

Supporting Information

Synthesis and Photochemical Properties of Axially Chiral Bis(dinaphthofuran)

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Chiral HPLC Chromatograms for Racemic and Enantiomerically Pure 4

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Results of DFT Calculations for Compounds *R*-4, 2, and 4

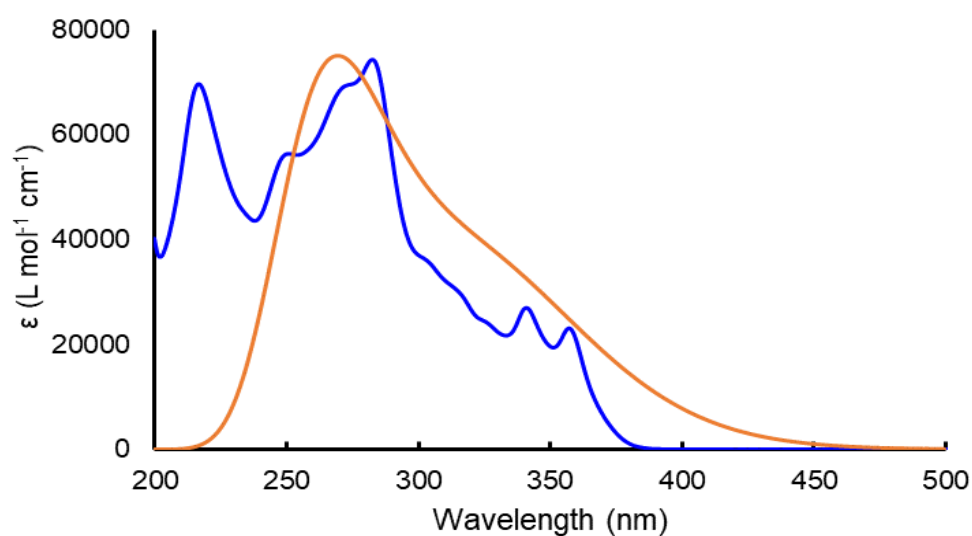
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(A)



(B)

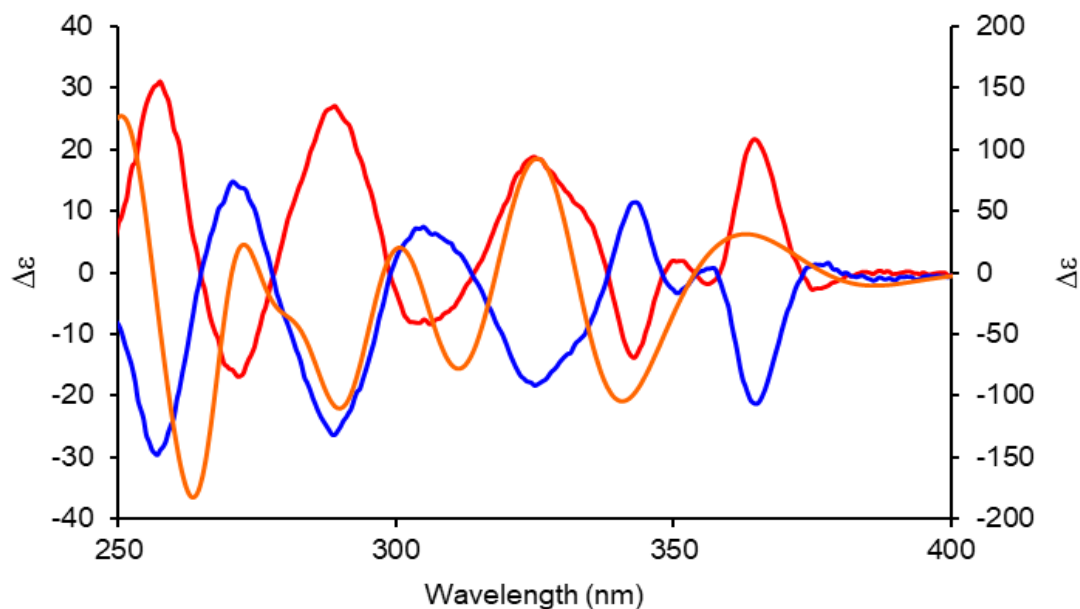


Figure S1. The experimental and theoretical UV-vis and CD spectra of compound **4**. (A) The experimental UV-vis spectrum of (–)-**4** (blue) in MeOH ($c = 1 \times 10^{-5}$ M, path length = 10 mm), and the theoretical spectrum of R-**4** (orange) calculated using TDDFT at the B3LYP/6-311++G(d,p) level.^{S1} (B) The experimental CD spectra of (+)-**4** (red) and (–)-**4** (blue) in MeOH ($c = 1 \times 10^{-5}$ M, path length = 10 mm), and the theoretical spectrum of R-**4** (orange) calculated using TDDFT at the same level.

Figure S2. ^1H NMR spectrum (400 MHz, $\text{DMSO-}d_6$) of compound **2**.

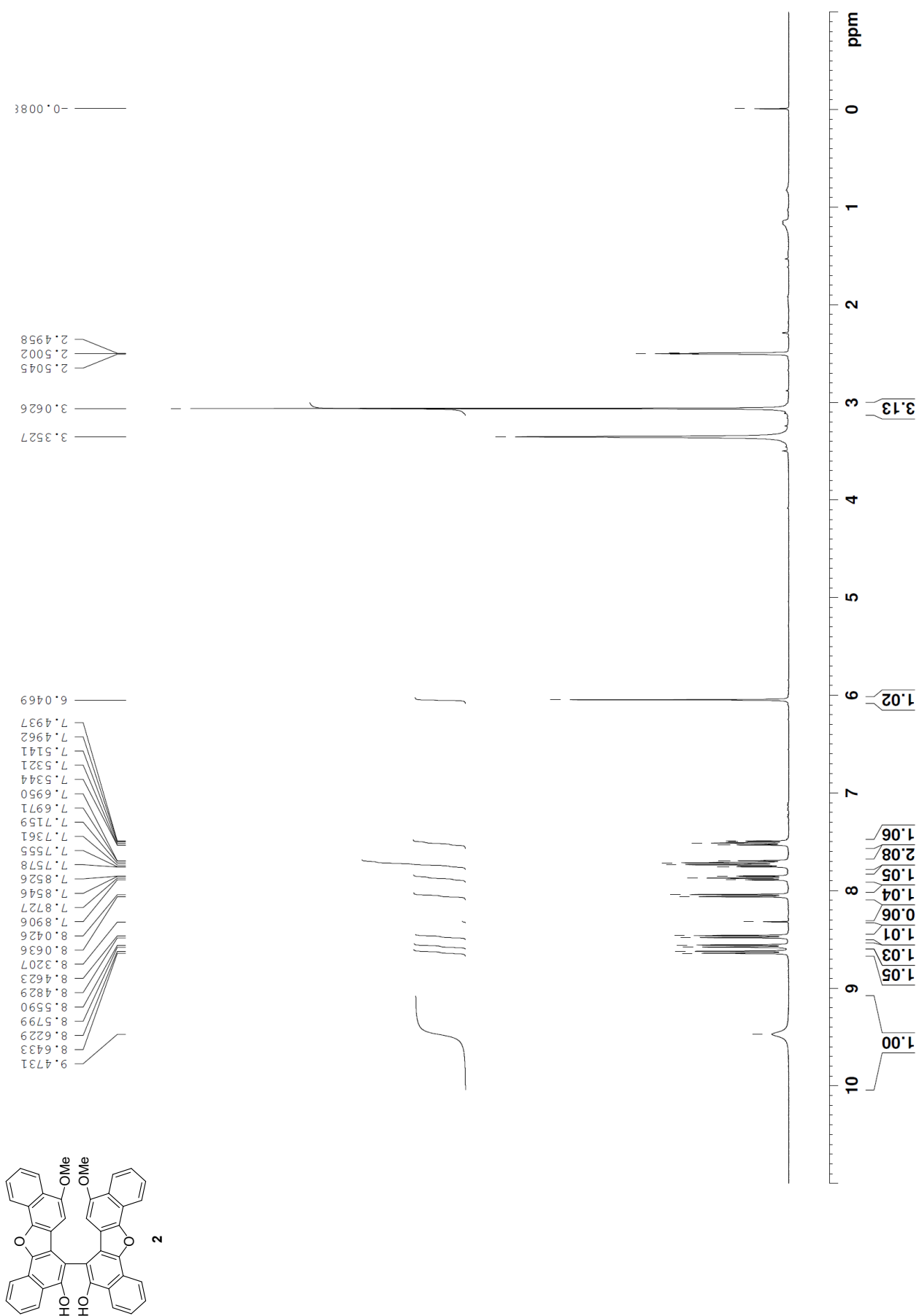


Figure S3. Zoom of ^1H NMR spectrum (400 MHz, $\text{DMSO-}d_6$) of compound **2** between 7 and 9 ppm.

