Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Colour-Responsive Fluorescent Oxy Radical Sensors

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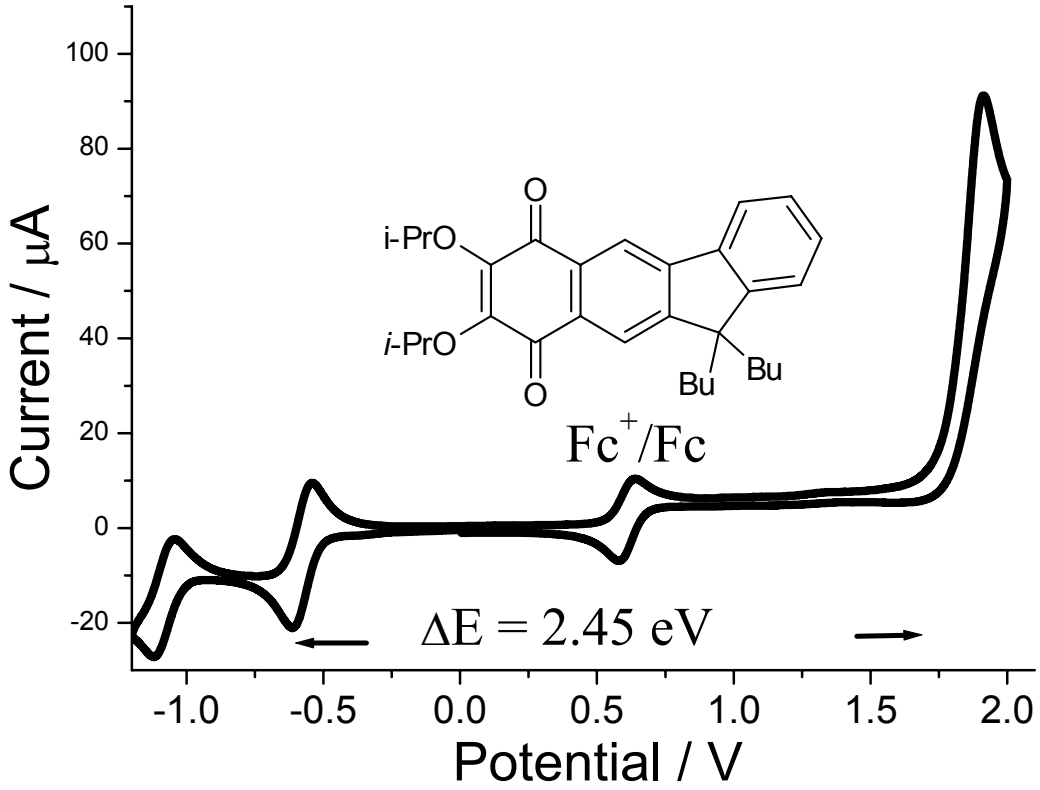
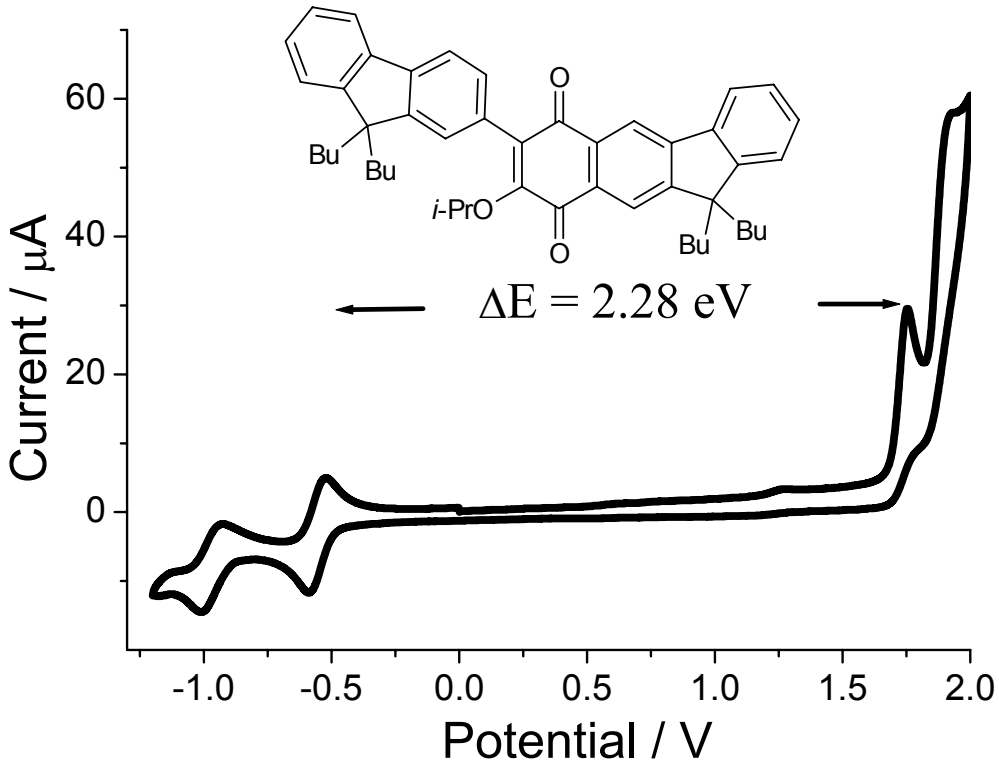
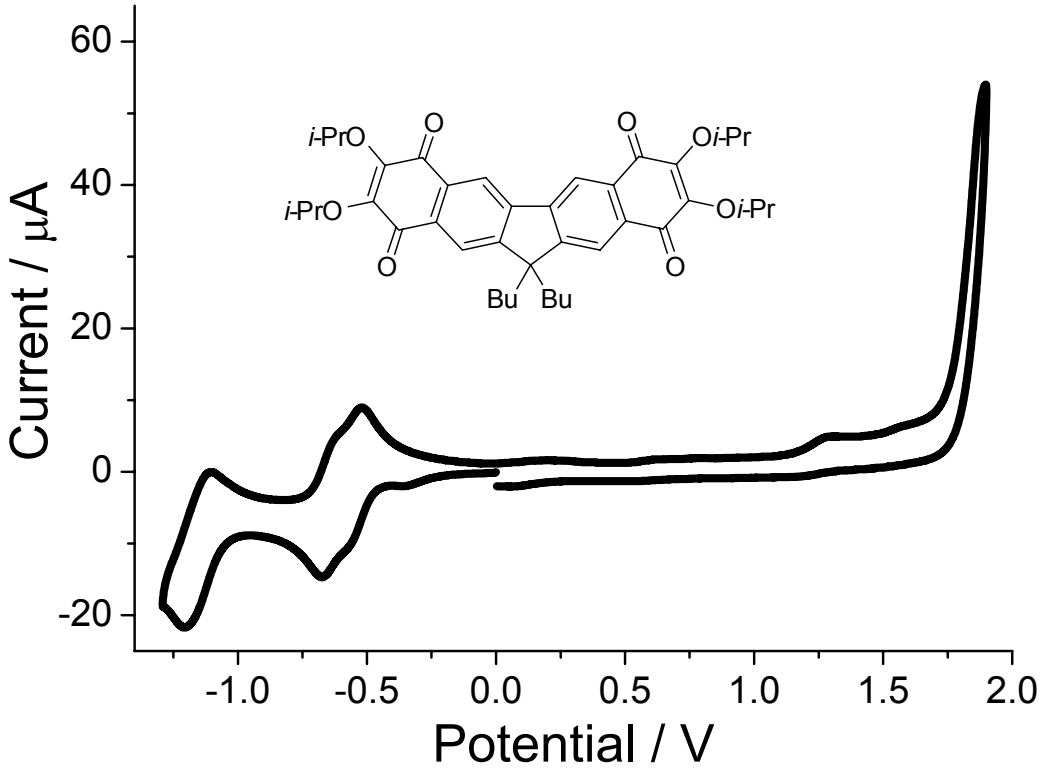


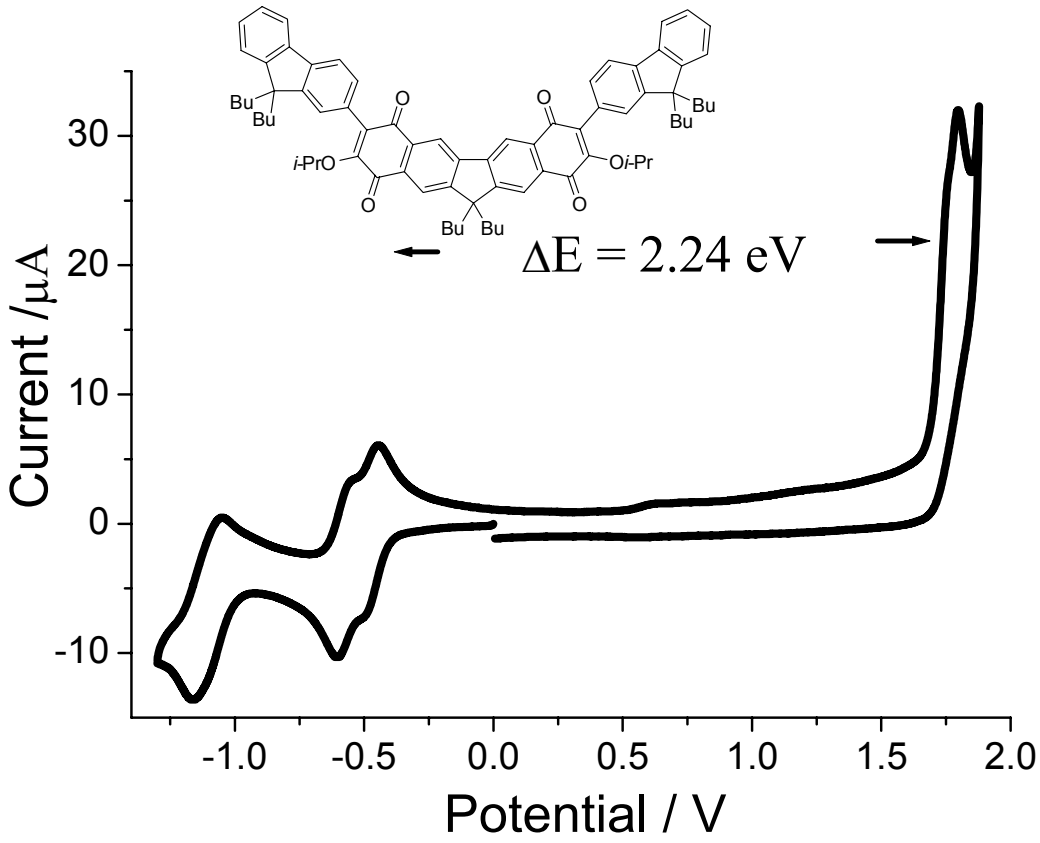
S1. Cyclic voltammogram for **Q1** in dry CH_3CN (0.2 M TBATFB) at a glassy carbon electrode at 50 mV s^{-1} using a silver wire reference.



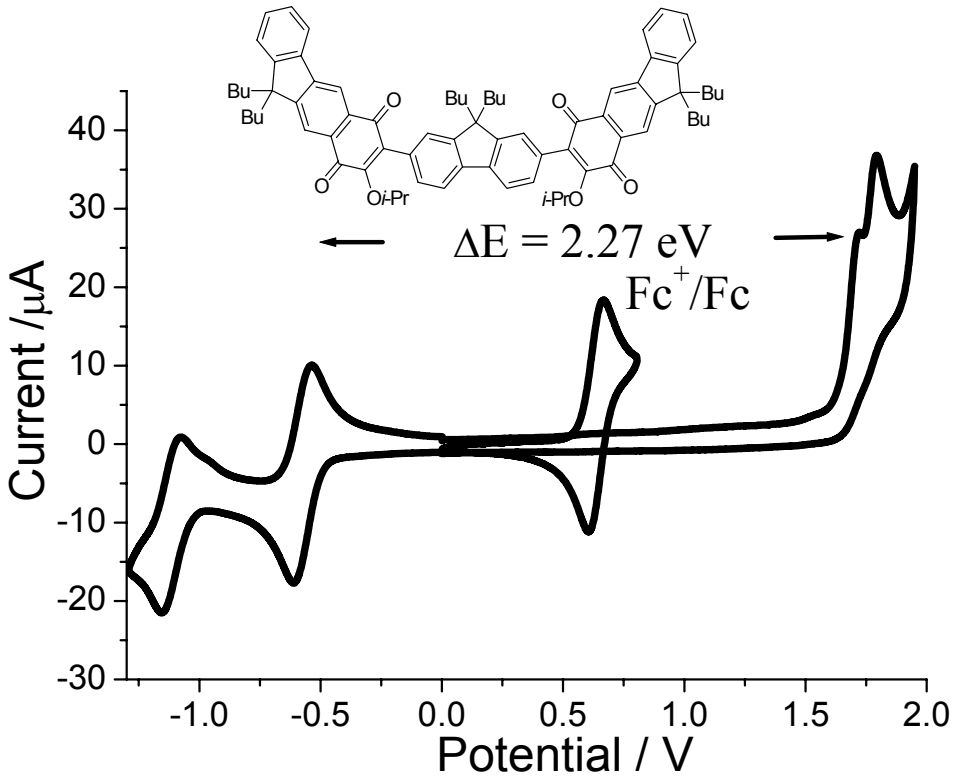
S2. Cyclic voltammogram for **Q2** in dry CH_3CN (0.2 M TBATFB) at a glassy carbon electrode at 50 mV s^{-1} using a silver wire reference.



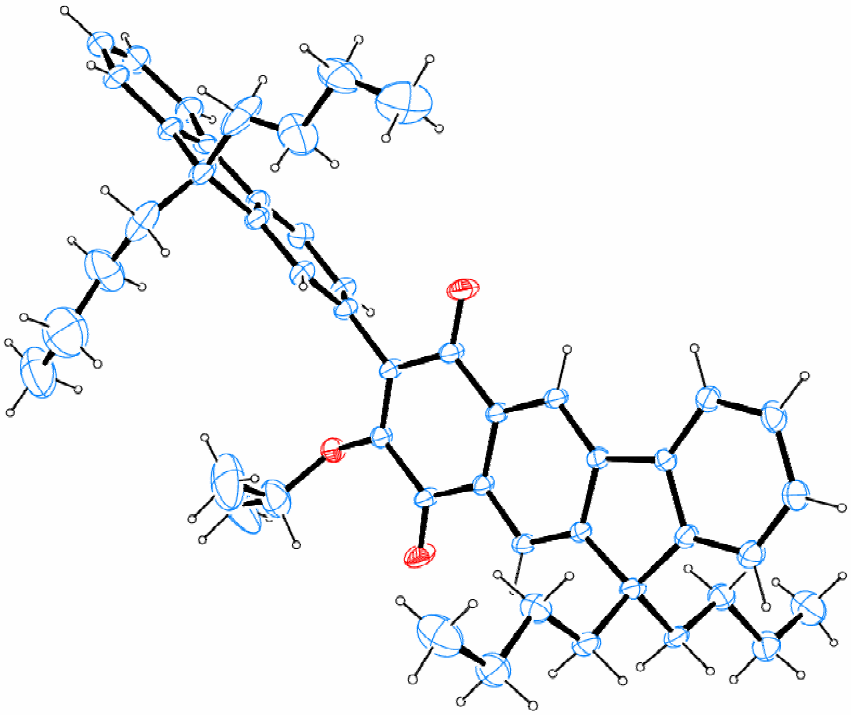
S3. Cyclic voltammogram for **Q3** in dry CH_3CN (0.2 M TBATFB) at a glassy carbon electrode at 50 mV s^{-1} using a silver wire reference.



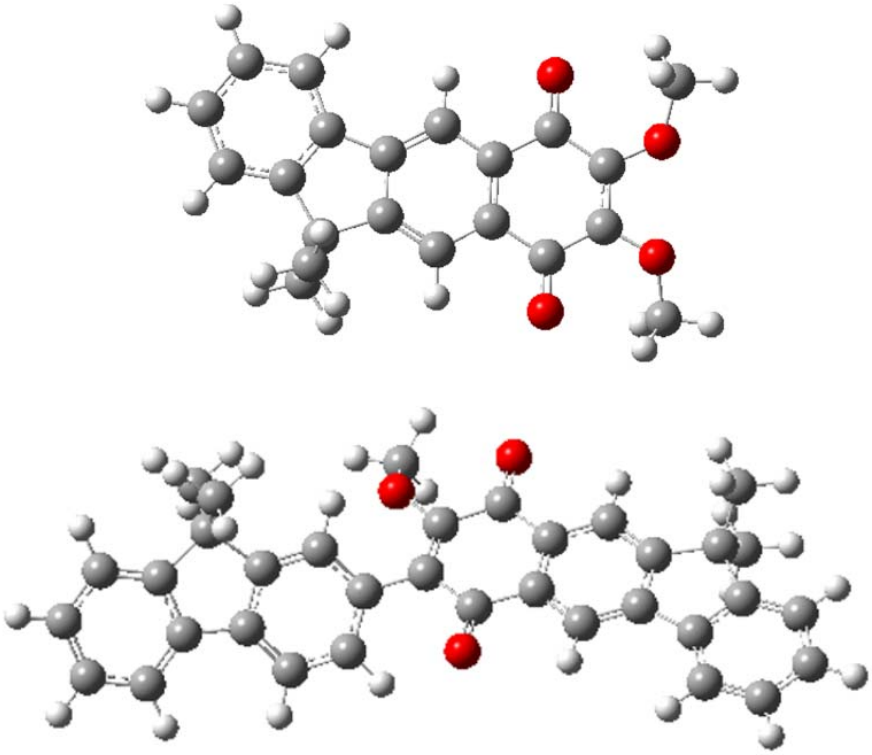
S4. Cyclic voltammogram for **Q4** in dry CH_3CN (0.2 M TBATFB) at a glassy carbon electrode at 50 mV s^{-1} using a silver wire reference.



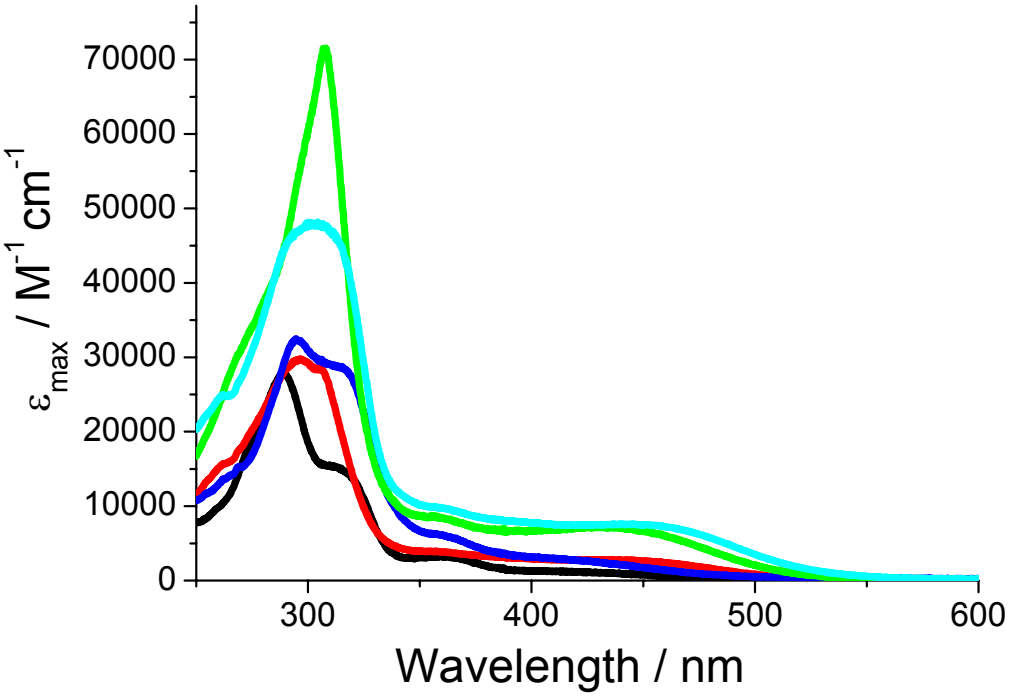
S5. Cyclic voltammogram for **Q5** in dry CH_3CN (0.2 M TBATFB) at a glassy carbon electrode at 50 mV s^{-1} using a silver wire reference.



S6. ORTEP for X-ray determined structure of 14B (Q2). Thermal ellipsoids are shown at 15% probability.



S7. Computer calculated structures for **Q1** (top) and **Q2** (bottom) using DFT (B3LYP) and the 6-311G basis set.

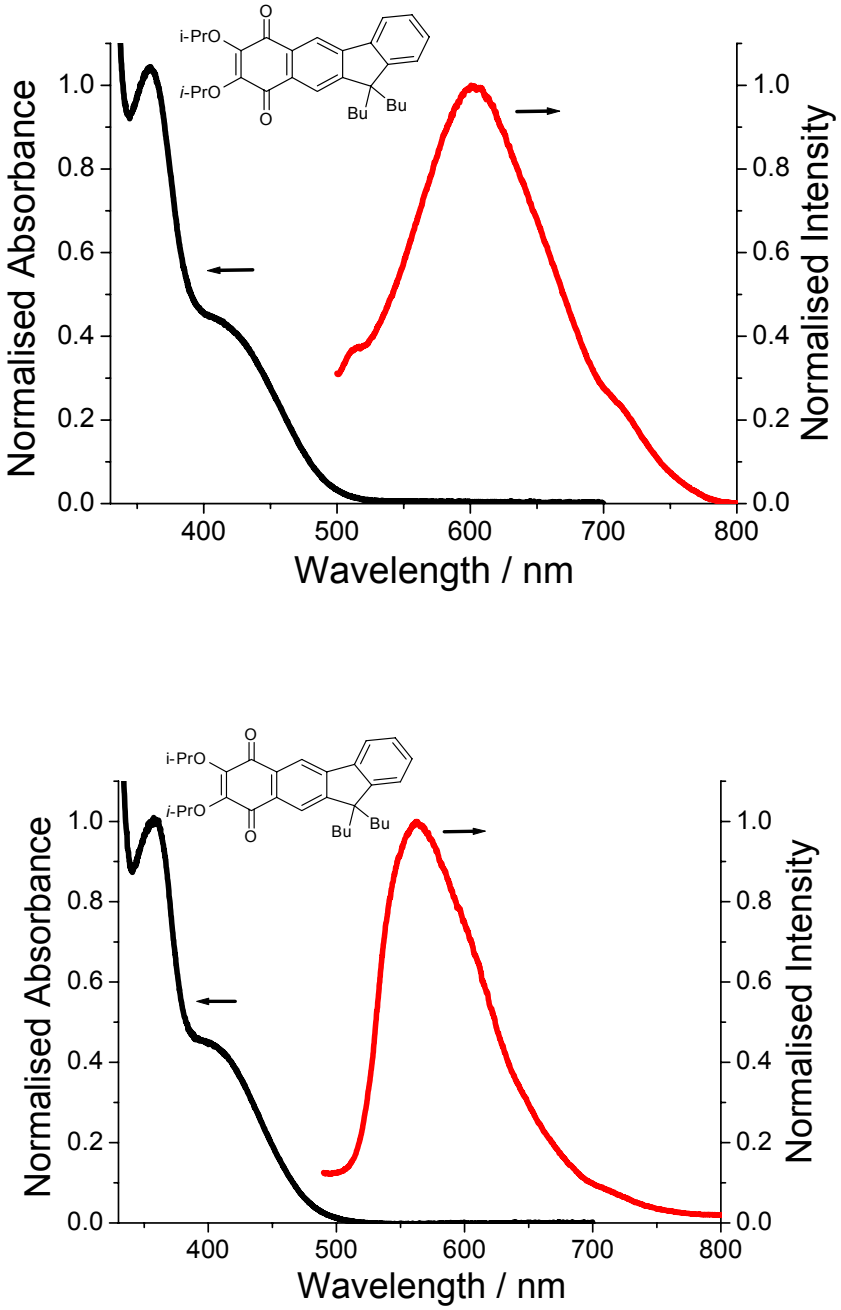


S8. Absorption spectra recorded for **Q1** (black), **Q2** (red), **Q3** (blue), **Q4** (green) and **Q5** (cyano) in MeCN.

