Electronic Supplementary Information for

4,9- and 4,10- Substituted Pyrenes: Synthesis, Successful Isolation, and Optoelectronic Properties

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Contents

Synthesis

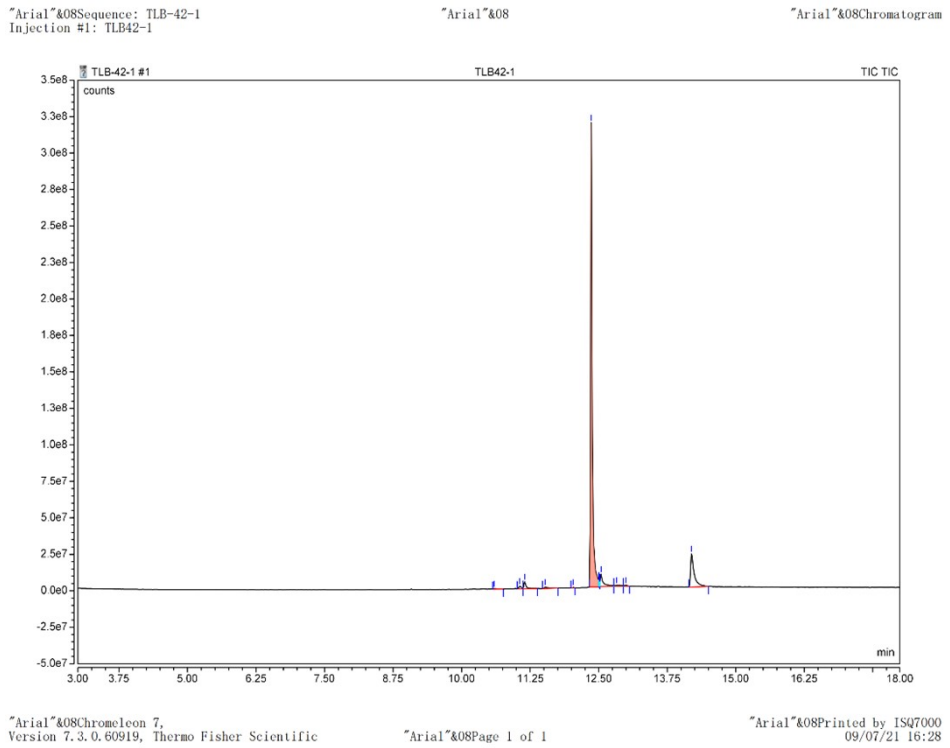


Figure S1. The gas chromatogram of 1,2,3,6,7,8-hexahydropyrene brominated with 2 eq of bromine.

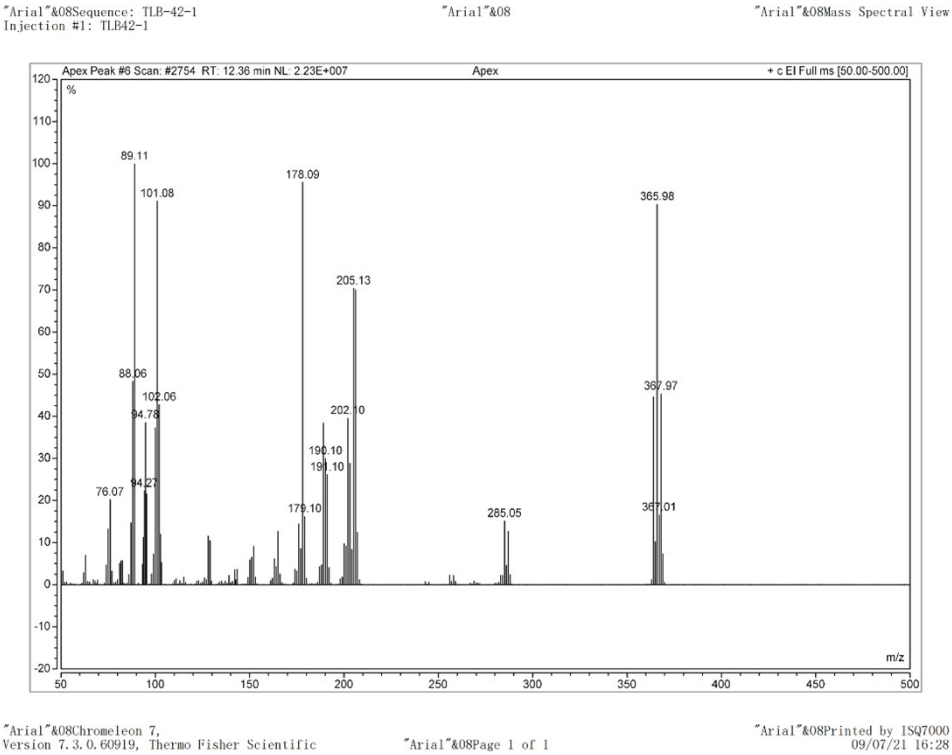


Figure S2. The mass spectrum at 12.5 minutes of the gas chromatograph in **Figure S1**.

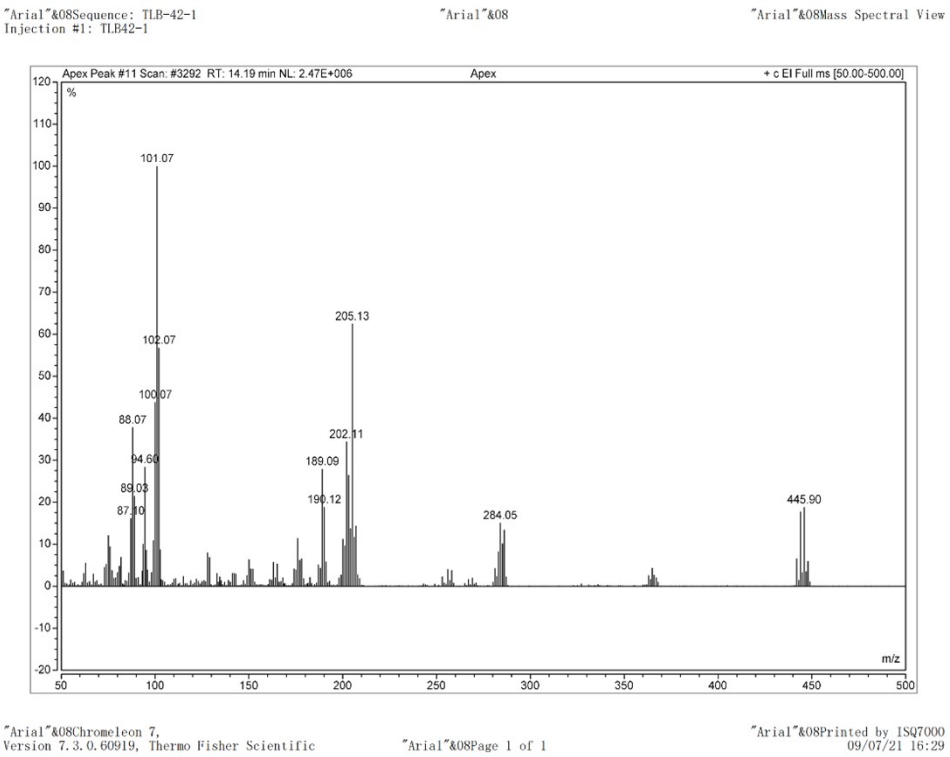


Figure S3. The mass spectrum at 14 minutes of the gas chromatograph in **Figure S1**.

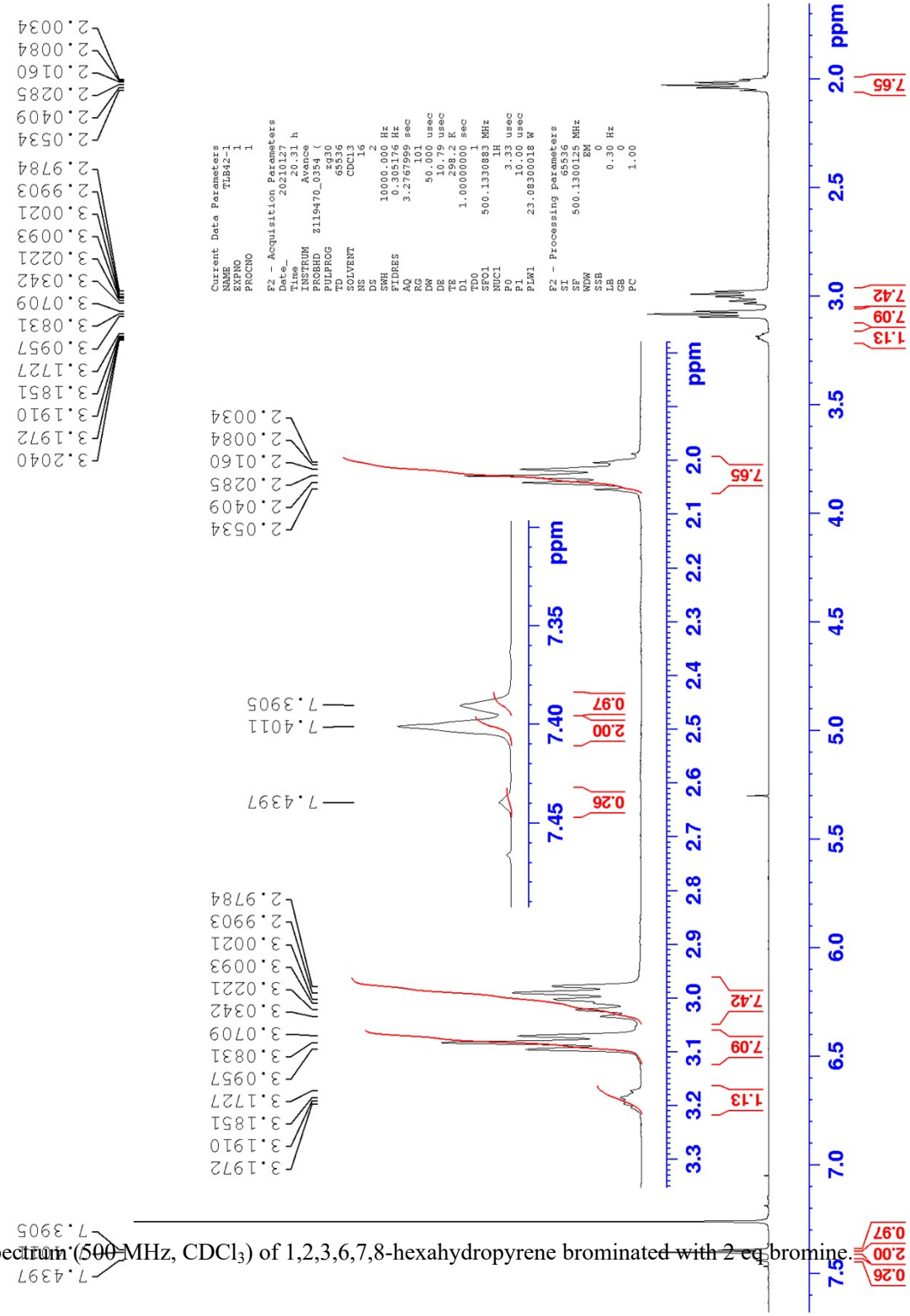


Figure S4. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of 1,2,3,6,7,8-hexahydropyrene brominated with 2 eq bromine.

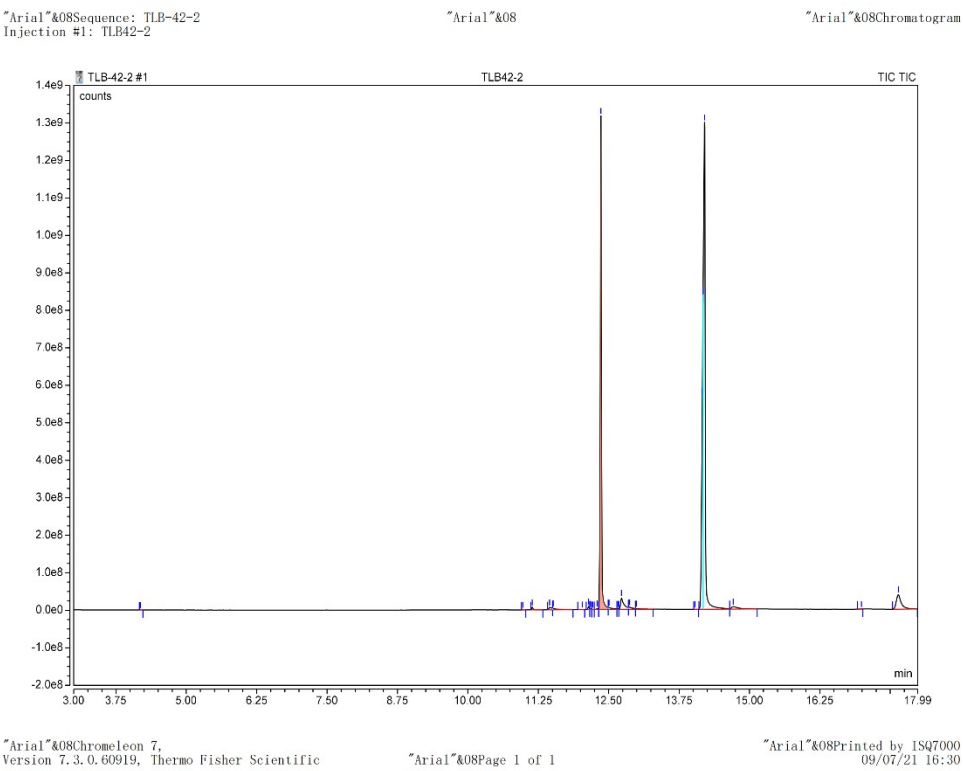


Figure S5. The gas chromatogram of 1,2,3,6,7,8-hexahydropyrene brominated with 3 eq bromine.

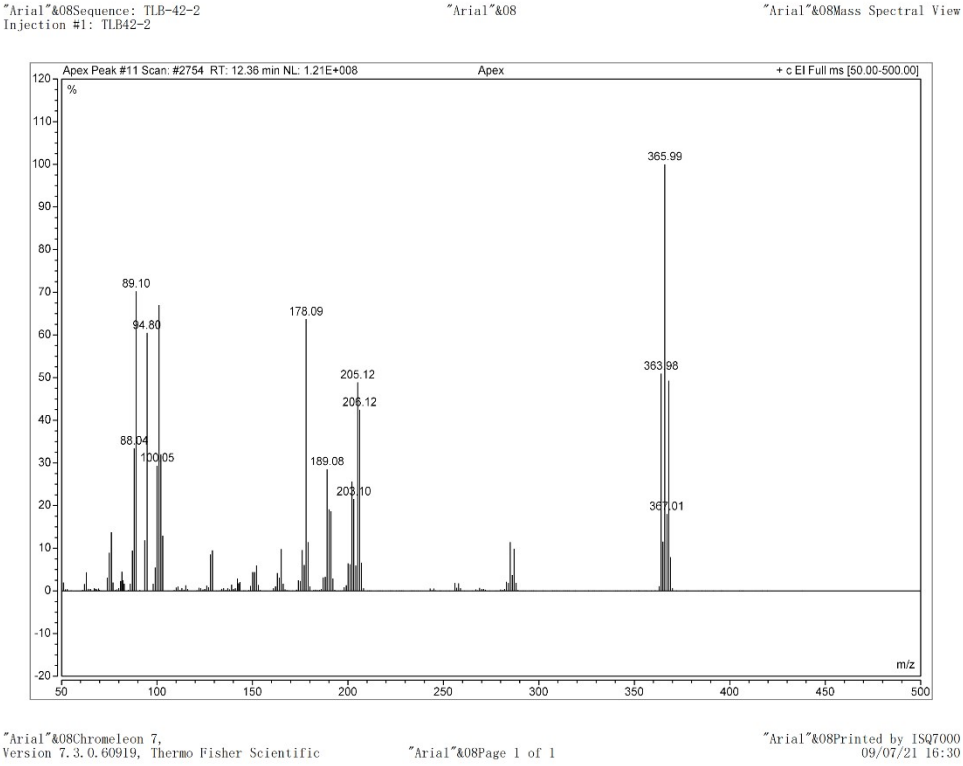


Figure S6. The mass spectrum at 12.5 minutes of the gas chromatograph shown in **Figure S5**.