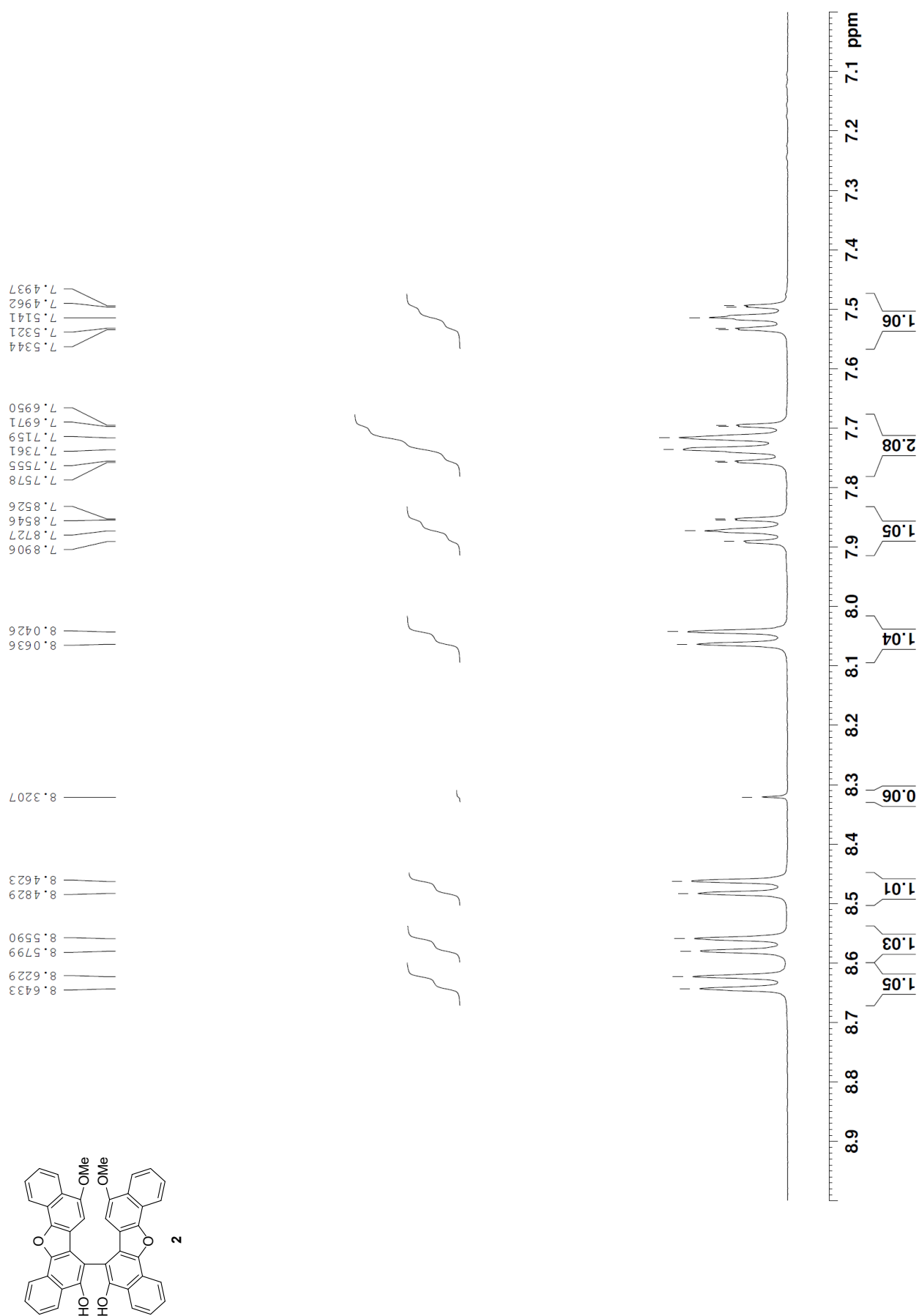


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of compound **2**.

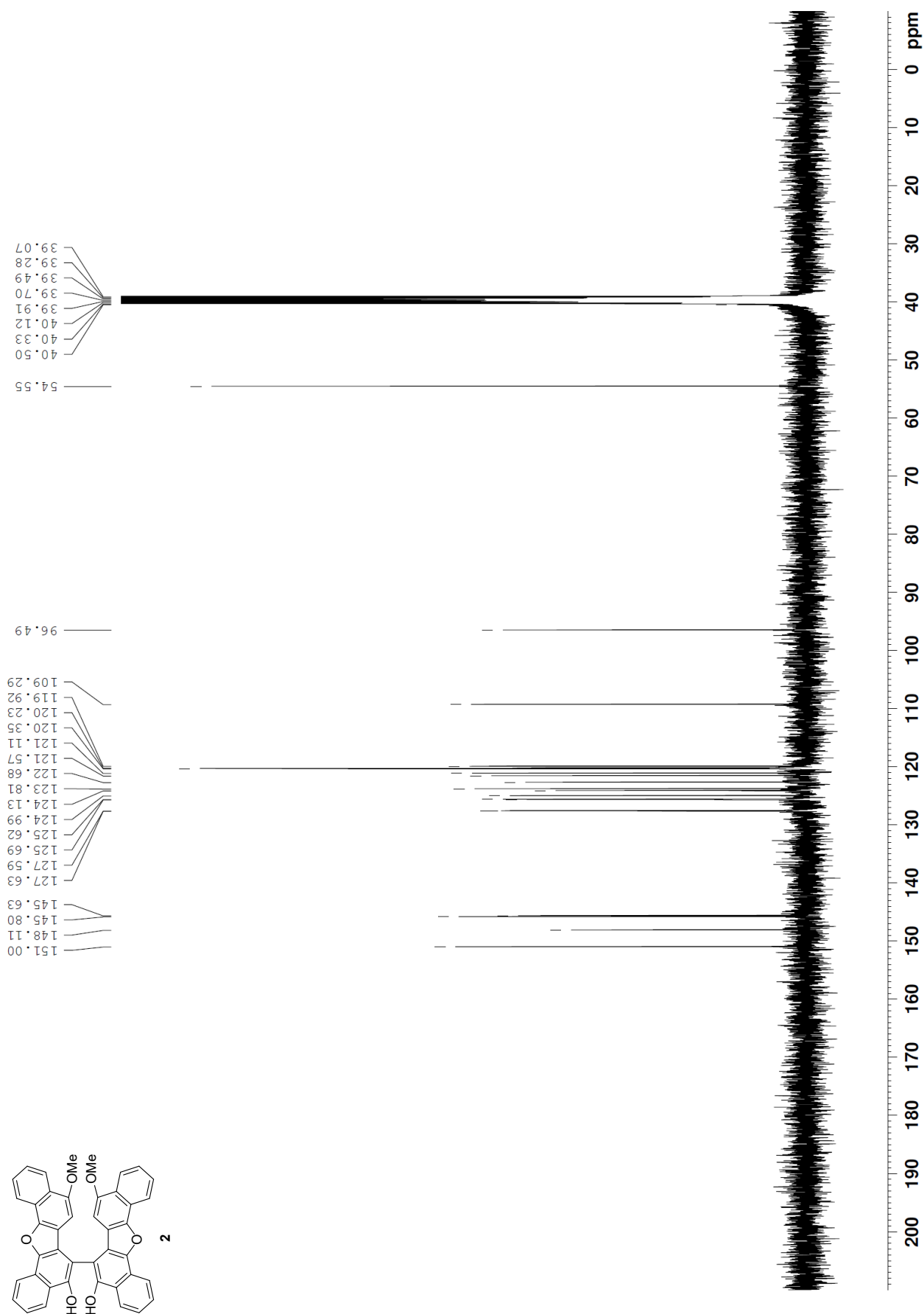


Figure S5. Zoom of $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of compound **2** between 115 and 135 ppm.

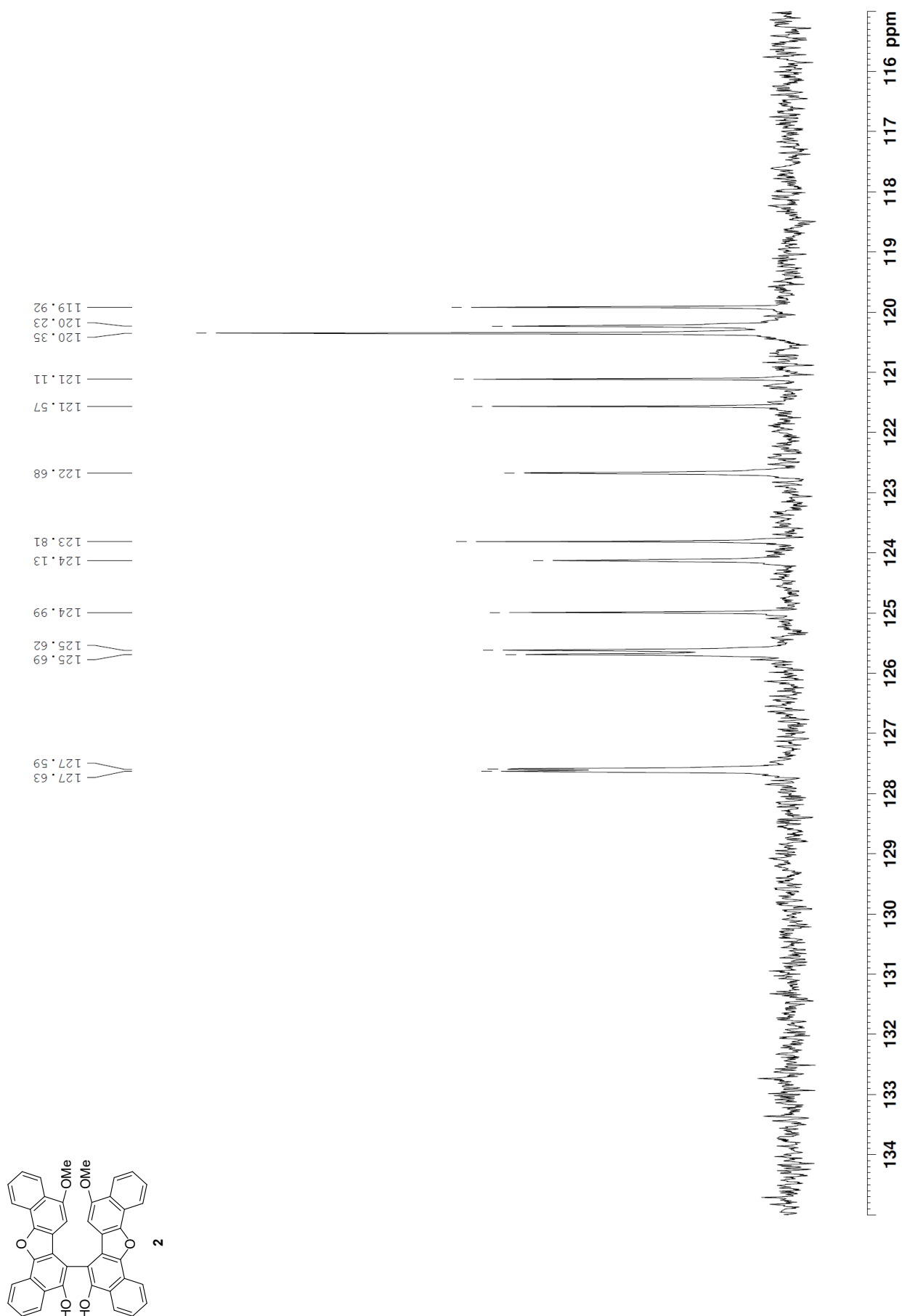


Figure S6. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **3**.

