	8.847
38	6.0473	-7.2218	38	6.018	-46.2022	38	6.0391	-4.0609
39	6.0697	-20.3993	39	6.0466	42.9985	39	6.047	2.9283
40	6.098	-23.2935	40	6.0772	36.4996	40	6.078	-2.2446
41	6.1061	4.5323	41	6.093	-1.1413	41	6.091	-11.7628
42	6.1112	11.5613	42	6.0959	0.8557	42	6.118	-7.0384
43	6.1274	19.5307	43	6.1082	10.6774	43	6.1451	1.0423
44	6.1401	-27.5343	44	6.1156	0.9545	44	6.1623	102.1881
45	6.1509	31.0593	45	6.1838	5.0834	45	6.194	15.9716
46	6.1718	65.1705	46	6.1909	-3.3027	46	6.2108	-0.4294
47	6.1895	2.8216	47	6.2168	-20.1645	47	6.226	0.7829
48	6.2412	12.5888	48	6.2366	-6.7472	48	6.2449	5.8976
49	6.2476	7.5383	49	6.2571	6.4568	49	6.2509	-0.2099
50	6.2757	13.3381	50	6.2641	-1.5468	50	6.2895	-11.5792
51	6.2869	-4.6521	51	6.27	-0.8261	51	6.2953	23.027
52	6.3016	-26.9657	52	6.28	-15.0737	52	6.316	28.4829
53	6.3201	-1.4211	53	6.3037	107.3293	53	6.3376	-11.4358
54	6.3435	2.2454	54	6.3106	16.5956	54	6.3591	-28.6462
55	6.352	23.7647	55	6.3206	-27.6141	55	6.3825	6.1323
56	6.3528	-23.8301	56	6.3546	13.5982	56	6.3919	21.4986
57	6.3646	-1.5382	57	6.3829	-6.5644	57	6.4134	4.6562
58	6.4032	-4.8103	58	6.4201	2.3568	58	6.4266	-23.0823
59	6.4127	9.3885	59	6.4282	7.402	59	6.4323	6.7865
60	6.4149	3.4909	60	6.4523	3.0602	60	6.4632	-4.5386
	(8*S*,2′*R*)-**1P-C16**			(8*S*,2′*R*)-**1P-C17**				
1	3.7628	-14.0659	1	3.8047	10.5648			
2	3.8122	17.4516	2	3.8696	-4.3414			
3	3.9998	1.5955	3	3.9309	0.5501			
4	4.2773	36.9934	4	4.2905	23.3102			
5	4.6262	21.5005	5	4.6067	-50.9091			
6	4.6508	-33.438	6	4.662	13.0949			
7	4.7445	-12.0531	7	4.7738	3.3436			
8	4.7675	-4.3264	8	4.842	-3.4311			
9	4.9435	1.7709	9	4.9785	-1.0912			
10	5.02	6.0067	10	5.097	-7.0929			
11	5.0882	-4.8355	11	5.2048	-2.6331			
12	5.1219	0.0189	12	5.2279	-1.0575			

13	5.1522	-5.613	13	5.2855	-3.4594			
14	5.2915	16.1041	14	5.3136	-3.9828			
15	5.322	-7.8137	15	5.3706	0.353			
16	5.3713	2.0204	16	5.3713	-0.8743			
17	5.4022	-3.1262	17	5.4286	-39.3358			
18	5.4266	-62.9842	18	5.4552	-2.9861			
19	5.4634	-1.5895	19	5.4889	-9.7347			
20	5.4776	0.2281	20	5.5166	10.0274			
21	5.4973	15.9518	21	5.5375	9.1981			
22	5.547	-26.1693	22	5.591	14.3631			
23	5.5823	-4.2307	23	5.6334	-71.9616			
24	5.5829	3.8452	24	5.67	4.243			
25	5.6064	6.9243	25	5.702	-11.9156			
26	5.6268	30.6786	26	5.7484	-9.005			
27	5.6345	-19.8723	27	5.7564	0.1213			
28	5.6854	24.1733	28	5.7759	21.6943			
29	5.6888	-7.6368	29	5.7902	-16.8136			
30	5.7384	27.155	30	5.8117	26.0373			