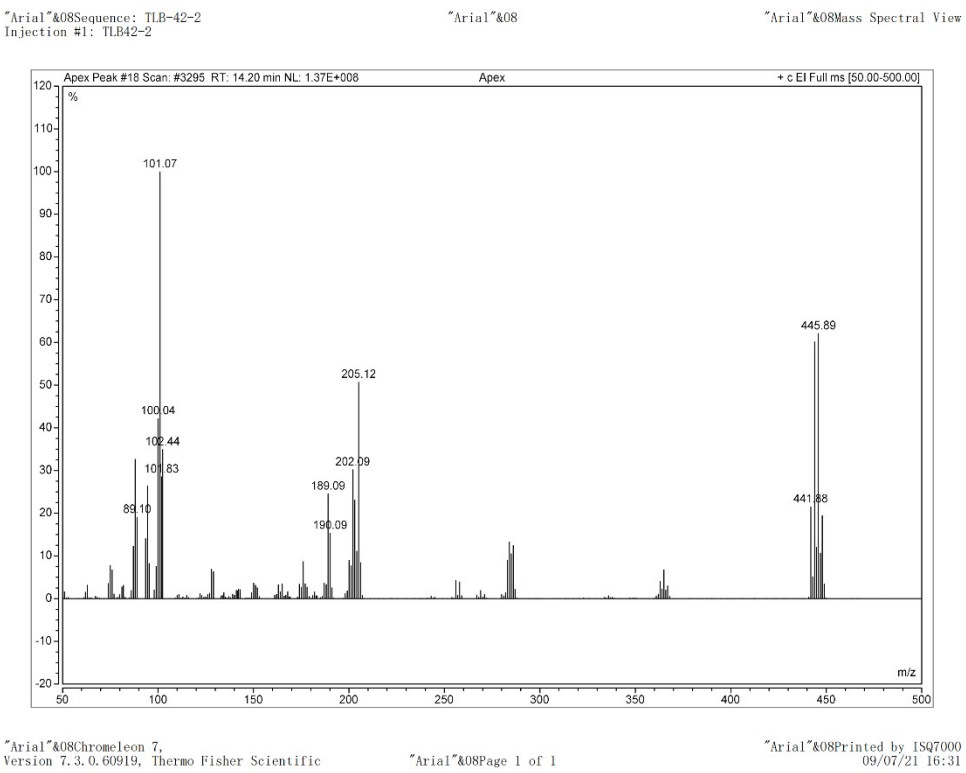


Figure S7. The mass spectrum at 14 minutes of the gas chromatograph shown in **Figure S5**.

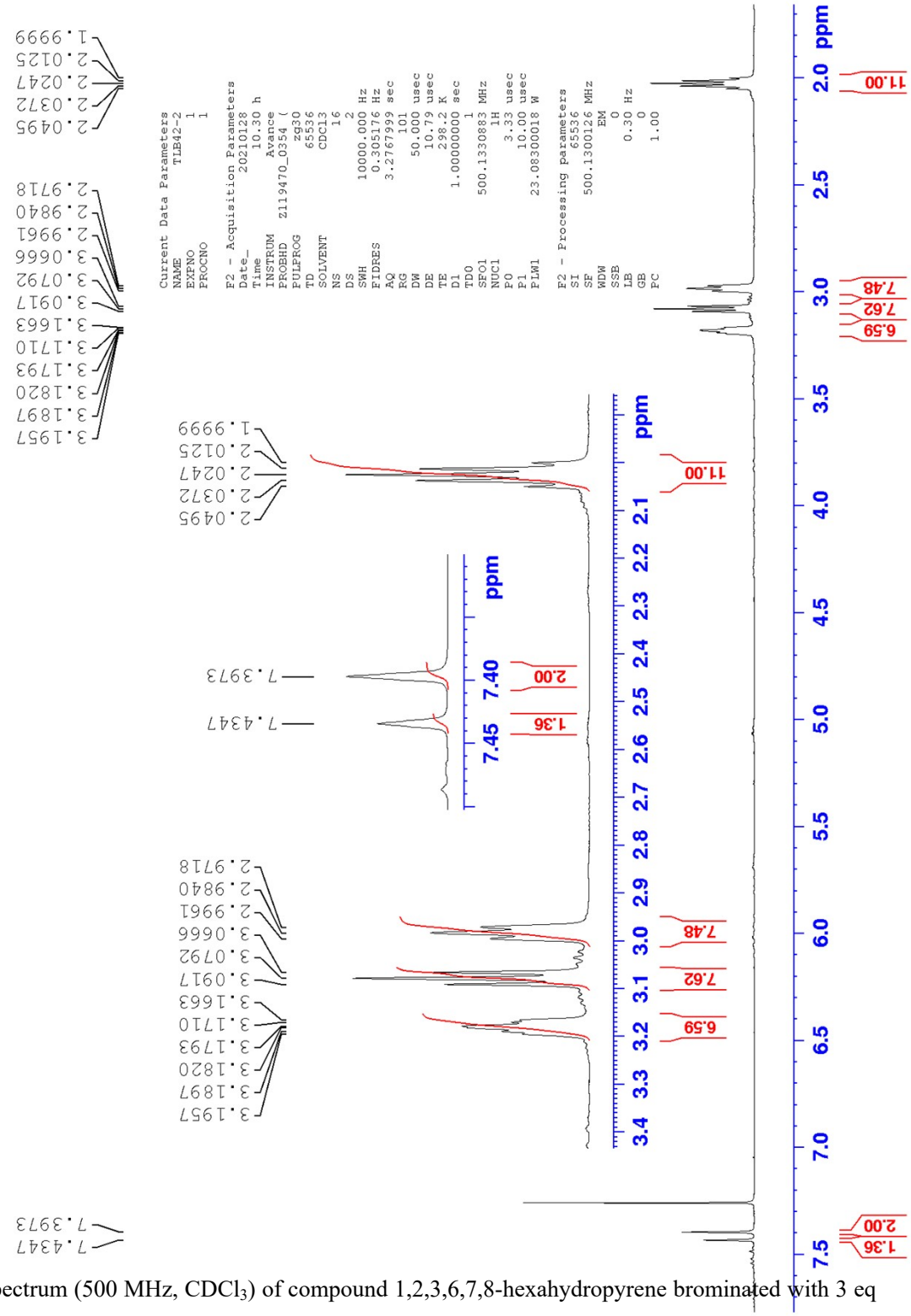


Figure S8. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound 1,2,3,6,7,8-hexahydropyrene brominated with 3 eq of bromine.

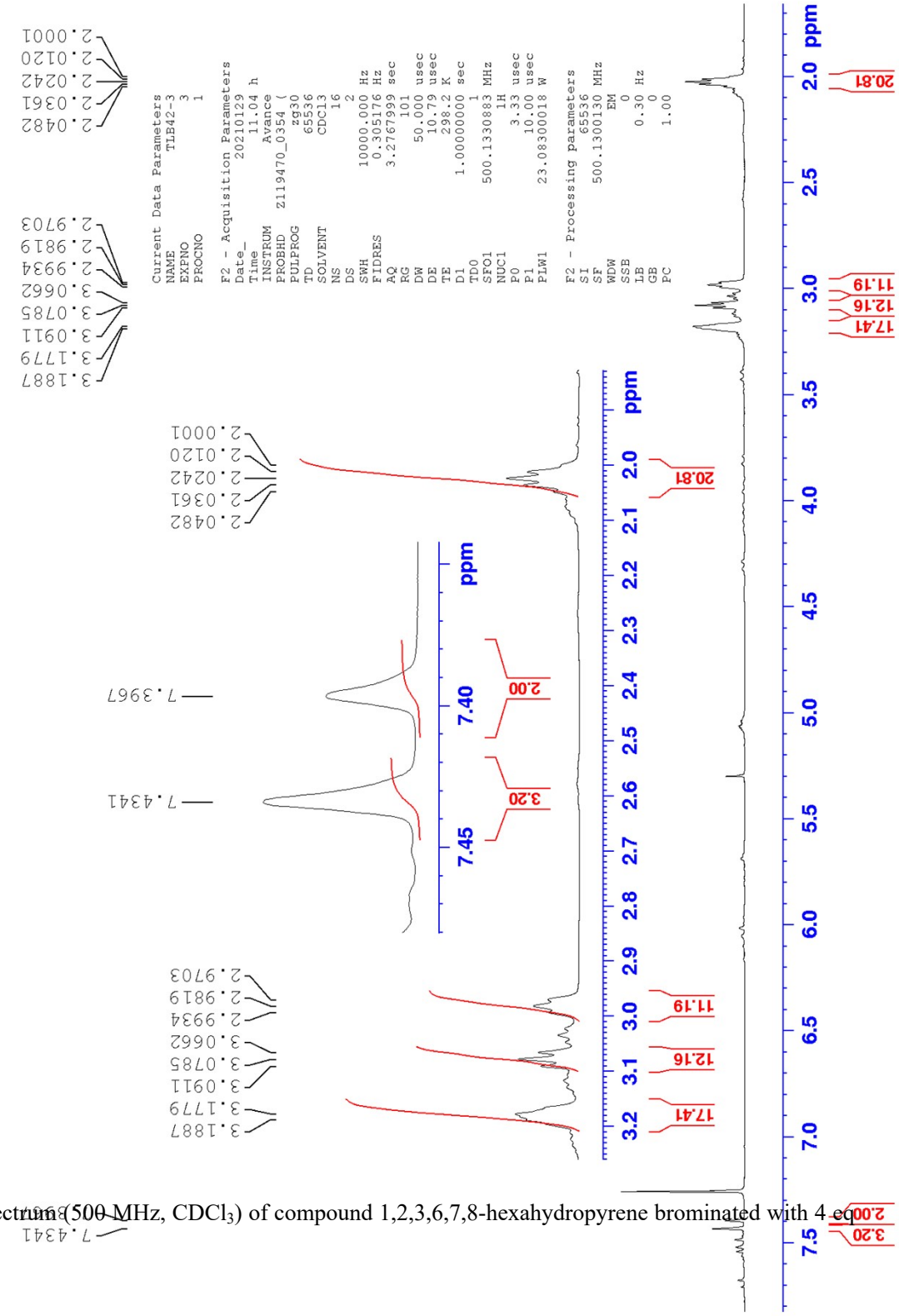


Figure S9. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound 1,2,3,6,7,8-hexahydropyrene brominated with 4 eq of bromine.

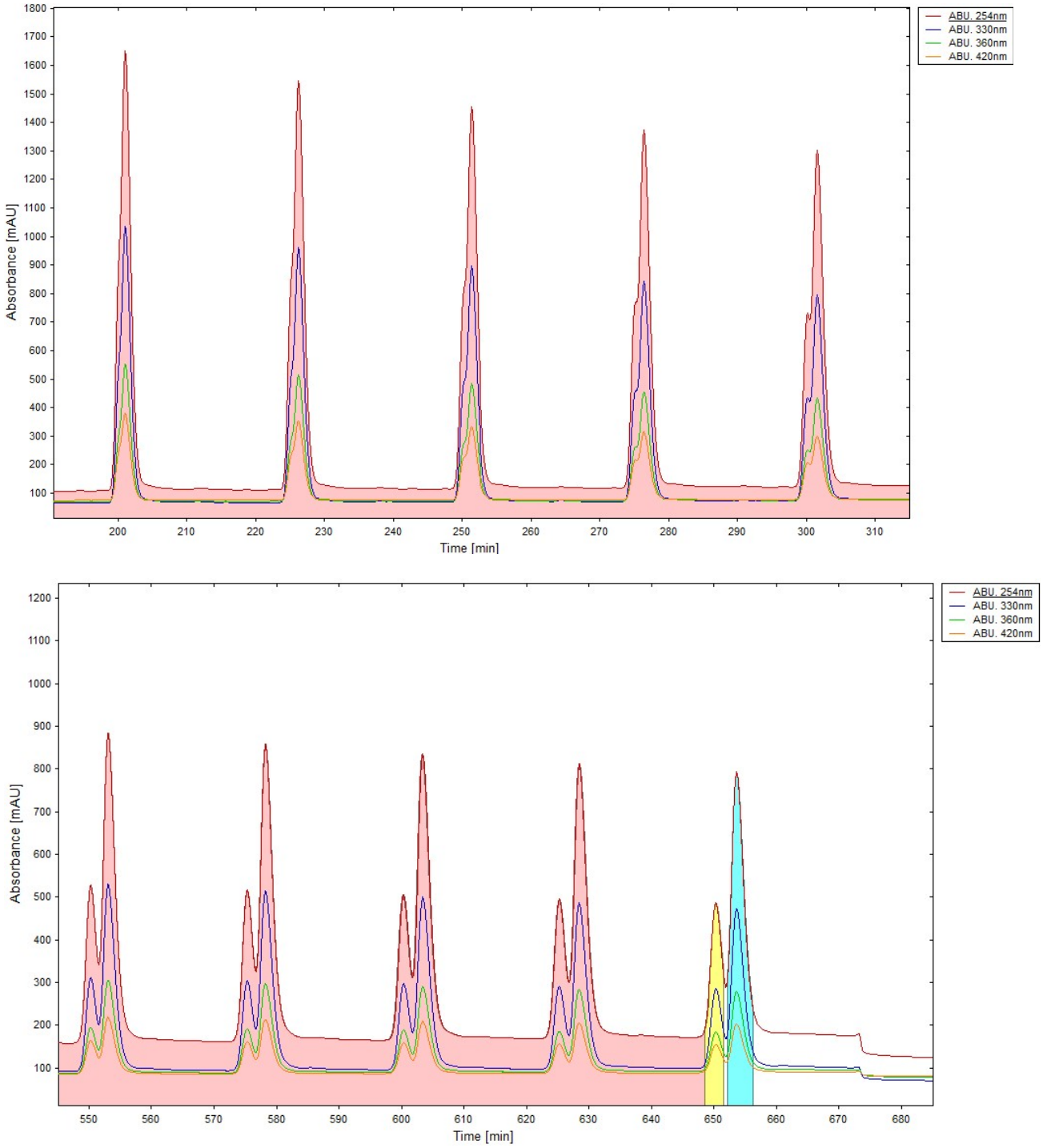


Figure S10. The separation of **1** and **2** on a Recycling Preparative SEC.

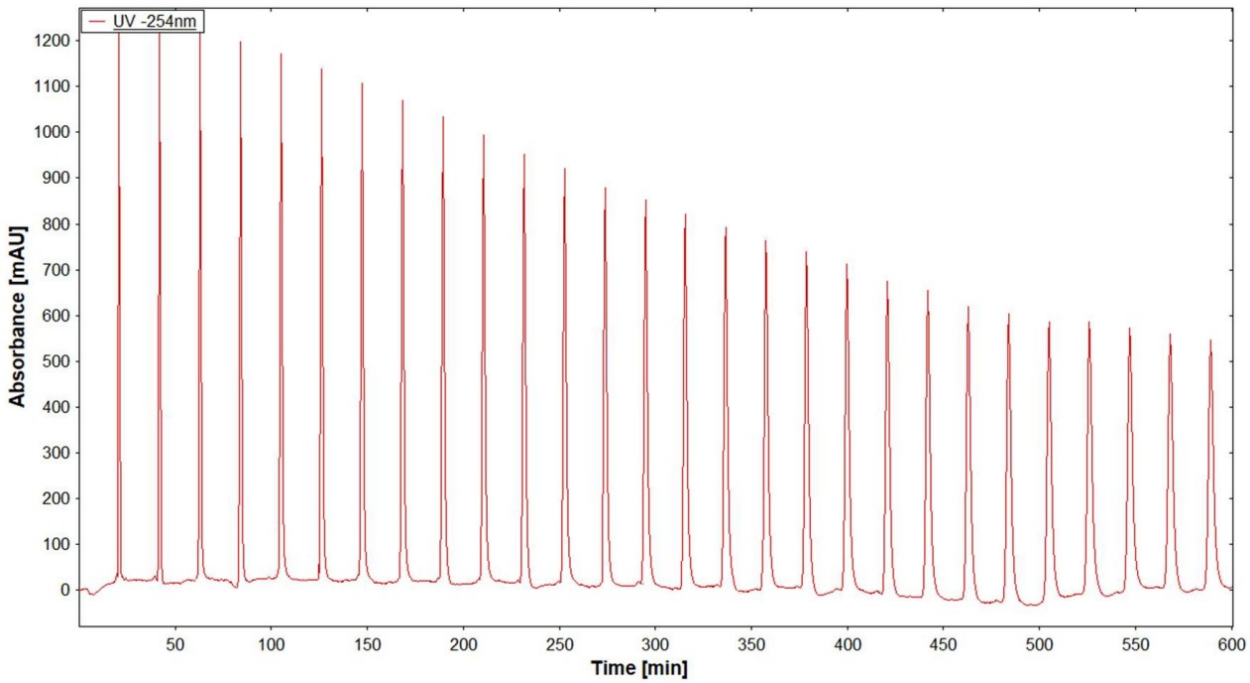


Figure S11. The separation of **3** and **6** by Recycling Preparative SEC.