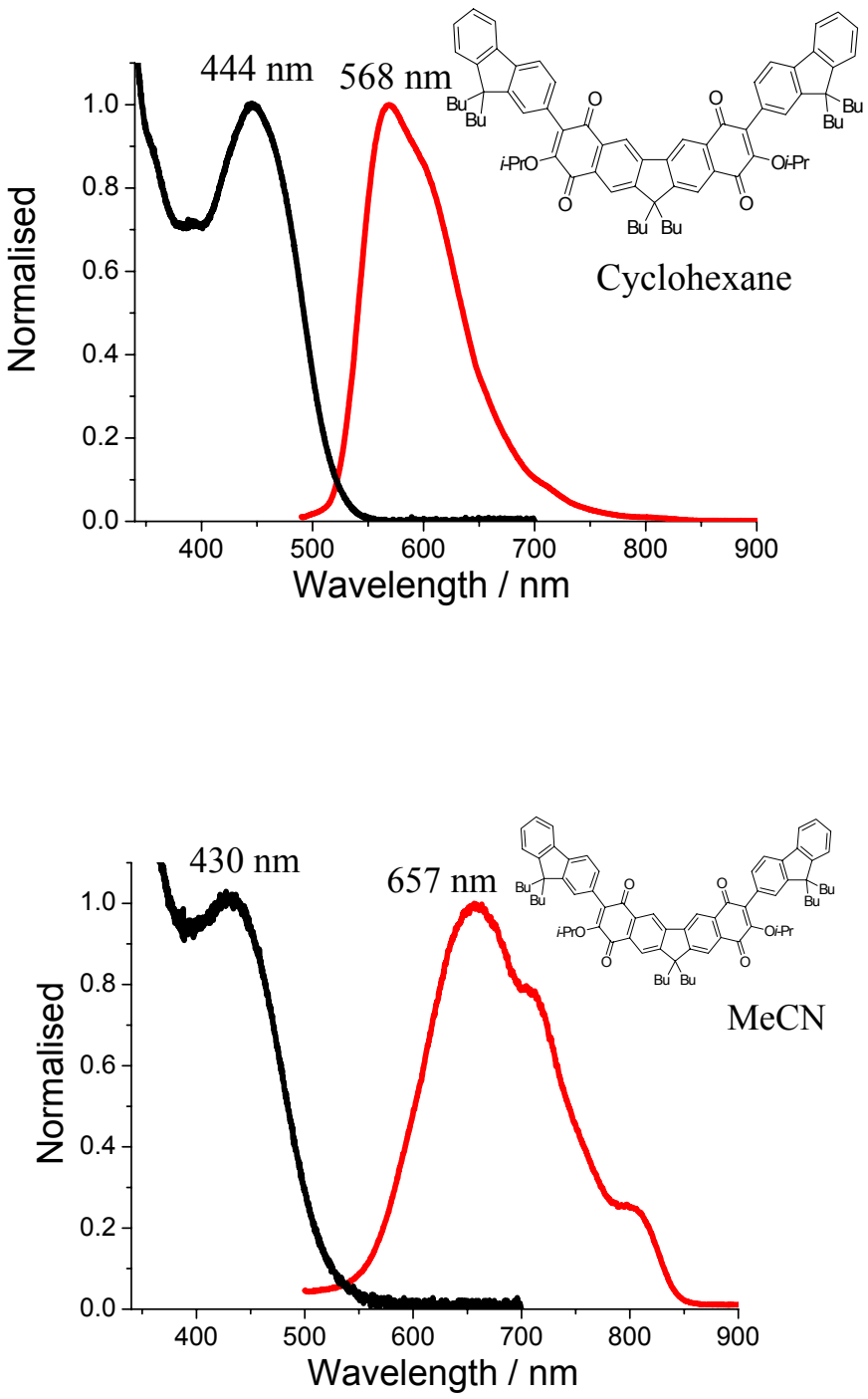
Table 2. Photophysical properties collected for **Q2** in a range of solvents.

Solvent	n[a]	ε[b]	λ_{ABS} / nm	λ_{EM} / nm	SS / cm^{-1}	λ_{tot} / eV
THF[c]	1.405	7.58	439	606	6277	0.39
EA[d]	1.372	6.02	439	606	6277	0.39
DCM[e]	1.431	9.1	446	632	6599	0.41 (0.47)[j]
MeTHF[f]	1.403	6.97	441	598	5954	0.37
Bu_2O	1.399	3.1	446	585	5328	0.33
DMF[g]	1.431	36.7	430	640	7631	0.47
MeCN	1.344	37.5	433	644	7567	0.47
CHX[h]	1.426	2.02	467	561	3588	0.22
Toluene	1.493	2.4	447	595	5564	0.34
Pentane	1.358	2.1	438	556	4845	0.30
CCl_4	1.460	2.2	459	587	4750	0.29

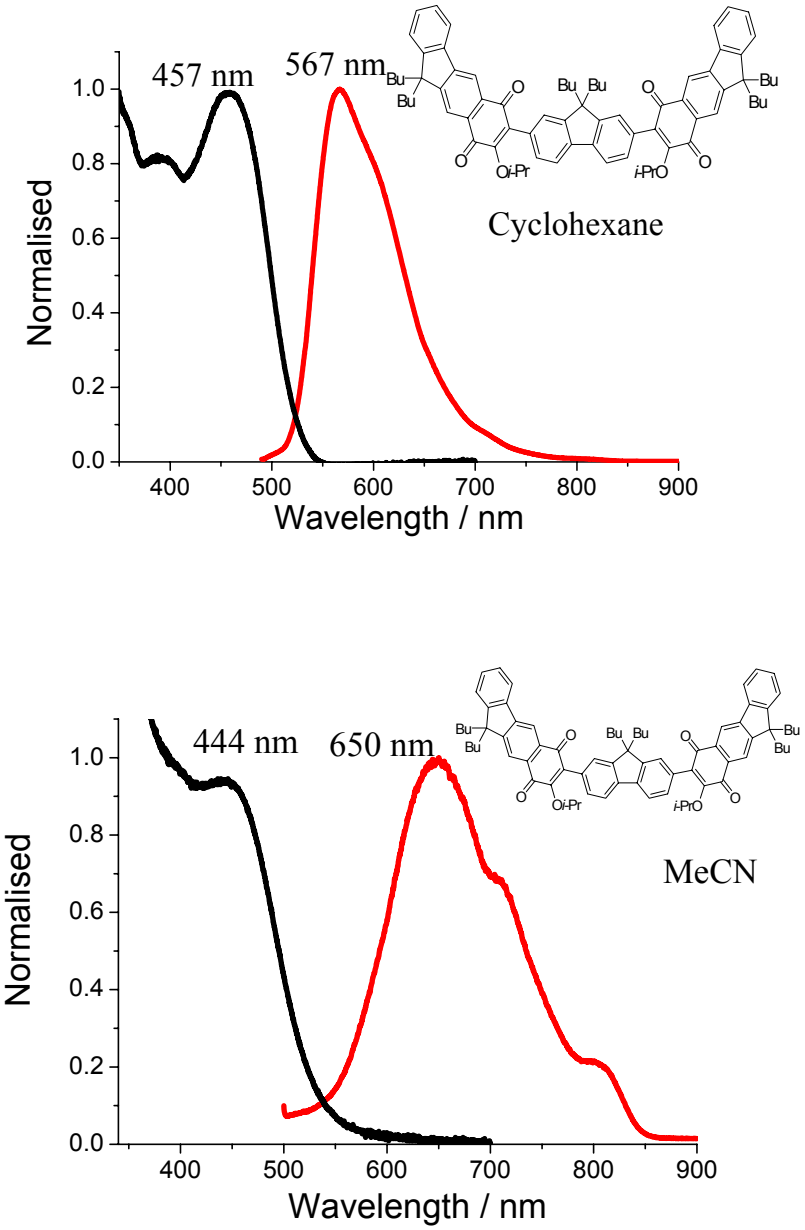
[a]refractive index, [b]dielectric constant, [c]Tetrahydrofuran, [d]ethyl acetate, [e]dichloromethane, [f]methyltetrahydrofuran, [g]N,N-dimethylformamide, [h]cyclohexane. [j]calculated by $\lambda_{tot} = \lambda_{ABS}$-ΔE



S9. Absorption and emission profiles recorded for **Q1** in MeCN (top) and cyclohexane (bottom).



S10. Absorption and emission profiles recorded for **Q4** in cyclohexane (top) and MeCN (bottom).



S11. Absorption and emission profiles recorded for **Q5** in cyclohexane (top) and MeCN (bottom)

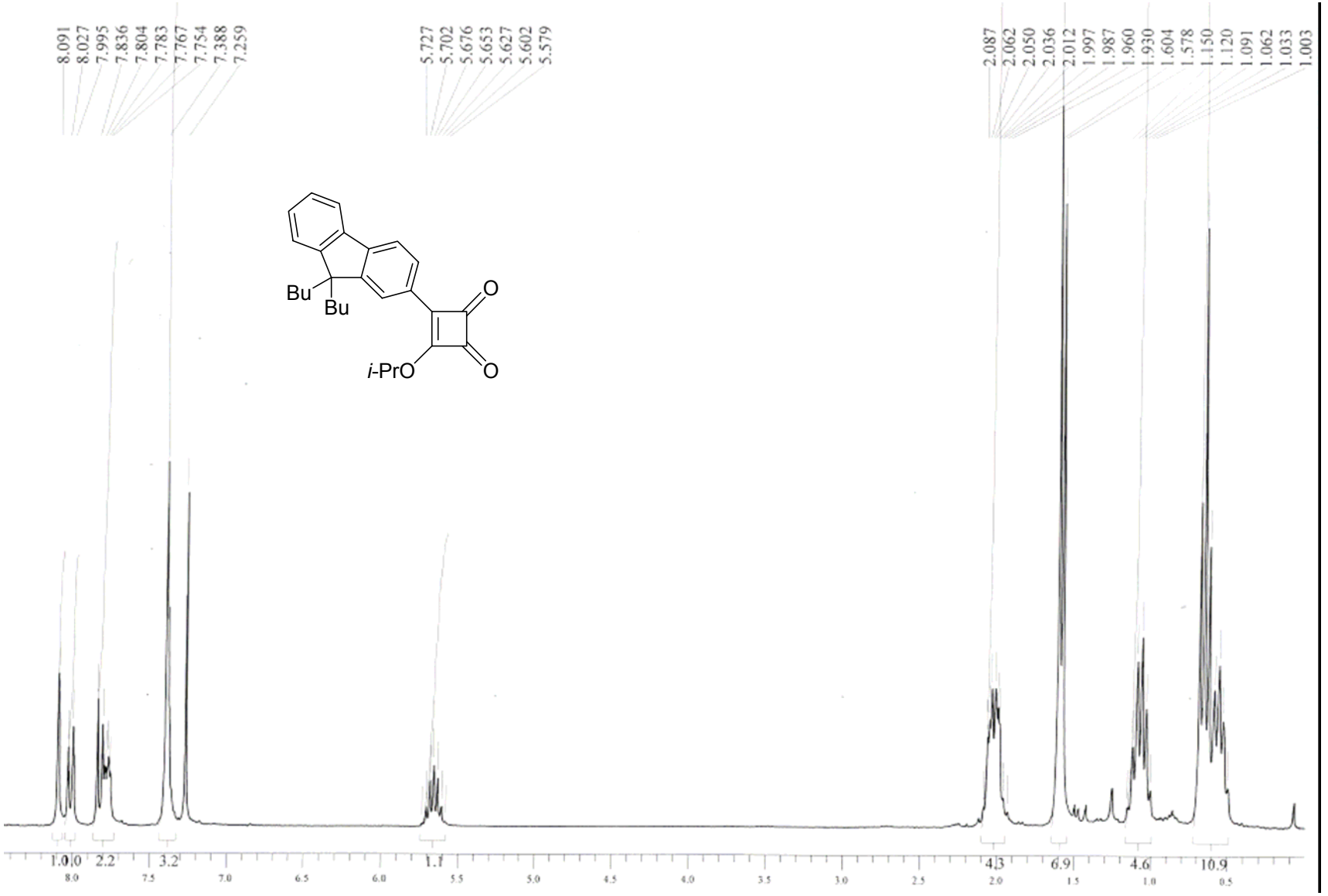


Figure S1. ^{1}H NMR spectrum of compound **8B**.

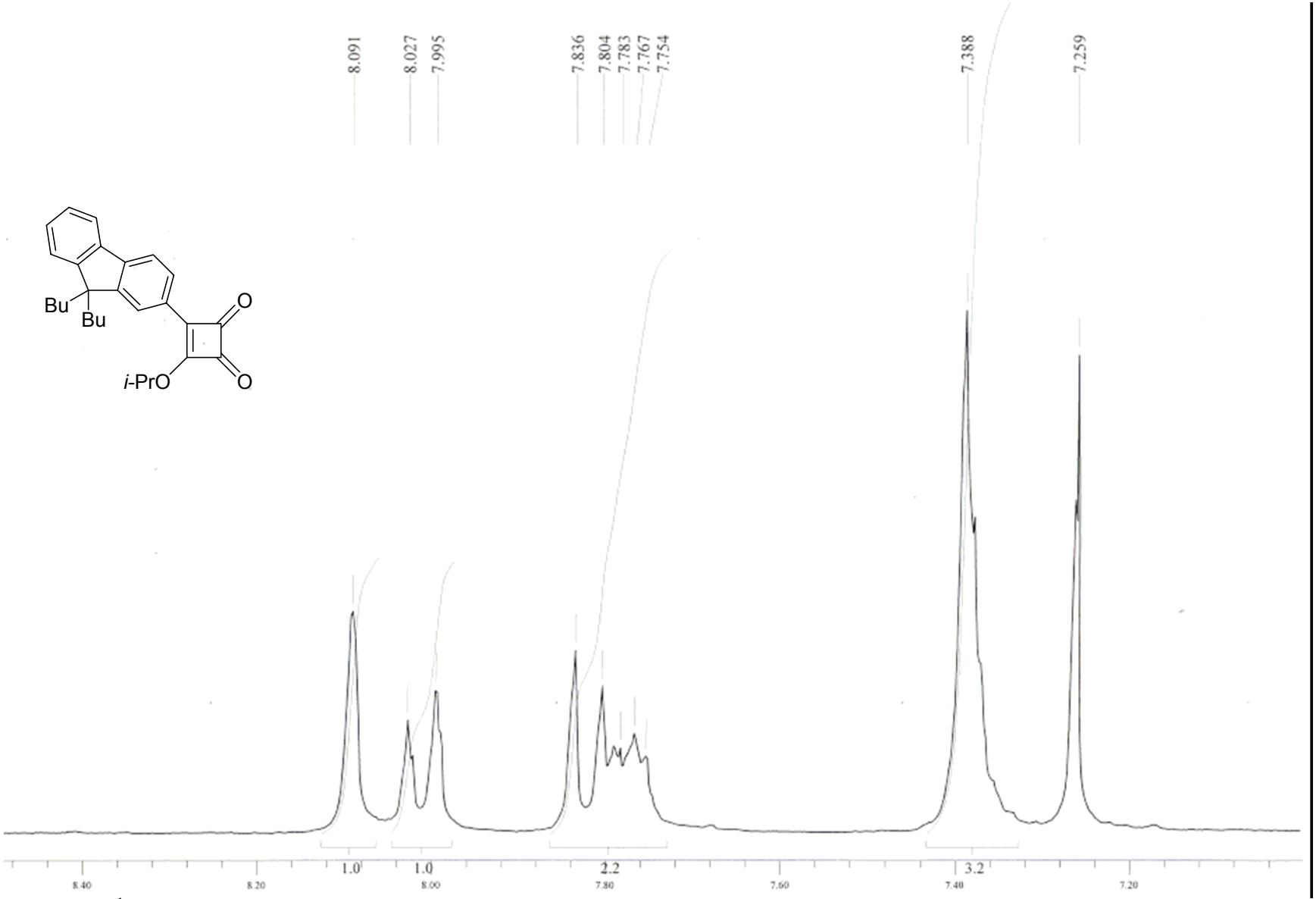


Figure S2. ^{1}H NMR spectrum of compound **8B** (8.5–7.0 ppm).

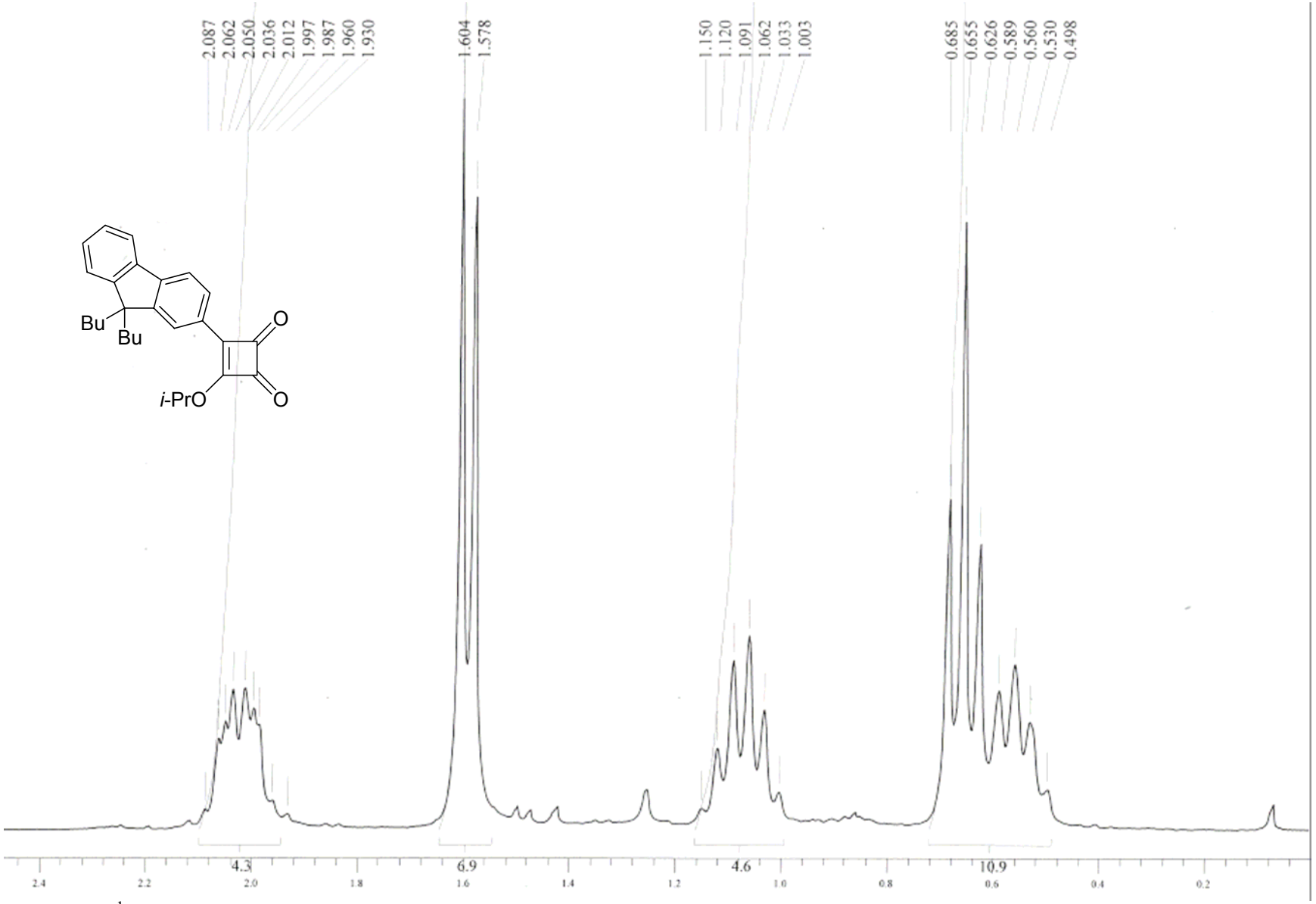


Figure S3. ^{1}H NMR spectrum of compound **8B** (2.5–0.0 ppm).

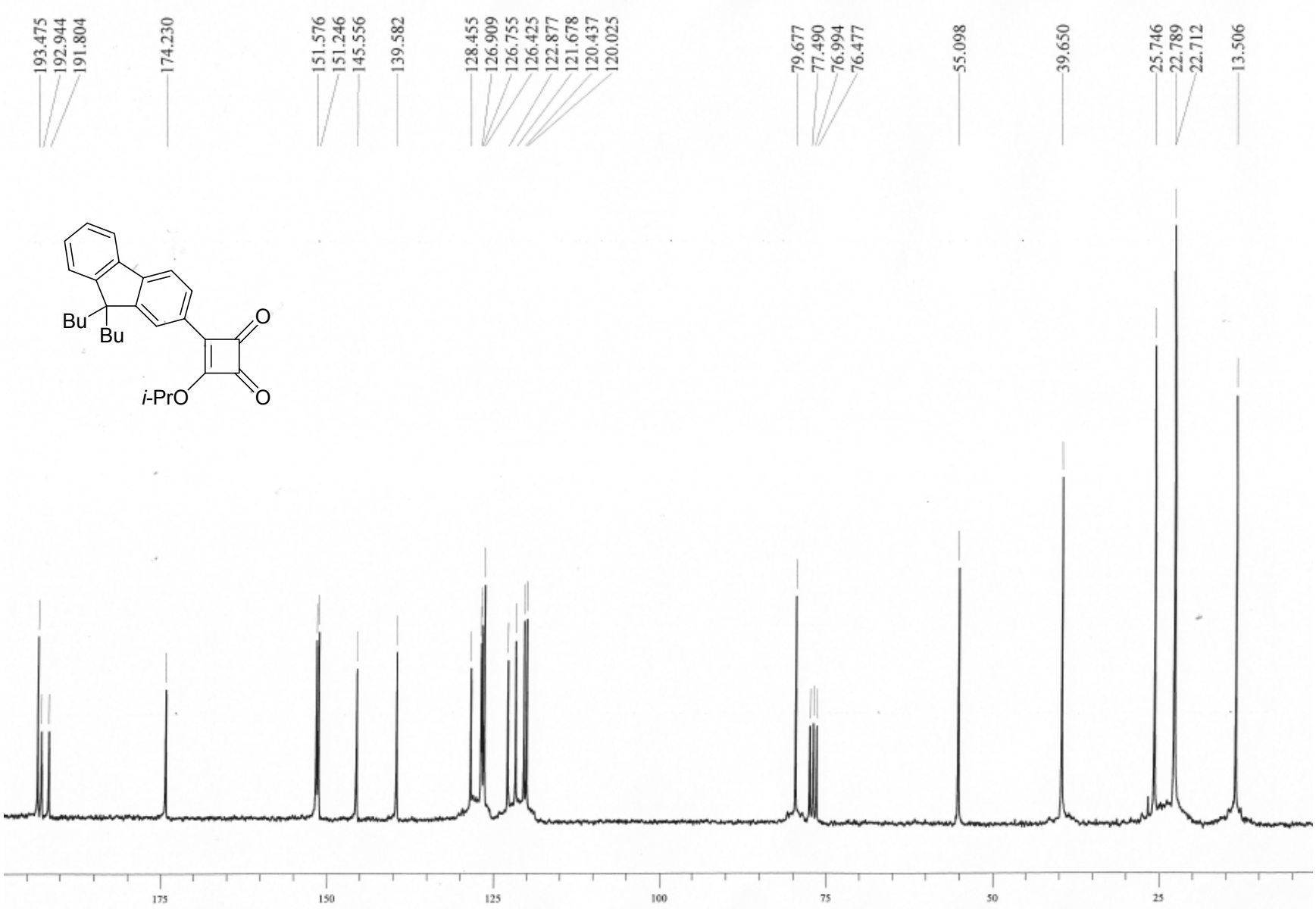


Figure S4. ^{13}C NMR spectrum of compound **8B**.