31	5.7495	-3.639	31	5.8167	-44.4338			
32	5.7977	-18.9632	32	5.866	1.115			
33	5.8003	-24.7411	33	5.8977	-45.885			
34	5.8285	-51.6725	34	5.9284	14.9187			
35	5.8482	9.0524	35	5.9654	-3.9255			
36	5.8938	57.2018	36	5.9864	-50.5231			
37	5.9225	-34.5187	37	6.0127	12.4992			
38	5.9299	5.1706	38	6.0463	-0.5887			
39	5.941	-3.4808	39	6.0562	7.4706			
40	5.9716	-13.0914	40	6.0718	3.0349			
41	6.0021	-35.9976	41	6.076	-14.4076			
42	6.0253	4.983	42	6.111	3.0482			
43	6.0316	10.9471	43	6.1369	5.7335			
44	6.0743	34.6478	44	6.1382	-30.5301			
45	6.0821	-33.314	45	6.1495	11.2695			
46	6.0862	19.2493	46	6.1597	47.5531			
47	6.1088	-3.9449	47	6.1907	46.0928			
48	6.1532	2.77	48	6.2236	-6.6926			
49	6.1709	-1.2149	49	6.2283	3.8313			
50	6.1907	-3.774	50	6.254	7.2459			
51	6.2188	2.5692	51	6.2573	21.8192			
52	6.2502	11.2442	52	6.2631	-4.1817			
53	6.2609	-4.5145	53	6.2847	-1.1115			
54	6.2952	20.856	54	6.303	-1.2936			
55	6.3034	47.7818	55	6.3513	-1.7673			
56	6.3188	-18.691	56	6.3537	8.7047			
57	6.33	-17.2915	57	6.361	1.1381			
58	6.3314	-2.7456	58	6.3753	-13.59			
59	6.3453	21.6239	59	6.4178	0.3846			
60	6.368	40.0144	60	6.4243	-2.6698			

* R(velocity) 10**-40 erg-esu-cm

Table S3. Calculated ECD data for compound **1**

NO	(8*S*,2′*R*)-**2M-C1**		NO	(8*S*,2′*R*)-**2M-C2**		NO	(8*S*,2′*R*)-**2M-C3**	
	Excitation energies(eV)	Rotatory Strengths*		Excitation energies(eV)	Rotatory Strengths*		Excitation energies(eV)	Rotatory Strengths*
1	3.7831	14.8943	1	3.8002	16.1159	1	3.7873	14.5297
2	3.8829	-7.9782	2	3.8841	-8.2524	2	3.893	-7.7376
3	4.0031	7.8063	3	4.0719	11.0076	3	4.0428	8.9192
4	4.406	12.1661	4	4.4517	13.2597	4	4.4544	15.6253
5	4.5389	-30.9729	5	4.5511	-10.0706	5	4.5296	-33.4251
6	4.6075	104.2811	6	4.6138	69.6826	6	4.5894	60.517
7	4.675	-77.9825	7	4.669	-76.7818	7	4.6833	-42.8344
8	4.8301	-5.0029	8	4.8328	-2.2644	8	4.7943	-7.1485
9	4.8329	-4.1548	9	4.8685	-6.4083	9	4.8223	-0.5201
10	4.898	-8.618	10	4.9175	0.4407	10	4.8728	-11.3445
11	4.9569	-0.2762	11	4.9458	-3.2918	11	4.9408	-0.0288
12	5.1061	-0.1441	12	5.0777	-21.2428	12	5.0953	-0.4779
13	5.184	-14.8663	13	5.1431	3.4297	13	5.1774	-4.5059
14	5.2517	-31.0477	14	5.2446	-22.2108	14	5.2651	-9.8603
15	5.3072	-0.5146	15	5.2684	-12.3345	15	5.319	0.6631
16	5.3171	-7.5552	16	5.2996	-0.7229	16	5.3394	-5.4369
17	5.4083	-35.1286	17	5.3833	0.3867	17	5.3612	-8.2132
18	5.4659	-15.5005	18	5.408	-16.636	18	5.4317	-56.4433