Electrochemistry

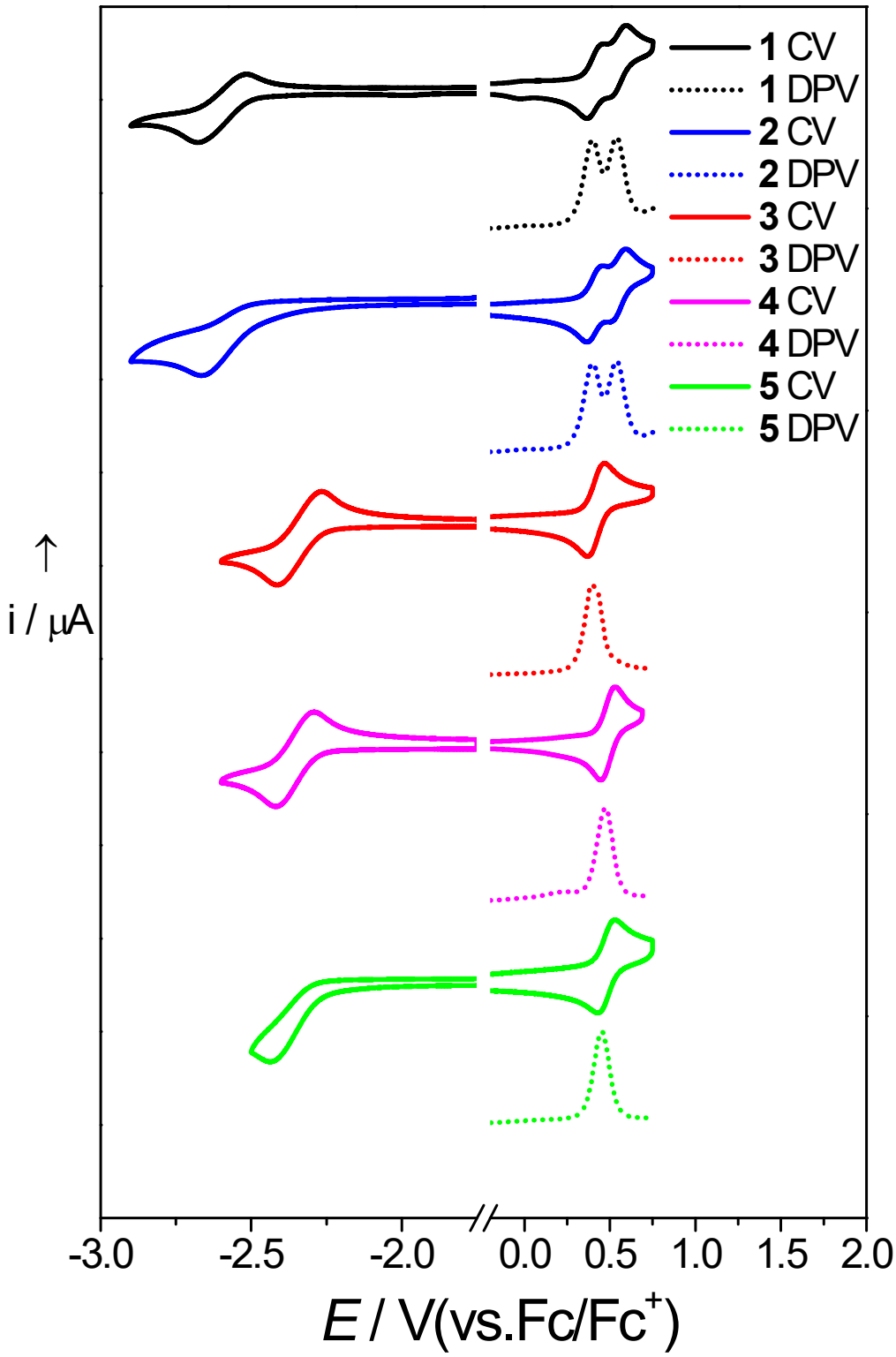


Figure S12. Cyclic voltammograms (solid line) and differential pulse voltammetry (dashed lined) of compounds **1**-**5**. The reduction potentials were measured in THF and the oxidation potentials were measured in dichloromethane.

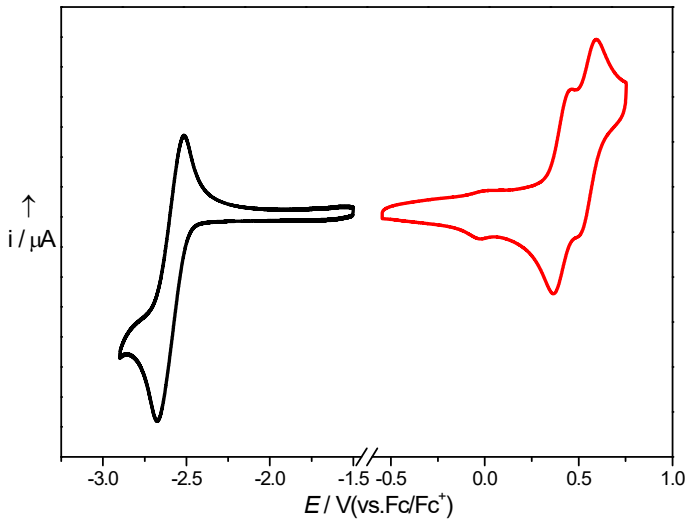


Figure S13. Cyclic voltammograms of compound **1** in THF (black) and dichloromethane (red).

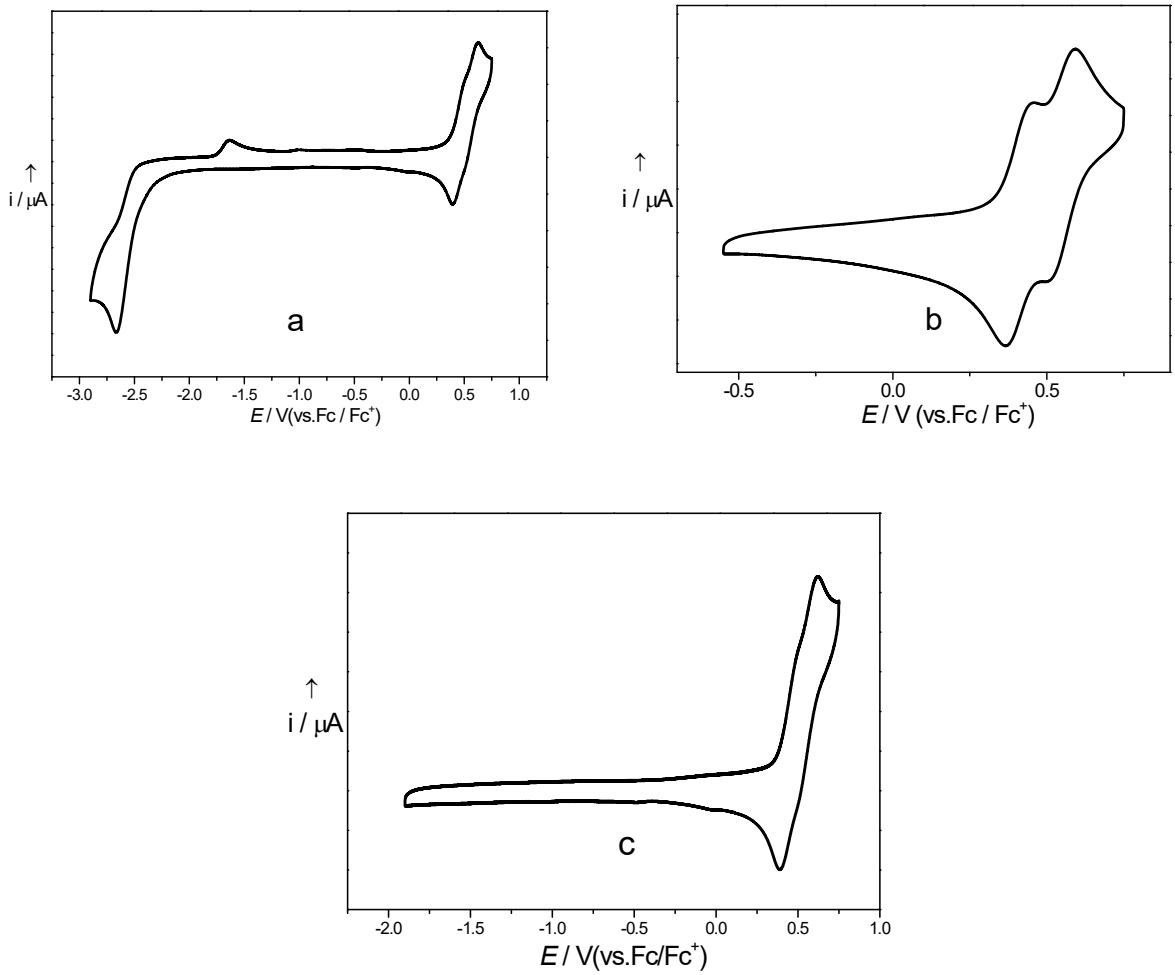


Figure S14. Cyclic voltammograms of compound **2** in THF (a and b) and dichloromethane (c).

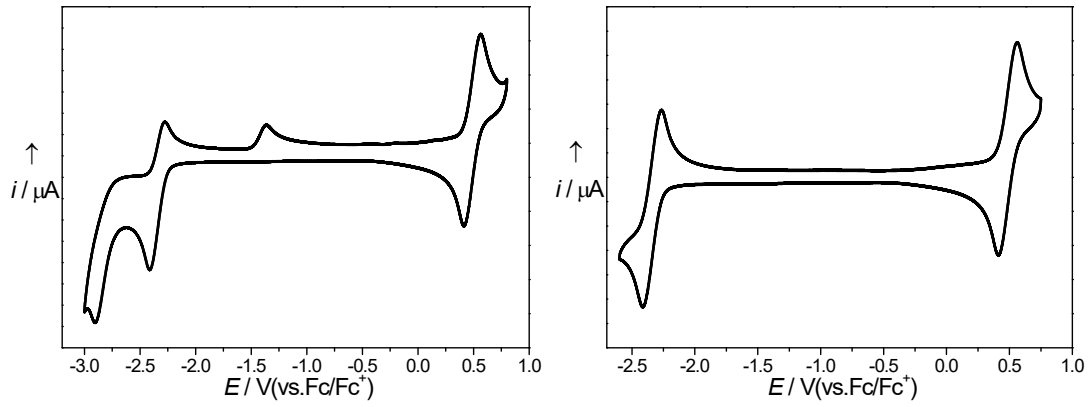


Figure S15. Cyclic voltammograms of compound **3** in THF.

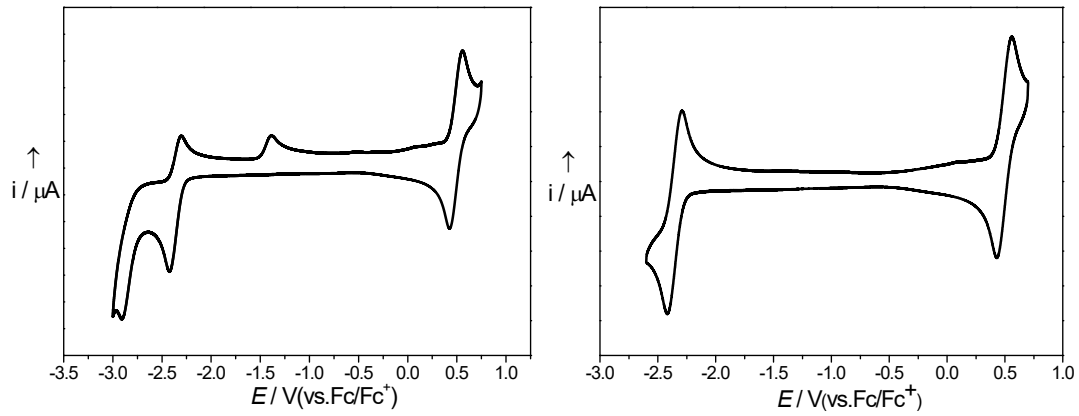


Figure S16. Cyclic voltammograms of compound **4** in THF.

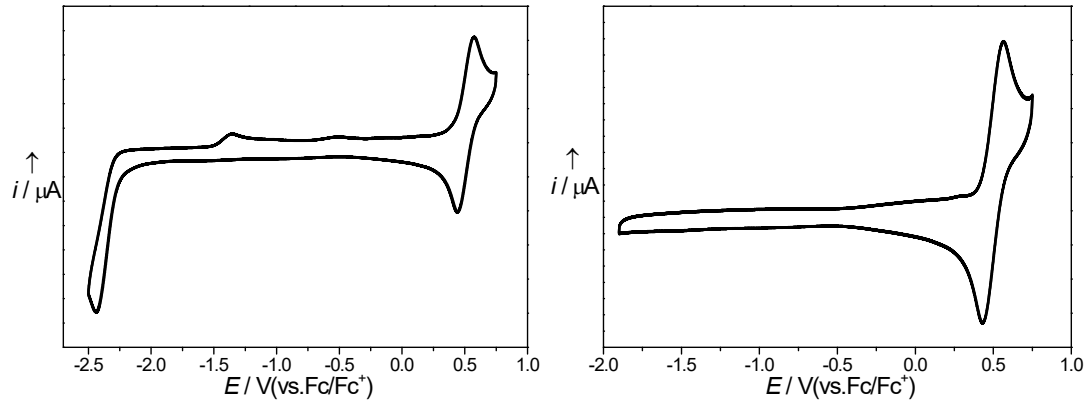


Figure S17. Cyclic voltammograms of compound **5** in THF.

Photophysics

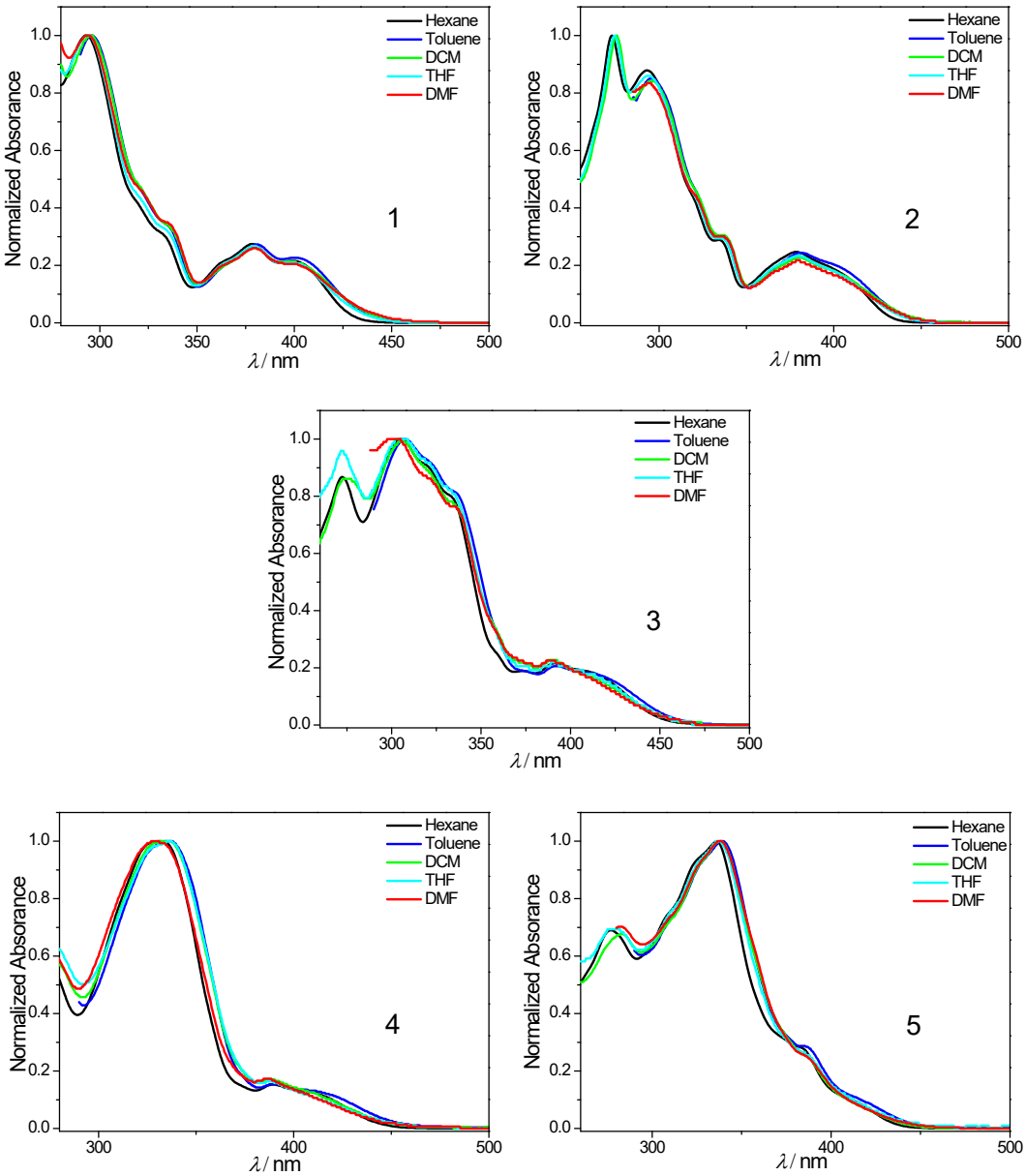


Figure S18. Absorption spectra of compounds **1-5** in hexane, toluene, DCM, THF and DMF.