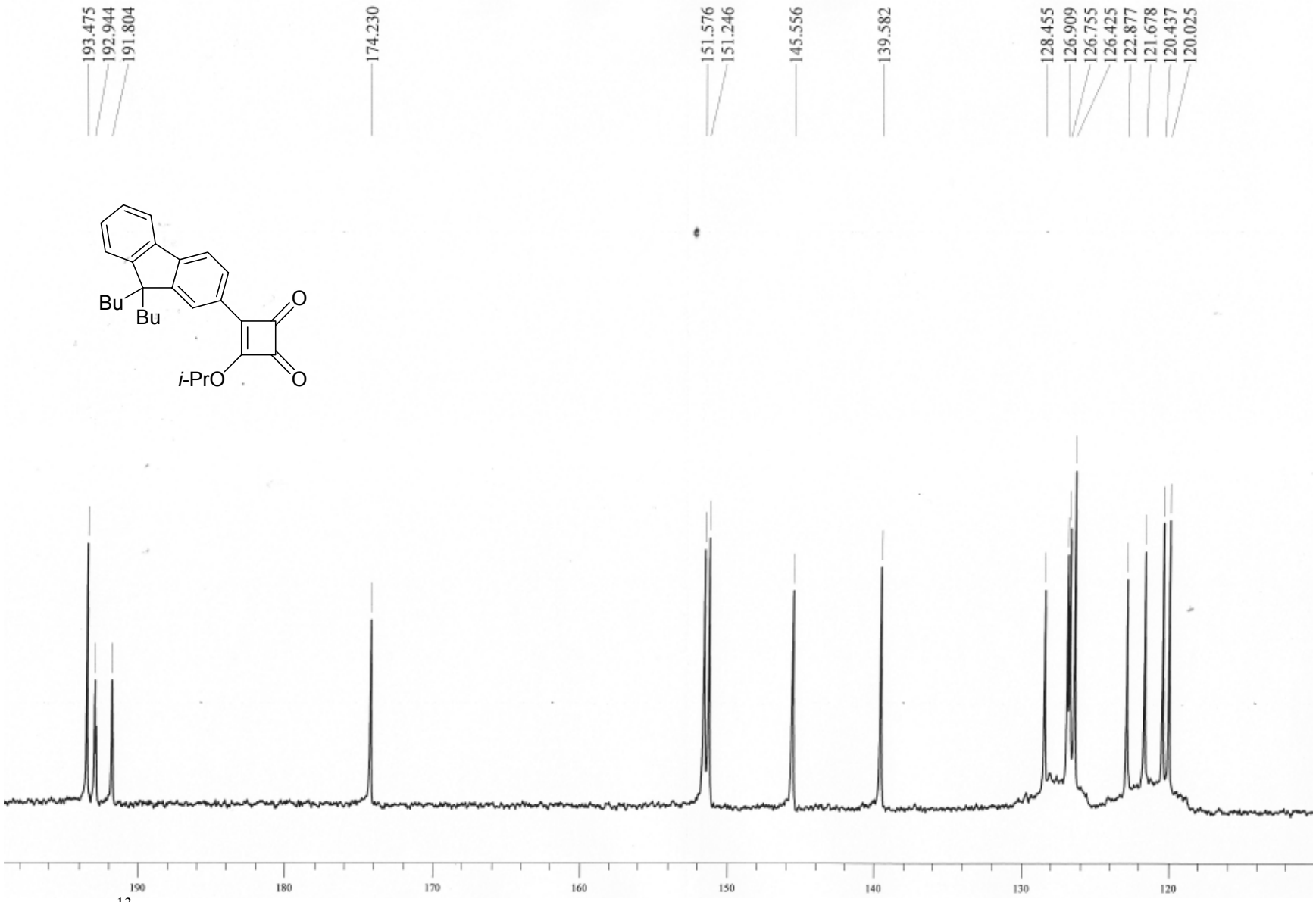


Figure S5. ^{13}C NMR spectrum of compound **8B** (200–110 ppm).

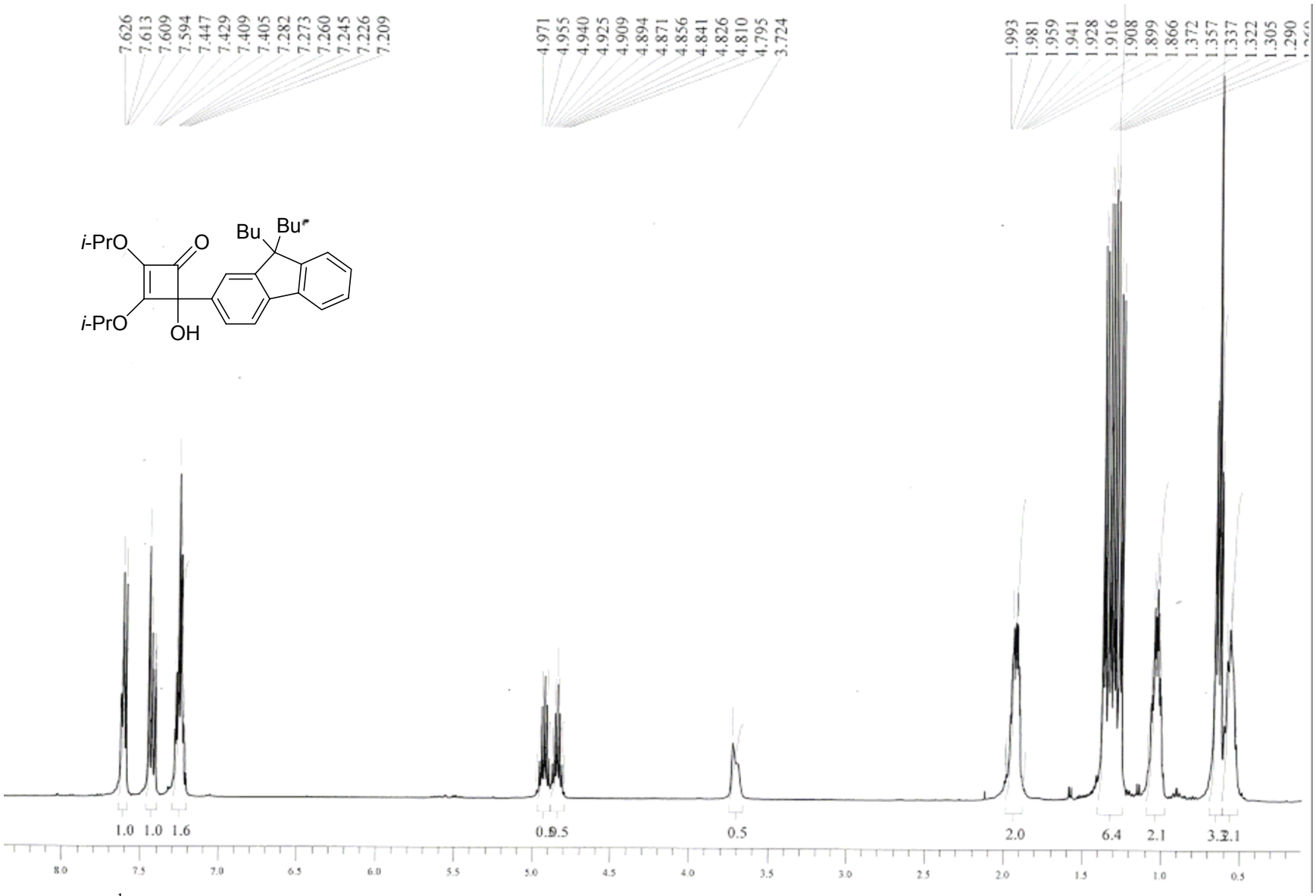


Figure S6. ^{1}H NMR spectrum of compound **9A**.

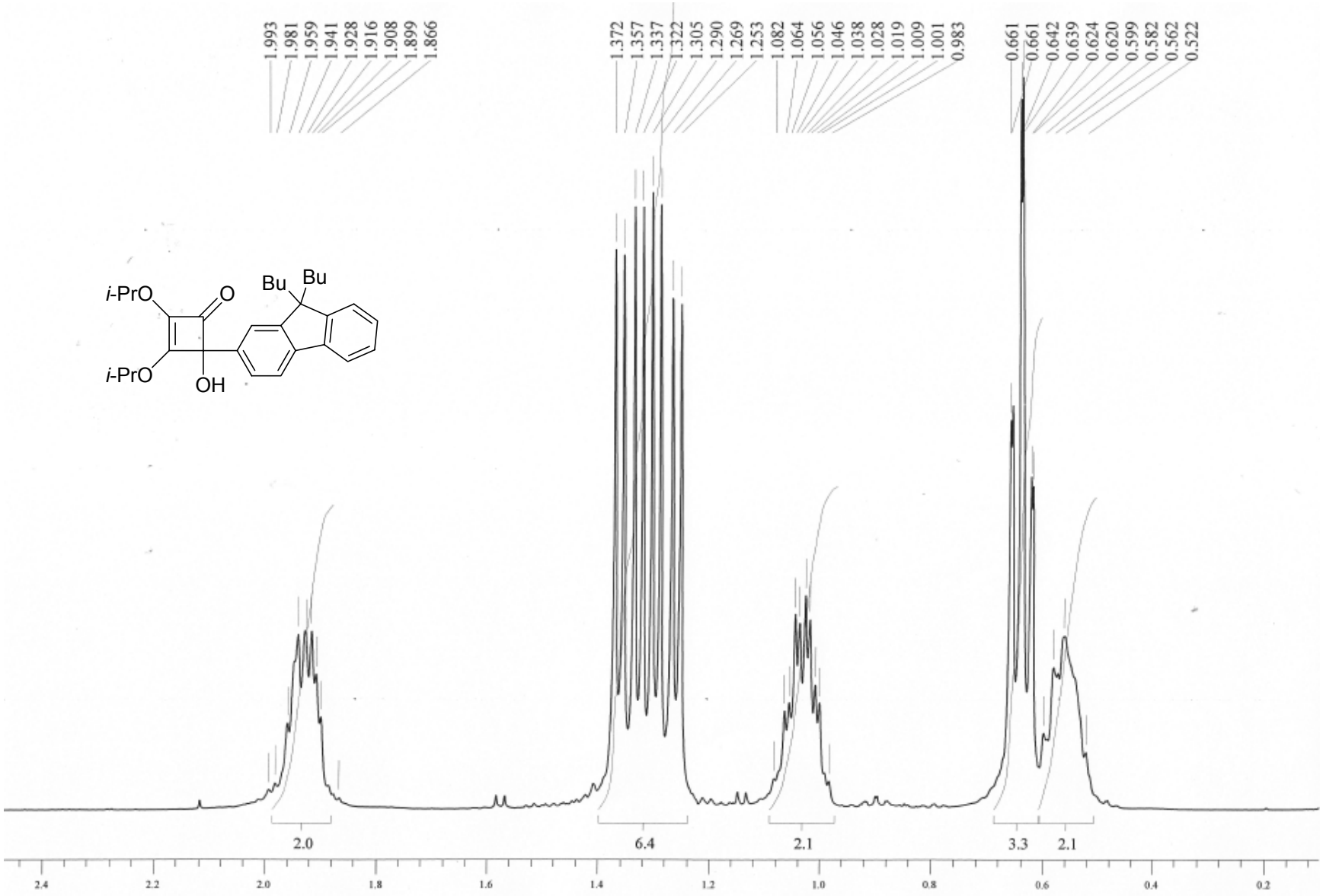


Figure S7. ^{1}H NMR spectrum of compound **9A** (2.5–0.0 ppm).

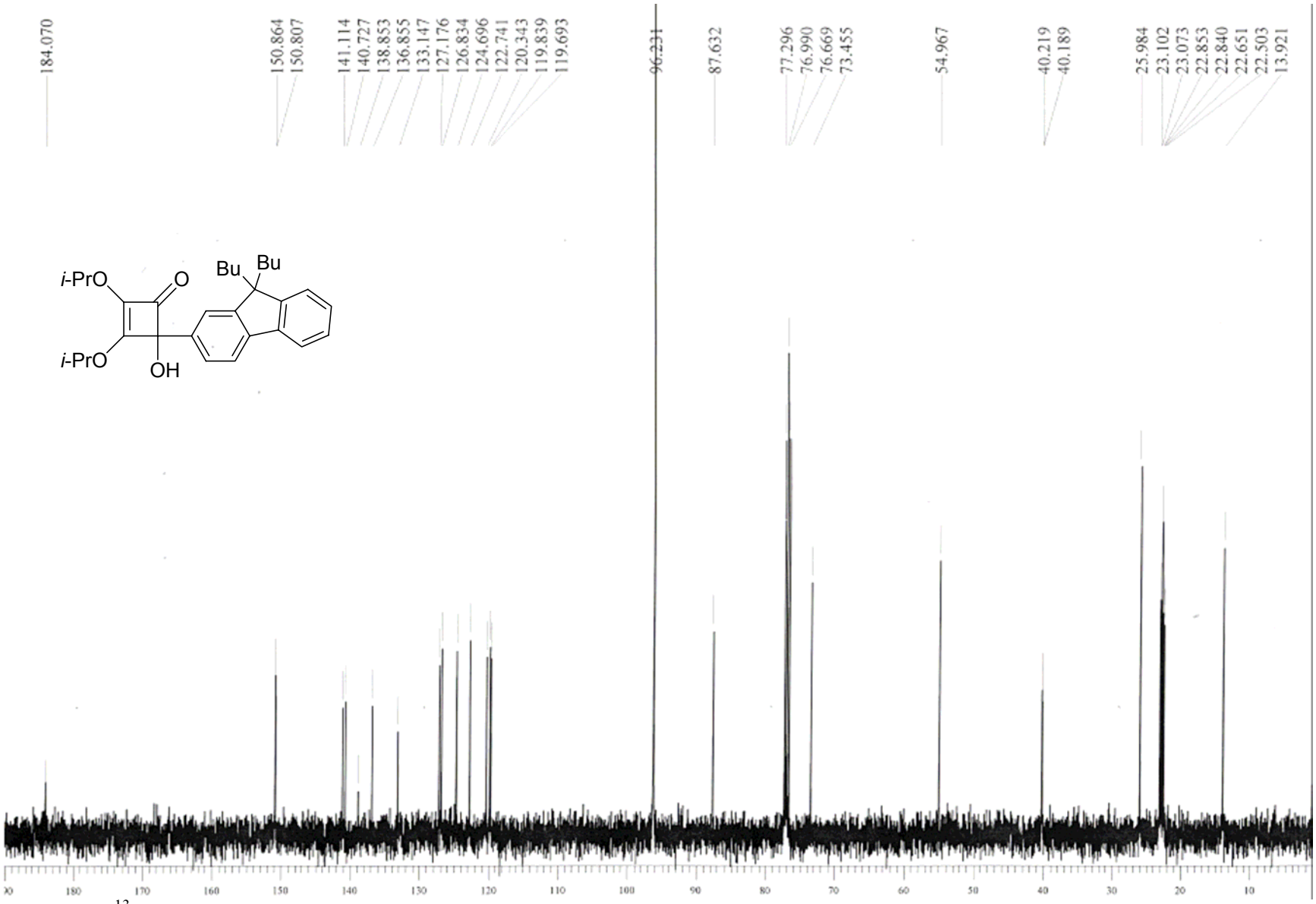


Figure S8. ^{13}C NMR spectrum of compound **9A**.

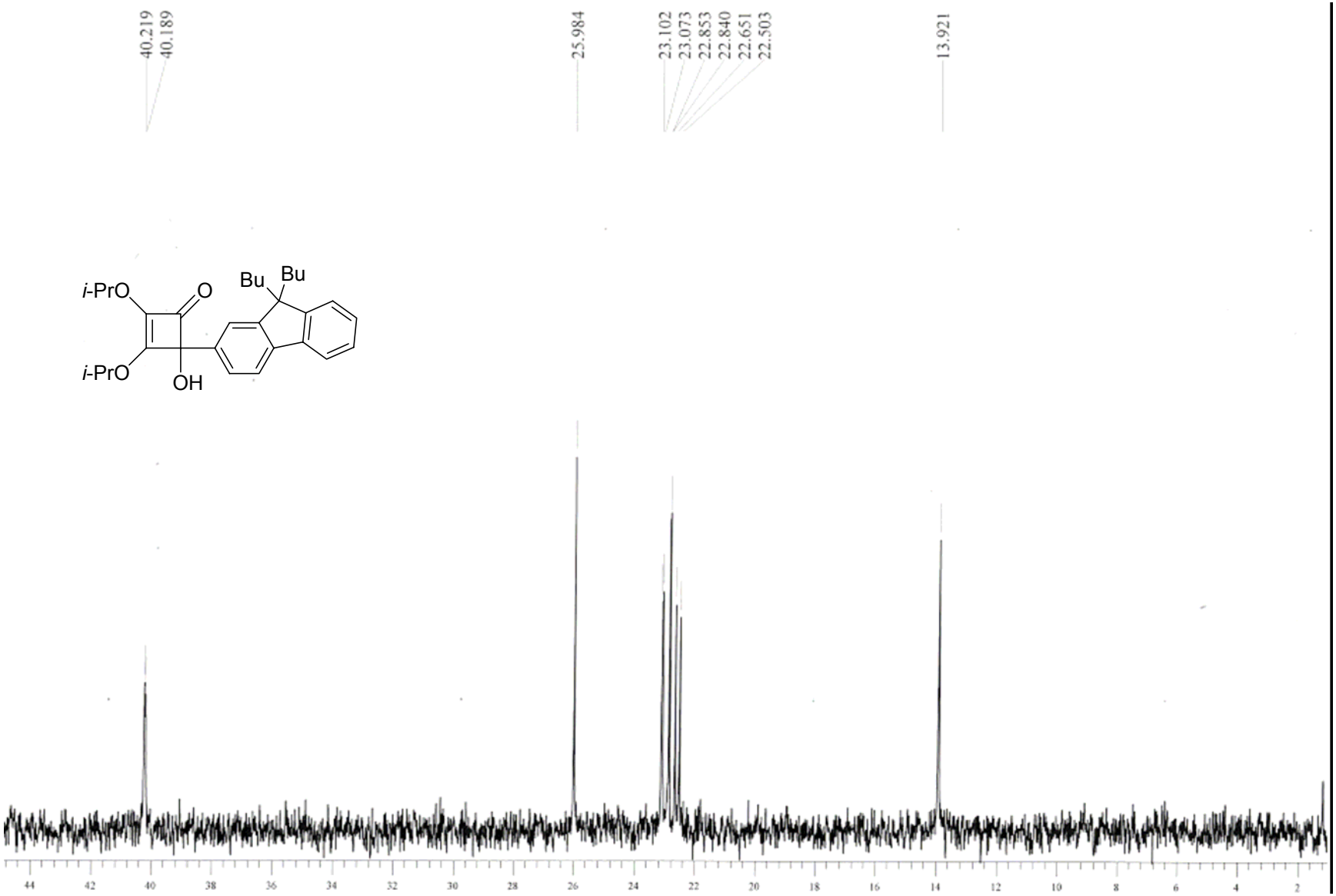


Figure S9. ^{13}C NMR spectrum of compound **9A** (45–0.0 ppm).

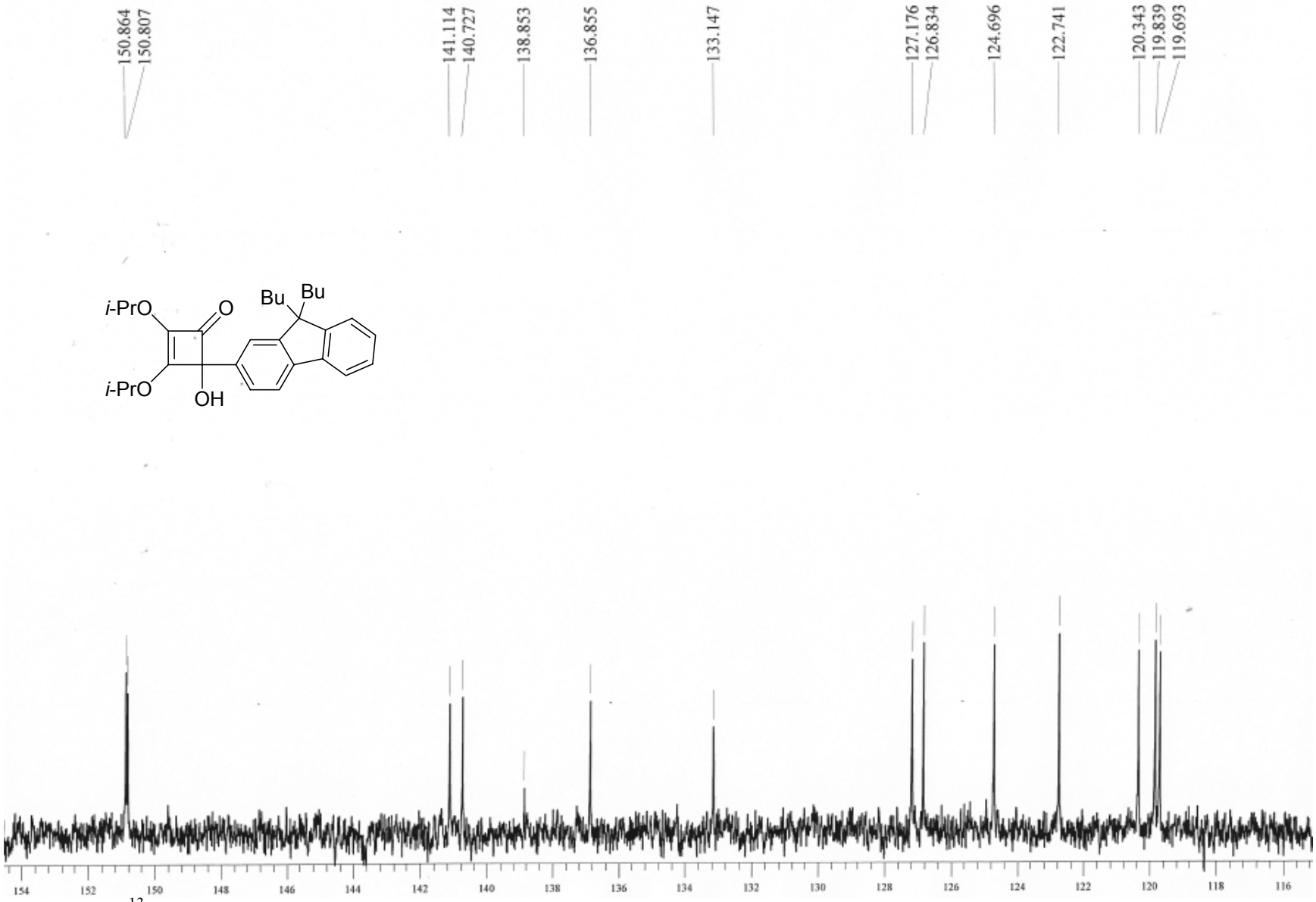


Figure S10. ^{13}C NMR spectrum of compound **9A** (155–115 ppm).