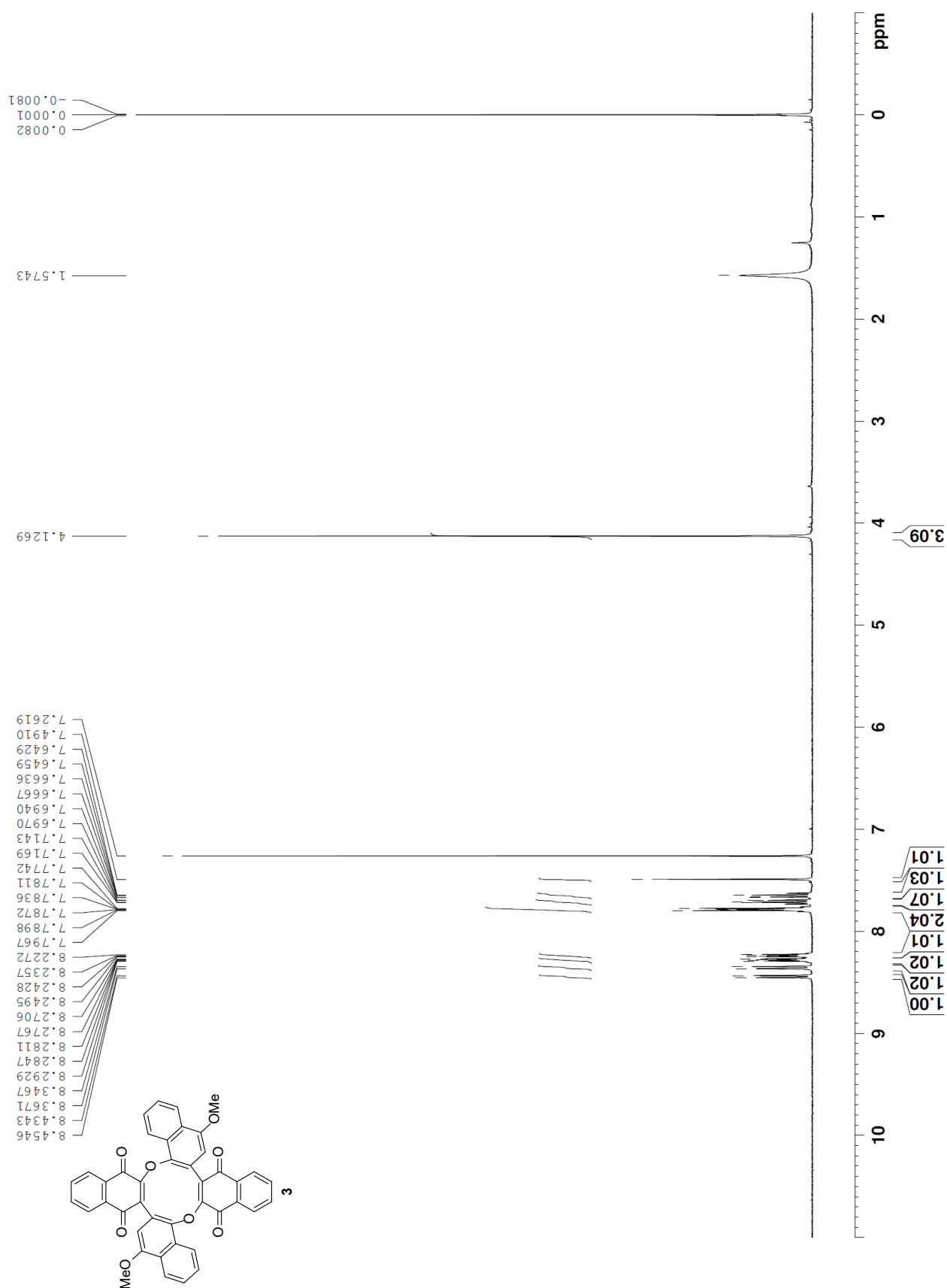


Figure S7. Zoom of ^1H NMR spectrum (400 MHz, CDCl_3) of compound **3** between 7 and 9 ppm.

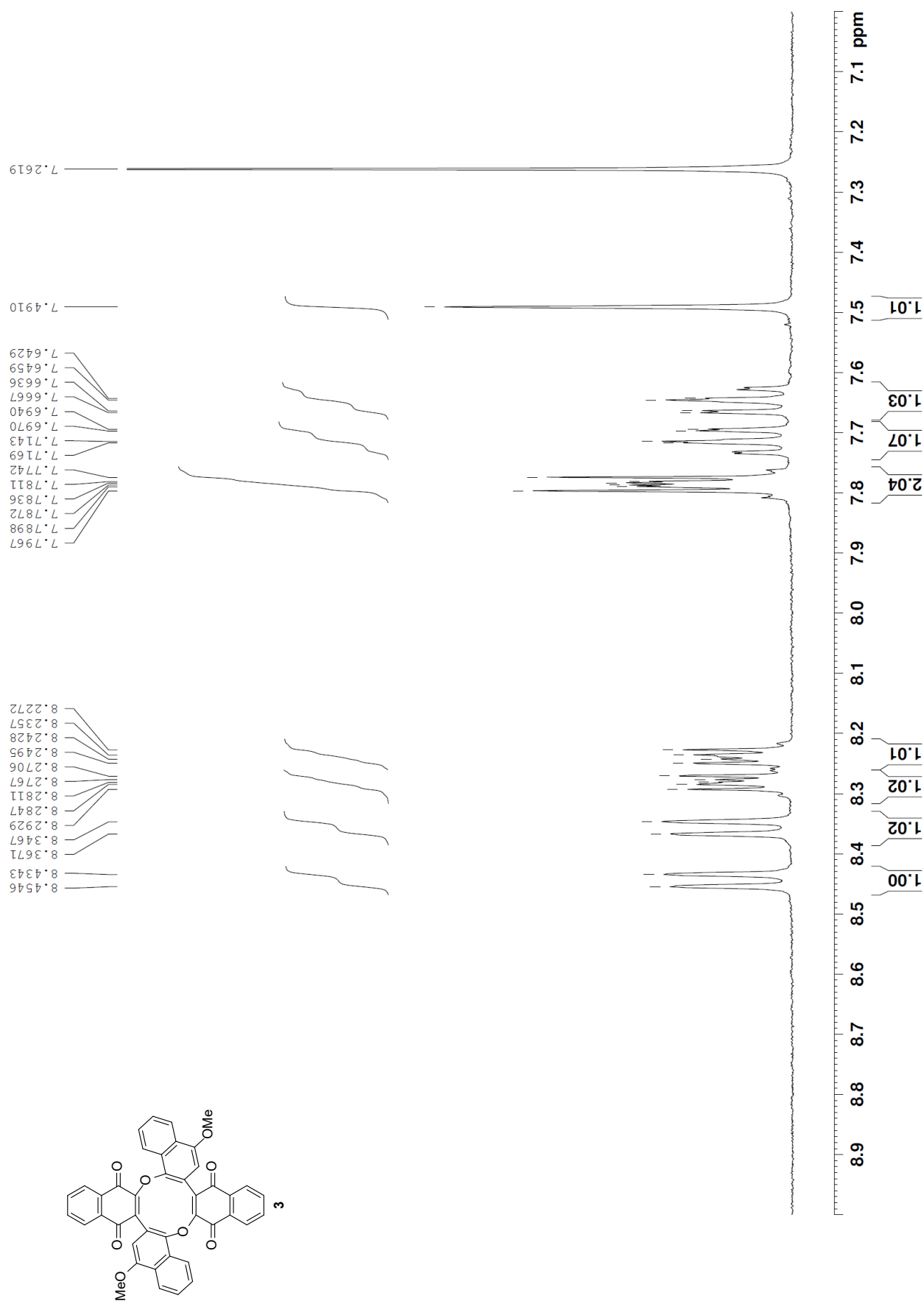


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, CDCl_3) of compound **3**.