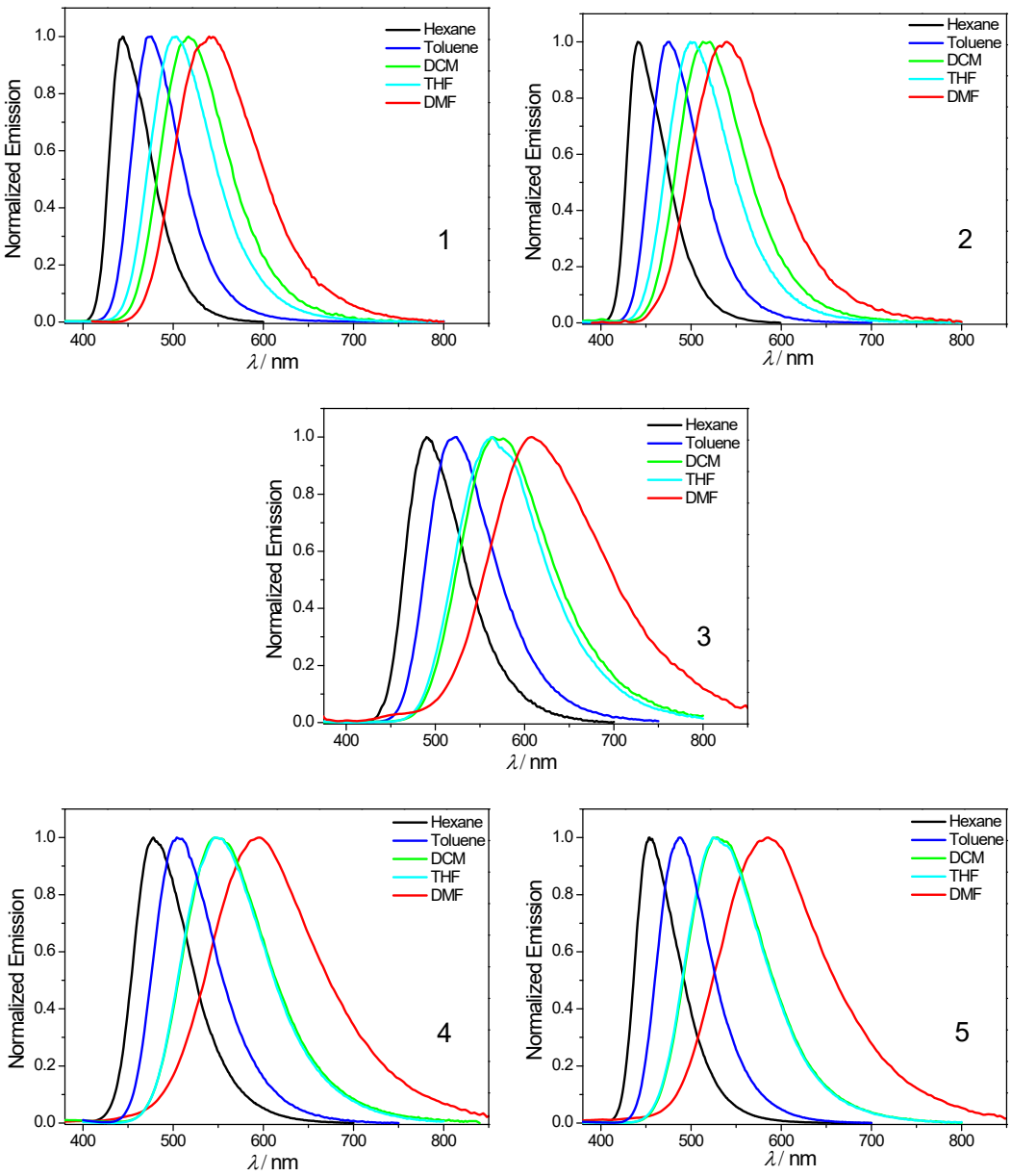


Figure S19. Fluorescence spectra of compounds **1-5** in hexane, toluene, DCM, THF, and DMF.

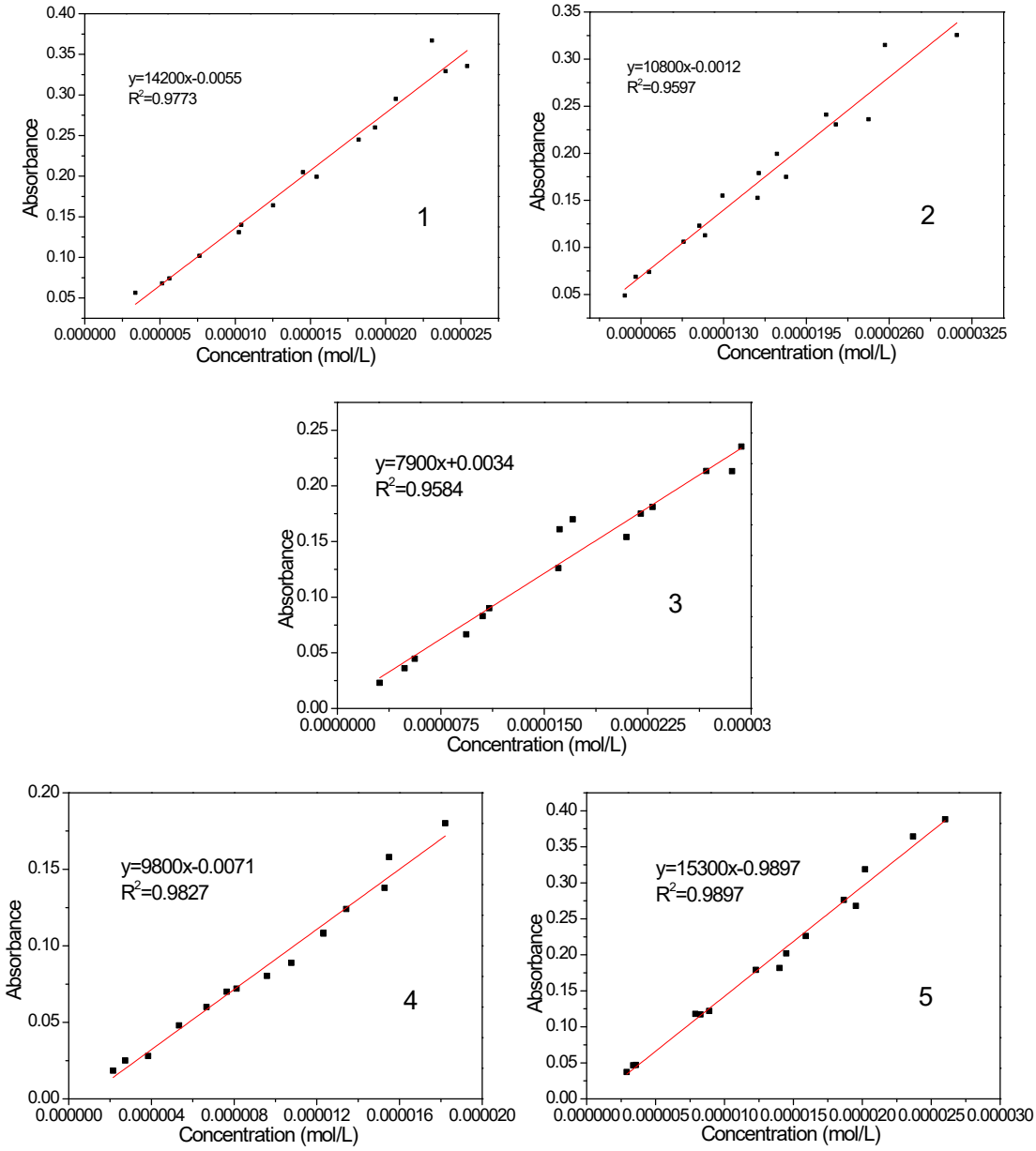


Figure S20. The absorbance dependence of compounds **1**-**5** in hexane on concentrations (**1** & **2** at 379 nm, **3** at 391 nm, **4** at 390 nm, and **5** at 385 nm). The slope of the fitted line (in red) is the molar extinction coefficient of the corresponding compound at designated wavelength.

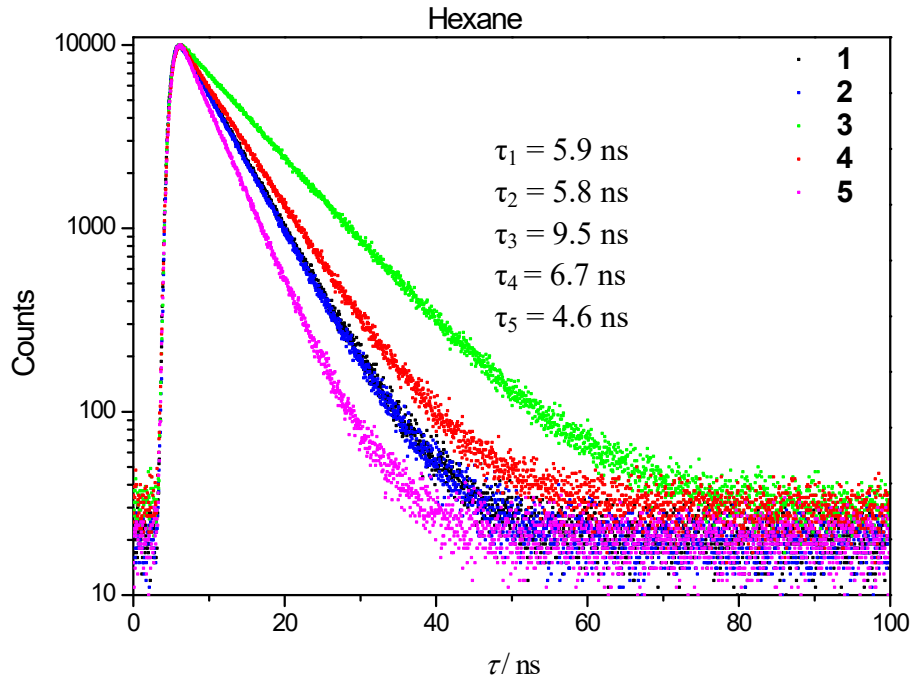


Figure S21. Fluorescence decay of compounds **1-5** in hexane (excited at 293.6 nm).

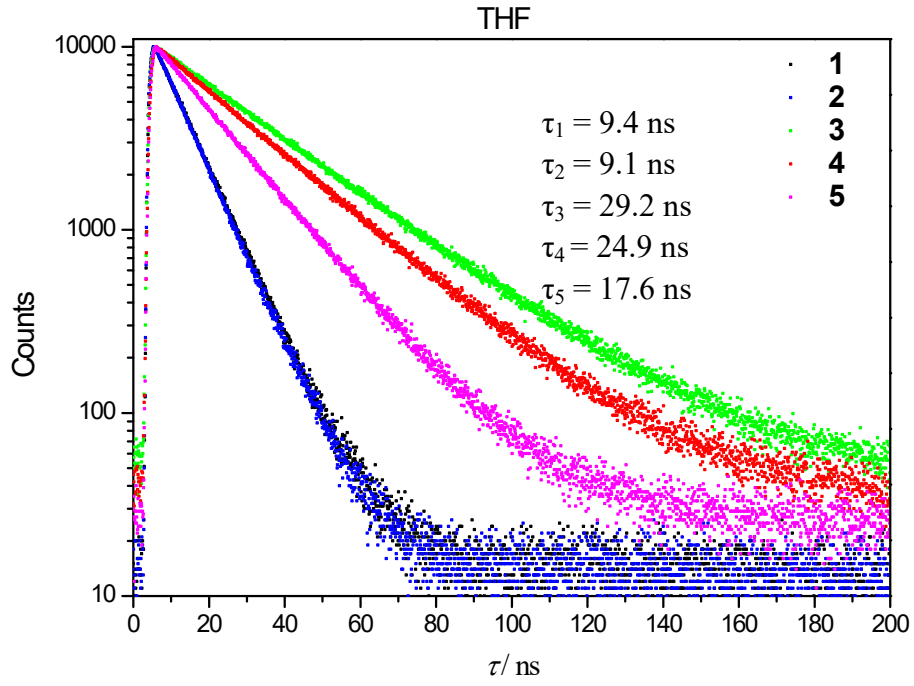


Figure S22. Fluorescence decay of compounds **1-5** in THF (excited at 293.6 nm).

Theoretical studies

Table S1. TD-DFT calculations results of compound **1** in gas phase.

Excited State	△*E* / eV	*l* / nm	Oscillator strength	Transitions	Contribution
S1	3.5430	349.94	0.3887	**HOMO→LUMO**	**88%**
S2	3.6126	343.20	0.0000	**HOMO-1→LUMO**	**89%**
S3	3.8910	318.65	0.0625	**HOMO-3→LUMO**	**26%**
				HOMO→LUMO+1	**44%**
S4	4.2046	294.88	0.1505	**HOMO-2→LUMO**	**71%**
S5	4.5208	274.25	0.0001	**HOMO-1→LUMO+1**	**45%**
				HOMO-1→LUMO+6	15%
				HOMO→LUMO+2	10%
				HOMO→LUMO+5	13%

Table S2. TD-DFT calculations results of compound **2** in gas phase.

Excited State	△*E* / eV	*l* / nm	Oscillator strength	Transitions	Contribution
S1	3.5706	347.24	0.1731	**HOMO-1→LUMO**	**84%**
S2	3.5887	345.48	0.2143	**HOMO →LUMO**	**91%**
S3	3.9280	315.64	0.0995	HOMO-3→LUMO	29%
				HOMO-2→LUMO+1	13%
				HOMO→LUMO+1	**49%**
S4	4.1670	297.54	0.0607	**HOMO-2→LUMO**	**82%**
S5	4.5406	273.06	0.0972	**HOMO-1→LUMO+1**	**43%**
				HOMO-1→LUMO+6	12%
				HOMO →LUMO+3	11%
				HOMO →LUMO+5	13%

Table S3. TD-DFT calculations results of compound **3** in gas phase.

Excited State	△*E* / eV	*l* / nm	Oscillator strength	Transitions	Contribution
S1	3.4919	355.07	0.3485	**HOMO →LUMO**	**82%**
S2	3.6946	335.58	0.0431	**HOMO-1→LUMO**	**48%**
				HOMO→LUMO+1	29%
S3	3.9734	312.03	0.0212	HOMO-3→LUMO	23%
				HOMO-2→LUMO	13%
				HOMO-1→LUMO+2	14%

				HOMO →LUMO+2	**24%**
S4	4.1197	300.95	0.0551	HOMO-3→LUMO	15%
				HOMO-2→LUMO	**44%**
				HOMO-2→LUMO+1	16%
S5	4.2242	293.51	0.1660	HOMO-1→LUMO	16%
				HOMO-1→LUMO+1	**38%**
				HOMO →LUMO+1	18%

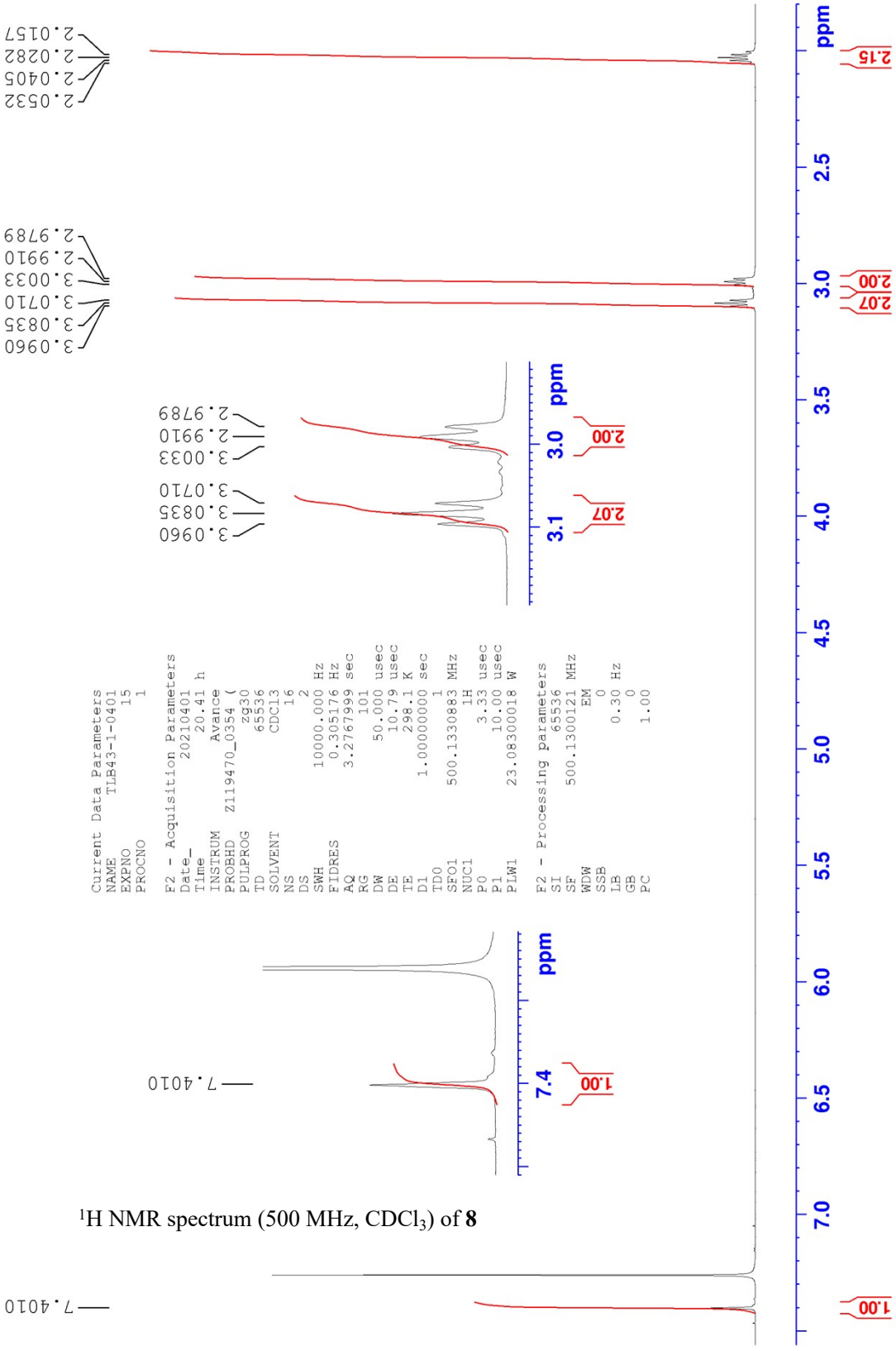
Table S4. TD-DFT calculations results of compound **4** in gas phase.