Figure S11. ^{1}H NMR spectrum of compound **13A**.

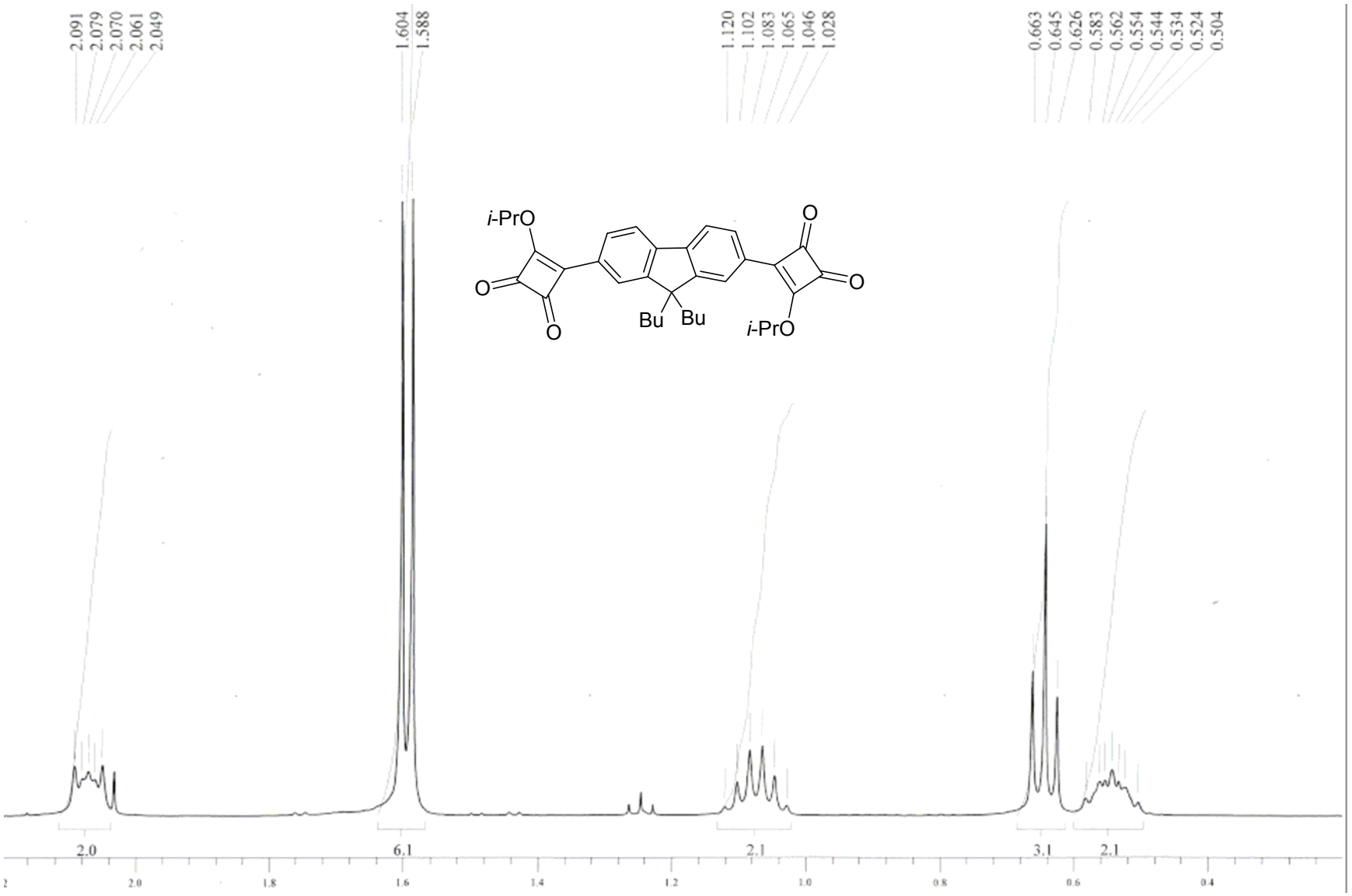


Figure S12. ^{1}H NMR spectrum of compound **13A** (2.2–0.0 ppm).

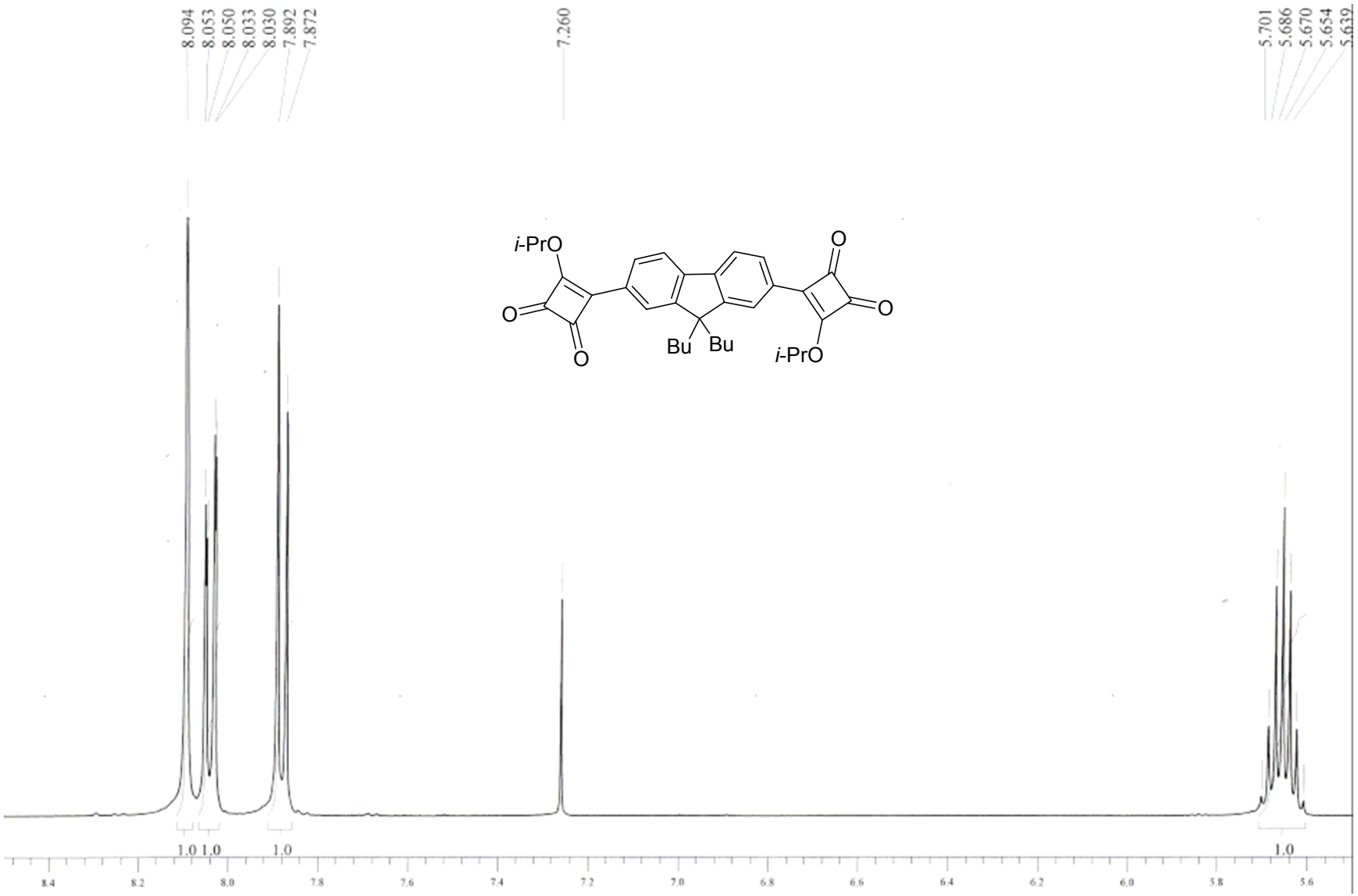


Figure S13. ^{1}H NMR spectrum of compound **13A** (8.5–5.5 ppm).

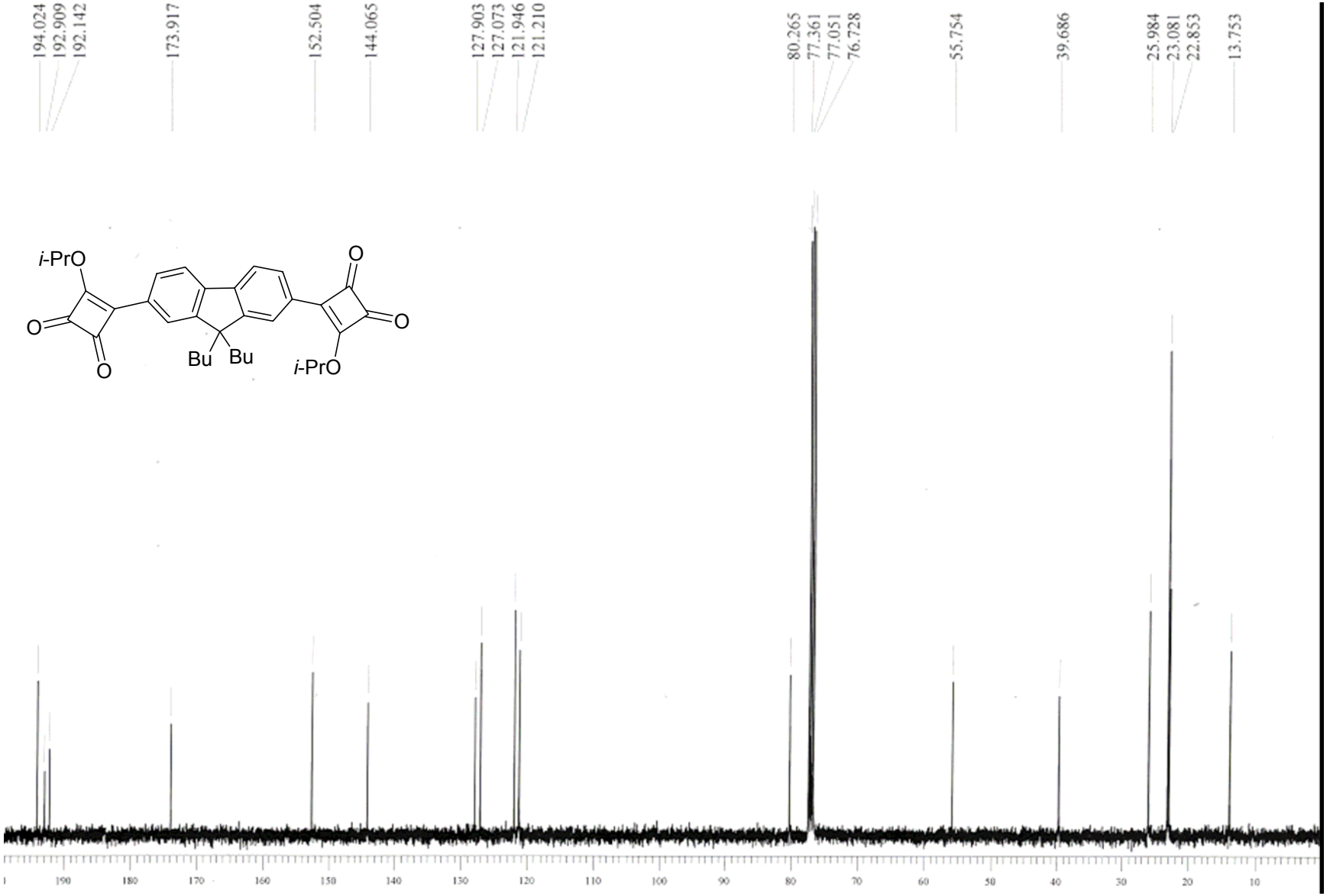


Figure S14. ^{13}C NMR spectrum of compound **13A**.

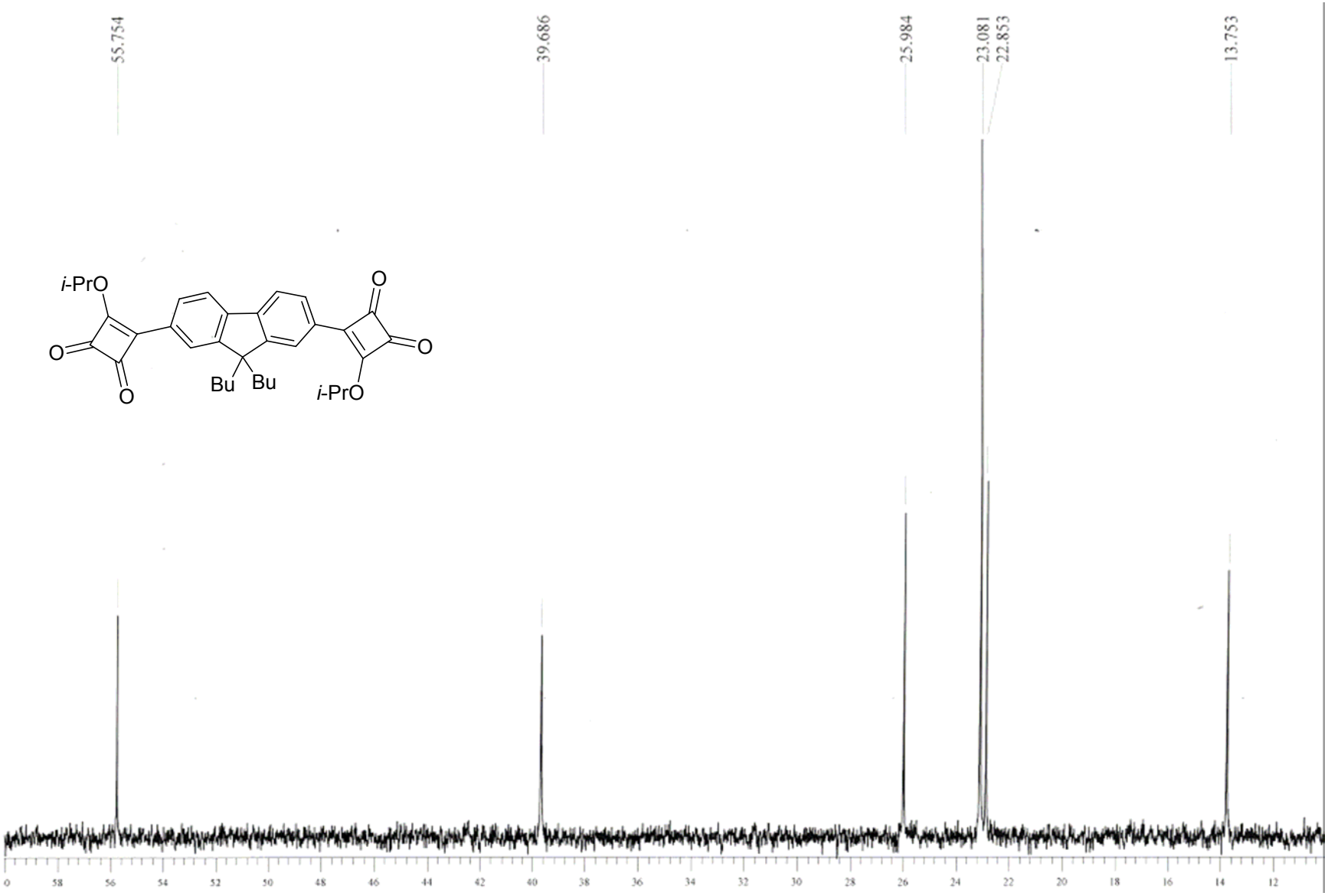


Figure S15. ^{13}C NMR spectrum of compound **13A** (60–0.0 ppm).

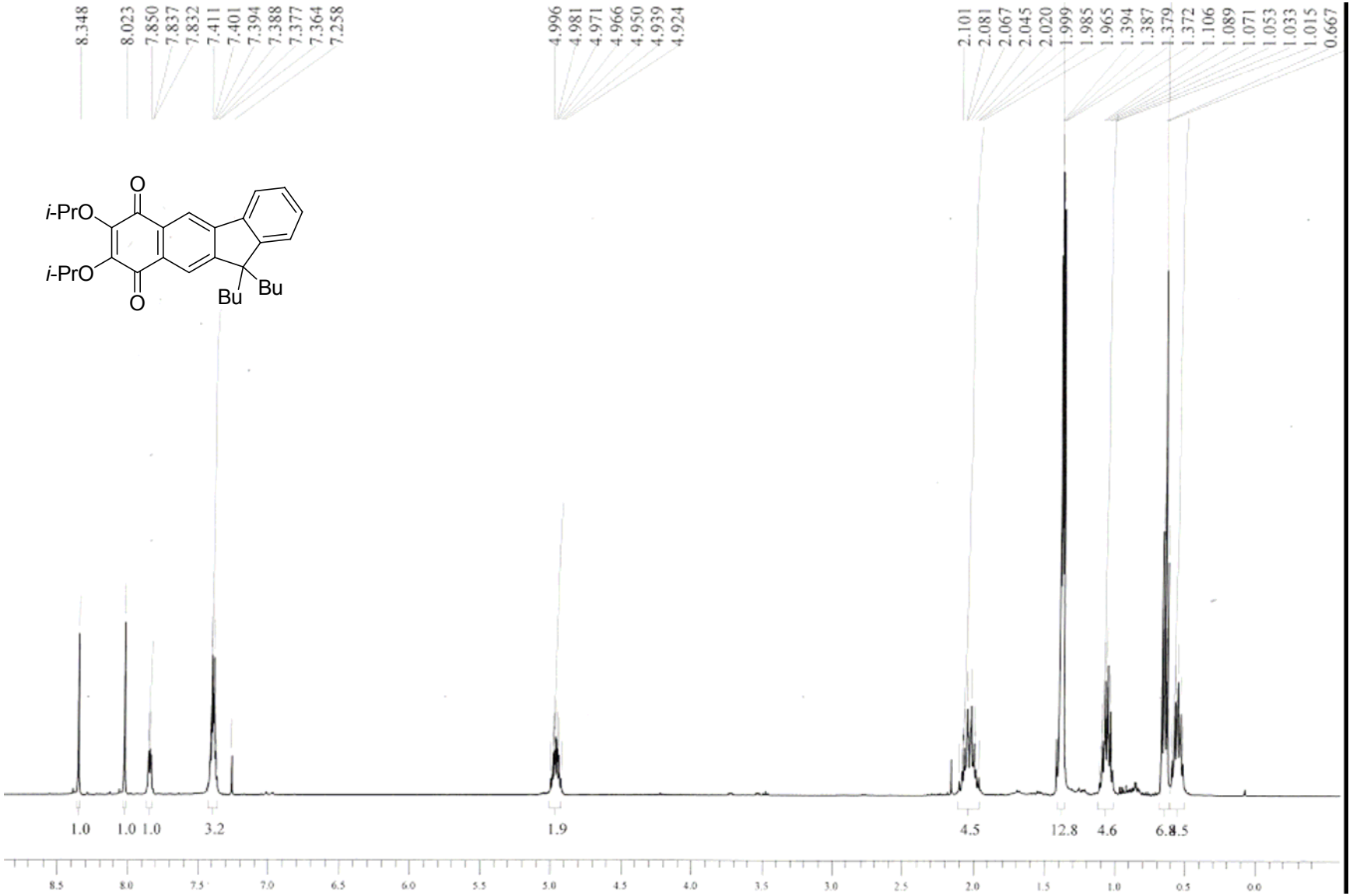


Figure S16. ^{1}H NMR spectrum of compound **Q1**.

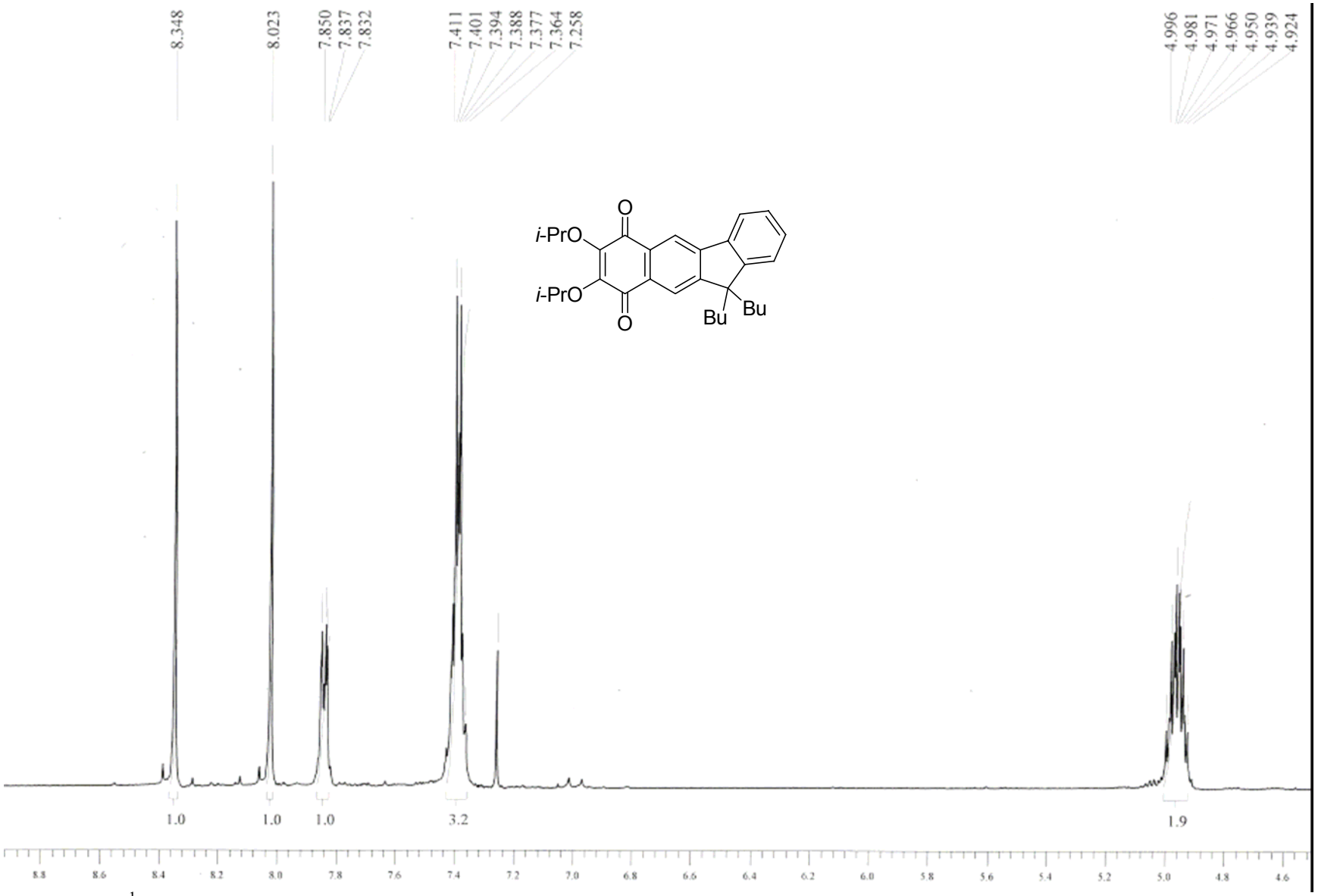


Figure S17. ^{1}H NMR spectrum of compound **Q1** (8.8–4.6 ppm).