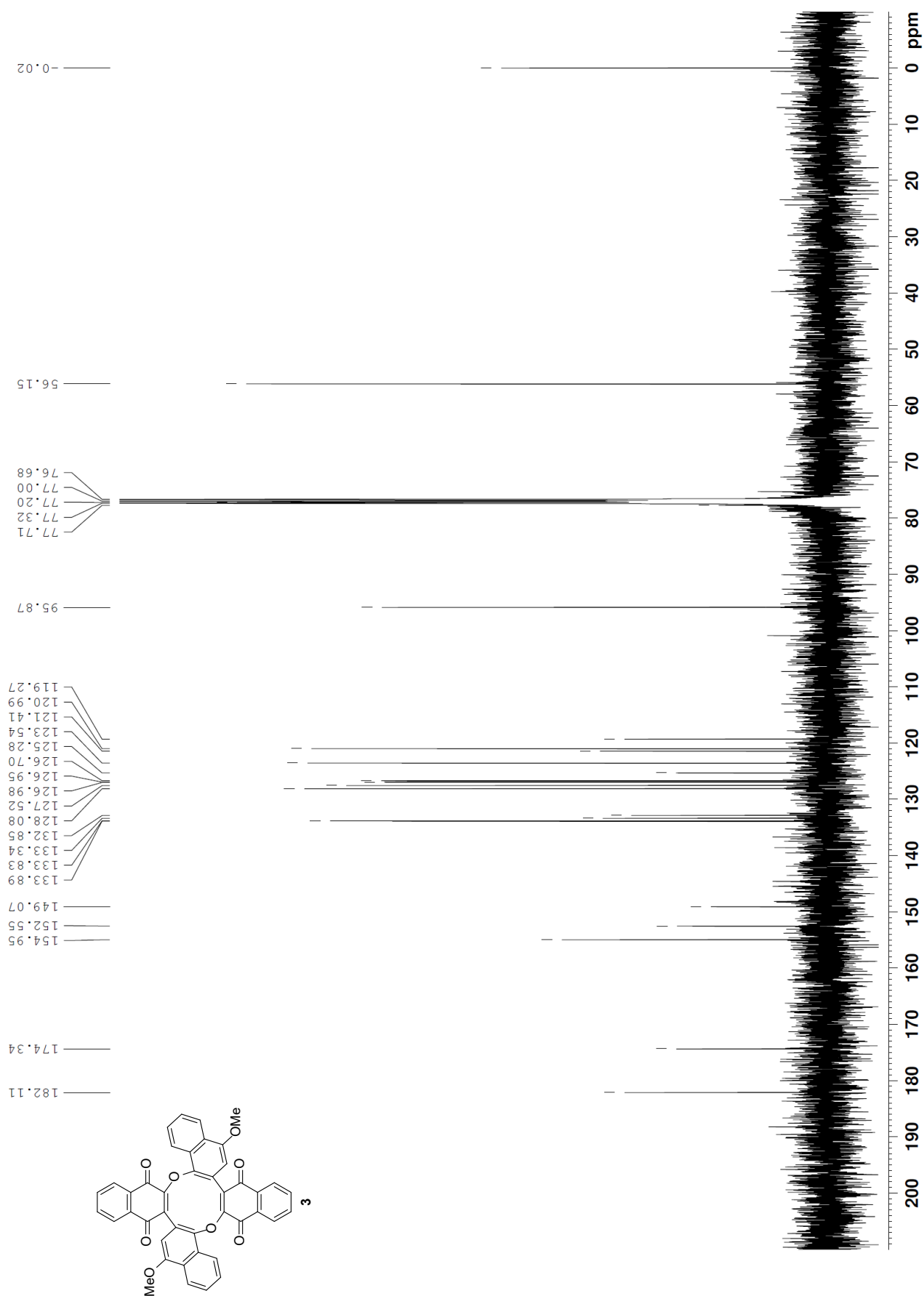


Figure S9. Zoom of $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, CDCl_3) of compound **3** between 115 and 135 ppm.

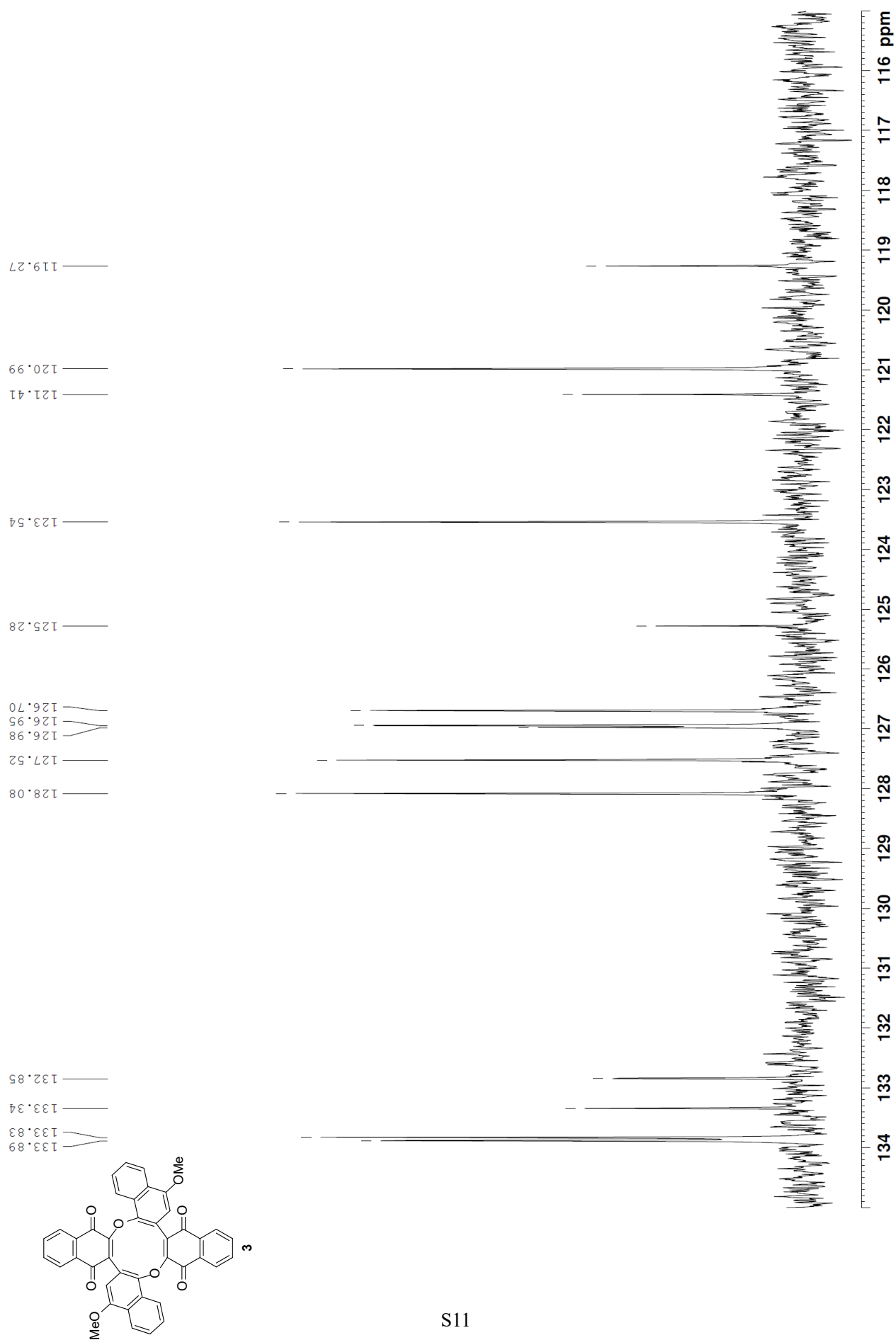




Figure S11. Zoom of ^1H NMR spectrum (400 MHz, CDCl_3) of compound **4** between 7 and 9 ppm.