Excited State	△E / eV	l / nm	Oscillator strength	Transitions	Contribution
S1	3.5104	353.19	0.3996	**HOMO →LUMO**	**78%**
S2	3.7052	334.63	0.0487	**HOMO-1→LUMO**	**48%**
				HOMO →LUMO+1	25%
S3	3.9716	312.18	0.0270	**HOMO-4→LUMO**	**26%**
				HOMO-1→LUMO	10%
				HOMO-1→LUMO+3	14%
				HOM0 →LUMO+3	16%
S4	4.1081	301.81	0.0752	**HOMO-3→LUMO**	**28%**
				HOMO-3→LUMO+1	11%
				HOMO-2→LUMO	**28%**
				HOMO-2→LUMO+1	12%
S5	4.1785	296.72	0.7321	HOMO →LUMO+2	67%

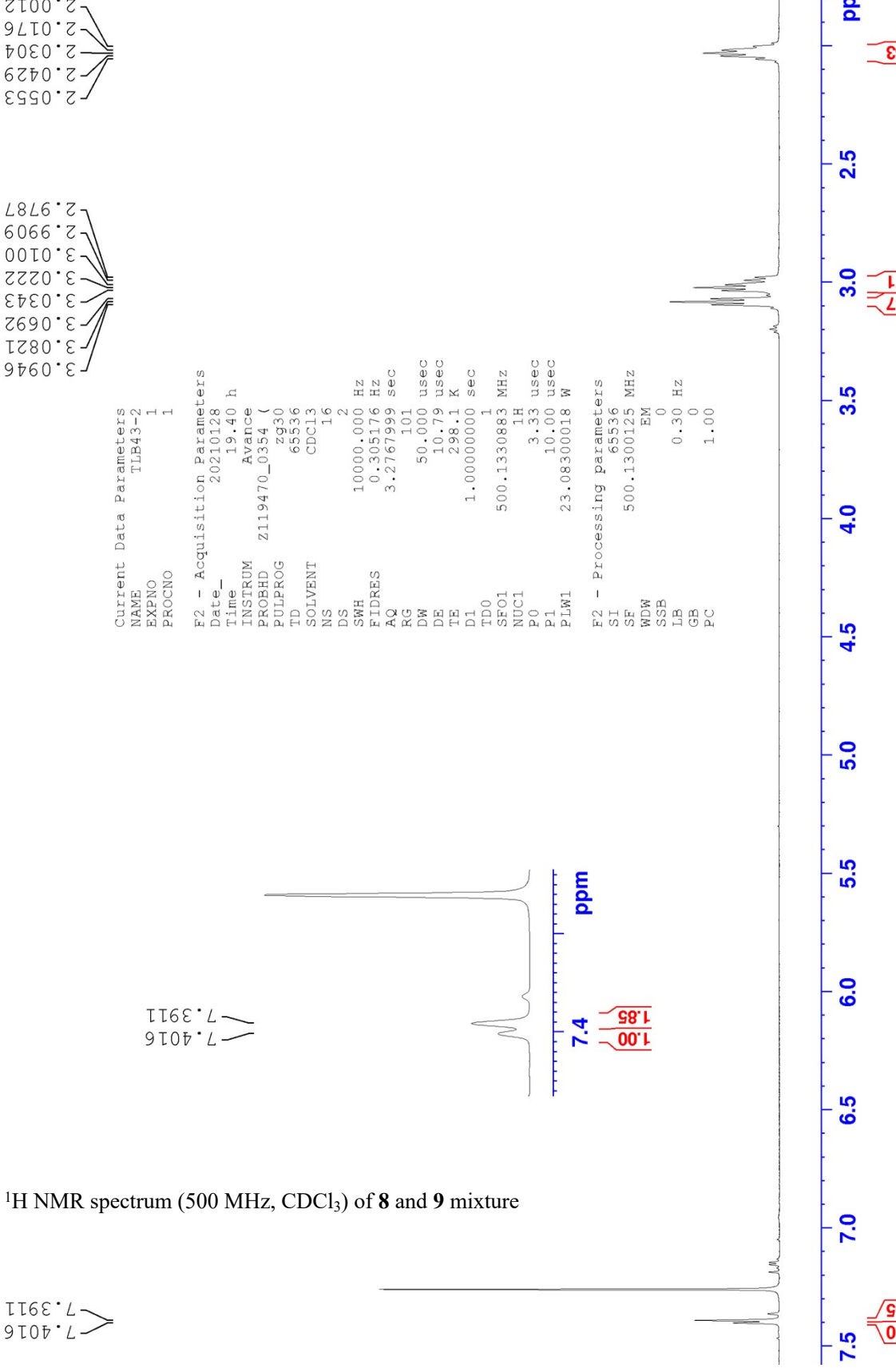
Table S5. TD-DFT calculations results of compound **5** in gas phase.

Excited State	△E / eV	l / nm	Oscillator strength	Transitions	Contribution
S1	3.5476	349.48	0.1952	**HOMO →LUMO**	**73%**
				HOMO →LUMO+1	10%
S2	3.7227	333.05	0.3563	**HOMO-1→LUMO**	**52%**
				HOMO →LUMO+1	26%
S3	3.9027	317.68	0.0523	**HOMO-4→LUMO**	**26%**
				HOMO-1→LUMO	12%
				HOMO-1→LUMO+1	10%
				HOMO-1→LUMO+3	11%
				HOMO →LUMO+3	11%
S4	4.1141	301.36	0.0638	HOMO-3→LUMO	29%
				HOMO-3→LUMO+1	12%
				HOMO-2→LUMO	**30%**
				HOMO-2→LUMO+1	12%
S5	4.1833	296.38	0.9432	**HOMO →LUMO+2**	**68%**

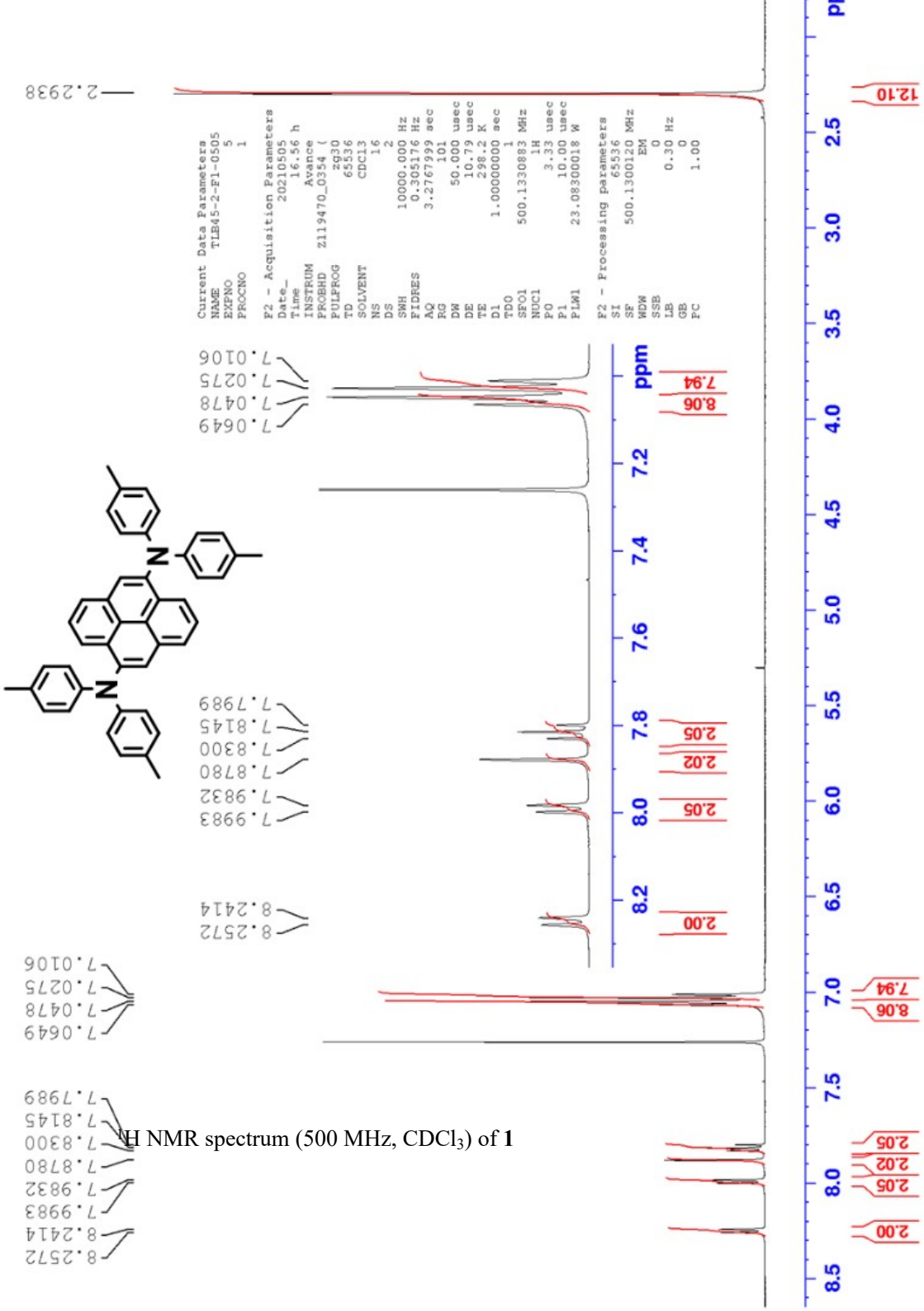
^{1}H and ^{13}C NM



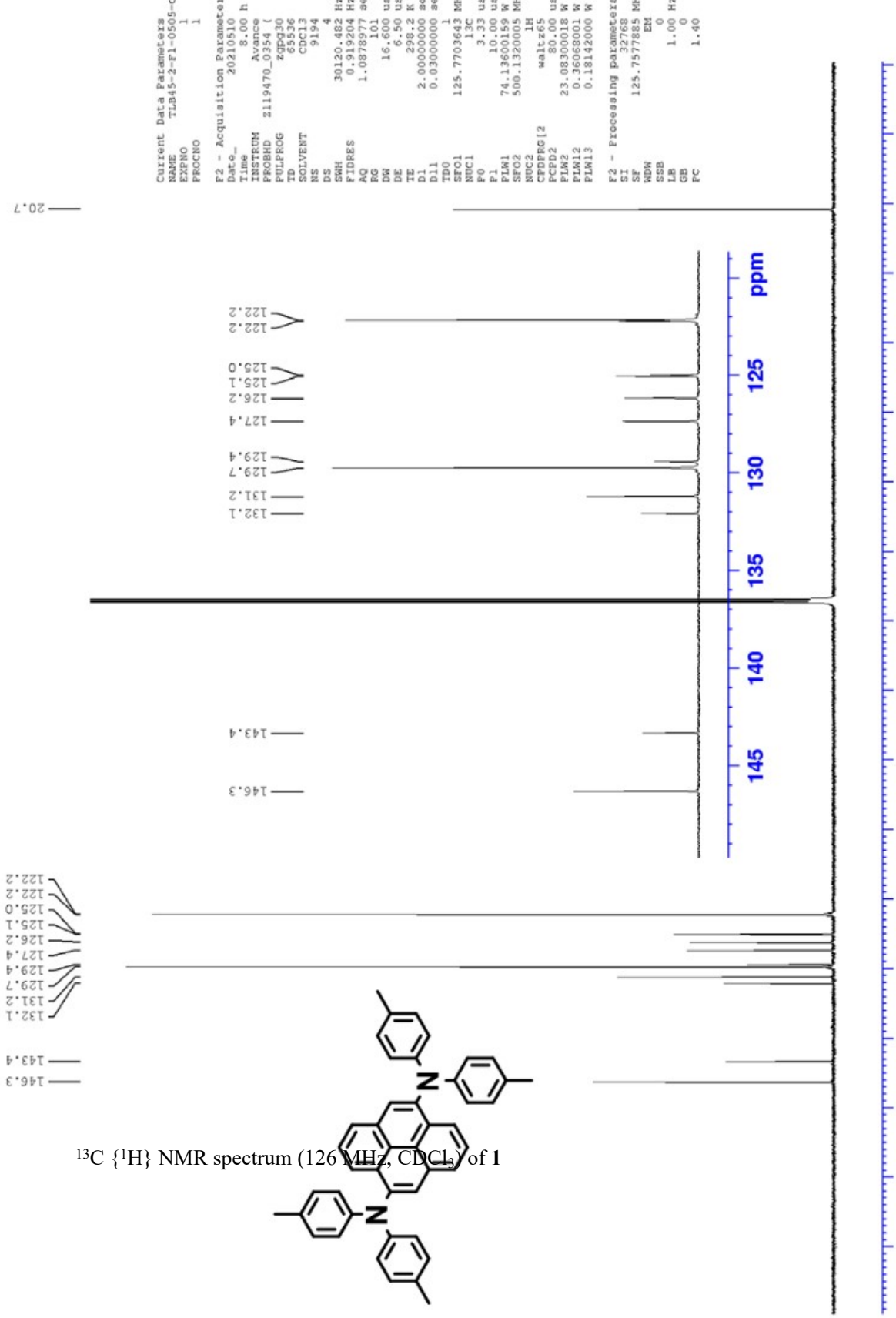
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **8**



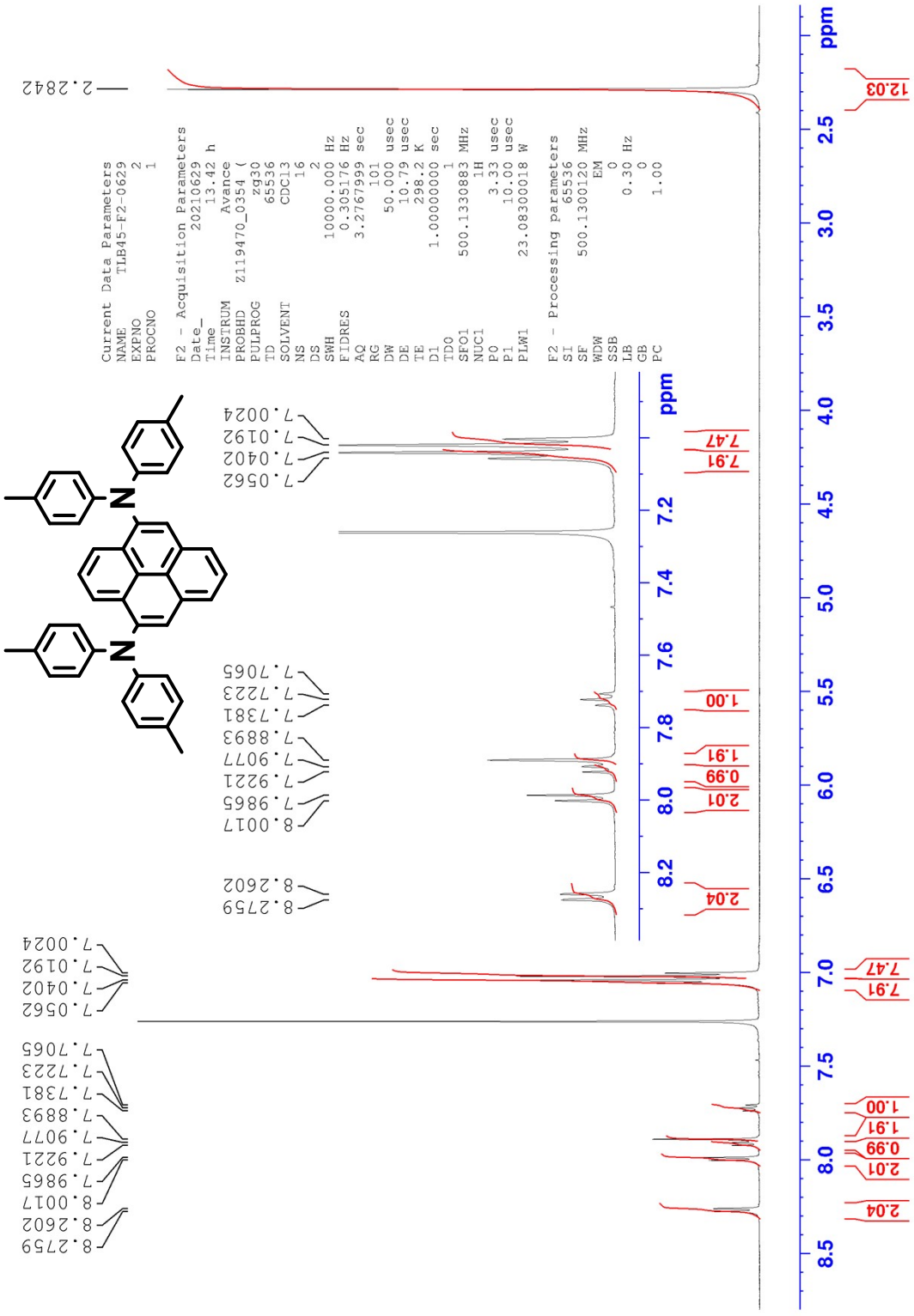
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **8** and **9** mixture