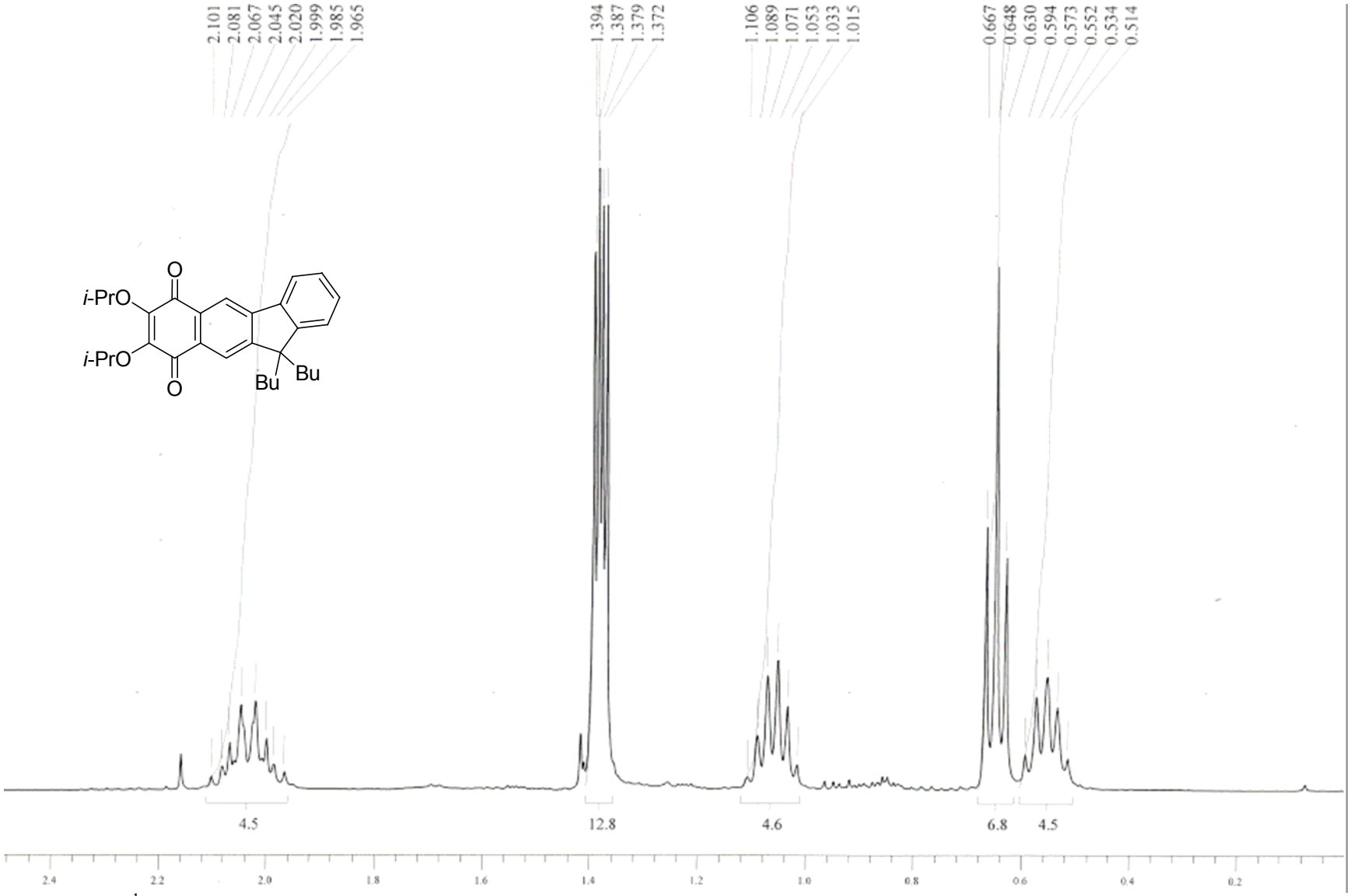


Figure S18. ^{1}H NMR spectrum of compound **Q1** (2.4–0.0 ppm).

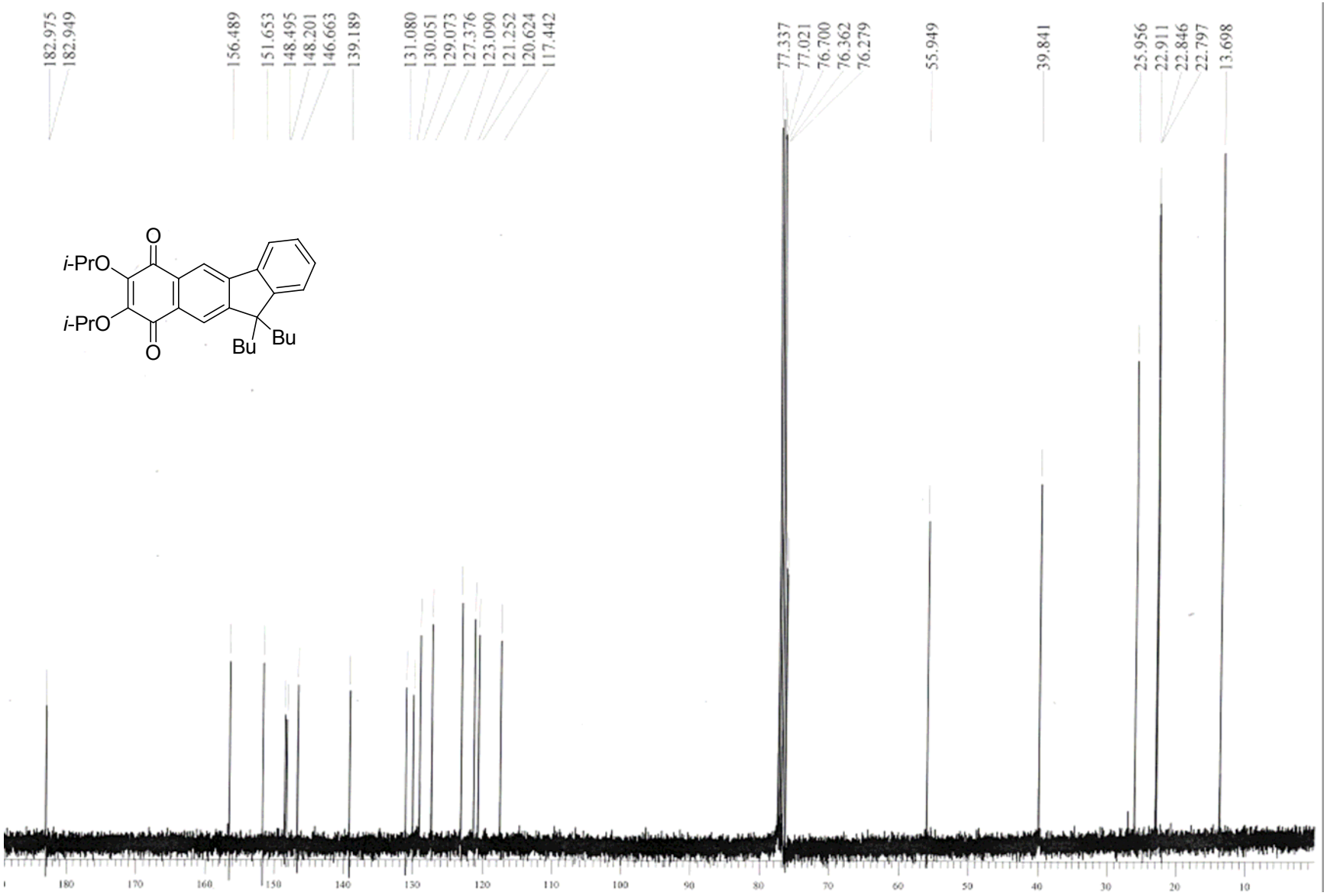


Figure S19. ^{13}C NMR spectrum of compound **Q1**.

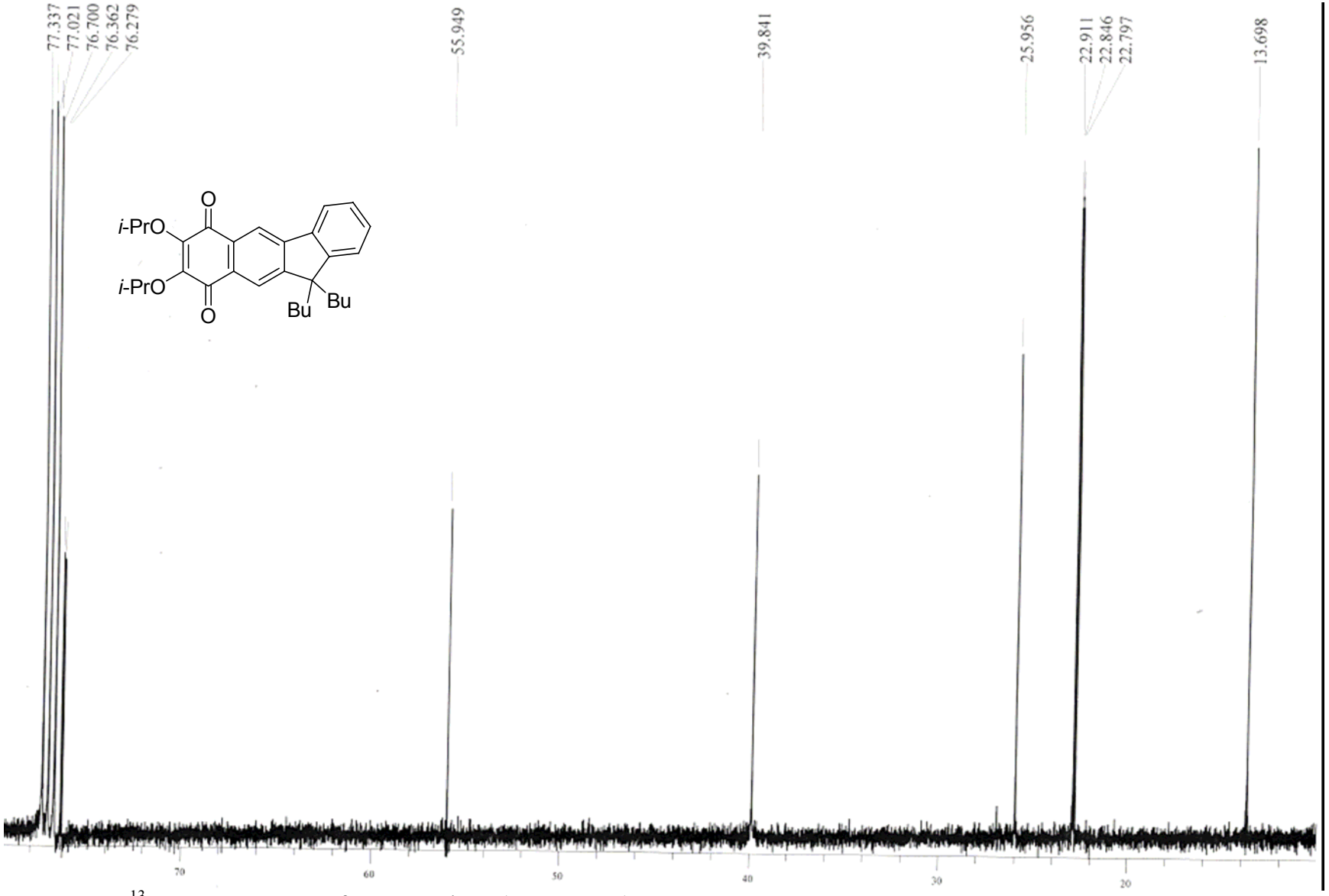


Figure S20. ^{13}C NMR spectrum of compound **Q1** (80–0.0 ppm).

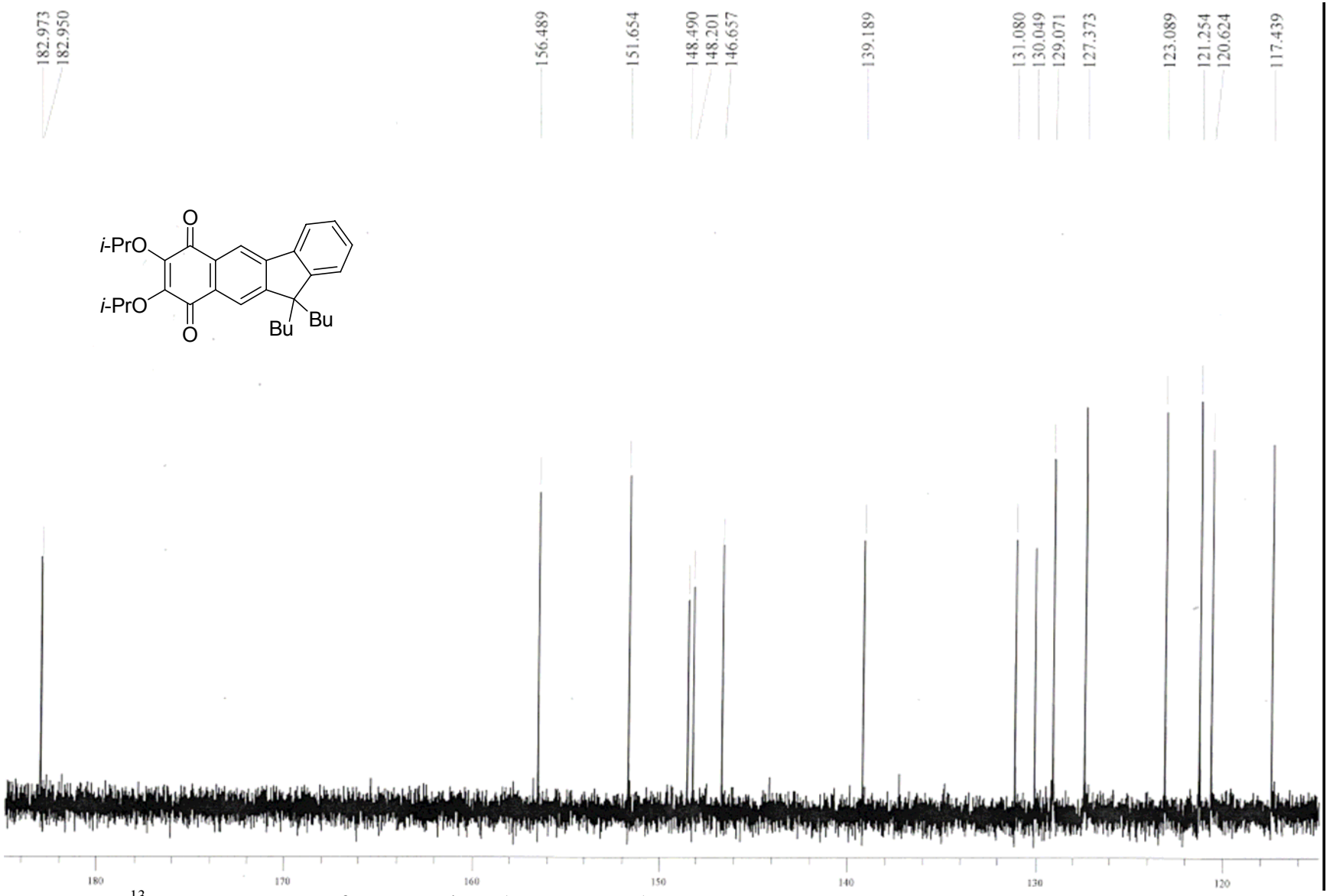


Figure S21. ^{13}C NMR spectrum of compound **Q1** (185–115 ppm).

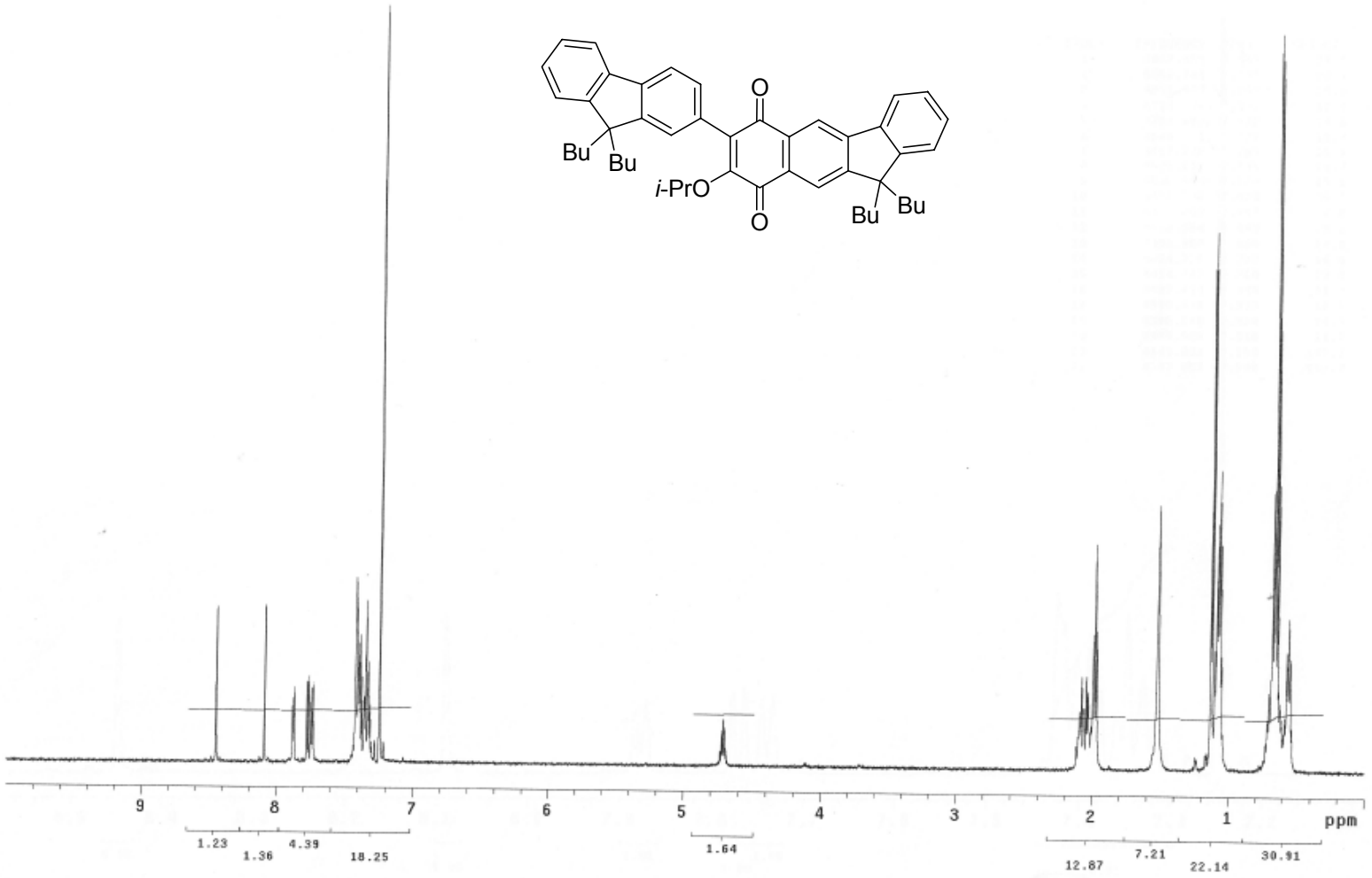


Figure S22. ^{1}H NMR spectrum of compound **Q2**.

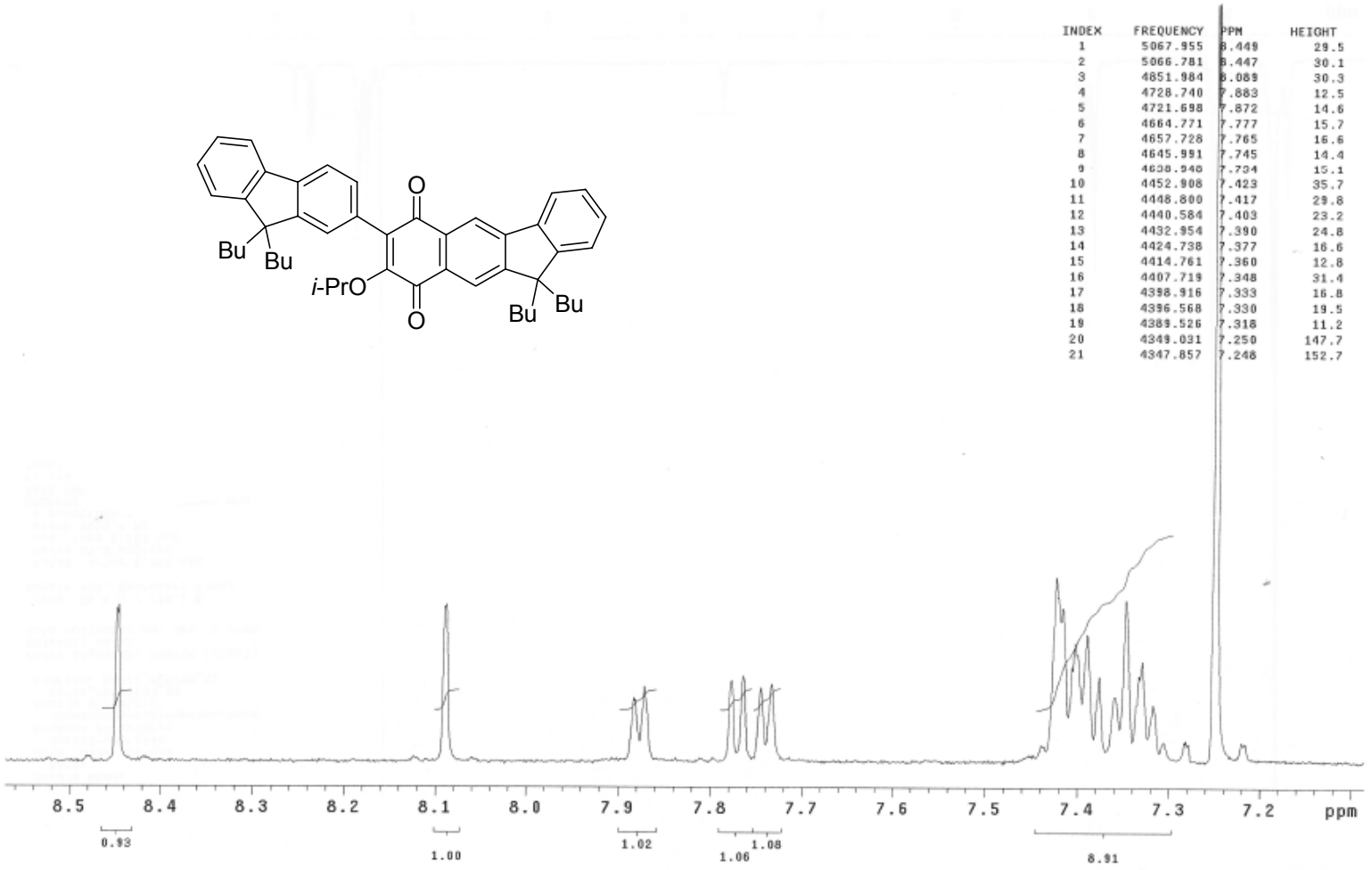


Figure S23. ^{1}H NMR spectrum of compound **Q2** (8.5–7.1 ppm).