19	5.4838	6.2617	19	5.4217	5.7186	19	5.4649	5.7835
20	5.5068	22.2505	20	5.4971	8.98	20	5.4812	-7.1013
21	5.5295	9.1748	21	5.5078	-5.5238	21	5.5053	17.3191
22	5.5423	11.0143	22	5.5389	-26.2965	22	5.5207	-5.8051
23	5.5629	1.252	23	5.5566	-15.928	23	5.5676	2.7445
24	5.5669	-9.8824	24	5.5667	21.0388	24	5.611	-3.2329
25	5.6102	-27.252	25	5.6255	-9.9465	25	5.6325	-22.7235
26	5.645	9.5599	26	5.6471	11.1198	26	5.6373	-10.8819
27	5.6593	-0.3163	27	5.662	-13.0654	27	5.6495	-24.9765
28	5.6801	-4.6018	28	5.6759	11.4618	28	5.6801	-0.0162
29	5.7139	-38.5333	29	5.7406	-28.3056	29	5.7215	10.2681
30	5.7483	-11.5547	30	5.7691	-41.1309	30	5.7439	6.7932
31	5.808	18.7555	31	5.8029	7.1619	31	5.7648	1.553
32	5.8363	12.3401	32	5.8104	-4.5179	32	5.8169	29.1699
33	5.8425	-62.2526	33	5.8291	30.096	33	5.8286	-28.6989
34	5.8477	-9.1278	34	5.8329	34.0017	34	5.8426	-7.0842
35	5.8584	-6.8565	35	5.8665	-6.5547	35	5.8506	-11.2446
36	5.8644	63.5862	36	5.8725	1.0755	36	5.8713	-7.735
37	5.882	30.8368	37	5.9134	30.2888	37	5.8847	-20.8433
38	5.9366	-4.663	38	5.9306	-2.9864	38	5.9276	-53.9592
39	5.9645	-20.0169	39	5.9497	-1.0521	39	5.9489	-13.4553
40	5.989	-29.2482	40	5.9674	-8.5725	40	5.9839	-11.9563
41	6.0347	-0.9534	41	5.999	-13.7719	41	5.9947	-19.4
42	6.0489	-3.8702	42	6.0336	-28.6671	42	6.0362	-12.8653
43	6.0705	-32.3499	43	6.0627	0.7958	43	6.0573	-65.8015

44	6.0805	9.712	44	6.0722	-7.5351	44	6.06	9.452
45	6.0911	-38.0694	45	6.0757	-100.416	45	6.0634	-66.6627
46	6.1132	1.2037	46	6.0838	9.6392	46	6.0844	11.6401
47	6.119	114.1441	47	6.117	-0.9283	47	6.1109	54.91
48	6.1282	-66.0838	48	6.1311	28.8561	48	6.1226	36.9839
49	6.1315	13.734	49	6.1612	83.323	49	6.127	8.5416
50	6.162	-22.5249	50	6.1751	-45.899	50	6.1521	-37.4247
51	6.1675	-9.4403	51	6.1913	2.6447	51	6.1633	-6.6688
52	6.1836	-15.3923	52	6.1969	23.8582	52	6.1719	-15.6907
53	6.189	36.4019	53	6.2136	-53.3094	53	6.1883	20.913
54	6.2044	-9.4303	54	6.2446	14.458	54	6.203	-7.6951
55	6.2359	-27.3617	55	6.2551	2.2194	55	6.2093	4.284
56	6.2621	23.9874	56	6.2697	-2.4888	56	6.2262	-11.6177
57	6.2824	5.9543	57	6.2781	-9.4892	57	6.2363	10.039
58	6.2944	6.5856	58	6.2986	28.5774	58	6.257	-4.1844
59	6.3338	72.7727	59	6.3287	13.4818	59	6.3168	-1.5973
60	6.3668	11.4735	60	6.349	-0.8886	60	6.3426	-1.9831
	(8*S*,2′*R*)-**2M-C4**			(8*S*,2′*R*)-**2M-C5**			(8*S*,2′*R*)-**2M-C6**	
1	3.7252	-11.6267	1	3.721	13.2346	1	3.8043	16.5149
2	3.8076	13.423	2	3.8877	-4.1839	2	3.8919	-8.6026