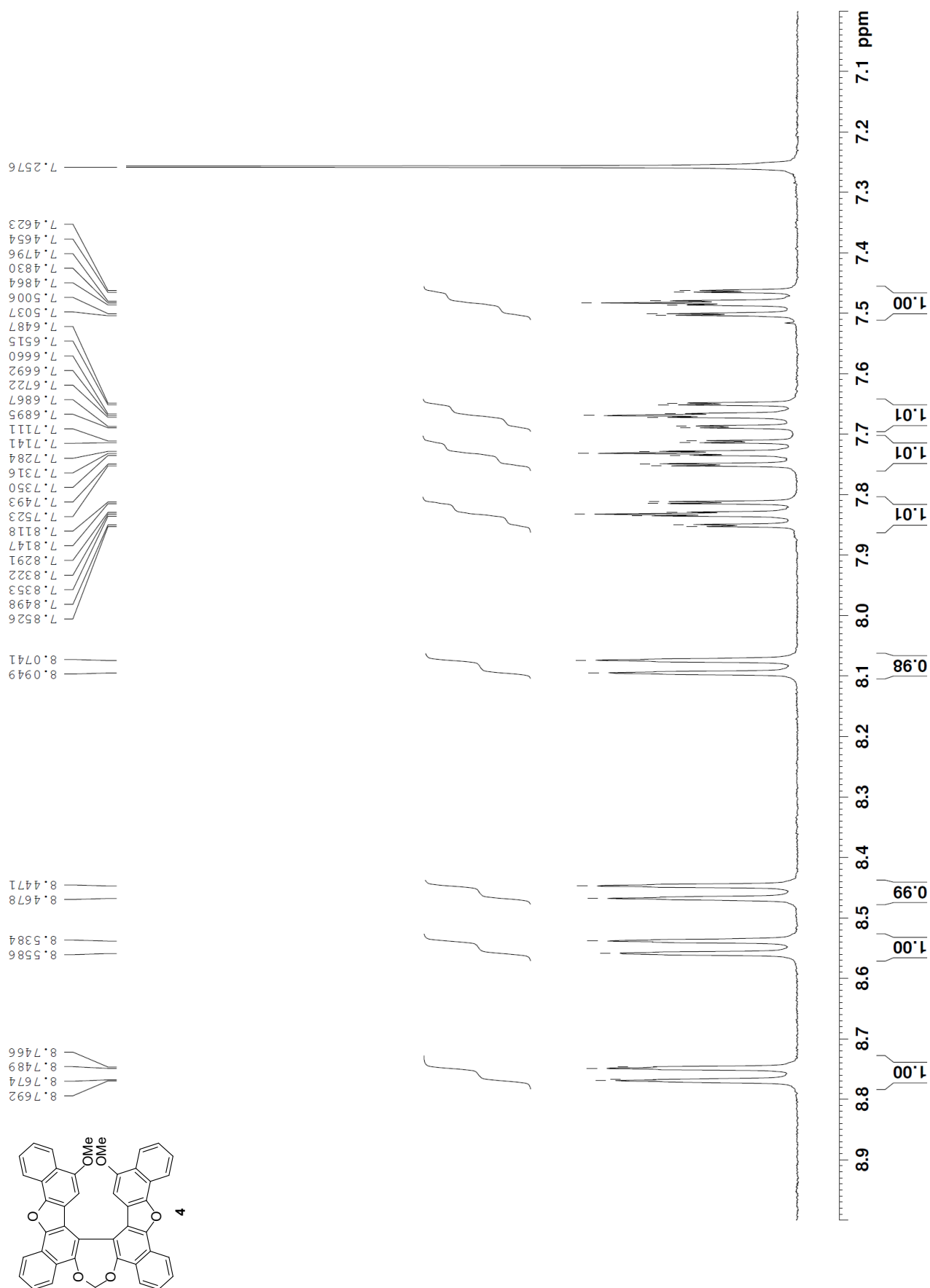


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, CDCl_3) of compound **4**.

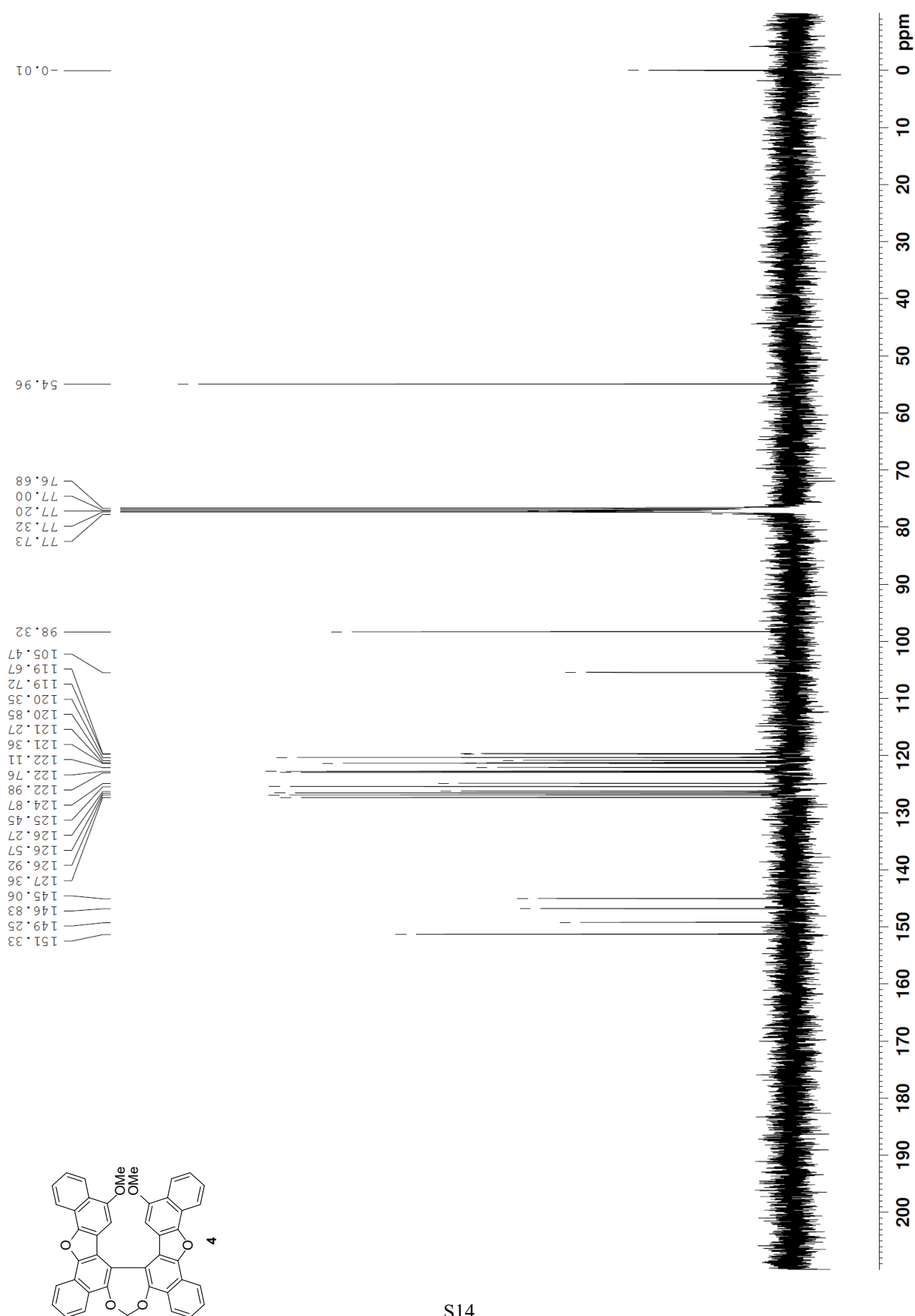
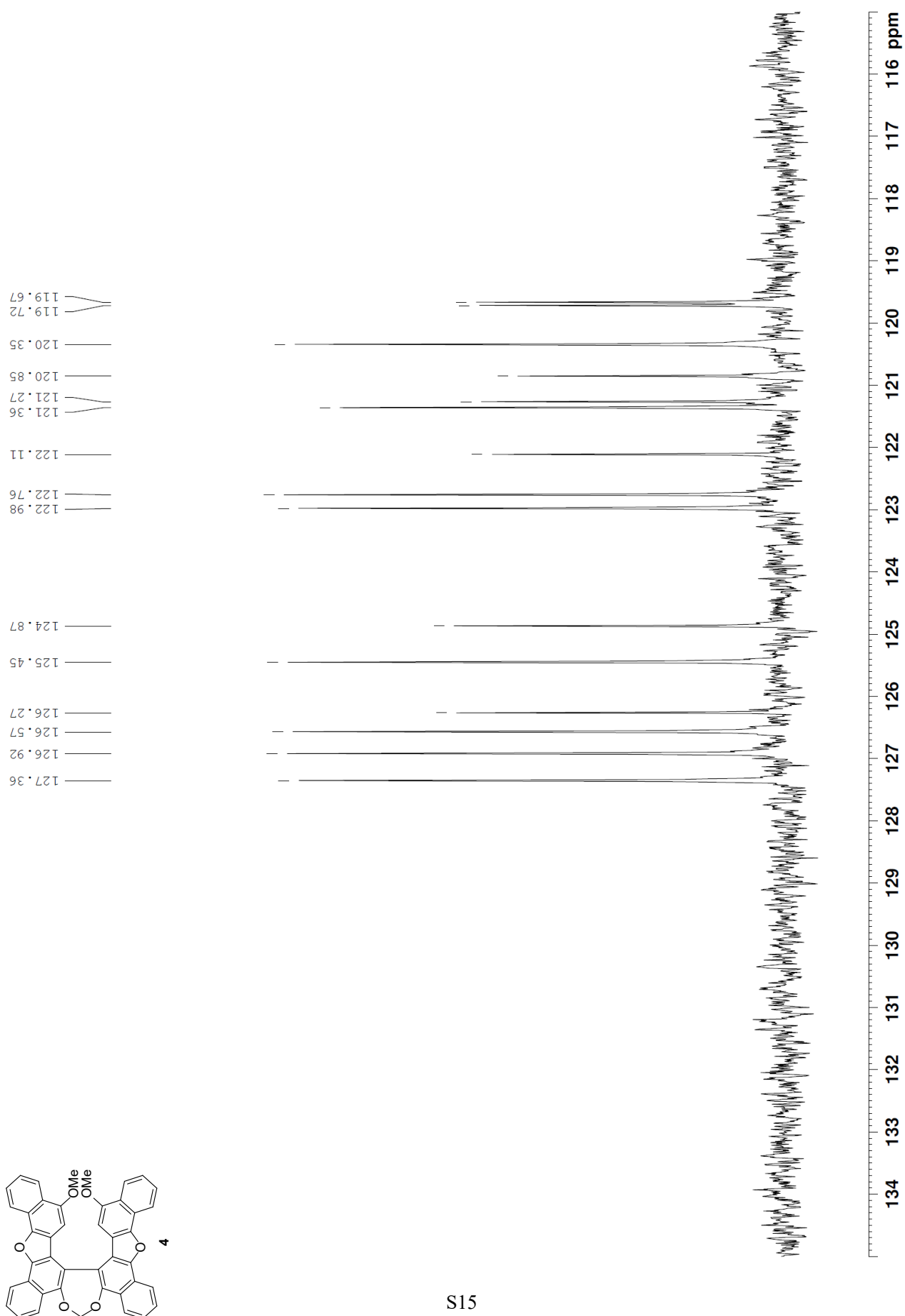


Figure S13. Zoom of $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, CDCl_3) of compound **4** between 115 and 135 ppm.