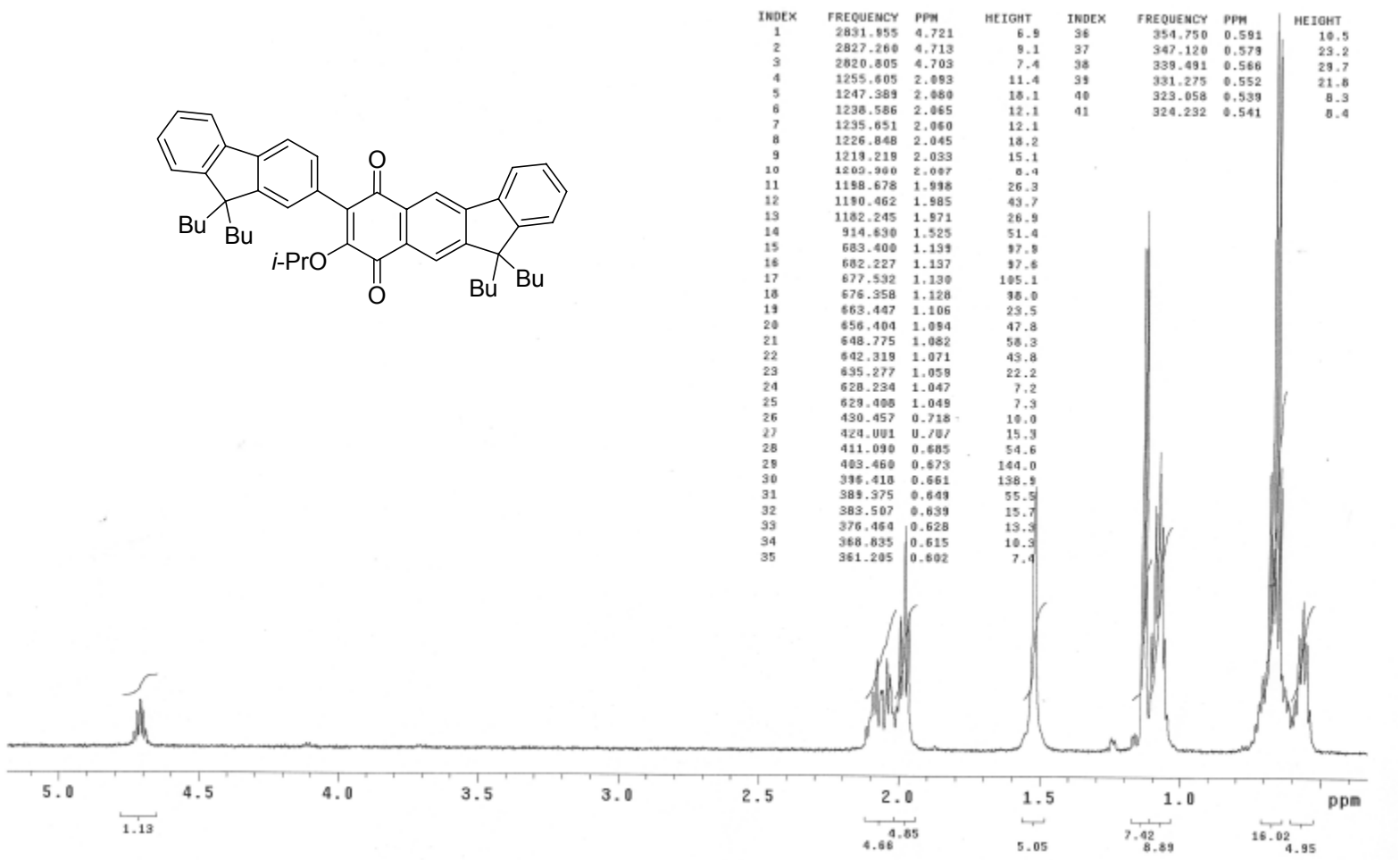


Figure S24. ^{1}H NMR spectrum of compound **Q2** (5.0–0.0 ppm).

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	27947.568	185.292	17.5	36	6021.170	39.920	69.3
2	27562.650	182.740	16.6	37	3923.087	26.010	75.2
3	23559.530	156.199	19.9	38	3917.307	25.972	89.5
4	23553.750	156.161	21.2	39	3483.819	23.098	112.0
5	22883.288	151.716	21.1	40	3458.387	22.929	90.9
6	22796.590	151.141	21.8	41	3422.552	22.691	91.2
7	22585.048	149.738	20.7	42	2083.940	13.816	100.1
8	22179.303	147.048	20.4	43	2072.381	13.740	90.8
9	21313.402	141.308	20.5				
10	21236.003	140.794	18.1				
11	21007.151	139.277	21.4				
12	20367.900	135.039	16.9				
13	19937.879	132.188	17.7				
14	19672.807	130.425	23.0				
15	19579.529	129.812	24.9				
16	19550.630	129.620	32.3				
17	19483.584	129.176	30.3				
18	19216.555	127.405	31.2				
19	19196.903	127.275	26.6				
20	19121.765	126.777	36.3				
21	18925.251	125.474	38.5				
22	18565.714	123.090	29.7				
23	18532.221	122.868	37.5				
24	18311.481	121.404	36.0				
25	18171.559	120.477	38.9				
26	18083.705	119.895	32.8				
27	17929.962	118.875	37.9				
28	17779.668	117.879	33.4				
29	11644.959	77.206	192.3				
30	11612.592	76.991	208.3				
31	11580.225	76.777	192.6				
32	11562.805	76.662	39.6				
33	8434.803	55.923	35.6				
34	8303.053	55.049	40.6				
35	6065.097	40.211	63.5				

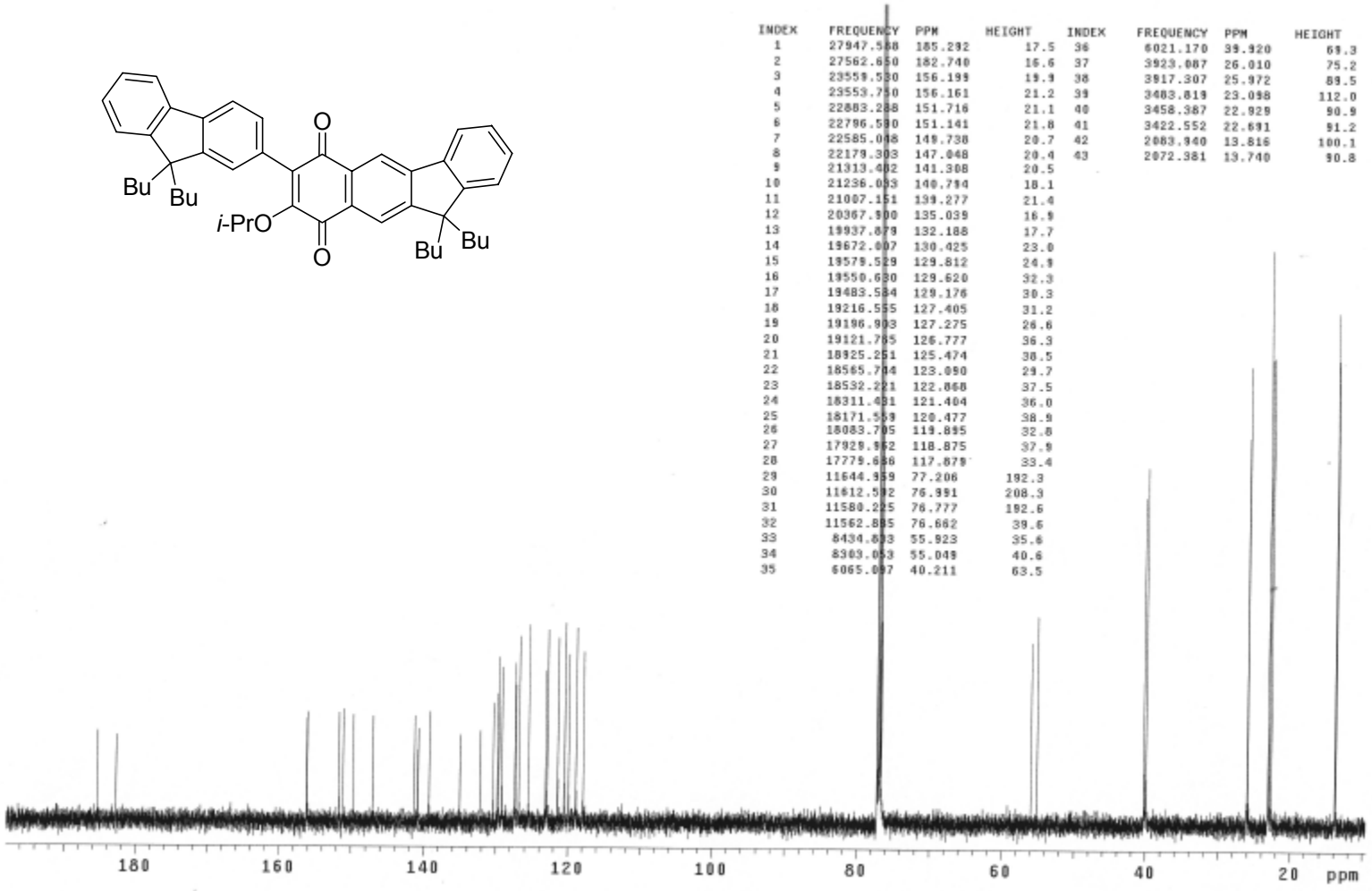


Figure S25. ^{13}C NMR spectrum of compound **Q2**.

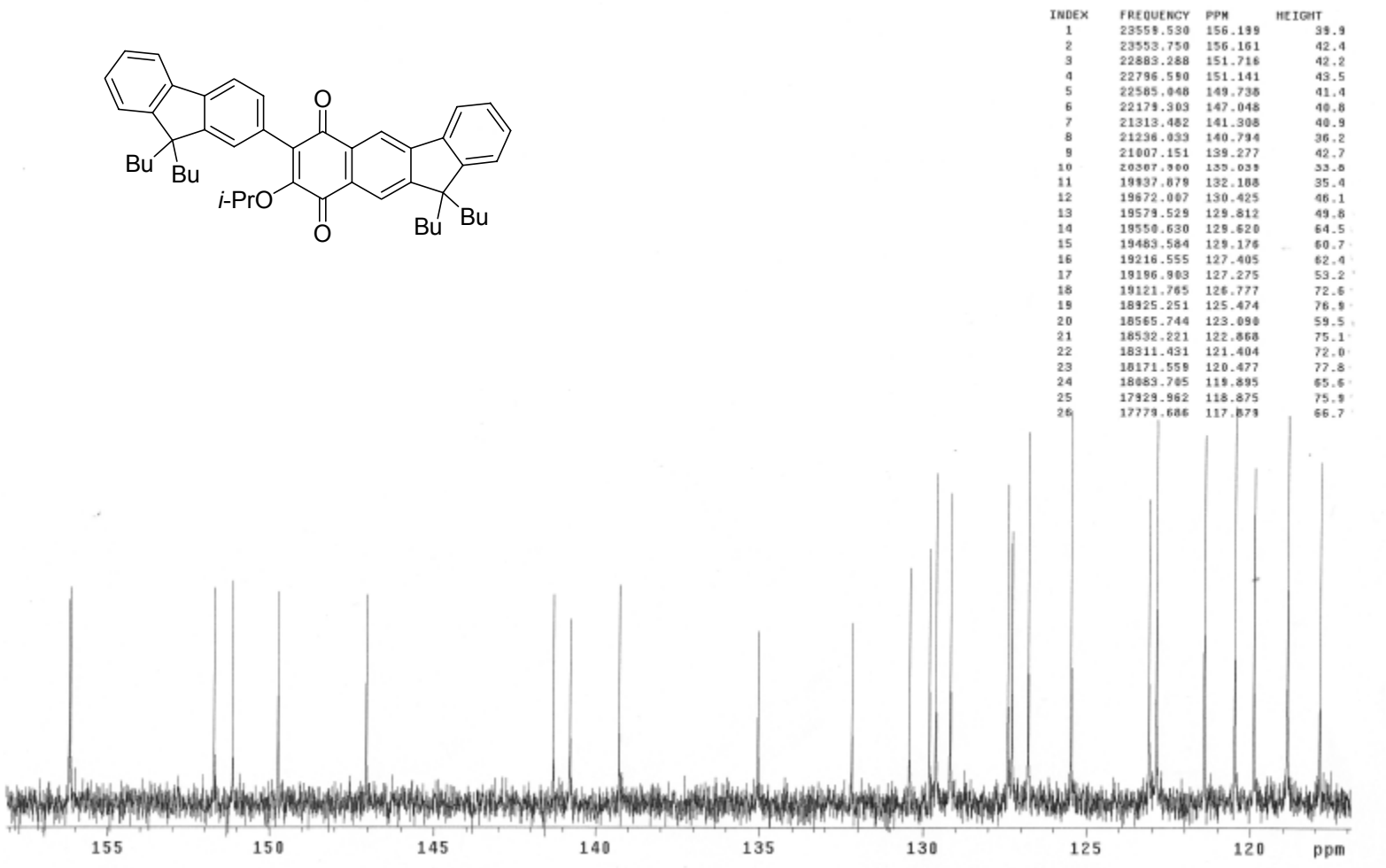


Figure S26. ^{13}C NMR spectrum of compound **Q2** (160–115 ppm).

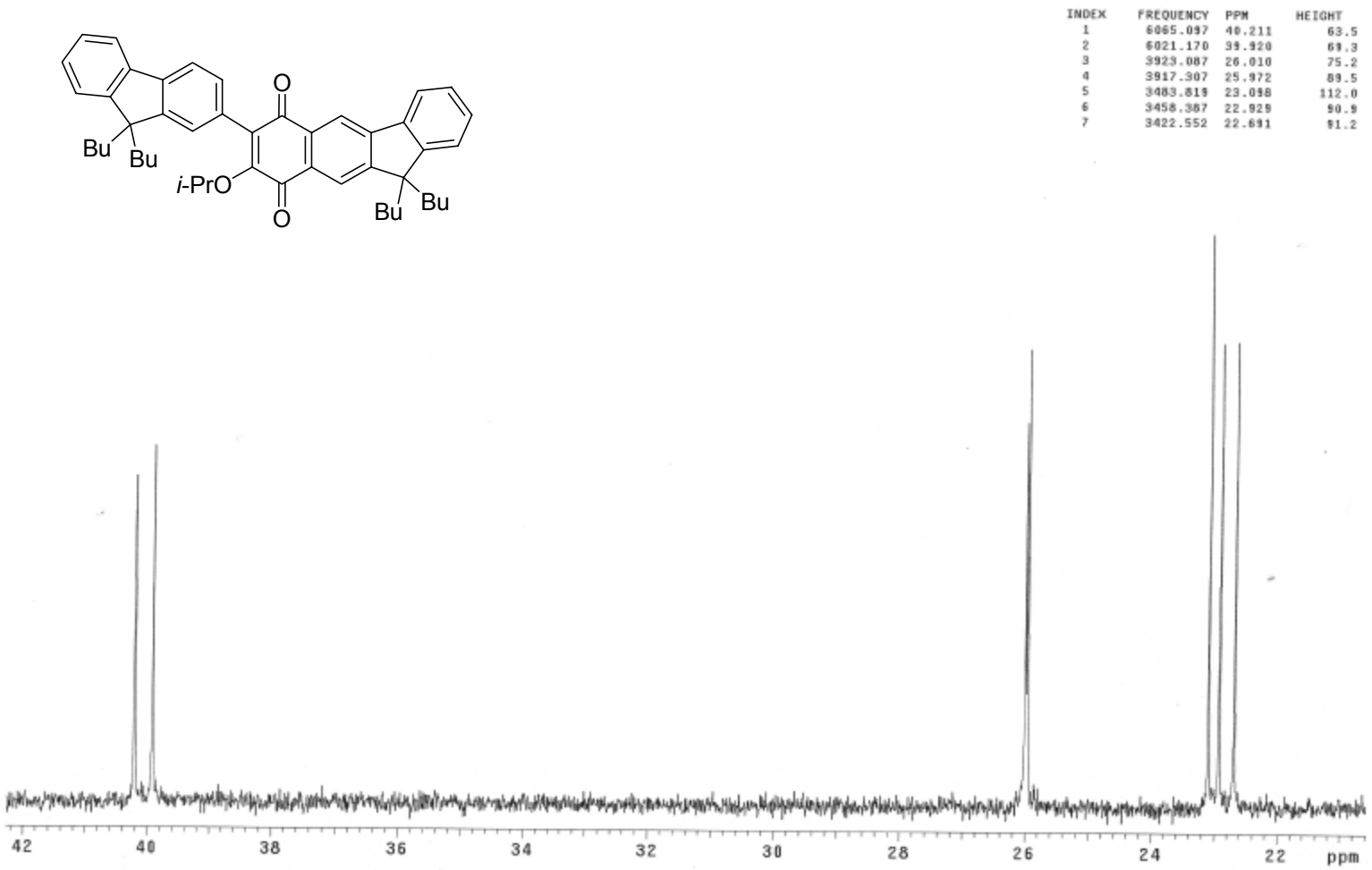


Figure S27. ^{13}C NMR spectrum of compound **Q2** (42–21 ppm).

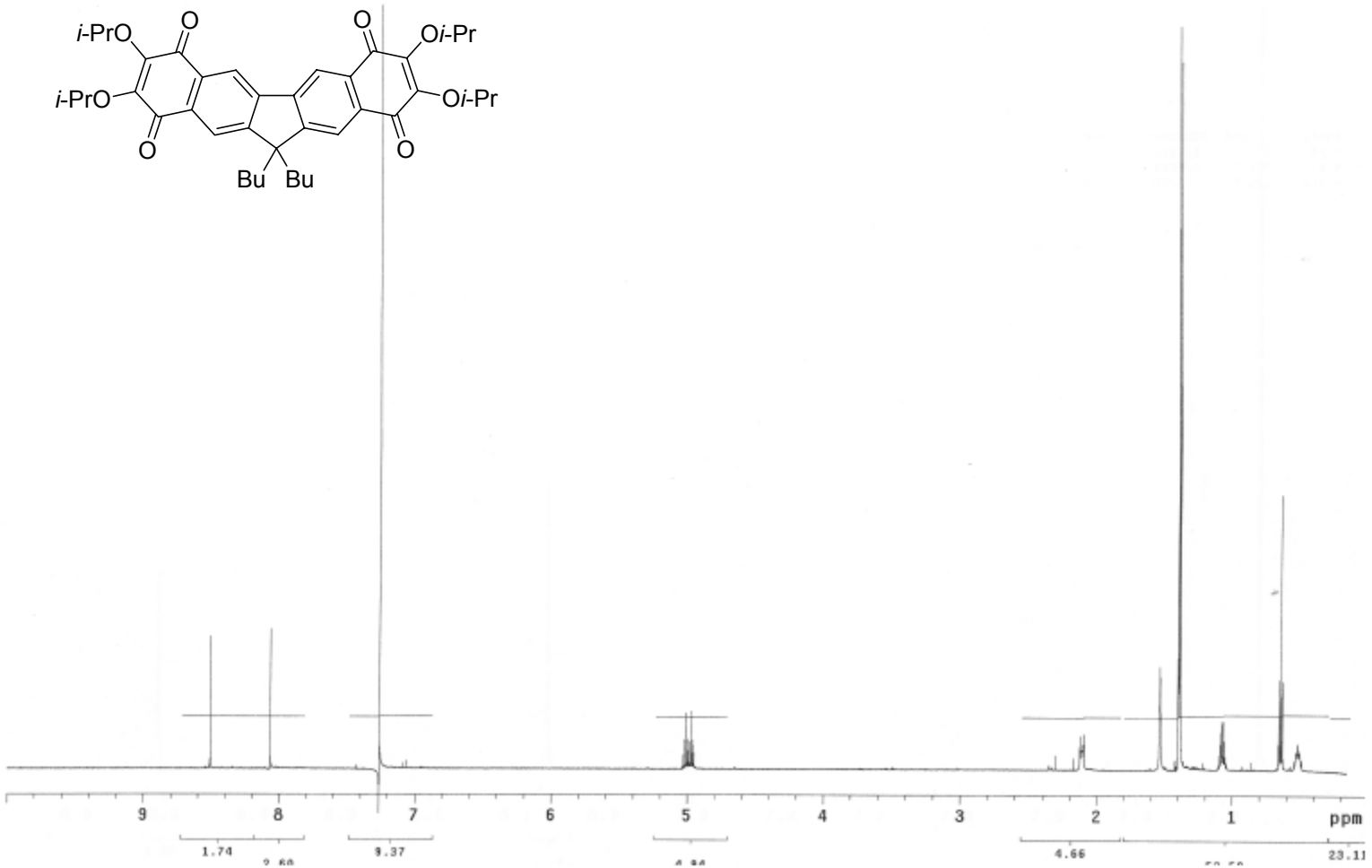


Figure S28. ^{1}H NMR spectrum of compound **Q3**.

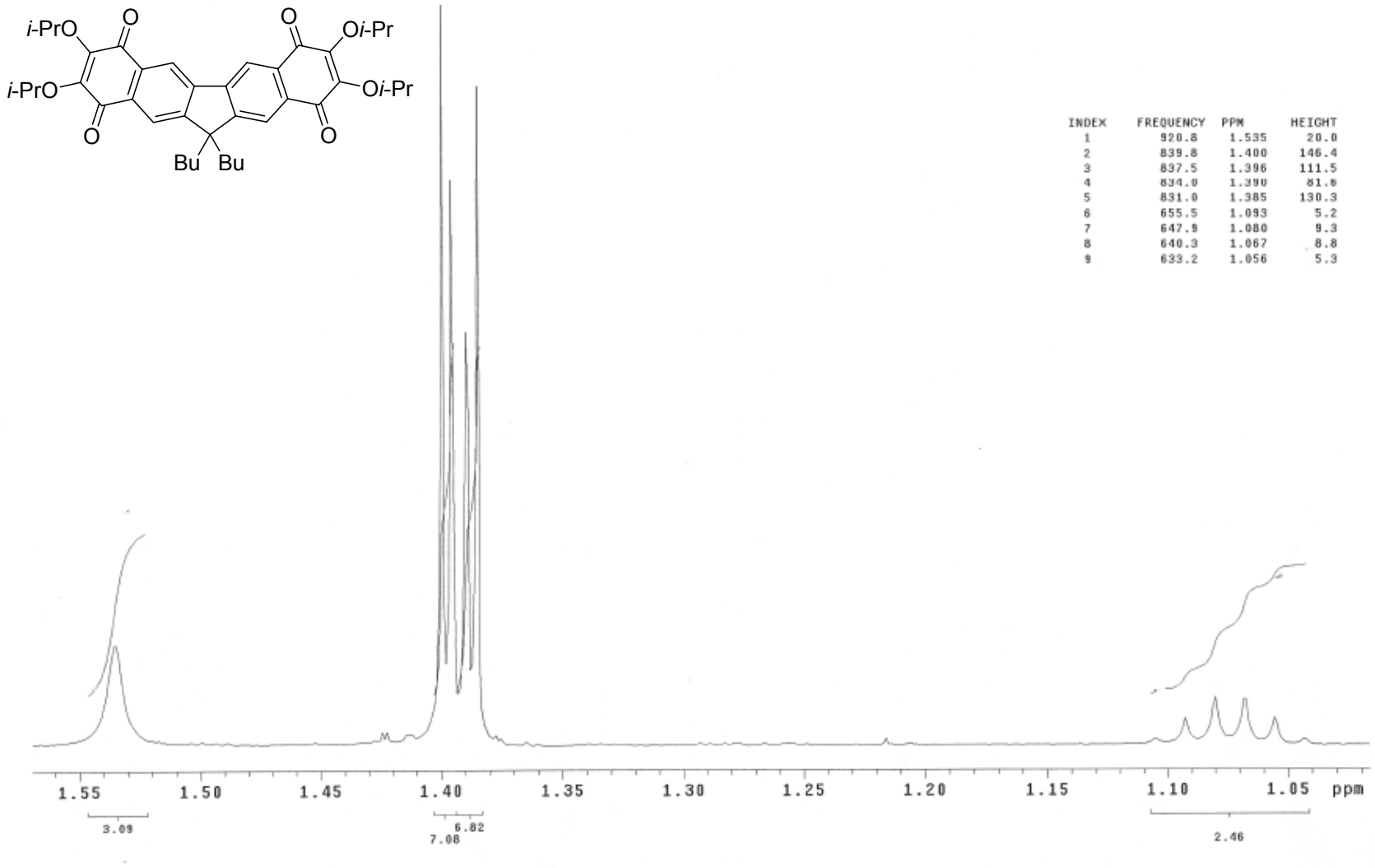
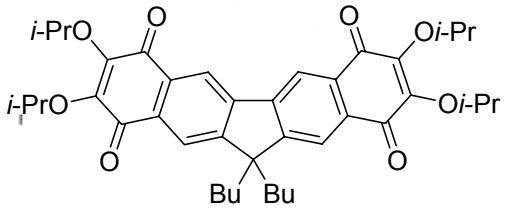


Figure S29. ^{1}H NMR spectrum of compound **Q3** (1.55–1.0 ppm).