3	3.9965	1.0691	3	3.9648	5.2196	3	4.112	12.362
4	4.3653	28.2307	4	4.2242	1.4554	4	4.4722	-0.4433
5	4.5556	20.8259	5	4.4362	11.4289	5	4.5561	30.8915
6	4.5898	26.8235	6	4.5639	17.5717	6	4.6263	1.4198
7	4.6652	-26.3975	7	4.6127	21.4972	7	4.68	-48.2139
8	4.6784	-48.0988	8	4.6966	-62.5746	8	4.8128	-3.1462
9	4.865	-0.5856	9	4.8058	-3.0691	9	4.8457	-9.5594
10	4.9359	8.397	10	4.8608	-4.3886	10	4.8941	0.7824
11	5.0106	0.0132	11	4.953	-0.3649	11	4.8982	1.8354
12	5.1344	-1.6536	12	5.0876	-2.8998	12	5.0602	-11.5999
13	5.1604	4.792	13	5.1029	-29.1638	13	5.1234	2.9788
14	5.291	-2.747	14	5.1946	4.7019	14	5.2272	-2.6341
15	5.3039	1.8755	15	5.2103	7.2717	15	5.2593	-6.595
16	5.3091	-17.9063	16	5.3301	-18.5068	16	5.2974	-1.1663
17	5.3395	24.4797	17	5.3724	-36.0224	17	5.344	-15.3974
18	5.4597	-22.0378	18	5.4323	-46.4947	18	5.3883	-0.4425
19	5.4996	-44.0411	19	5.4849	-0.4098	19	5.3943	7.0152
20	5.5187	12.3272	20	5.5199	-12.7597	20	5.4655	-7.5666
21	5.5425	-11.2978	21	5.532	-0.4554	21	5.501	4.8001
22	5.5626	13.6397	22	5.5414	29.681	22	5.5067	-2.3102
23	5.5787	-2.3865	23	5.5677	11.14	23	5.5714	-52.9755
24	5.5959	6.509	24	5.5764	-11.1914	24	5.5984	-8.8588
25	5.6259	20.5605	25	5.6059	7.3262	25	5.6276	-40.2646
26	5.6446	-6.0897	26	5.6498	-4.2776	26	5.6541	8.8131
27	5.6868	15.6352	27	5.6583	0.673	27	5.6722	-1.5786
28	5.6901	-3.9096	28	5.6739	-3.3124	28	5.6927	-0.0457
29	5.7074	-2.2524	29	5.6827	-3.631	29	5.7194	-10.89
30	5.717	-4.96	30	5.7147	-11.3302	30	5.7449	-10.0831
31	5.7367	-15.156	31	5.7406	-13.0218	31	5.7476	14.7107

32	5.7546	-36.3633	32	5.7672	30.373	32	5.7798	10.7367
33	5.8057	-46.4165	33	5.8207	-2.6914	33	5.8117	26.7944
34	5.8414	6.3841	34	5.8295	-84.4407	34	5.8291	11.9971
35	5.8462	0.3382	35	5.8524	-26.1825	35	5.8554	7.9487
36	5.8738	73.6144	36	5.8603	-8.3121	36	5.8594	13.5452
37	5.8884	0.0142	37	5.8903	2.0758	37	5.8829	-40.7223
38	5.9284	-31.1054	38	5.9061	0.9939	38	5.9083	1.5222
39	5.9538	20.1486	39	5.9355	18.9757	39	5.9219	-91.1399
40	5.992	-30.2946	40	5.969	39.1738	40	5.9395	-17.8897
41	6.0034	41.0165	41	5.9937	-6.2812	41	5.9536	-47.2846
42	6.0268	-3.2521	42	6.0245	2.6872	42	6.0071	1.4111
43	6.042	-6.308	43	6.0452	27.6143	43	6.0416	-8.7704
44	6.072	-20.5208	44	6.0663	0.6625	44	6.0545	-94.1725
45	6.0827	6.6985	45	6.0814	2.072	45	6.0605	12.2831
46	6.1303	1.0774	46	6.1009	70.0879	46	6.0898	33.7245
47	6.1364	0.1683	47	6.1184	-10.2787	47	6.1085	29.5162
48	6.1418	3.9378	48	6.1286	-3.6988	48	6.1231	-2.1331