Chiral HPLC Chromatogram for Racemic and Enantiomerically Pure 4

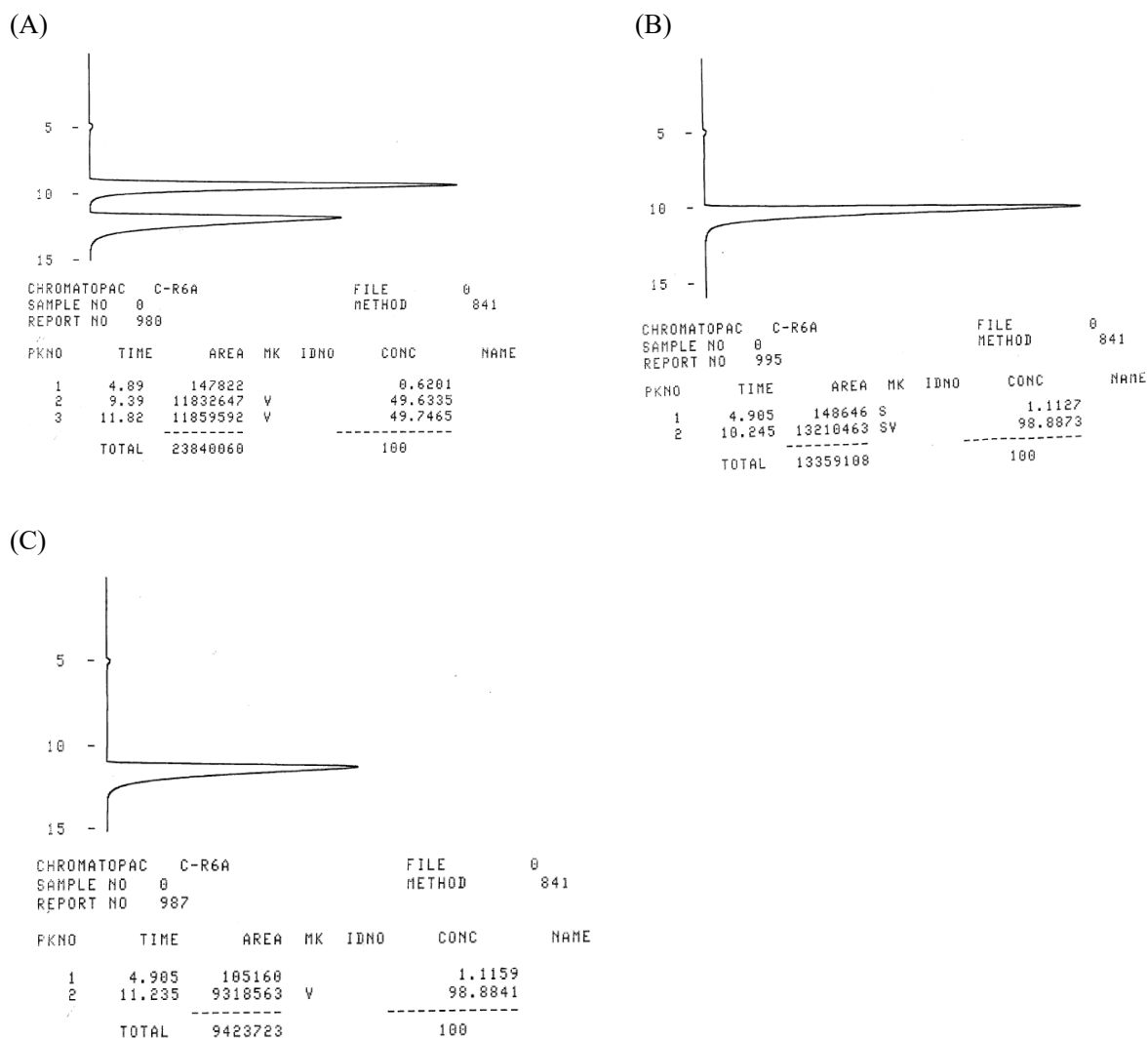
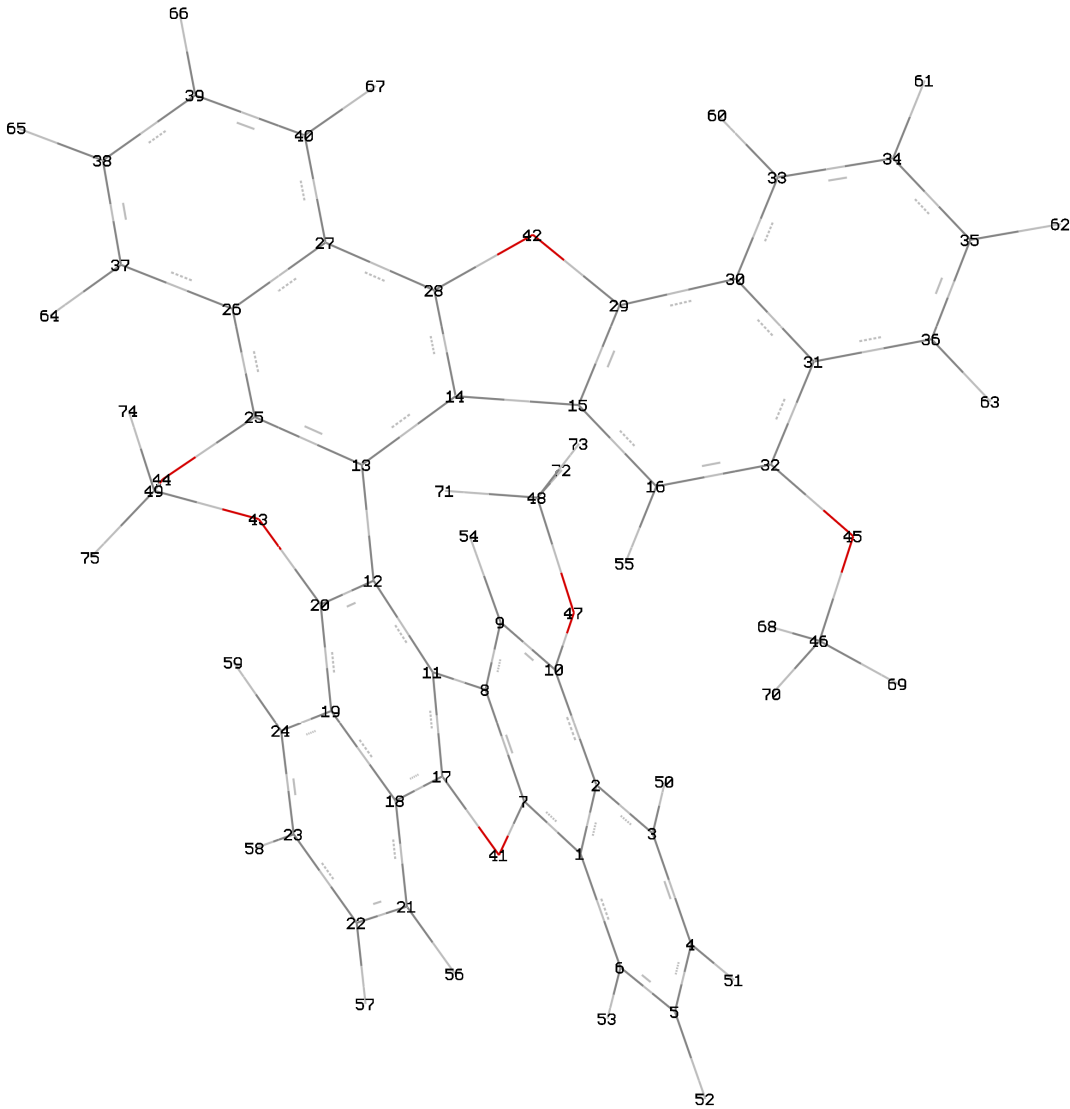


Figure S14. Chiral HPLC chromatograms for (±)-4, *S*-(+)-4, and *R*-(-)-4. (A) (±)-4, (B) *S*-(+)-4, (C) *R*-(-)-4. Conditions: CHIRALPAK IB column (4.6 × 250 mm), mobile phase, hexane/CHCl₃/2-propanol = 85:14:1, flow rate, 1.0 mL/min; temperature, rt; detection at UV 254 nm, *t_R* = 10.2 min for *S*-(+)-4 and *t_R* = 11.2 min for *R*-(-)-4.

Results of DFT Calculations for Compounds *R*-4, 2, and 4

Table S1. Total Energy, Number of Imaginary Frequencies, and Atom Coordinates for Compound *R*-4 Optimized by DFT/B3LYP/6-311++G(d,p) Level^{S1}