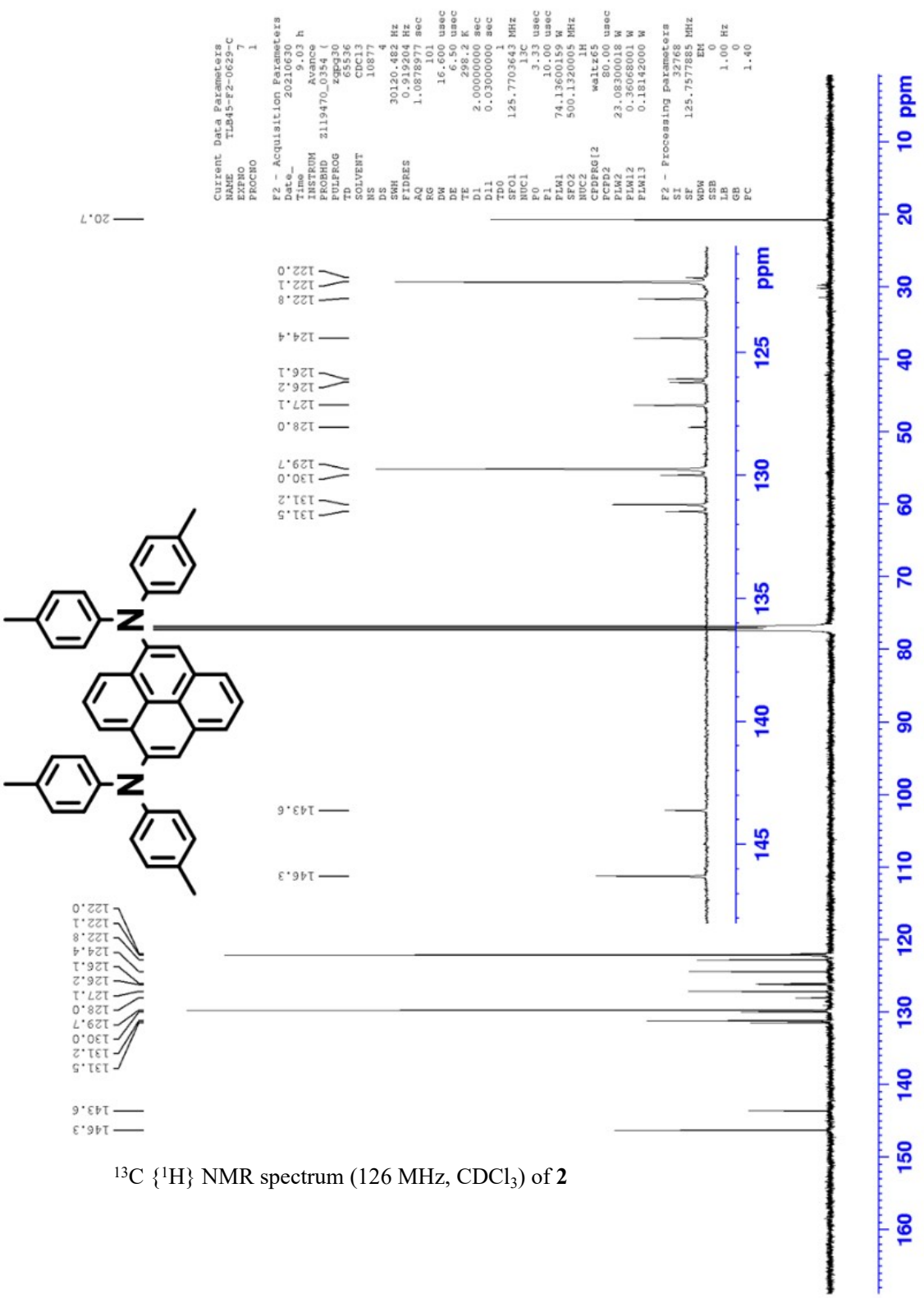
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **1**



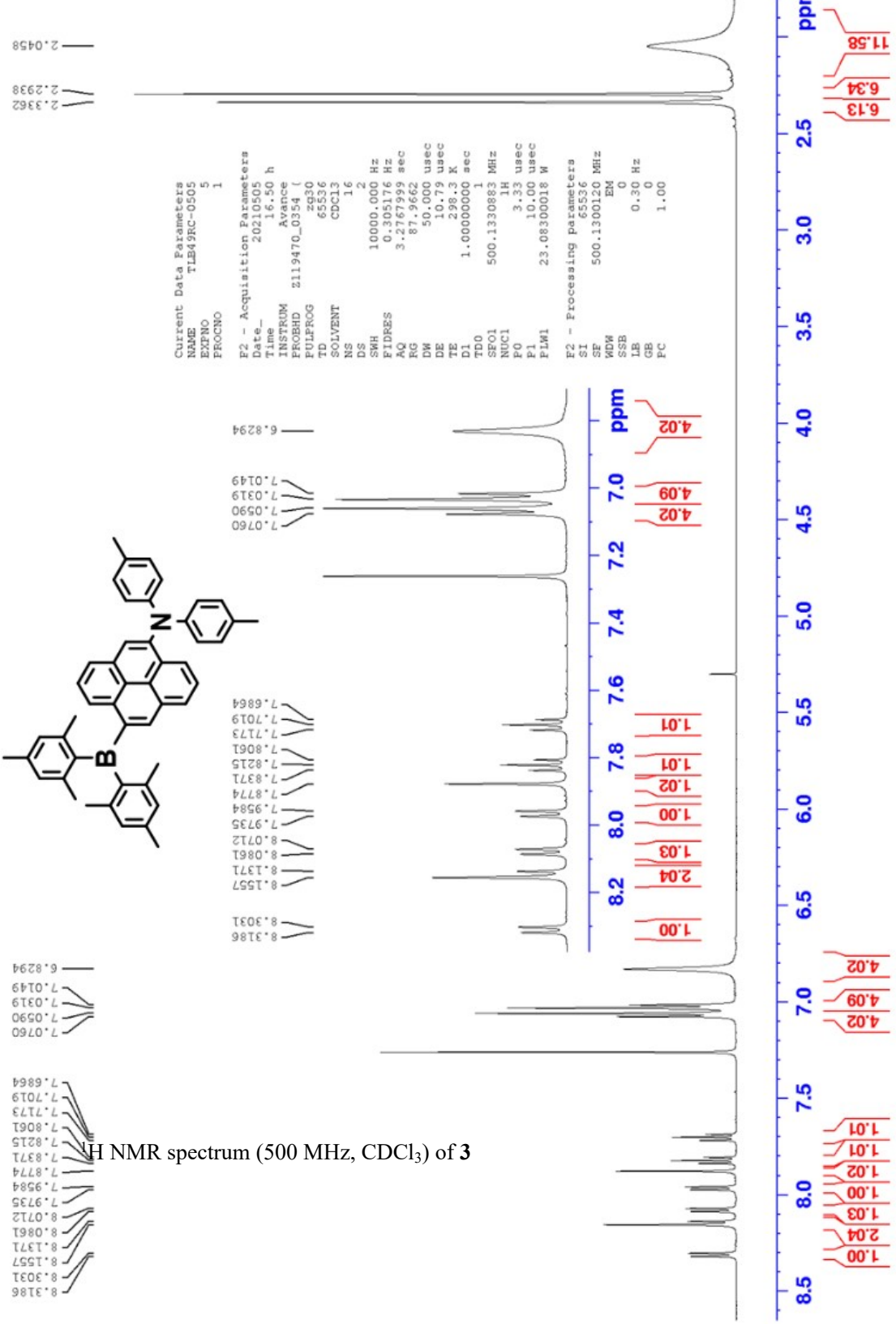
^{13}C {^{1}H} NMR spectrum (126 MHz, $CDCl_3$) of **1**



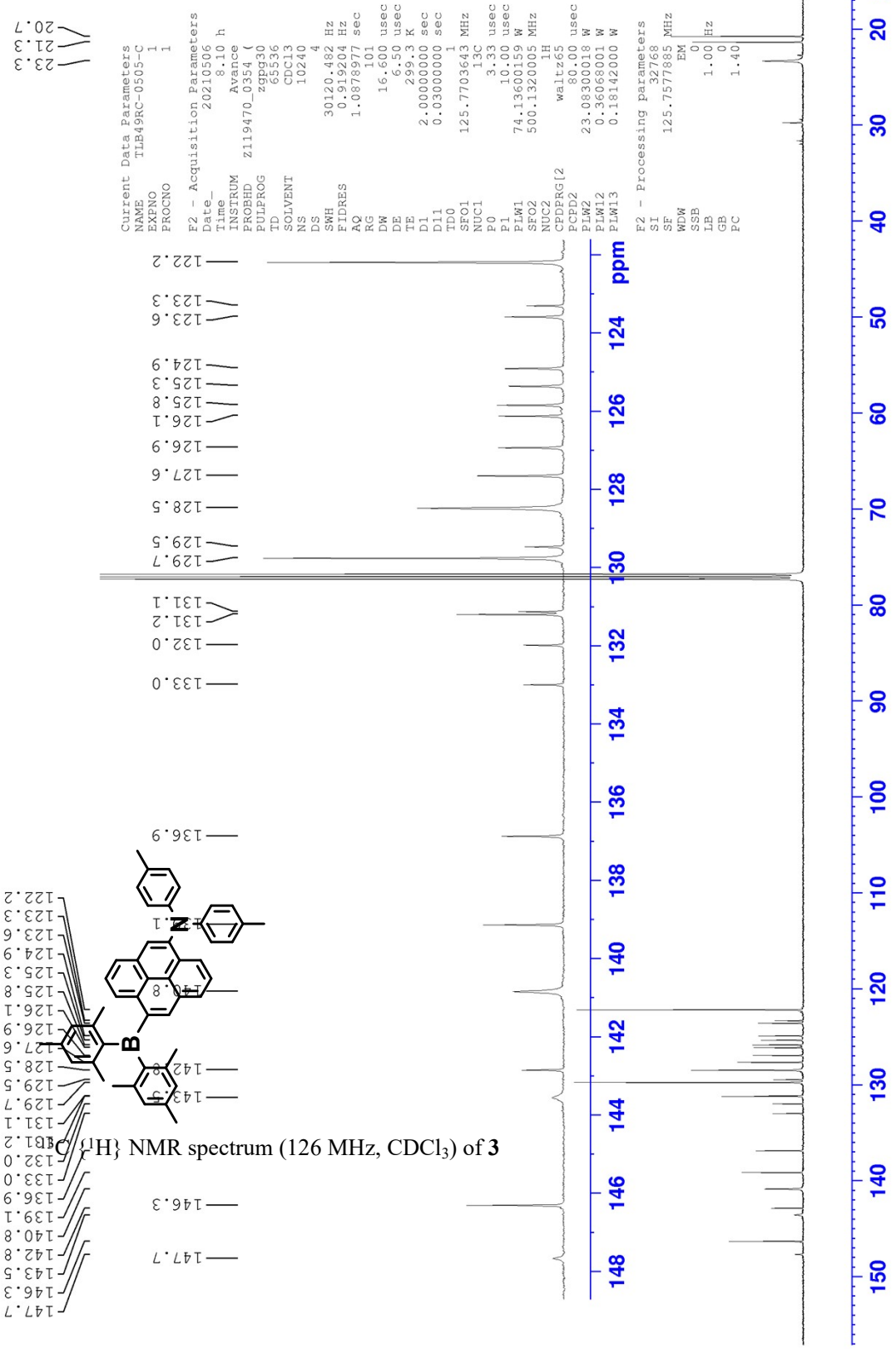
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **2**



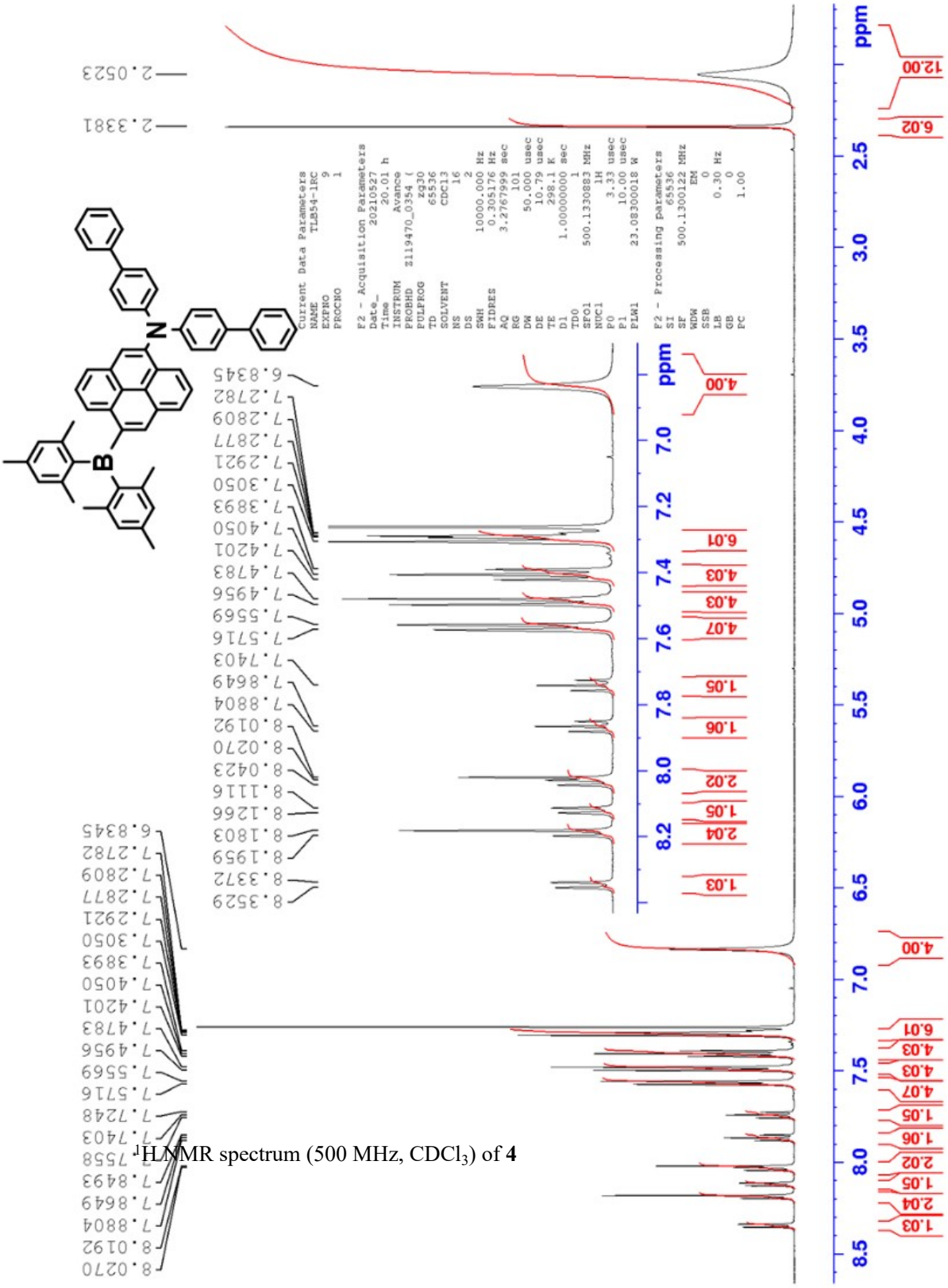
^{13}C {^{1}H} NMR spectrum (126 MHz, $CDCl_3$) of **2**



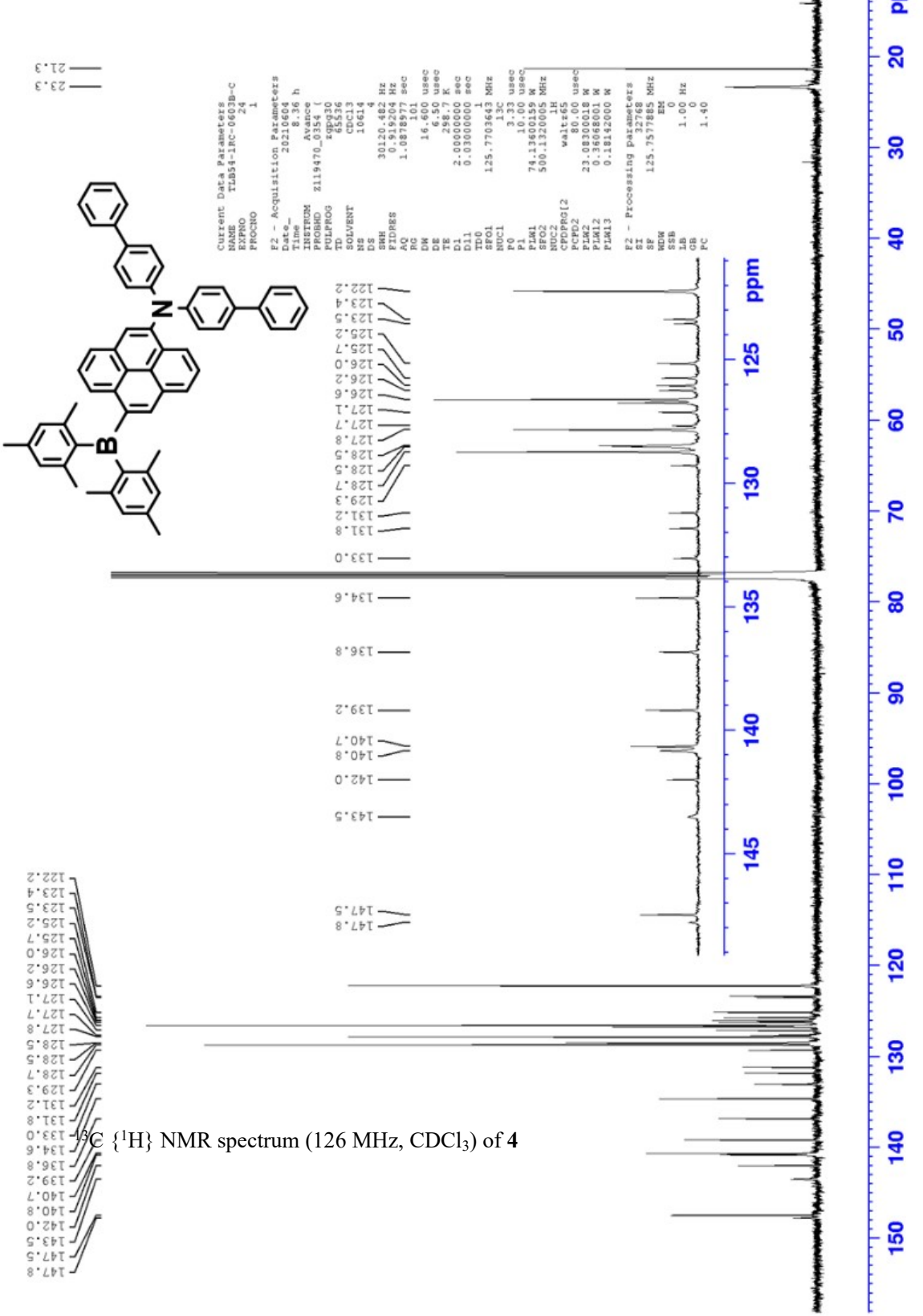
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **3**