49	6.1529	46.837	49	6.1585	-3.0038	49	6.1509	17.3441
50	6.1715	-16.7081	50	6.1673	11.0886	50	6.1659	-24.0021
51	6.1812	35.8834	51	6.1751	12.4978	51	6.1724	-29.8699
52	6.1915	-117.409	52	6.1868	13.7749	52	6.1849	-40.4422
53	6.1987	17.0344	53	6.1904	-2.27	53	6.1875	40.5048
54	6.2186	7.8264	54	6.1995	15.8853	54	6.2132	-3.4357
55	6.2262	-3.5158	55	6.2019	-14.2196	55	6.2262	-2.8514
56	6.2383	37.7231	56	6.2201	-9.0721	56	6.2487	20.212
57	6.253	-5.1159	57	6.2626	-22.6463	57	6.2581	3.5429
58	6.3104	14.2389	58	6.3087	5.6782	58	6.2782	-9.3528
59	6.3224	-10.5472	59	6.3122	-1.9578	59	6.2981	-8.8599
60	6.352	-19.1353	60	6.3461	-24.1204	60	6.3243	-4.26
	(8*S*,2′*R*)-**2P-C1**			(8*S*,2′*R*)-**2P-C2**			(8*S*,2′*R*)-**2P-C3**	
1	3.7716	8.1327	1	3.7579	8.5685	1	3.7907	11.5944
2	3.8543	0.7366	2	3.889	-1.7034	2	3.875	-3.5204
3	3.9462	-1.9453	3	3.9923	0.5229	3	3.9909	0.1163
4	4.179	8.0555	4	4.2128	7.9484	4	4.2736	16.5432
5	4.4569	8.6465	5	4.4483	10.4017	5	4.5021	-17.412
6	4.6092	-8.0577	6	4.5788	-3.3391	6	4.6138	9.3072
7	4.6745	1.2891	7	4.6434	-8.6909	7	4.6706	0.2232
8	4.7309	-8.8892	8	4.7262	-14.3168	8	4.7745	-12.0316
9	4.8561	0.0669	9	4.8607	0.108	9	4.8679	0.0877
10	5.0052	-11.9458	10	4.933	-9.5954	10	4.9945	-8.2911
11	5.0826	-0.2406	11	5.0466	-1.082	11	5.0734	-1.2856
12	5.1355	-29.1628	12	5.125	-3.4435	12	5.1373	-25.7565
13	5.1839	-0.2947	13	5.1441	-24.7673	13	5.2209	2.1453
14	5.2531	-6.6767	14	5.2393	-8.4258	14	5.2314	3.2685
15	5.2871	-0.1295	15	5.2512	5.6578	15	5.2785	-3.3338
16	5.3598	45.1254	16	5.3497	2.4991	16	5.3984	-29.6524
17	5.3788	-122.993	17	5.3716	-45.1032	17	5.4174	-63.6132
18	5.4815	6.5152	18	5.4991	-7.2186	18	5.5091	-30.7047
19	5.4949	9.8937	19	5.524	-8.5263	19	5.5264	2.222

20	5.5298	-2.9916	20	5.5345	-20.3151	20	5.5461	20.372
21	5.5417	-29.2098	21	5.5393	-32.1345	21	5.5626	10.8445
22	5.5796	-23.9035	22	5.5725	0.873	22	5.564	-15.6286
23	5.6157	1.9236	23	5.5867	-17.081	23	5.6162	-3.1325
24	5.6374	-4.6488	24	5.6392	41.506	24	5.6241	2.7564
25	5.6547	9.4823	25	5.653	0.9759	25	5.6439	4.4536
26	5.6694	60.645	26	5.6557	-0.6869	26	5.6805	31.3044
27	5.7045	-1.8141	27	5.6784	10.1692	27	5.7078	9.0611
28	5.7293	-9.2261	28	5.7044	-3.2505	28	5.7231	-3.7429
29	5.7441	2.7671	29	5.7409	0.2561	29	5.7528	-4.5293
30	5.7649	-11.3039	30	5.7654	-16.549	30	5.7861	-74.8392
31	5.8038	-4.0513	31	5.7819	5.8035	31	5.8047	20.3421
32	5.8183	-21.7449	32	5.7912	3.7362	32	5.8162	-2.0611