R-4

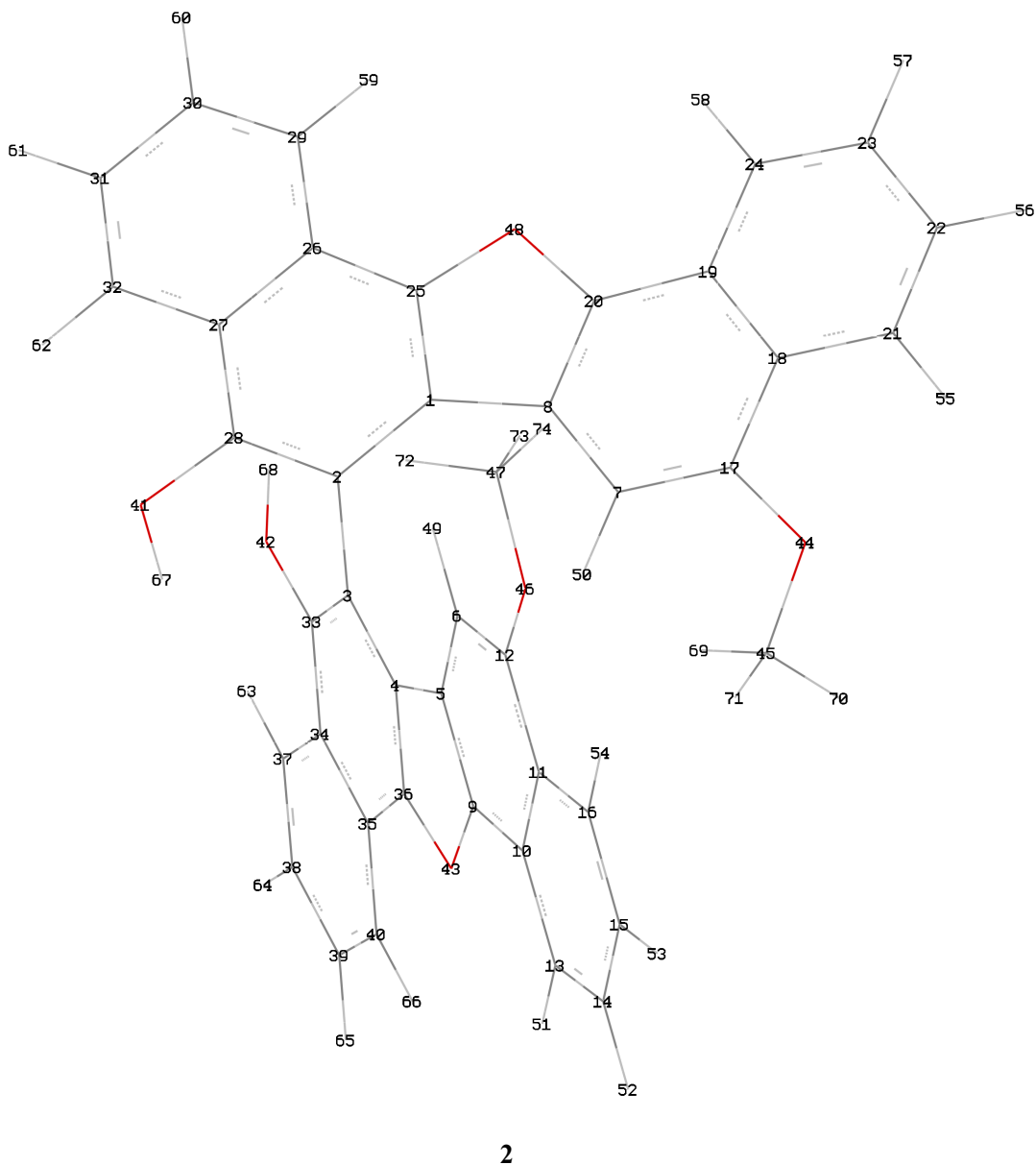
Total energy [E(RB3LPY)] = -2106.12797083 au. Number of imaginary frequencies = 0.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.213215	-2.177937	-1.538470
2	6	0	-2.196620	-2.824488	-2.308061
3	6	0	-2.522585	-4.024663	-2.980835
4	6	0	-3.791445	-4.557836	-2.897455
5	6	0	-4.790919	-3.912501	-2.139695

6	6	0	-4.509086	-2.742209	-1.471297
7	6	0	-2.835185	-0.986421	-0.884917
8	6	0	-1.564289	-0.437714	-0.944766
9	6	0	-0.562599	-1.077987	-1.723338
10	6	0	-0.879561	-2.241427	-2.384816
11	6	0	-1.627979	0.773890	-0.147506
12	6	0	-0.718791	1.828050	0.181006
13	6	0	0.718916	1.827993	-0.181059
14	6	0	1.628027	0.773785	0.147490
15	6	0	1.564248	-0.437816	0.944747
16	6	0	0.562512	-1.078012	1.723334
17	6	0	-2.946690	0.854960	0.290823
18	6	0	-3.484134	1.927594	1.030738
19	6	0	-2.590180	3.012550	1.293686
20	6	0	-1.240459	2.931894	0.830518
21	6	0	-4.822844	1.993438	1.484477
22	6	0	-5.261539	3.094196	2.184791
23	6	0	-4.381851	4.165382	2.456635
24	6	0	-3.076033	4.127056	2.020601
25	6	0	1.240676	2.931794	-0.830577
26	6	0	2.590407	3.012370	-1.293693
27	6	0	3.484287	1.927367	-1.030705
28	6	0	2.946763	0.854769	-0.290807
29	6	0	2.835098	-0.986621	0.884902
30	6	0	3.213046	-2.178166	1.538456
31	6	0	2.196402	-2.824642	2.308050
32	6	0	0.879387	-2.241469	2.384811
33	6	0	4.508871	-2.742528	1.471286
34	6	0	4.790620	-3.912846	2.139688
35	6	0	3.791102	-4.558106	2.897442
36	6	0	2.522276	-4.024837	2.980820
37	6	0	3.076362	4.126855	-2.020593
38	6	0	4.382194	4.165104	-2.456563
39	6	0	5.261814	3.093859	-2.184681
40	6	0	4.823028	1.993132	-1.484393
41	8	0	-3.688087	-0.215480	-0.131309
42	8	0	3.688068	-0.215733	0.131312
43	8	0	-0.398618	3.994082	1.114557
44	8	0	0.398894	3.994022	-1.114676

45	8	0	0.001238	-2.941542	3.159126
46	6	0	-1.330227	-2.456652	3.281612
47	8	0	-0.001475	-2.941560	-3.159152
48	6	0	1.330092	-2.456905	-3.281481
49	6	0	0.000119	4.771904	-0.000114
50	1	0	-1.755562	-4.517094	-3.563384
51	1	0	-4.024257	-5.479147	-3.419227
52	1	0	-5.785442	-4.340818	-2.084632
53	1	0	-5.270960	-2.239083	-0.888202
54	1	0	0.424848	-0.648844	-1.786754
55	1	0	-0.424905	-0.648799	1.786745
56	1	0	-5.491229	1.168342	1.270623
57	1	0	-6.287560	3.140697	2.531735
58	1	0	-4.738812	5.022928	3.015564
59	1	0	-2.396822	4.941344	2.237332
60	1	0	5.270788	-2.239465	0.888194
61	1	0	5.785115	-4.341226	2.084623
62	1	0	4.023836	-5.479433	3.419219
63	1	0	1.755223	-4.517216	3.563373
64	1	0	2.397200	4.941176	-2.237350
65	1	0	4.739243	5.022625	-3.015475
66	1	0	6.287851	3.140315	-2.531586
67	1	0	5.491344	1.167988	-1.270506
68	1	0	-1.349516	-1.464008	3.743780
69	1	0	-1.846414	-3.166583	3.925736
70	1	0	-1.828492	-2.417293	2.307673
71	1	0	1.349617	-1.464268	-3.743651
72	1	0	1.846229	-3.166929	-3.925542
73	1	0	1.828243	-2.417633	-2.307480
74	1	0	0.823583	5.387624	0.372389
75	1	0	-0.823408	5.387529	-0.372631

Table S2. Total Energy, Number of Imaginary Frequencies, and Atom Coordinates for 2 Optimized by DFT/B3LYP/6-31G(d,p) Level^{S1}



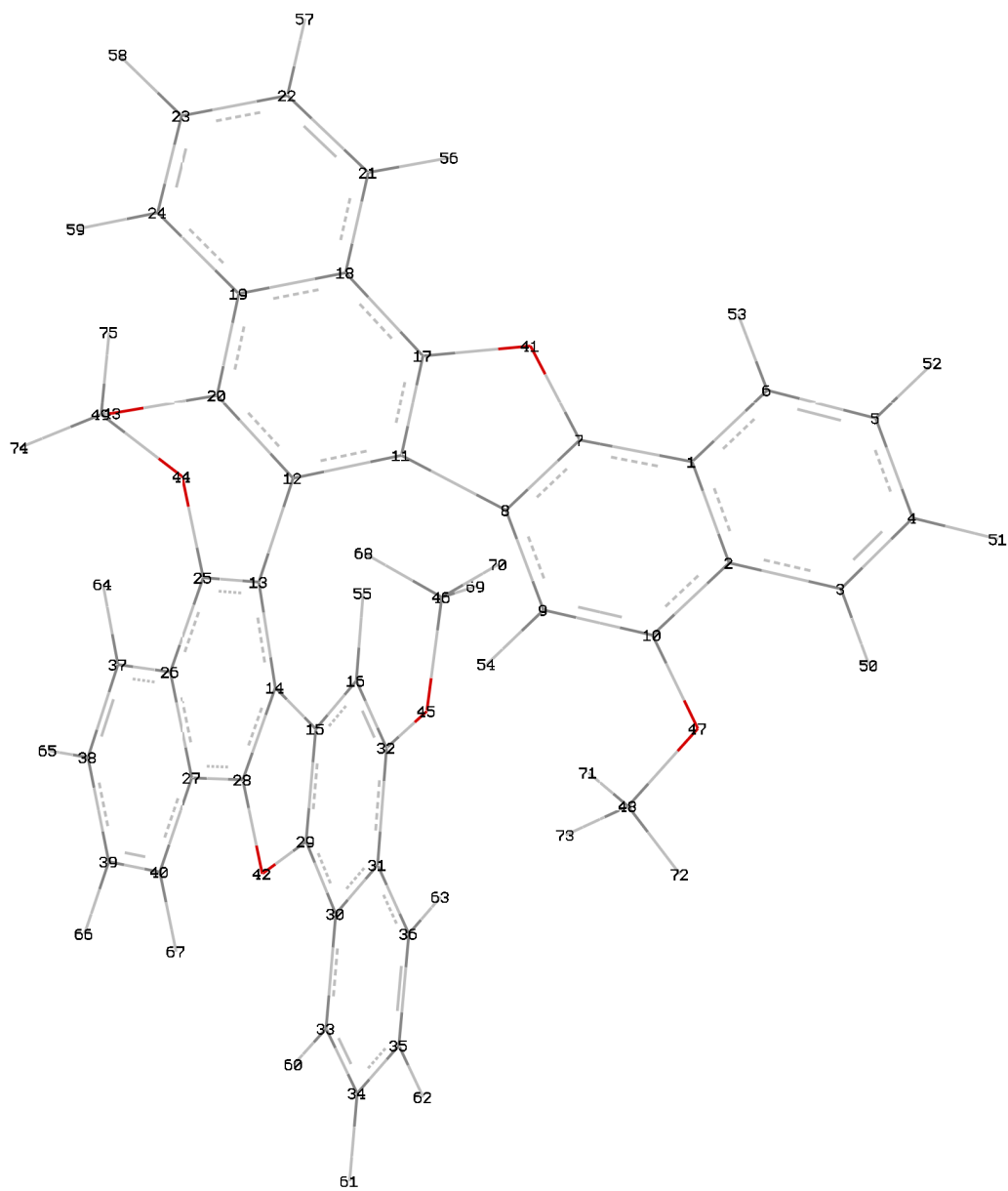
Total energy [E(RB3LPY)] = -2067.56997166 au. Number of imaginary frequencies = 0.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.698677	0.832426	0.002243
2	6	0	0.668644	1.767270	-0.334137
3	6	0	-0.668644	1.767270	0.334137
4	6	0	-1.698677	0.832426	-0.002243
5	6	0	-1.818457	-0.248061	-0.958745