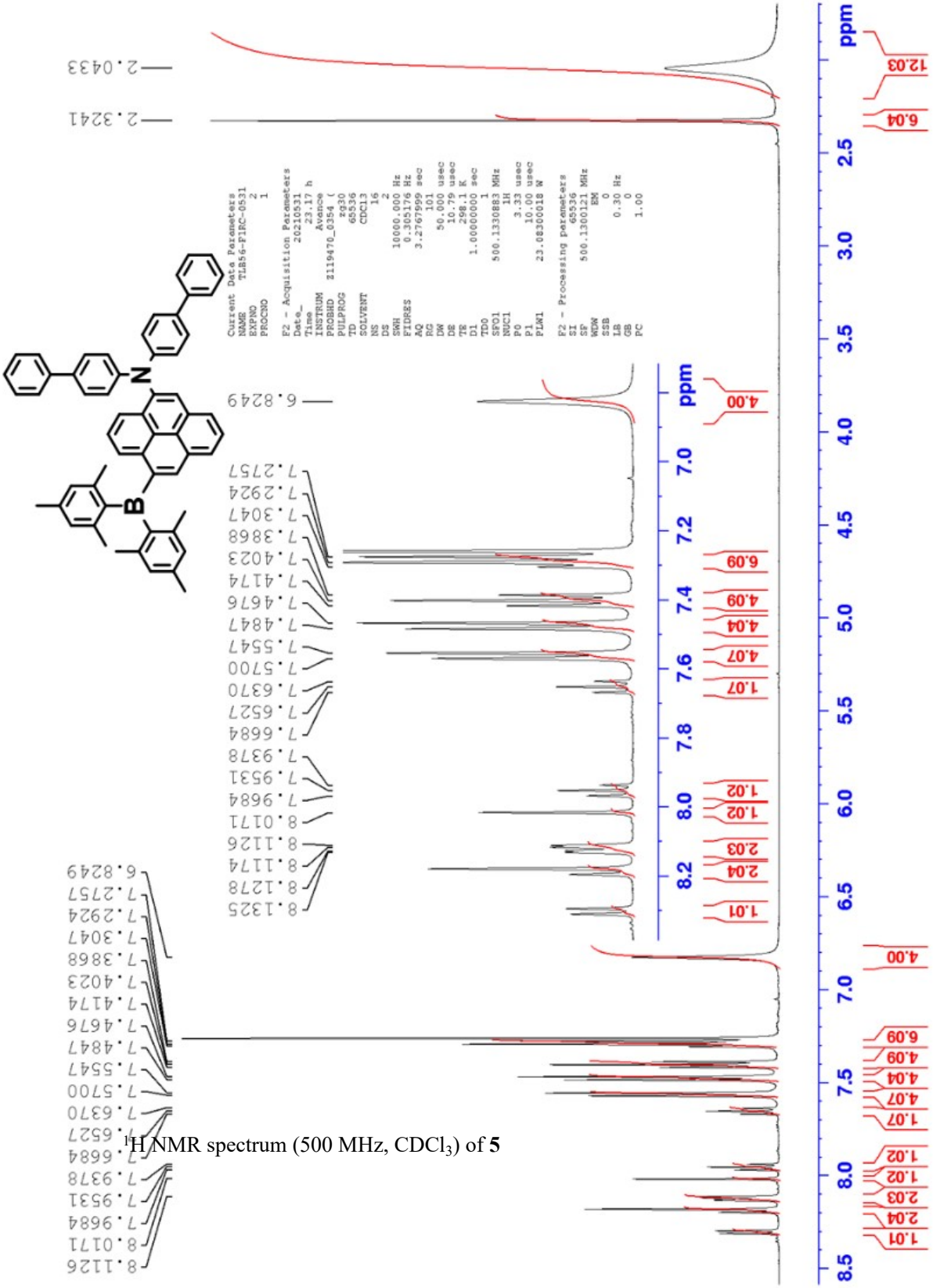
$^{13}C\{^1H\}$ NMR spectrum (126 MHz, $CDCl_3$) of **3**



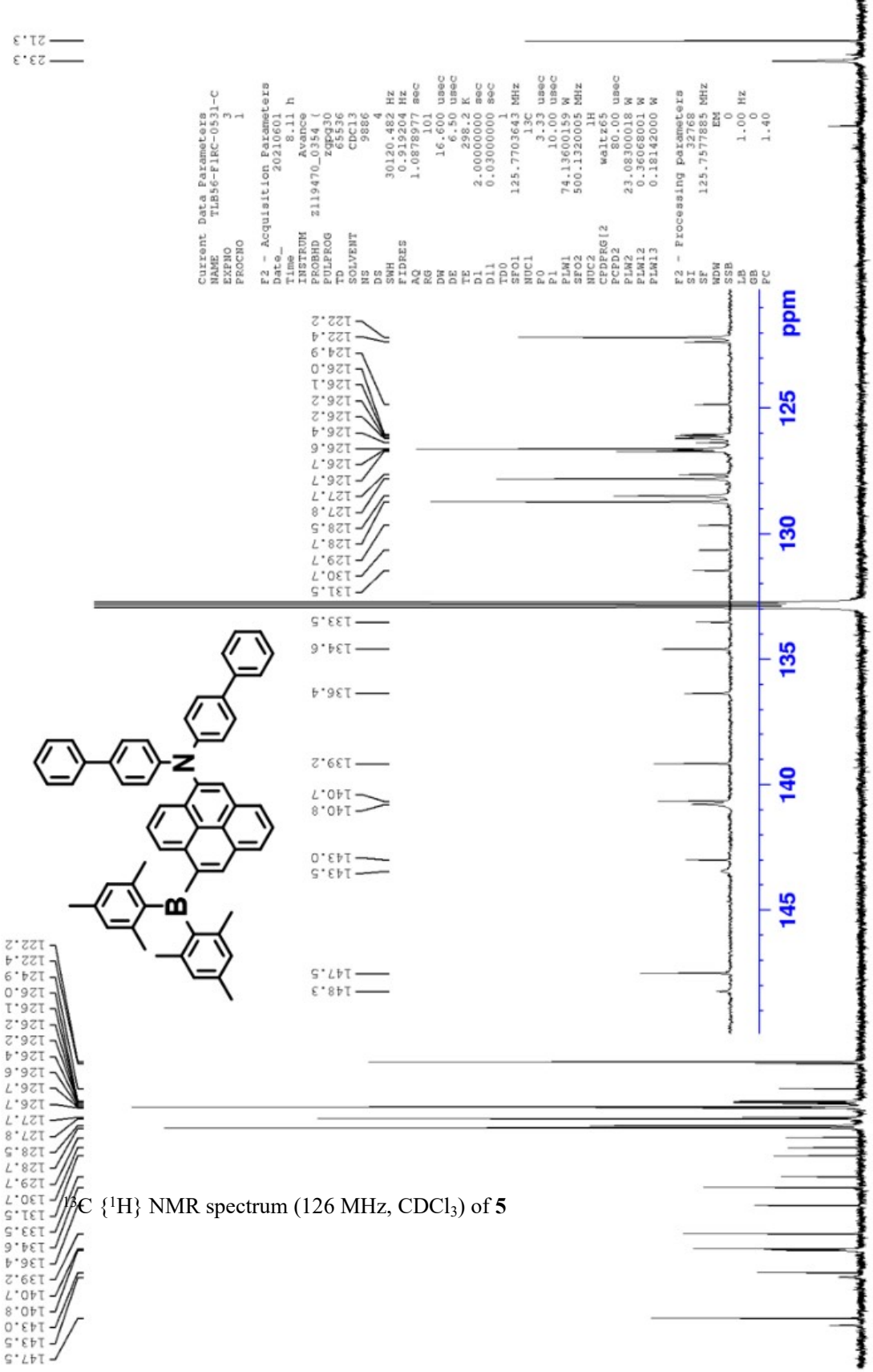
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **4**



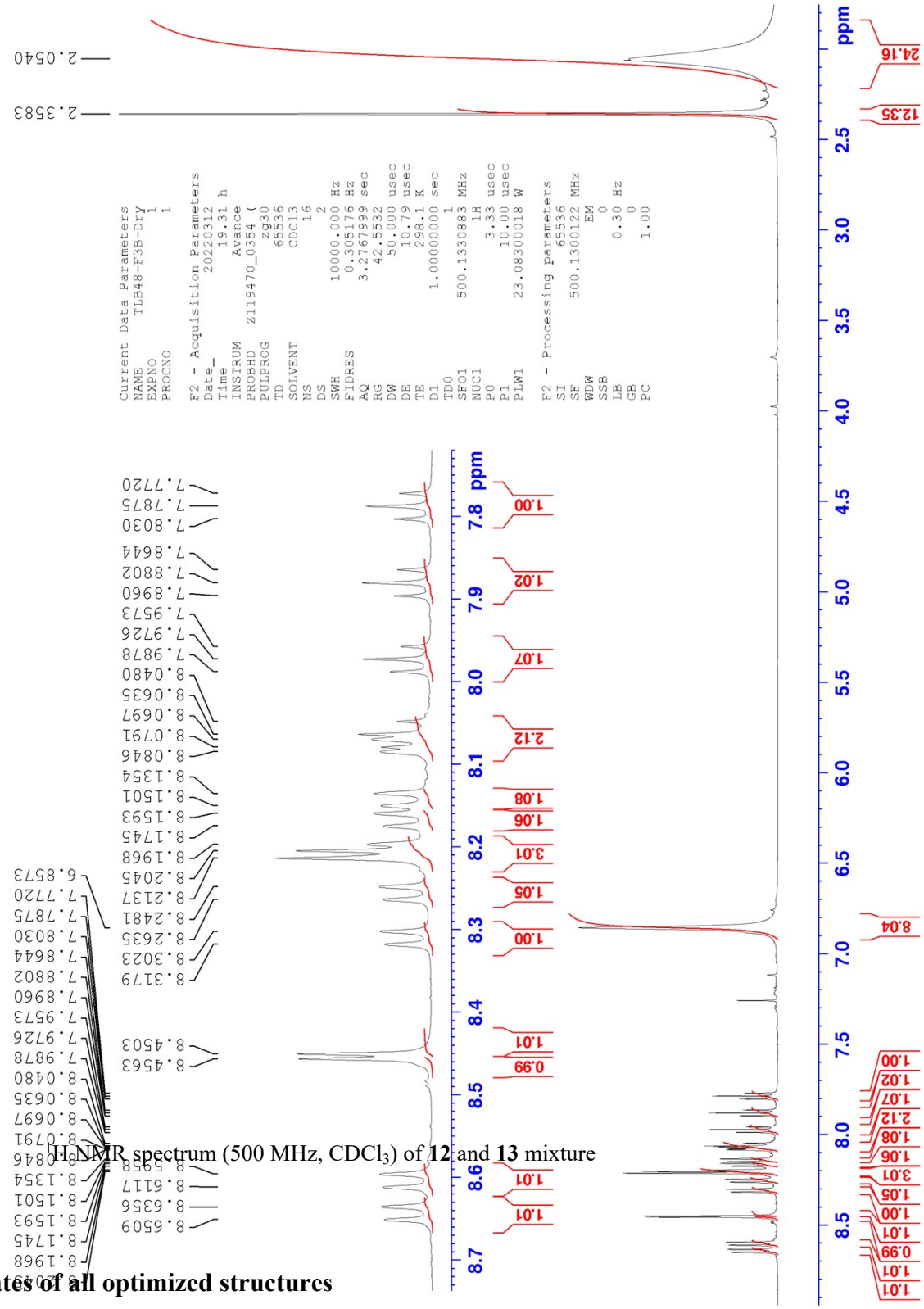
^{13}C {^{1}H} NMR spectrum (126 MHz, $CDCl_3$) of **4**



^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **5**



^{13}C {^{1}H} NMR spectrum (126 MHz, $CDCl_3$) of **5**



^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **12** and **13** mixture

Cartesian coordinates of all optimized structures

1

DFT B3LYP/6-31G(d), gas phase, S_0

E(total): -1807.935273 hartree

Imaginary Freq = 0

Dipole Moment = 0.028826 Debye

Symbol	X / Å	Y / Å	Z / Å
C	1.0263	-2.6644	2.059
C	1.985	-1.8733	1.4297

C	1.6058	-0.801	0.6105
C	0.2226	-0.5358	0.4196
C	-0.7438	-1.3471	1.0675
C	-0.3288	-2.4067	1.8862
C	2.5764	0.0525	-0.0696
C	-0.22	0.5374	-0.4213
C	0.7464	1.3486	-1.0693
C	2.1403	1.0792	-0.868
C	0.3314	2.4082	-1.888
H	1.084	3.0342	-2.3904
C	-1.0237	2.6659	-2.0608
C	-1.9824	1.8749	-1.4315
C	-1.6032	0.8026	-0.6122
C	-2.5738	-0.0509	0.068
C	-2.1377	-1.0777	0.8663
H	-2.855	-1.7279	1.3952
H	1.3475	-3.5003	2.6989
H	3.051	-2.1022	1.5886
H	-1.0814	-3.0327	2.3886
H	2.8576	1.7295	-1.3968
H	-1.3449	3.5017	-2.7008
H	-3.0484	2.1038	-1.5904
N	3.9669	-0.2329	0.088
C	4.7628	-0.2067	-1.0885
C	6.0007	0.4682	-1.1451
C	4.332	-0.919	-2.2318
C	6.7793	0.4163	-2.2962
H	6.3628	1.0371	-0.2741
C	5.1201	-0.9541	-3.375
H	3.3658	-1.4473	-2.2208
C	6.3525	-0.2926	-3.4229
H	7.7432	0.9476	-2.319
H	4.7686	-1.5137	-4.2555
C	4.5693	0.104	1.329
C	5.7689	-0.5337	1.7211
C	3.9728	1.0209	2.221
C	6.3346	-0.2629	2.9606
H	6.2612	-1.2462	1.0408
C	4.5497	1.2735	3.4609
H	3.0392	1.5358	1.9442
C	5.734	0.6385	3.8467
H	7.269	-0.7685	3.2492
H	4.0664	1.9883	4.1445
C	7.1921	-0.354	-4.6403

H	7.8485	-1.2603	-4.6065
H	6.559	-0.4162	-5.5596
H	7.8469	0.5483	-4.7224
C	6.3353	0.9038	5.1729
H	5.9418	0.1727	5.9239
H	7.4478	0.801	5.1358
H	6.0871	1.9348	5.5266
N	-3.9643	0.2346	-0.0893
C	-4.7602	0.2082	1.0872
C	-5.9987	-0.4656	1.1432
C	-4.3287	0.9193	2.231
C	-6.7772	-0.4139	2.2944
H	-6.3613	-1.0334	0.2718
C	-5.1168	0.9542	3.3743
H	-3.3621	1.4468	2.2203
C	-6.3497	0.2937	3.4217
H	-7.7416	-0.9443	2.3168
H	-4.7648	1.5128	4.2552
C	-4.5669	-0.1008	-1.3305
C	-5.7661	0.5382	-1.7221
C	-3.9702	-1.0159	-2.2242
C	-6.3319	0.2691	-2.9618
H	-6.2574	1.251	-1.0414
C	-4.5472	-1.2667	-3.4645
H	-3.0357	-1.5301	-1.9489
C	-5.7323	-0.6326	-3.8486
H	-7.2645	0.7774	-3.2512
H	-4.062	-1.9783	-4.1502
C	-7.1893	0.3549	4.6391
H	-7.845	1.2617	4.606
H	-7.8447	-0.5469	4.7206
H	-6.5561	0.416	5.5584
C	-6.3517	-0.9182	-5.1622
H	-7.1125	-1.7327	-5.0575
H	-6.8653	-0.0114	-5.5668
H	-5.5845	-1.2504	-5.9043

2

DFT B3LYP/6-31G(d), gas phase, S_0
E(total): -1807.935286 hartree
Imaginary Freq = 0
Dipole Moment = 0.114157 Debye