INDEX	FREQUENCY	PPM	HEIGHT
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2	3011.3	5.020	20.6
3	3005.4	5.010	44.2
4	2999.5	5.001	20.9
5	2994.2	4.992	13.9
6	2993.1	4.990	13.9
7	2988.4	4.982	24.3
8	2981.9	4.971	42.7
9	2976.1	4.962	24.4
10	2969.6	4.951	11.2
11	1411.4	2.353	4.2
12	1384.4	2.308	12.4
13	1302.9	2.172	11.7
14	1275.3	2.126	28.5
15	1267.1	2.112	20.1
16	1263.0	2.106	15.0
17	1258.3	2.098	25.1

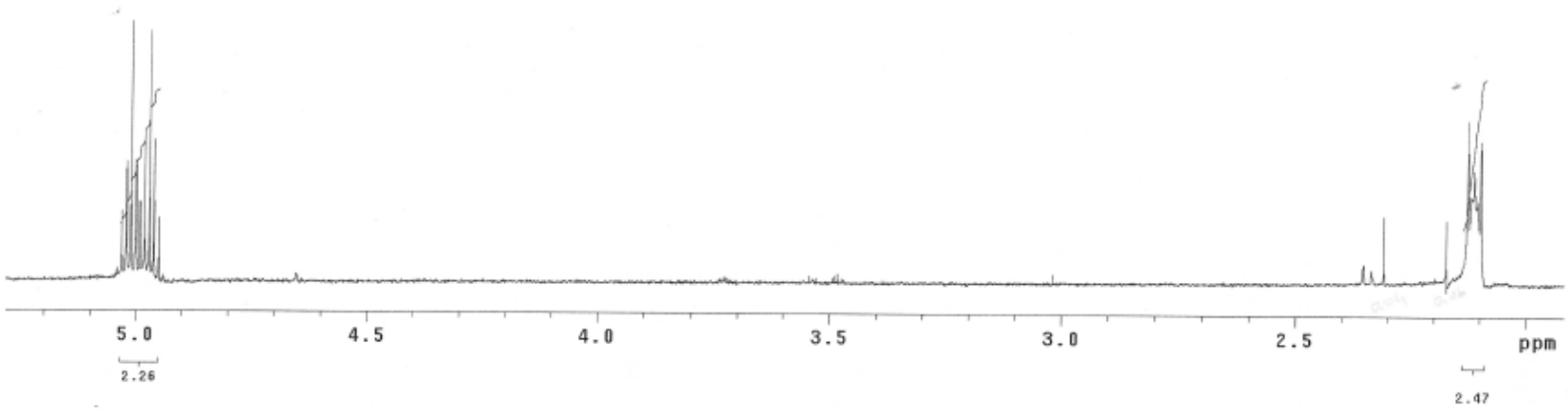
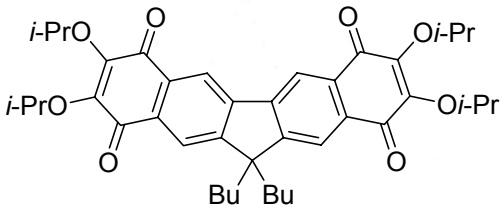


Figure S30. ^{1}H NMR spectrum of compound **Q3** (5.5–2.0 ppm).



INDEX	FREQUENCY	PPM	HEIGHT
1	394.4	0.657	38.9
2	386.8	0.645	103.7
3	384.4	0.641	5.0
4	379.7	0.633	31.0
5	326.3	0.544	4.0
6	318.7	0.531	7.2
7	314.6	0.524	7.1
8	310.5	0.518	10.0
9	306.3	0.511	7.0
10	302.2	0.504	5.8
11	58.1	0.097	7.4

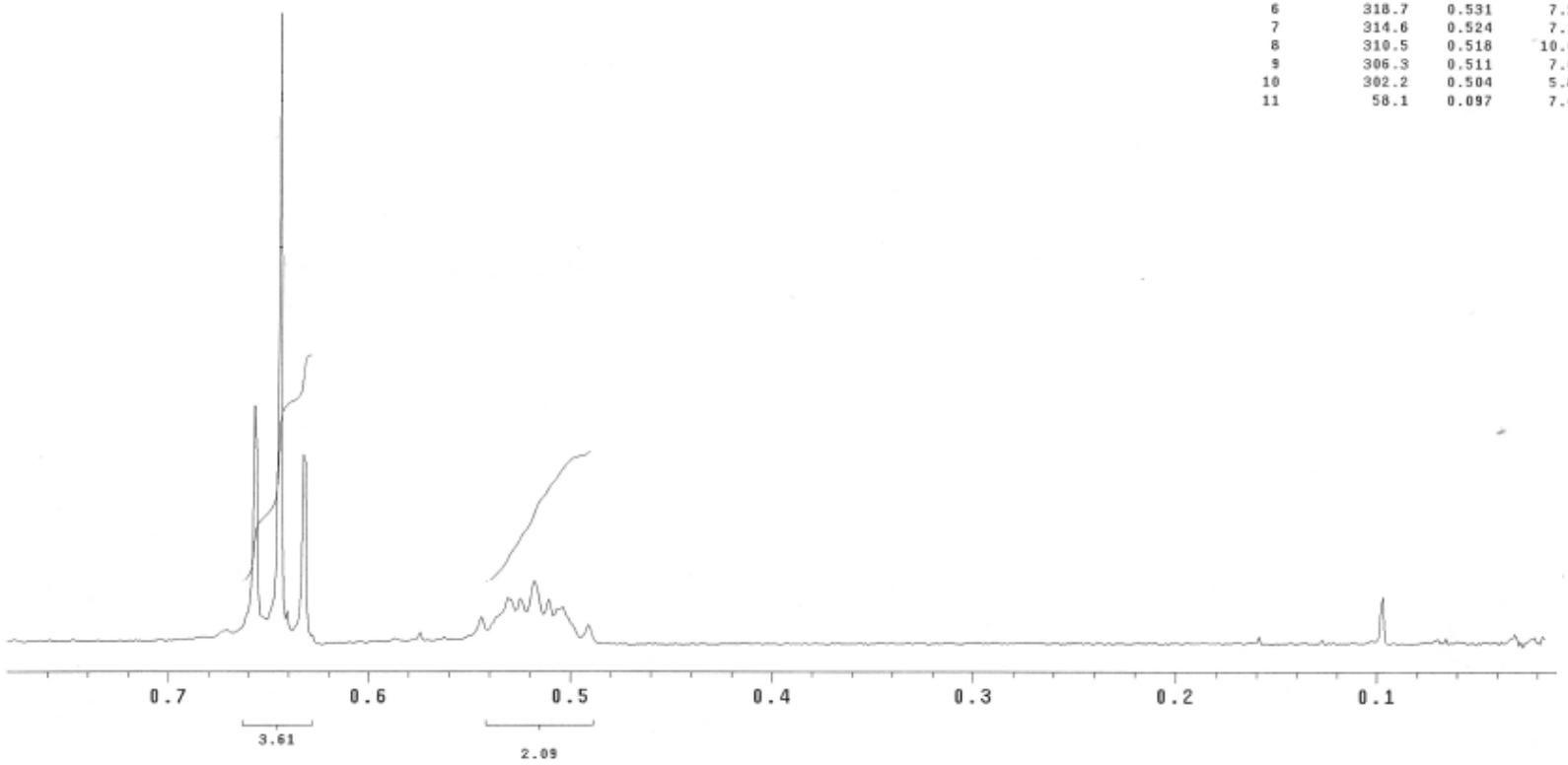


Figure S31. ^{1}H NMR spectrum of compound **Q3** (0.8–0.0 ppm).

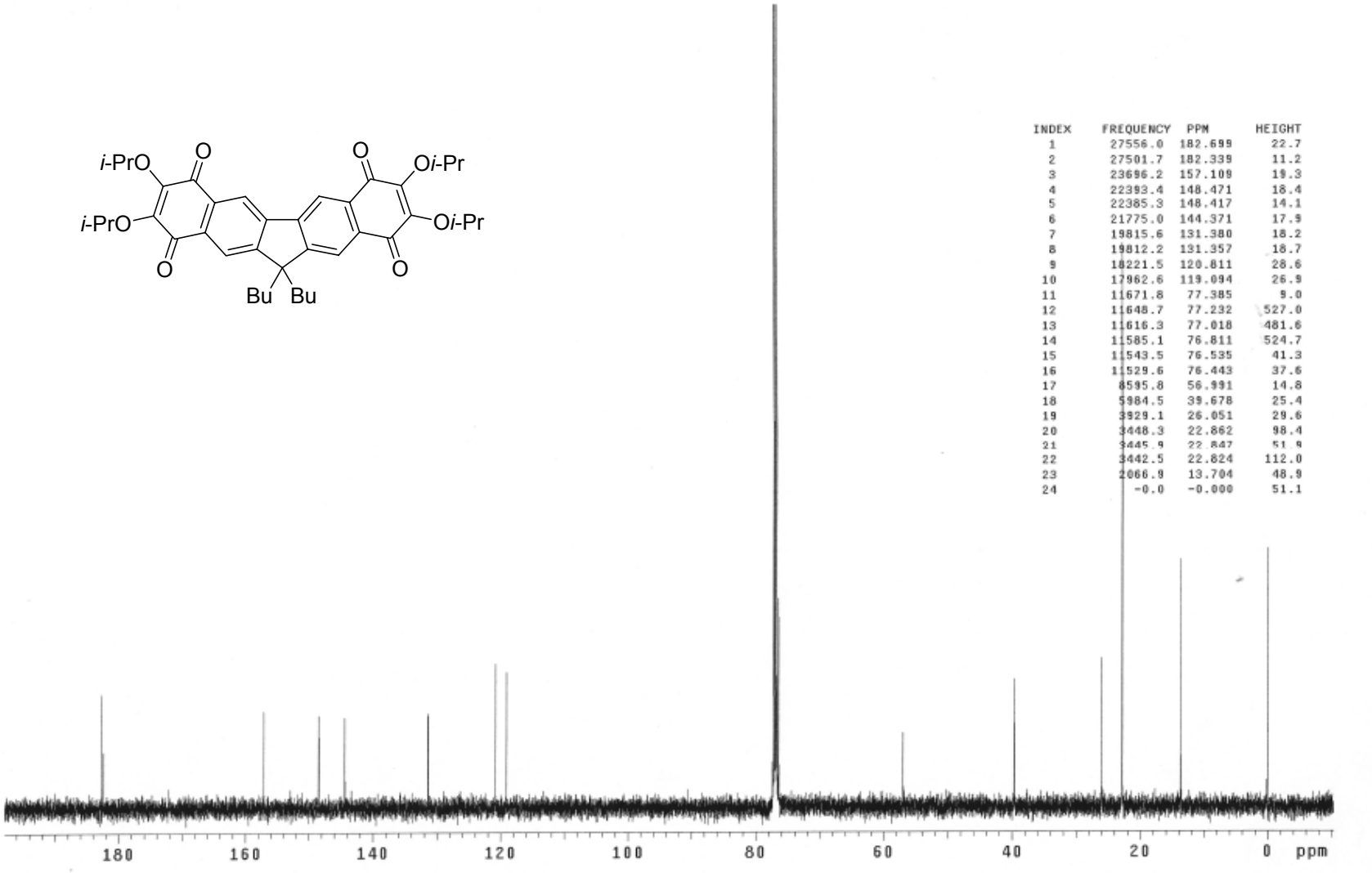


Figure S32. ^{13}C NMR spectrum of compound **Q3**.

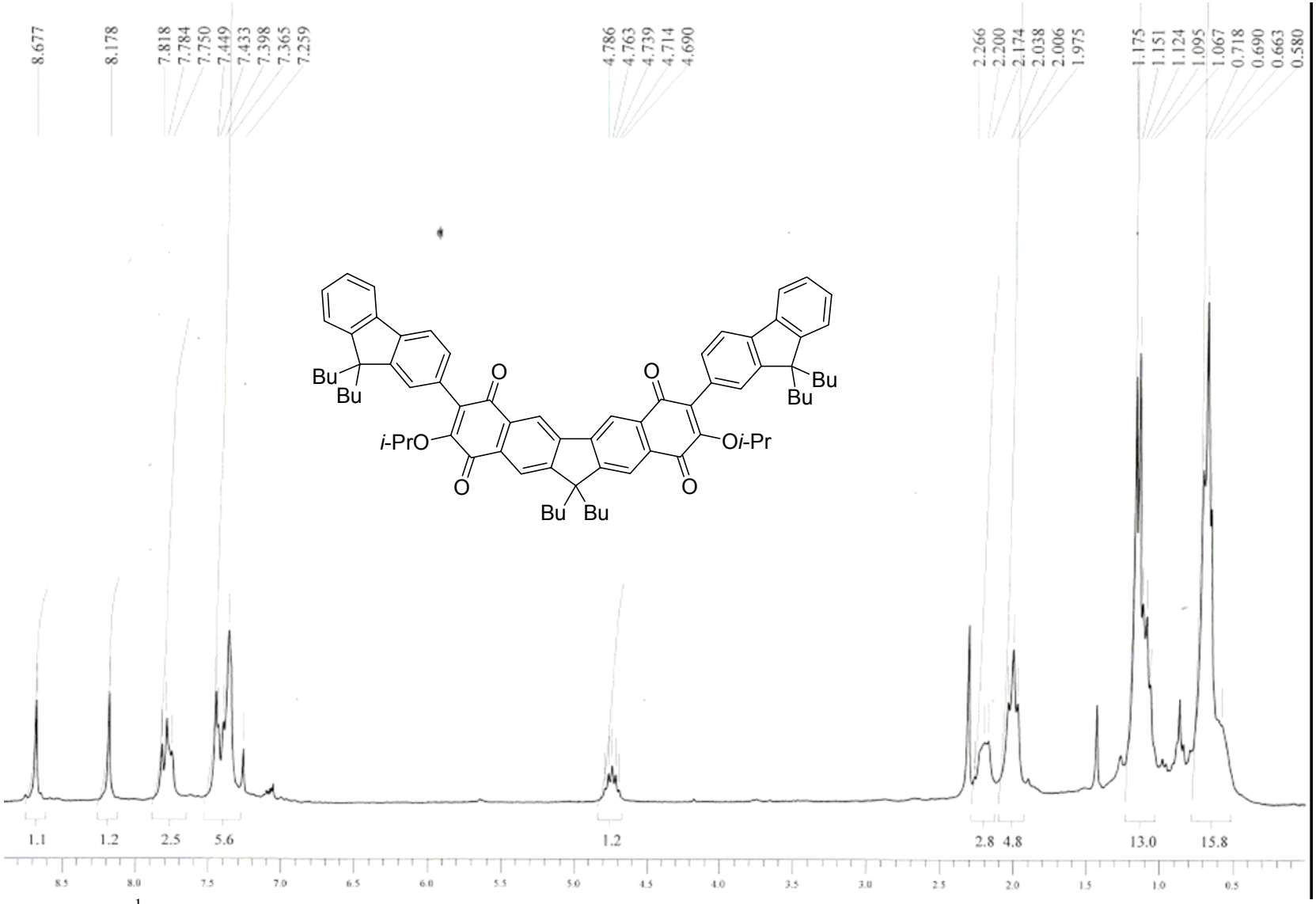


Figure S33. ^{1}H NMR spectrum of compound **Q4**.

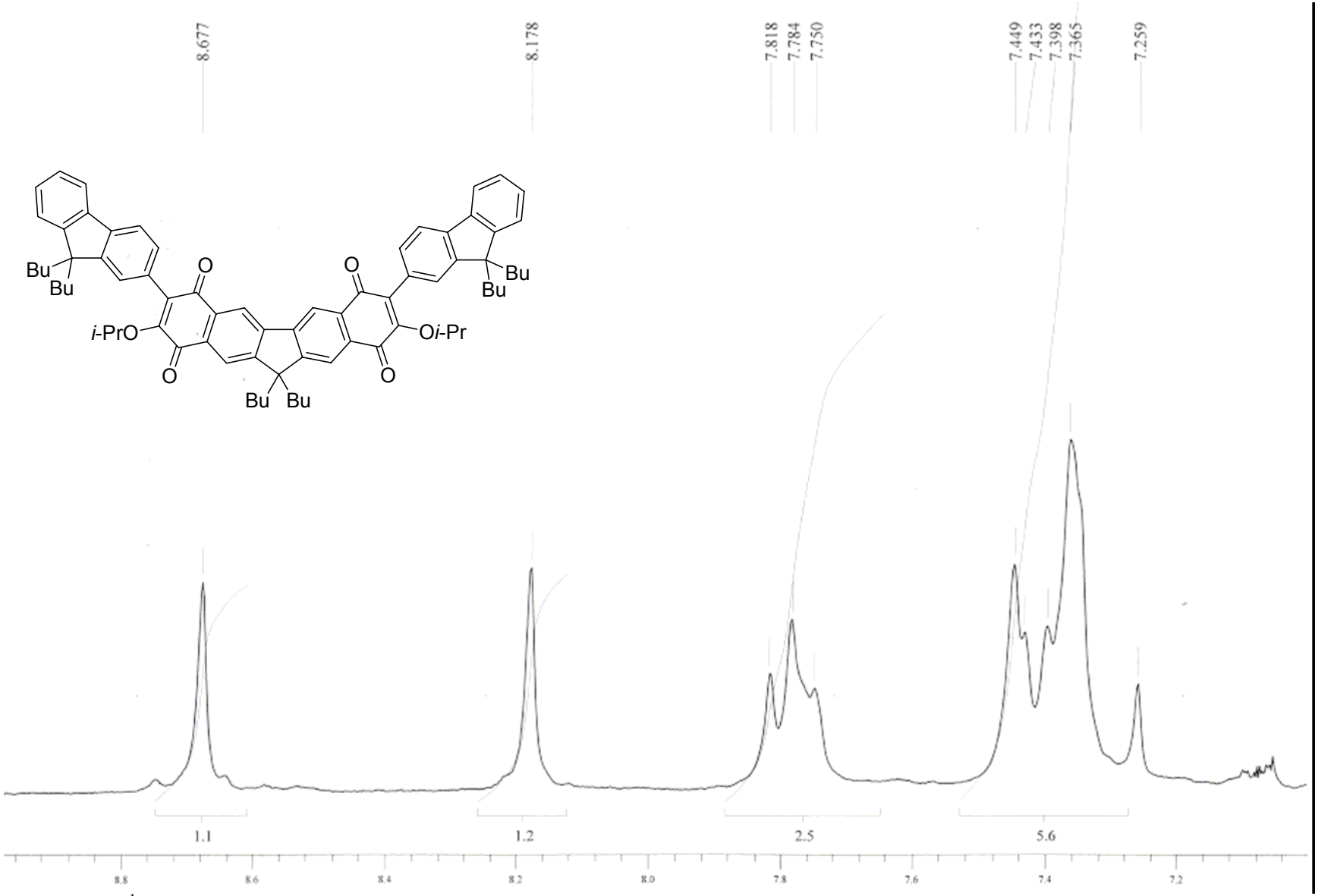


Figure S34. ^{1}H NMR spectrum of compound **Q4** (9.0–7.0 ppm).

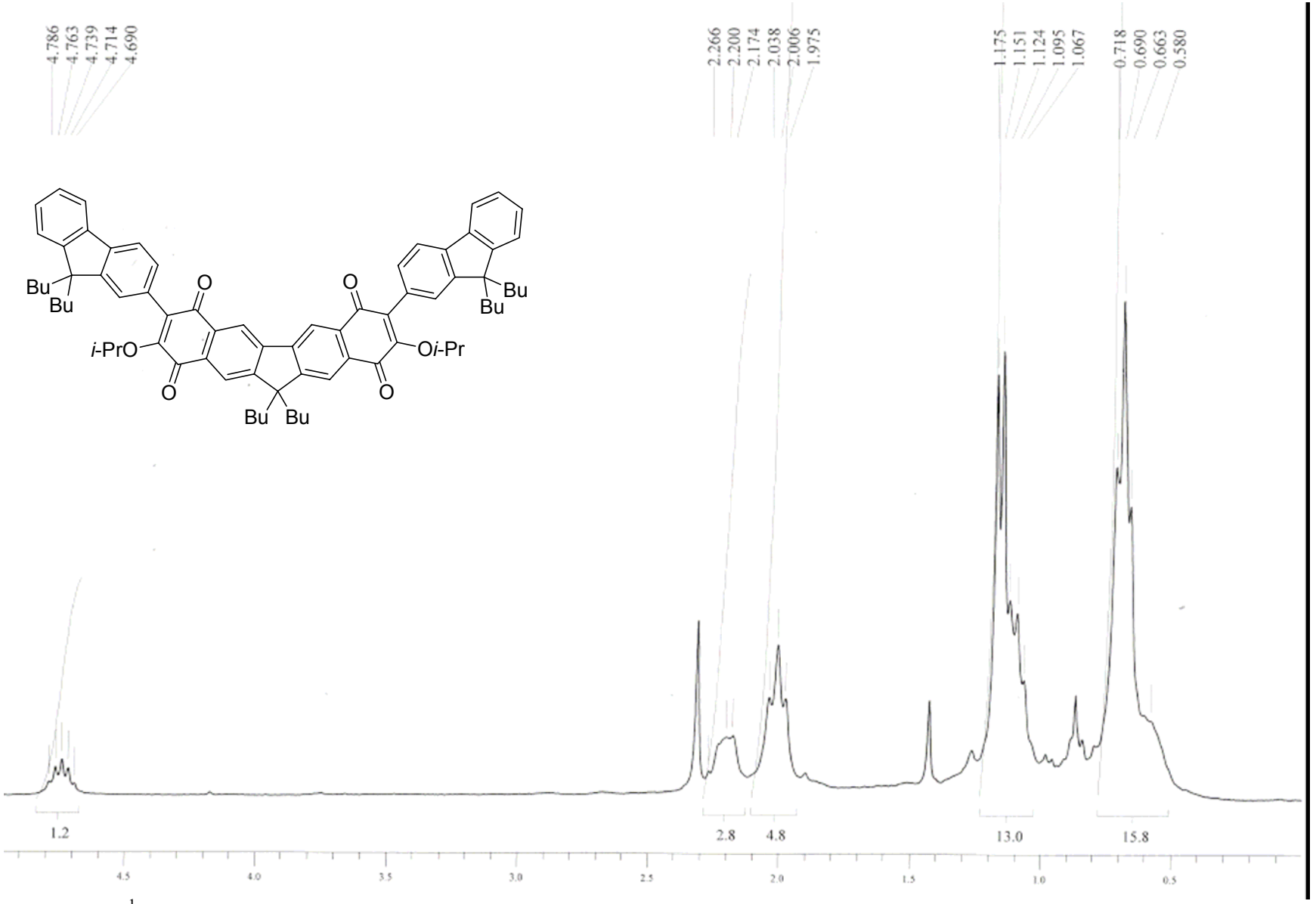


Figure S35. ^{1}H NMR spectrum of compound **Q4** (5.0–0.0 ppm).