6	6	0	-0.958814	-0.814433	-1.939117
7	6	0	0.958814	-0.814433	1.939117
8	6	0	1.818457	-0.248061	0.958745
9	6	0	-3.096775	-0.760586	-0.778324
10	6	0	-3.622068	-1.841550	-1.520653
11	6	0	-2.751777	-2.411240	-2.505317
12	6	0	-1.423771	-1.872474	-2.689412
13	6	0	-4.923374	-2.370045	-1.341470
14	6	0	-5.353194	-3.430927	-2.110026
15	6	0	-4.500115	-3.998759	-3.081472
16	6	0	-3.227421	-3.499499	-3.274830
17	6	0	1.423771	-1.872473	2.689412
18	6	0	2.751777	-2.411240	2.505317
19	6	0	3.622068	-1.841549	1.520653
20	6	0	3.096775	-0.760586	0.778324
21	6	0	3.227421	-3.499499	3.274830
22	6	0	4.500115	-3.998759	3.081472
23	6	0	5.353194	-3.430927	2.110026
24	6	0	4.923374	-2.370045	1.341470
25	6	0	2.917885	0.873159	-0.666865
26	6	0	3.231655	1.797520	-1.687366
27	6	0	2.203050	2.734025	-2.028172
28	6	0	0.941554	2.689714	-1.337912
29	6	0	4.472771	1.842671	-2.368278
30	6	0	4.687348	2.781029	-3.355304
31	6	0	3.674974	3.705308	-3.698179
32	6	0	2.457833	3.682640	-3.048068
33	6	0	-0.941555	2.689714	1.337912
34	6	0	-2.203051	2.734025	2.028172
35	6	0	-3.231655	1.797520	1.687366
36	6	0	-2.917885	0.873159	0.666865
37	6	0	-2.457833	3.682640	3.048068
38	6	0	-3.674974	3.705308	3.698179
39	6	0	-4.687348	2.781029	3.355304
40	6	0	-4.472772	1.842671	2.368278
41	8	0	0.020327	3.612379	-1.735757
42	8	0	-0.020327	3.612379	1.735757
43	8	0	-3.782158	-0.090234	0.208027
44	8	0	0.695968	-2.503701	3.657026

45	6	0	-0.628387	-2.053473	3.898824
46	8	0	-0.695967	-2.503701	-3.657026
47	6	0	0.628388	-2.053473	-3.898823
48	8	0	3.782158	-0.090234	-0.208027
49	1	0	0.036320	-0.415479	-2.075534
50	1	0	-0.036320	-0.415479	2.075534
51	1	0	-5.570139	-1.925320	-0.592315
52	1	0	-6.352283	-3.832442	-1.968294
53	1	0	-4.848659	-4.834625	-3.680652
54	1	0	-2.570737	-3.933631	-4.019212
55	1	0	2.570737	-3.933631	4.019212
56	1	0	4.848659	-4.834625	3.680653
57	1	0	6.352284	-3.832441	1.968294
58	1	0	5.570139	-1.925320	0.592315
59	1	0	5.244278	1.129416	-2.098069
60	1	0	5.641136	2.811041	-3.873801
61	1	0	3.857479	4.438094	-4.478263
62	1	0	1.677669	4.389049	-3.306607
63	1	0	-1.677669	4.389049	3.306607
64	1	0	-3.857479	4.438094	4.478263
65	1	0	-5.641136	2.811041	3.873800
66	1	0	-5.244278	1.129416	2.098068
67	1	0	-0.799838	3.450119	-1.242137
68	1	0	0.799838	3.450119	1.242136
69	1	0	-0.643178	-1.008391	4.232775
70	1	0	-1.023254	-2.691523	4.690508
71	1	0	-1.255691	-2.152162	3.004257
72	1	0	0.643178	-1.008391	-4.232775
73	1	0	1.023254	-2.691523	-4.690508
74	1	0	1.255691	-2.152162	-3.004257

Table S3. Total Energy, Number of Imaginary Frequencies, and Atom Coordinates for 4 Optimized by DFT/B3LYP/6-31G(d,p) Level ^{S1}



4

Total energy [E(RB3LPY)] = -2105.65494312 au. Number of imaginary frequencies = 0.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.399989	3.289539	-2.180569
2	6	0	2.190107	2.297831	-2.845330
3	6	0	2.840572	2.651718	-4.051329
4	6	0	2.718098	3.924547	-4.572044

5	6	0	1.940562	4.899095	-3.908618
6	6	0	1.291746	4.589203	-2.732267
7	6	0	0.770558	2.882616	-0.983242
8	6	0	0.873676	1.607206	-0.443438
9	6	0	1.671735	0.631688	-1.101781
10	6	0	2.307668	0.976691	-2.274549
11	6	0	0.089014	1.639734	0.778515
12	6	0	-0.205296	0.713240	1.830585
13	6	0	0.205296	-0.713240	1.830585
14	6	0	-0.089014	-1.639734	0.778515
15	6	0	-0.873676	-1.607206	-0.443438
16	6	0	-1.671735	-0.631688	-1.101781
17	6	0	-0.389256	2.947136	0.871272
18	6	0	-1.137073	3.458551	1.953549
19	6	0	-1.368937	2.548688	3.034591
20	6	0	-0.870815	1.210796	2.940169
21	6	0	-1.625624	4.785440	2.031769
22	6	0	-2.329313	5.197888	3.142863
23	6	0	-2.569756	4.302520	4.210812
24	6	0	-2.099850	3.007028	4.159404
25	6	0	0.870815	-1.210796	2.940169
26	6	0	1.368937	-2.548688	3.034591
27	6	0	1.137073	-3.458551	1.953549
28	6	0	0.389256	-2.947136	0.871272
29	6	0	-0.770558	-2.882616	-0.983242
30	6	0	-1.399989	-3.289539	-2.180569
31	6	0	-2.190107	-2.297831	-2.845330
32	6	0	-2.307668	-0.976691	-2.274549
33	6	0	-1.291746	-4.589203	-2.732267
34	6	0	-1.940562	-4.899095	-3.908618
35	6	0	-2.718098	-3.924547	-4.572044
36	6	0	-2.840572	-2.651718	-4.051329
37	6	0	2.099850	-3.007028	4.159404
38	6	0	2.569756	-4.302520	4.210812
39	6	0	2.329313	-5.197888	3.142863
40	6	0	1.625624	-4.785440	2.031769
41	8	0	0.000000	3.709110	-0.198584
42	8	0	0.000000	-3.709110	-0.198584
43	8	0	-1.128760	0.354775	3.999798

44	8	0	1.128760	-0.354775	3.999798
45	8	0	-3.094154	-0.125577	-2.996409
46	6	0	-3.234436	1.209810	-2.534758
47	8	0	3.094154	0.125577	-2.996409
48	6	0	3.234436	-1.209810	-2.534758
49	6	0	0.000000	0.000000	4.776149
50	1	0	3.437400	1.902184	-4.557126
51	1	0	3.223837	4.179613	-5.498517
52	1	0	1.854348	5.897293	-4.327734
53	1	0	0.692591	5.330264	-2.213443
54	1	0	1.766748	-0.358082	-0.680581
55	1	0	-1.766748	0.358082	-0.680581
56	1	0	-1.434906	5.464207	1.207221
57	1	0	-2.703510	6.215684	3.199609
58	1	0	-3.131109	4.639289	5.077189
59	1	0	-2.291155	2.313077	4.969893
60	1	0	-0.692591	-5.330264	-2.213443
61	1	0	-1.854348	-5.897293	-4.327734
62	1	0	-3.223837	-4.179613	-5.498517
63	1	0	-3.437400	-1.902184	-4.557126
64	1	0	2.291155	-2.313077	4.969893
65	1	0	3.131109	-4.639289	5.077189
66	1	0	2.703510	-6.215684	3.199609
67	1	0	1.434906	-5.464207	1.207221
68	1	0	-3.710867	1.245198	-1.546954
69	1	0	-3.873022	1.713613	-3.261544
70	1	0	-2.264760	1.720012	-2.484666
71	1	0	3.710867	-1.245198	-1.546954
72	1	0	3.873022	-1.713613	-3.261544
73	1	0	2.264760	-1.720012	-2.484666
74	1	0	-0.342132	-0.836749	5.396135
75	1	0	0.342132	0.836749	5.396135

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