33	5.8309	-3.9275	33	5.8245	5.4871	33	5.8427	1.6276
34	5.8586	-36.0969	34	5.8575	-0.9141	34	5.8727	-15.3316
35	5.8821	11.8139	35	5.87	13.7859	35	5.9092	11.0967
36	5.893	-1.8735	36	5.8752	-64.5664	36	5.9151	22.503
37	5.928	1.1038	37	5.9099	10.2777	37	5.9436	-1.5362
38	5.9619	-1.9414	38	5.9349	-6.3969	38	5.9658	18.7103
39	5.977	15.4399	39	5.9644	-4.0575	39	5.9905	-5.9417
40	5.9819	2.6397	40	5.9841	31.8288	40	6.0063	-33.3944
41	5.9977	-5.1134	41	6.001	-34.783	41	6.026	-66.726
42	6.0271	-65.1174	42	6.0295	-3.4085	42	6.0429	-27.5915
43	6.061	3.3715	43	6.0437	11.7597	43	6.0682	19.3687
44	6.073	-6.2885	44	6.0953	16.9873	44	6.1171	-5.5443
45	6.0957	-22.5714	45	6.0982	-20.406	45	6.1258	7.0757
46	6.1234	8.3076	46	6.1116	-6.5102	46	6.1332	-15.0139
47	6.1297	13.9515	47	6.1302	-16.0785	47	6.1387	-12.0496
48	6.1586	4.5002	48	6.139	9.8636	48	6.1472	11.978
49	6.1764	4.4369	49	6.149	6.6985	49	6.1643	9.4292
50	6.1793	-5.4725	50	6.1787	61.1369	50	6.1774	29.4005
51	6.1867	-5.6947	51	6.2096	55.0861	51	6.1972	-7.0746
52	6.2039	23.3089	52	6.2251	6.2764	52	6.2102	-30.5226
53	6.2427	2.3584	53	6.2362	10.8489	53	6.2248	73.1709
54	6.275	-0.5422	54	6.2579	16.0518	54	6.268	-10.0033
55	6.2814	48.3611	55	6.262	-3.2586	55	6.2753	24.9802
56	6.2941	-8.8642	56	6.2876	-17.731	56	6.2952	88.4429
57	6.3047	38.9198	57	6.2931	-10.5046	57	6.3221	-0.4084
58	6.3165	8.5051	58	6.3072	-10.9917	58	6.3347	0.1098
59	6.329	19.8265	59	6.3235	-19.835	59	6.3542	-24.3279
60	6.3364	18.9994	60	6.3575	-32.5251	60	6.3657	9.3358
	(8*S*,2′*R*)-**2P-C4**			(8*S*,2′*R*)-**2P-C5**			(8*S*,2′*R*)-**2P-C6**	
1	3.7792	11.7506	1	3.7724	-2.8728	1	3.7722	-2.8378
2	3.894	-3.79	2	3.8553	6.5866	2	3.8553	6.5562
3	4.0521	0.7284	3	4.0765	1.6301	3	4.0766	1.6295
4	4.3129	18.3775	4	4.326	40.4163	4	4.3261	40.4519
5	4.482	-9.8533	5	4.6008	22.612	5	4.6007	22.2736
6	4.5747	-0.3222	6	4.6205	5.3465	6	4.6205	5.8222
7	4.6353	-10.7004	7	4.6465	-29.9402	7	4.6464	-30.0736

8	4.7788	-7.9141	8	4.7352	-14.4015	8	4.7352	-14.4012
9	4.8711	0.4515	9	4.8241	-2.8886	9	4.8239	-2.8831
10	4.9202	-7.6839	10	4.9137	7.3866	10	4.9135	7.3779
11	5.0346	-0.535	11	4.9652	0.418	11	4.9651	0.4132
12	5.0937	-15.2004	12	5.0719	-1.8317	12	5.0717	-1.8418
13	5.1946	1.7869	13	5.0945	-11.3443	13	5.0945	-11.3231
14	5.2114	-10.6554	14	5.1681	2.5773	14	5.1682	2.5629
15	5.2647	-8.0892	15	5.2648	2.9954	15	5.2648	3.0266
16	5.3757	-48.6752	16	5.3519	-9.8566	16	5.3518	-9.9182