Symbol	X / Å	Y / Å	Z / Å

C	-0.00014	-3.1417	3.5814
C	1.21031	-2.69753	3.05276
C	1.23385	-1.79205	1.97821
C	-0.00005	-1.32799	1.43342
C	-1.234	-1.79202	1.97813
C	-1.21055	-2.6975	3.05268
C	2.45883	-1.29867	1.42547
C	0	-0.41665	0.33482
C	1.23859	0.0242	-0.23353
C	2.48035	-0.42729	0.37211
C	1.2115	0.84399	-1.3719
H	2.14479	1.16439	-1.8194
C	0.0001	1.23834	-1.93313
C	-1.21135	0.84401	-1.37199
C	-1.23855	0.02423	-0.23361
C	-2.48037	-0.42723	0.37195
C	-2.45893	-1.29861	1.4253
H	-3.39809	-1.63351	1.85666
H	3.39796	-1.6336	1.85688
H	-0.00018	-3.8425	4.41199
H	2.15101	-3.04948	3.46873
H	-2.15129	-3.04942	3.46859
H	0.00014	1.86307	-2.82217
H	-2.1446	1.16442	-1.81957
N	3.7275	0.01794	-0.16479
N	-3.72746	0.01803	-0.16505
C	-4.70768	-0.96045	-0.49703
C	-6.03626	-0.85198	-0.06252
C	-4.34506	-2.0755	-1.26967
C	-6.97203	-1.82692	-0.40674
H	-6.33479	-0.0047	0.54639
C	-5.28564	-3.04938	-1.58891
H	-3.31976	-2.17353	-1.61337
C	-6.62095	-2.9442	-1.17288
H	-7.99621	-1.72068	-0.05522
H	-4.97708	-3.90504	-2.18602
C	-4.08325	1.38896	-0.05492
C	-4.94217	1.98079	-0.999
C	-3.56237	2.19435	0.96682
C	-5.27127	3.32835	-0.90588
H	-5.34612	1.37759	-1.80604
C	-3.88804	3.54929	1.03428
H	-2.89916	1.76005	1.70767
C	-4.75145	4.14513	0.11008

H	-5.93687	3.75986	-1.65092
H	-3.46441	4.15147	1.83519
C	4.70758	-0.96058	-0.49707
C	6.03622	-0.85233	-0.06251
C	4.34486	-2.07544	-1.26985
C	6.97186	-1.82728	-0.40686
H	6.33479	-0.00522	0.54661
C	5.28538	-3.04939	-1.58924
H	3.31953	-2.17336	-1.61351
C	6.62066	-2.9444	-1.17326
H	7.99604	-1.72124	-0.05524
H	4.97672	-3.90496	-2.18643
C	4.08335	1.38882	-0.05462
C	4.94245	1.98062	-0.99856
C	3.56236	2.19425	0.96705
C	5.27161	3.32817	-0.90537
H	5.34647	1.37742	-1.80557
C	3.8881	3.54916	1.03458
H	2.89901	1.75998	1.70778
C	4.7517	4.14496	0.11052
H	5.93735	3.75965	-1.65032
H	3.46437	4.15135	1.83542
C	7.64338	-3.98723	-1.55945
H	7.22192	-4.9982	-1.5203
H	8.011	-3.8315	-2.58293
H	8.51302	-3.95982	-0.89435
C	5.12628	5.60554	0.20468
H	6.15307	5.73639	0.5722
H	5.07116	6.09951	-0.77283
H	4.46295	6.1442	0.88922
C	-5.1259	5.60575	0.20409
H	-5.06926	6.09998	-0.77321
H	-6.15319	5.73669	0.57014
H	-4.46345	6.1441	0.88973
C	-7.64352	-3.98736	-1.55859
H	-7.22512	-4.99915	-1.50825
H	-8.51801	-3.95239	-0.90029
H	-8.00286	-3.83886	-2.58606

3

DFT B3LYP/6-31G(d), gas phase, S_0
E(total): -1935.314857 hartree
Imaginary Freq = 0
Dipole Moment = 0.298436 Debye

Symbol	X / Å	Y / Å	Z / Å
C	1.5689	1.2105	-3.1287
C	2.5032	0.7759	-2.1907
C	2.0934	0.2793	-0.9457
C	0.7036	0.2132	-0.6557
C	-0.2383	0.662	-1.6177
C	0.208	1.1598	-2.8492
C	3.0357	-0.1862	0.0686
C	0.23	-0.3025	0.5949
C	1.1682	-0.7492	1.5598
C	2.5693	-0.6711	1.2643
C	0.7161	-1.2521	2.7875
H	1.4449	-1.5996	3.5349
C	-0.6473	-1.3119	3.0571
C	-1.5756	-0.8773	2.1151
C	-1.163	-0.3724	0.874
C	-2.1008	0.0913	-0.1235
C	-1.6381	0.5981	-1.3024
H	-2.3446	0.976	-2.0617
H	1.9148	1.5984	-4.0988
H	3.5745	0.8321	-2.442
H	-0.5245	1.5102	-3.5917
H	3.2659	-1.0341	2.0388
H	-0.9968	-1.7094	4.022
H	-2.6523	-0.9445	2.3416
B	-3.6389	0.0349	0.0825
N	4.432	-0.1569	-0.2315
C	5.1829	-1.3154	0.1027
C	6.4188	-1.2423	0.7797
C	4.7078	-2.5868	-0.2949
C	7.1531	-2.3961	1.0319
H	6.8144	-0.2685	1.1088
C	5.4519	-3.7289	-0.0284
H	3.7416	-2.6762	-0.8157
C	6.6828	-3.6506	0.633
H	8.1163	-2.317	1.559
H	5.0663	-4.7101	-0.3453
C	5.0797	1.1064	-0.2207
C	6.2964	1.2763	-0.9212
C	4.512	2.2277	0.4218
C	6.9072	2.5226	-0.9743
H	6.7654	0.4171	-1.4258
C	5.1342	3.4694	0.351

H	3.5647	2.1286	0.9751
C	6.3368	3.6337	-0.3426
H	7.853	2.6369	-1.526
H	4.6713	4.3332	0.8525
C	-4.3534	-1.2638	0.537
C	-5.1409	-1.296	1.704
C	-4.2284	-2.4381	-0.2274
C	-5.7703	-2.4821	2.0952
C	-4.8719	-3.6146	0.1742
C	-5.6415	-3.6485	1.3374
H	-6.3812	-2.4973	3.0109
H	-4.7656	-4.5233	-0.4378
C	-4.4335	1.3229	-0.2636
C	-5.259	1.3779	-1.4007
C	-4.3066	2.4674	0.5428
C	-5.9515	2.5534	-1.7081
C	-5.0082	3.6349	0.2238
C	-5.836	3.6866	-0.8992
H	-6.5966	2.5868	-2.5993
H	-4.9007	4.5223	0.8659
C	7.0033	4.9541	-0.3973
H	7.5608	5.0809	-1.3579
H	6.2587	5.7832	-0.3087
H	7.7339	5.049	0.4456
C	7.4753	-4.8733	0.8933
H	8.1214	-5.1055	0.009
H	8.1374	-4.741	1.7842
H	6.8071	-5.7507	1.0766
C	-6.5896	4.9198	-1.2233
H	-6.7185	5.0307	-2.3282
H	-7.6057	4.8792	-0.7553
H	-6.0622	5.8259	-0.8359
C	-5.3946	0.216	-2.3127
H	-4.5079	0.1608	-2.9948
H	-5.4523	-0.7417	-1.7349
H	-6.3137	0.3024	-2.9428
C	-3.4444	2.4785	1.7511
H	-4.0752	2.5592	2.6723
H	-2.8297	1.5453	1.827
H	-2.7502	3.3551	1.7241
C	-6.3028	-4.9012	1.7695
H	-7.2693	-4.6843	2.2876
H	-6.5109	-5.5675	0.8965
H	-5.6404	-5.4549	2.4823

C	-5.3237	-0.0944	2.5548
H	-4.3727	0.1577	3.0897
H	-5.6152	0.7883	1.9303
H	-6.1194	-0.2593	3.3225
C	-3.4287	-2.4896	-1.4773
H	-2.4871	-3.0689	-1.3023
H	-4.007	-2.9984	-2.2885
H	-3.1499	-1.4668	-1.8345

4

DFT B3LYP/6-31G(d), gas phase, S_0
E(total): -2318.794595 hartree
Imaginary Freq = 0
Dipole Moment = 0.796406 Debye

Symbol	X / Å	Y / Å	Z / Å
C	-1.884	-3.0484	1.3034
C	-0.5258	-2.7483	1.2873
C	-0.0838	-1.5205	0.7759
C	-1.0264	-0.5866	0.2761
C	-2.4144	-0.8965	0.3018
C	-2.8168	-2.1369	0.8165
C	1.3124	-1.1938	0.743
C	-0.5629	0.6642	-0.2483
C	0.8215	0.9851	-0.2709
C	1.7682	0.0027	0.2502
C	1.2213	2.2282	-0.78
H	2.2879	2.5029	-0.8041
C	0.2826	3.135	-1.268
C	-1.0728	2.8255	-1.2591
C	-1.5093	1.5948	-0.7506
C	-2.9031	1.2487	-0.7294
C	-3.3572	0.0698	-0.2149
H	-3.6125	1.9839	-1.1475
H	2.0124	-1.9443	1.1474
H	-2.2259	-4.0132	1.7077
H	0.2065	-3.4714	1.6764
H	-3.89	-2.3872	0.8494
H	0.6205	4.1042	-1.6652
H	-1.8086	3.5435	-1.6515
N	3.1584	0.3309	0.2628
B	-4.8916	-0.1698	-0.208
C	3.865	0.0927	1.4692
C	5.1341	-0.5251	1.4891

C	3.3085	0.5239	2.6961
C	5.8203	-0.6887	2.6866
H	5.5943	-0.8787	0.5528
C	4.0056	0.3501	3.8842
H	2.3144	0.9976	2.7145
C	5.2702	-0.2548	3.8993
H	6.8132	-1.165	2.6779
H	3.5532	0.6892	4.8294
C	3.8566	0.3005	-0.9703
C	5.0666	1.0185	-1.1135
C	3.3452	-0.3836	-2.0949
C	5.7261	1.0485	-2.3351
H	5.4933	1.5561	-0.2521
C	4.0153	-0.3397	-3.3118
H	2.4027	-0.9489	-2.0181
C	5.2131	0.3728	-3.4511
H	6.6697	1.6092	-2.4249
H	3.593	-0.8714	-4.1789
C	5.9141	0.4108	-4.7319
C	5.9946	-0.738	-5.5326
C	6.516	1.5965	-5.1781
C	6.6649	-0.6998	-6.7533
H	5.5315	-1.6753	-5.1893
C	7.1835	1.6303	-6.4006
H	6.4524	2.5057	-4.5616
C	7.2602	0.4833	-7.1904
H	6.7249	-1.6068	-7.3726
H	7.6497	2.5659	-6.7431
H	7.788	0.5118	-8.1545
C	5.9974	-0.4299	5.1539
C	5.9838	0.5776	6.1296
C	6.7189	-1.6073	5.3995
C	6.6791	0.4092	7.3251
H	5.4268	1.5083	5.9444
C	7.411	-1.772	6.5974
H	6.7307	-2.4072	4.6439
C	7.3935	-0.765	7.5622
H	6.6647	1.2064	8.0828
H	7.9716	-2.7003	6.7817
H	7.9409	-0.8964	8.5067
C	-5.6476	0.1355	-1.5289
C	-5.4627	-0.6876	-2.6533
C	-6.4957	1.2524	-1.6332
C	-6.1296	-0.4049	-3.8503

C	-7.1529	1.5235	-2.8375
C	-6.9797	0.6979	-3.9512
H	-5.9768	-1.0597	-4.7215
H	-7.8161	2.3991	-2.9095
C	-5.6404	-0.6176	1.0736
C	-5.5739	0.1702	2.2372
C	-6.4018	-1.8019	1.1002
C	-6.2483	-0.2256	3.3981
C	-7.0627	-2.1869	2.271
C	-6.9917	-1.4059	3.4271
H	-6.1877	0.4046	4.2985
H	-7.6529	-3.1162	2.2821
C	-7.6858	-1.8314	4.6642
H	-7.9387	-0.9518	5.3058
H	-8.631	-2.3779	4.424
H	-7.0259	-2.5167	5.2543
C	-4.8061	1.4398	2.2928
H	-3.8841	1.2995	2.9119
H	-4.4958	1.7826	1.2742
H	-5.4228	2.247	2.7613
C	-6.5234	-2.6777	-0.0912
H	-6.7974	-2.0755	-0.9949
H	-5.5526	-3.1952	-0.3003
H	-7.3073	-3.4601	0.06
C	-6.6924	2.1811	-0.4935
H	-5.8234	2.8839	-0.4196
H	-7.6215	2.7887	-0.6234
H	-6.7714	1.6188	0.4719
C	-4.5743	-1.876	-2.6124
H	-3.9918	-1.9219	-1.6569
H	-5.1814	-2.8125	-2.6986
H	-3.8501	-1.8485	-3.4644
C	-7.6962	0.9834	-5.2156
H	-8.7018	0.4916	-5.2028
H	-7.8471	2.0828	-5.3501
H	-7.1278	0.5939	-6.0957

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DFT B3LYP/6-31G(d), gas phase, S_0
E(total): -2318.794324 hartree
Imaginary Freq = 0
Dipole Moment = 0.878698 Debye

Symbol	X / Å	Y / Å	Z / Å

C	-0.6857	-2.0768	0.2409
C	0.4506	-1.2961	0.4342
C	0.3905	0.0965	0.291
C	-0.8502	0.7034	-0.0484
C	-2.0086	-0.1008	-0.2435
C	-1.8999	-1.4906	-0.0968
C	1.5562	0.9546	0.4919
C	-0.9432	2.1265	-0.1892
C	0.1985	2.9397	0.0202
C	1.4438	2.3154	0.358
C	0.092	4.3308	-0.1173
H	0.978	4.9618	0.0486
C	-1.125	4.9127	-0.4628
C	-2.2522	4.1234	-0.6747
C	-2.1772	2.7303	-0.5403
C	-3.3191	1.887	-0.7537
C	-3.2593	0.5331	-0.5984
H	-4.2639	2.3751	-1.0484
H	-0.6211	-3.1692	0.3594
H	1.3981	-1.7908	0.7001
H	-2.7919	-2.1232	-0.2362
H	-1.1959	6.0057	-0.5697
H	-3.2094	4.5906	-0.9509
B	-4.5716	-0.2705	-0.8131
C	-5.3779	0.0516	-2.0999
C	-4.8758	-0.3199	-3.3592
C	-6.5987	0.7463	-2.0302
C	-5.5927	-0.0146	-4.5212
C	-7.3021	1.0468	-3.201
C	-6.8083	0.6684	-4.452
H	-5.1894	-0.3163	-5.4997
H	-8.2589	1.5872	-3.1365
C	-5.0903	-1.2819	0.2413
C	-5.3391	-0.8568	1.5591
C	-5.331	-2.6285	-0.0928
C	-5.8106	-1.7623	2.5166
C	-5.794	-3.5221	0.8785
C	-6.0364	-3.0993	2.1876
H	-6.0032	-1.4119	3.5421
H	-5.9758	-4.5735	0.6078
C	-6.5145	-4.0583	3.21
H	-7.0957	-3.5364	4.0095
H	-7.1681	-4.8398	2.7499

H	-5.6417	-4.57	3.6892
C	-5.1231	0.5464	1.9937
H	-4.1945	0.6124	2.6153
H	-5.0111	1.2383	1.1218
H	-5.9847	0.9001	2.6132
C	-5.0985	-3.1462	-1.4636
H	-5.5829	-2.4801	-2.2225
H	-4.0022	-3.1886	-1.6881
H	-5.5163	-4.1762	-1.5834
C	-7.1555	1.2006	-0.7326
H	-7.0045	0.4253	0.0614
H	-6.6431	2.1415	-0.406
H	-8.2501	1.411	-0.8147
C	-3.5914	-1.0499	-3.5027
H	-3.0407	-1.1099	-2.5293
H	-3.7808	-2.0926	-3.8636
H	-2.9338	-0.5359	-4.2473
C	-7.5565	1.0019	-5.6859
H	-8.6583	1.0022	-5.4973
H	-7.263	2.0205	-6.0459
H	-7.3369	0.2673	-6.4993
H	2.3117	2.9768	0.5183
N	2.796	0.3482	0.8615
C	3.4937	0.9224	1.9543
C	4.884	1.1642	1.9164
C	2.791	1.2276	3.1435
C	5.5415	1.6759	3.0288
H	5.4613	0.9437	1.0045
C	3.4623	1.7413	4.2449
H	1.7036	1.0613	3.1995
C	4.8446	1.9712	4.2073
H	6.6282	1.8481	2.9804
H	2.8963	1.9757	5.1602
C	5.5426	2.5086	5.3724
C	5.207	2.076	6.6637
C	6.5574	3.464	5.2155
C	5.8748	2.589	7.7737
H	4.4173	1.3215	6.7978
C	7.221	3.9755	6.3287
H	6.8241	3.8156	4.2075
C	6.8822	3.5395	7.6094
H	5.6063	2.2411	8.782
H	8.0135	4.7265	6.1953
H	7.4075	3.9437	8.4866

C	3.52	-0.3426	-0.1419
C	4.4817	-1.3131	0.2236
C	3.2661	-0.1337	-1.5153
C	5.1512	-2.0415	-0.7507
H	4.7058	-1.4932	1.2869
C	3.9417	-0.8744	-2.4779
H	2.5202	0.612	-1.8336
C	4.8929	-1.8356	-2.1131
H	5.9	-2.7892	-0.4457
H	3.7206	-0.7028	-3.5431
C	5.6019	-2.6074	-3.1305
C	6.0346	-1.9936	-4.3152
C	5.8594	-3.9724	-2.9363
C	6.7118	-2.7315	-5.2837
H	5.8437	-0.9218	-4.475
C	6.5352	-4.7066	-3.9086
H	5.5179	-4.4658	-2.014
C	6.9633	-4.0887	-5.0834
H	7.0496	-2.2403	-6.2081
H	6.7297	-5.7773	-3.7482
H	7.4972	-4.6696	-5.8492