17	5.412	41.5884	17	5.3877	-38.3479	17	5.3876	-38.2206
18	5.4688	-53.83	18	5.4399	-4.1081	18	5.4398	-4.3383
19	5.5159	8.5713	19	5.457	29.0693	19	5.4569	29.2933
20	5.5311	-16.1256	20	5.467	-12.9507	20	5.467	-13.0339
21	5.5557	-16.4488	21	5.4745	8.7471	21	5.4745	8.793
22	5.5842	-14.9609	22	5.5369	-32.0785	22	5.5368	-31.8685
23	5.599	19.5988	23	5.5597	5.8721	23	5.5597	5.7819
24	5.6079	5.4316	24	5.5864	43.5229	24	5.5865	43.4274
25	5.6476	-3.5787	25	5.5948	-2.9865	25	5.5947	-2.9746
26	5.6734	0.0726	26	5.617	-15.8767	26	5.6171	-15.9056
27	5.6965	8.69	27	5.6487	7.0684	27	5.6486	6.2552
28	5.72	4.2035	28	5.6519	10.9973	28	5.6518	11.8047
29	5.7564	0.7557	29	5.6733	-3.5284	29	5.6733	-3.5233
30	5.781	-60.7322	30	5.6962	-0.0486	30	5.6961	-0.3328
31	5.811	41.2746	31	5.7215	3.9891	31	5.7215	4.1742
32	5.8151	-34.8988	32	5.7392	16.2763	32	5.7392	16.2054
33	5.8394	-12.1436	33	5.7558	4.0777	33	5.7559	4.0985
34	5.8575	7.0538	34	5.7948	-47.0567	34	5.7949	-46.9953
35	5.8818	7.7575	35	5.8309	3.4457	35	5.8308	3.3574
36	5.9109	10.381	36	5.837	4.1729	36	5.8371	4.0829
37	5.9258	5.0815	37	5.8562	-11.2617	37	5.8561	-10.9352
38	5.9463	-2.6889	38	5.8659	-47.158	38	5.8661	-47.6493
39	5.9701	-7.0687	39	5.8971	47.1834	39	5.8971	47.8569
40	6.0027	4.9061	40	5.9341	-19.8857	40	5.9342	-19.8952
41	6.019	-27.1275	41	5.9526	-9.0942	41	5.9528	-9.0346
42	6.0279	19.8834	42	5.9596	6.3313	42	5.9599	6.1423
43	6.0611	-5.0753	43	5.9737	-5.5012	43	5.9739	-5.6303
44	6.0727	-28.5825	44	6.0086	-9.5654	44	6.0085	-9.5413
45	6.0868	-3.0808	45	6.027	-0.1645	45	6.0271	-0.313
46	6.1257	-6.766	46	6.0489	-77.0084	46	6.0489	-76.8976
47	6.1319	37.3151	47	6.0736	26.2807	47	6.0737	26.2131
48	6.1497	-1.2554	48	6.0815	5.0858	48	6.0815	5.2572
49	6.1529	40.7282	49	6.1039	-13.9805	49	6.1038	-13.9859
50	6.1893	-0.968	50	6.1202	0.6575	50	6.1201	0.6325
51	6.2089	9.7246	51	6.1394	0.0342	51	6.1395	0.052
52	6.2274	-31.4927	52	6.1535	114.4109	52	6.1536	114.432
53	6.2369	-4.5615	53	6.173	-7.8246	53	6.1731	-7.8523
54	6.255	7.6282	54	6.2069	2.263	54	6.207	2.241
55	6.2794	59.7614	55	6.2236	-5.5989	55	6.2237	-5.4395
56	6.3112	-1.2714	56	6.2431	1.0665	56	6.243	1.0873

57	6.3184	-10.3164	57	6.2502	-2.9147	57	6.2501	-3.1322
58	6.3429	5.0568	58	6.2578	13.2498	58	6.2578	13.4384
59	6.361	3.1621	59	6.2749	27.0874	59	6.2751	27.0223
60	6.3698	-6.7822	60	6.284	-1.5716	60	6.2842	-1.7185

* R(velocity) 10**-40 erg-esu-cm

Table S4. Calculated ECD data for compound **2**