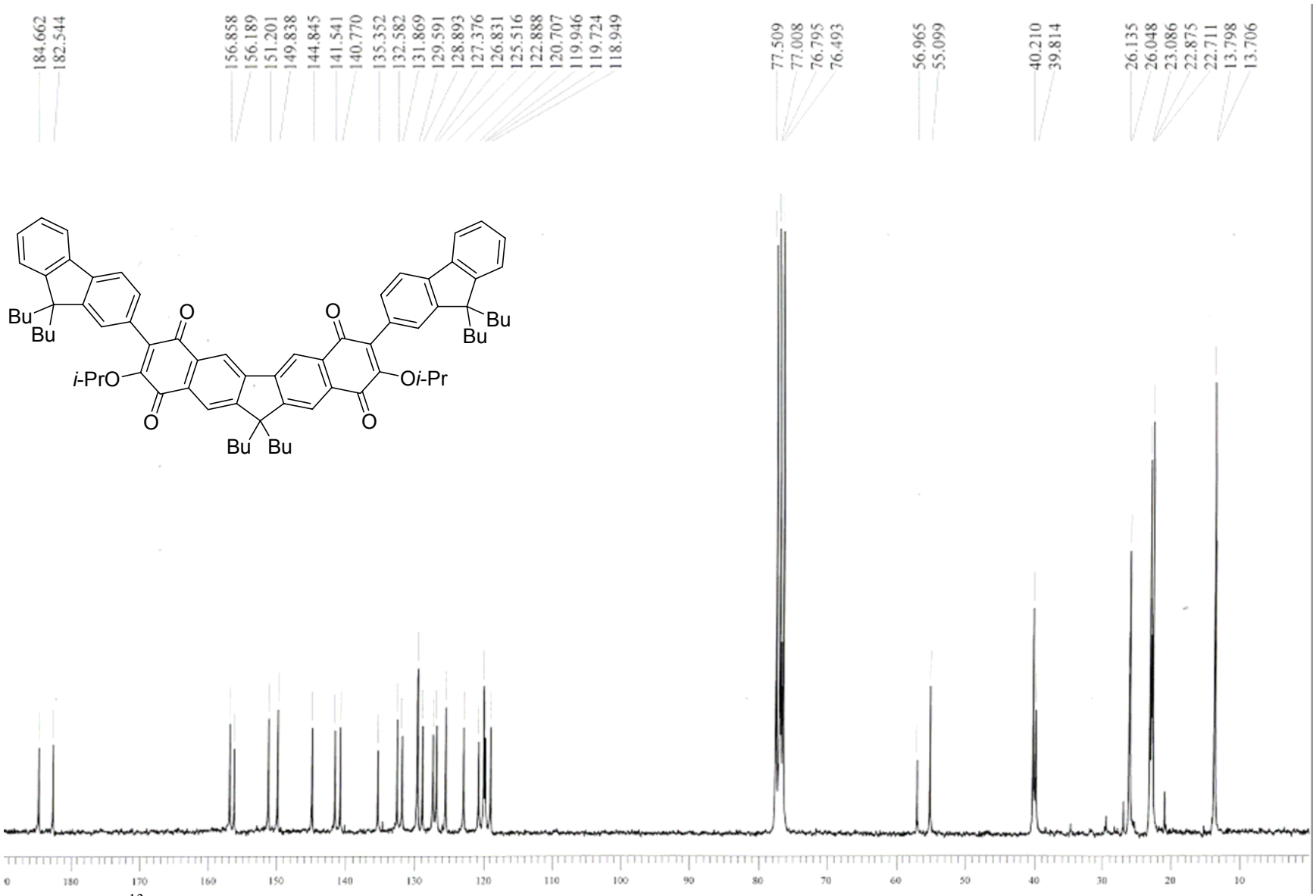


Figure S36. ^{13}C NMR spectrum of compound **Q4**.

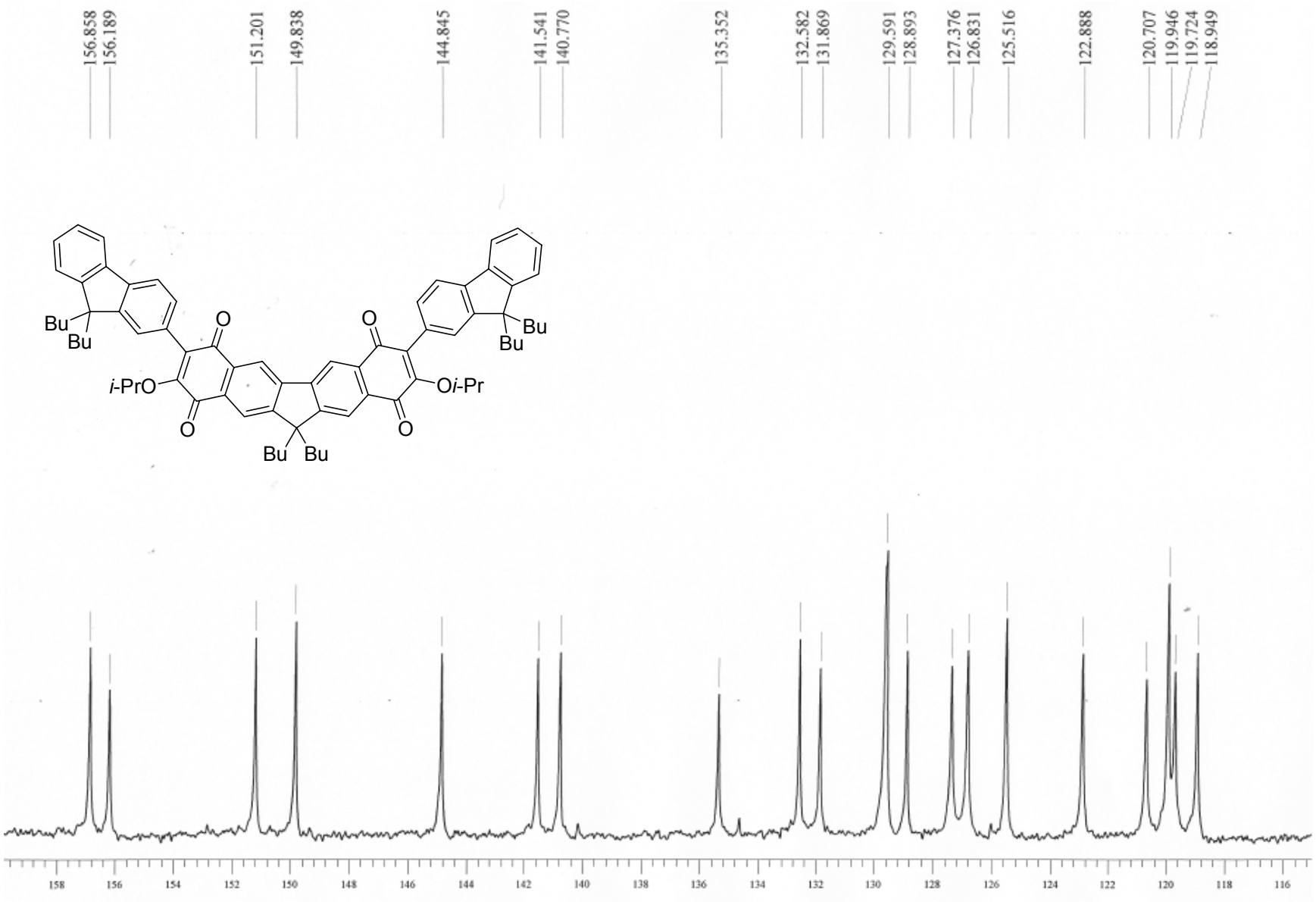


Figure S37. ^{13}C NMR spectrum of compound **Q4** (160–115 ppm).

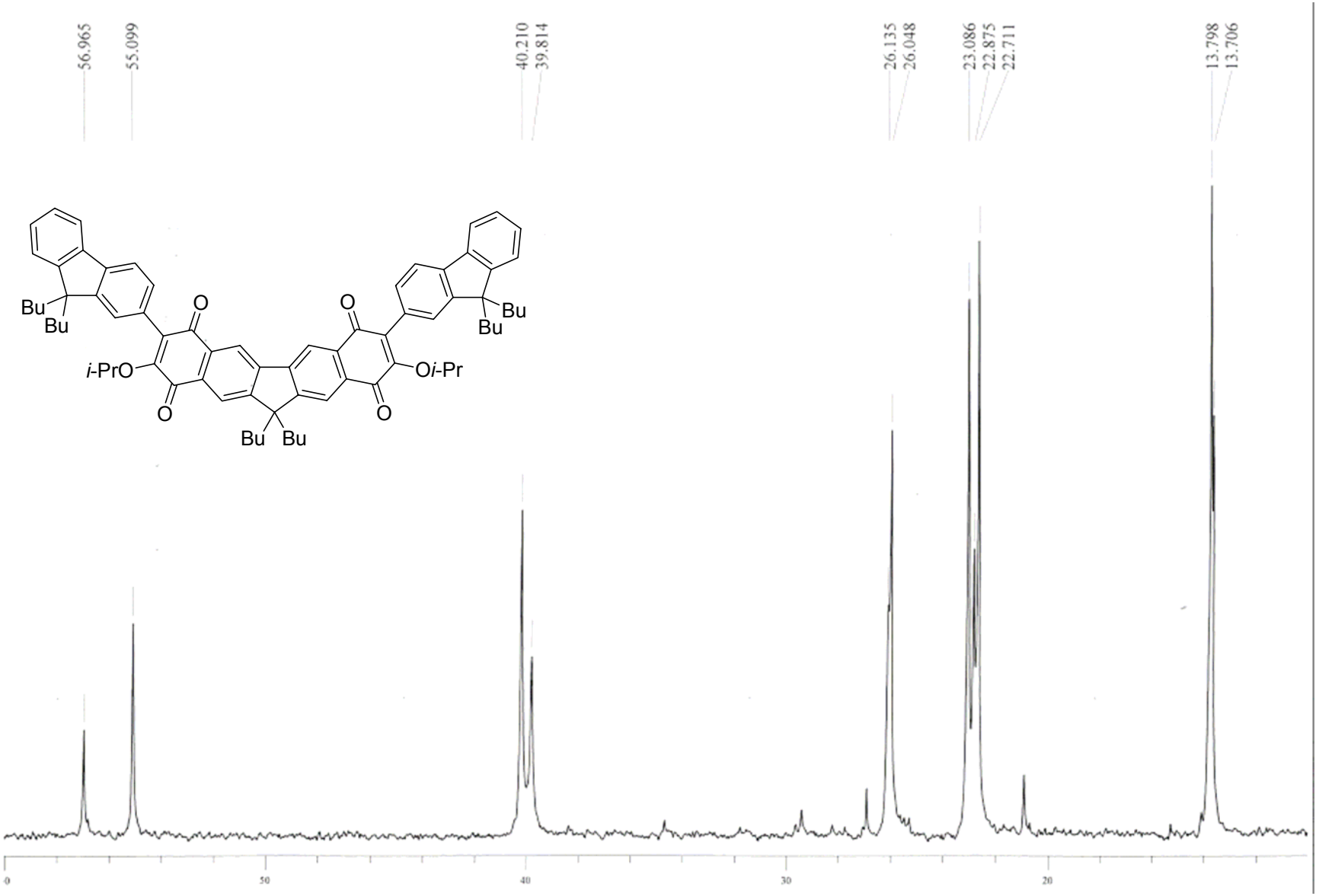


Figure S38. ^{13}C NMR spectrum of compound **Q4** (60–0.0 ppm).

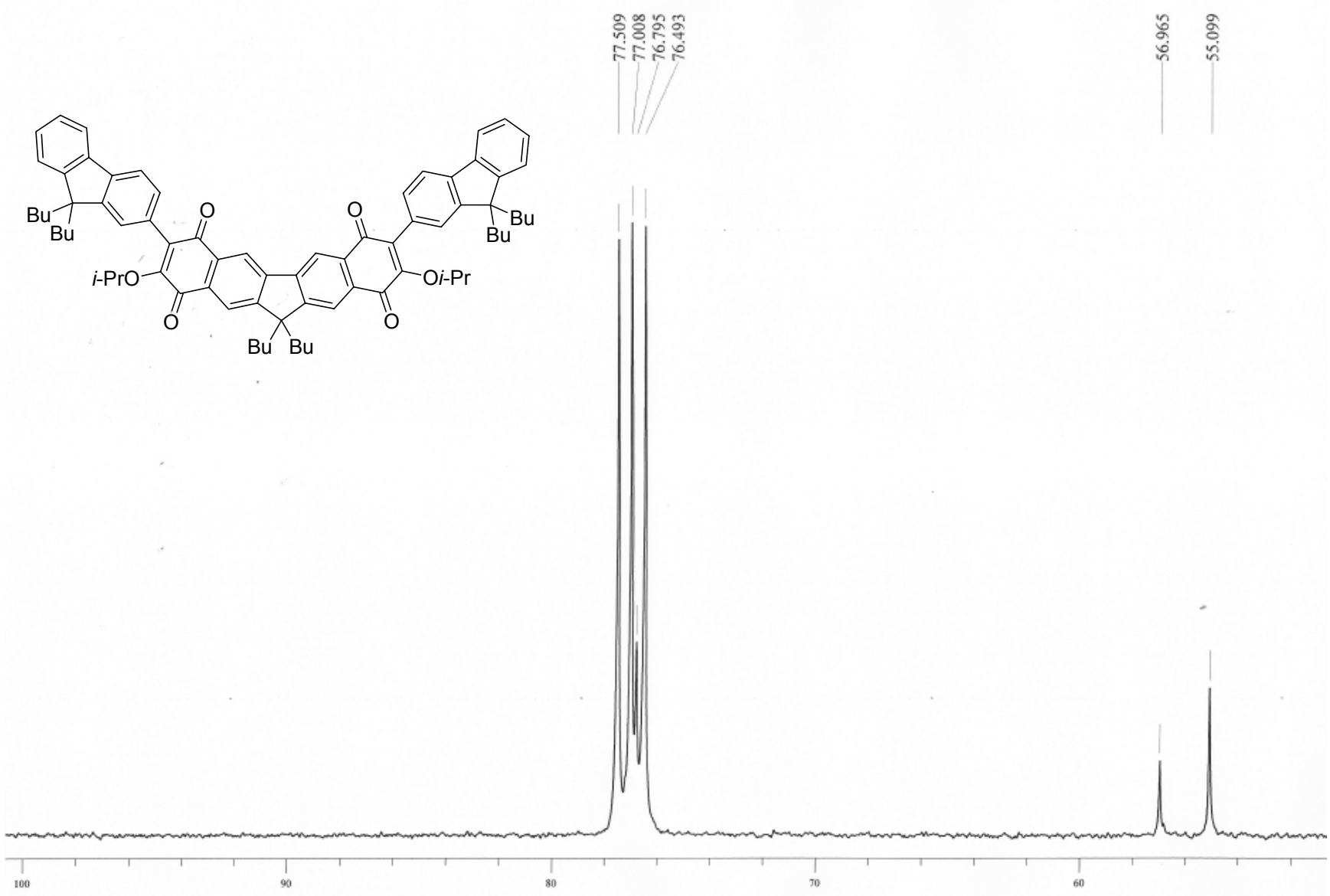


Figure S39. ^{13}C NMR spectrum of compound **Q4** (100–50 ppm).

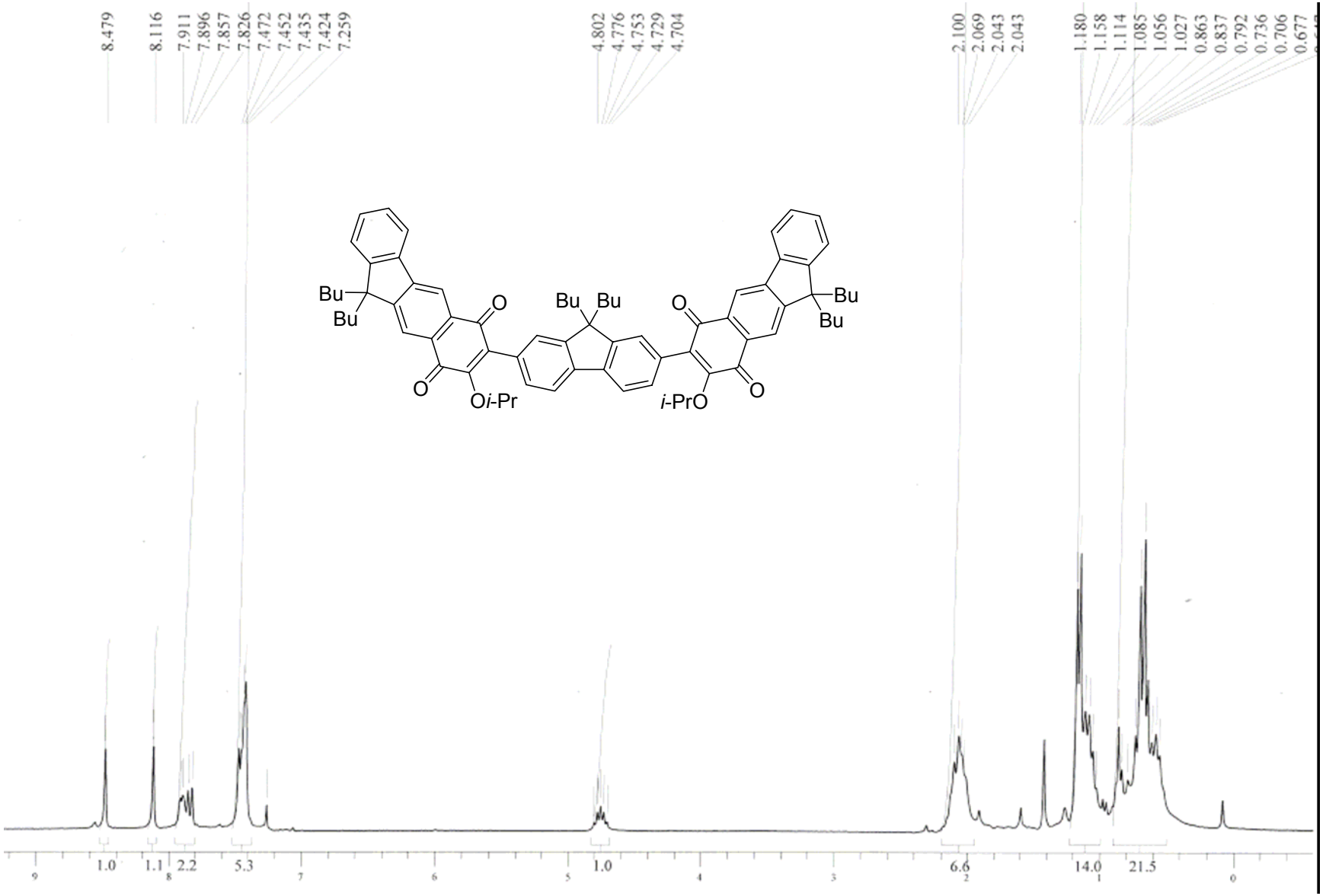


Figure S40. ^{1}H NMR spectrum of compound **Q5**.

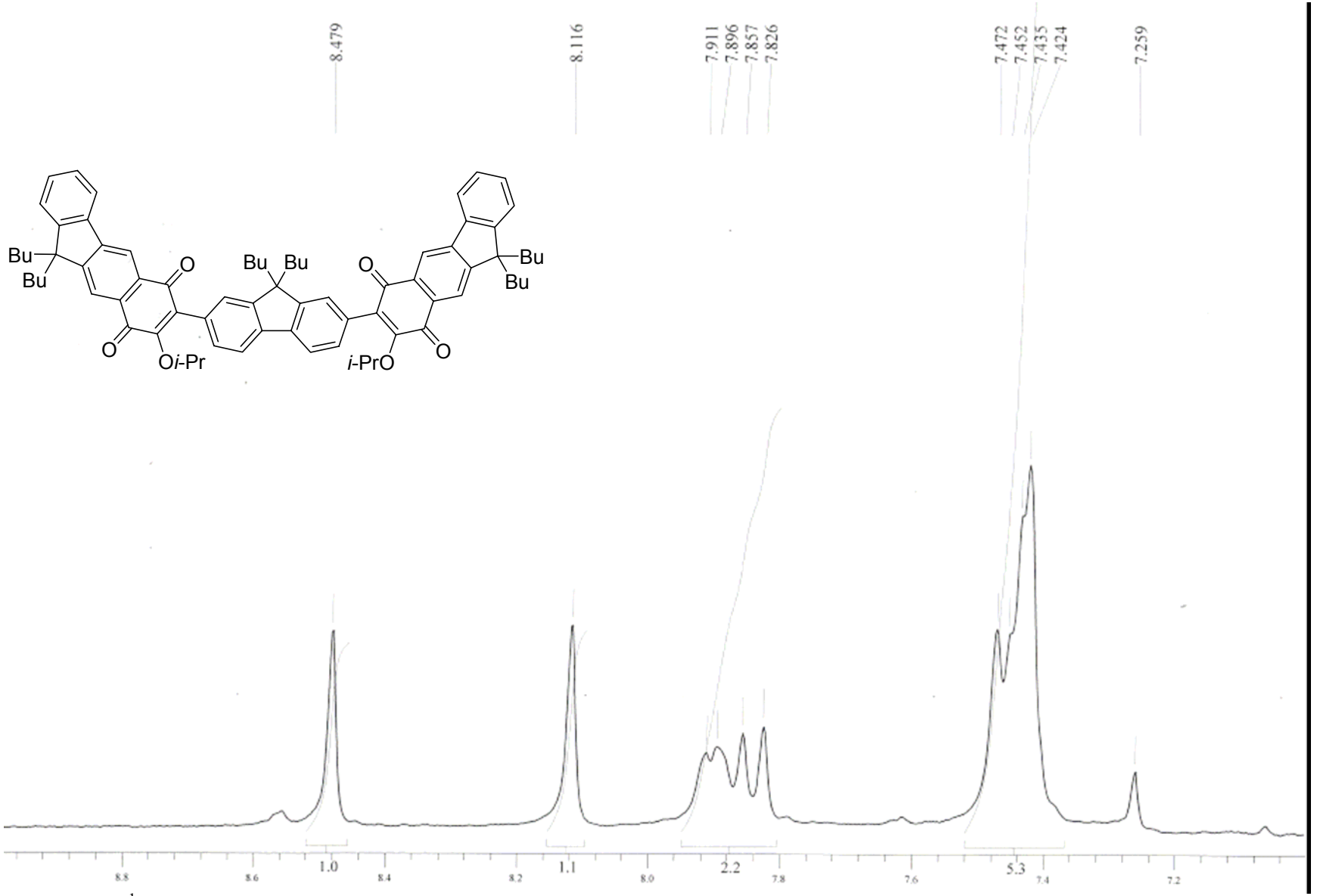


Figure S41. ^{1}H NMR spectrum of compound **Q5** (9.0–7.0 ppm).

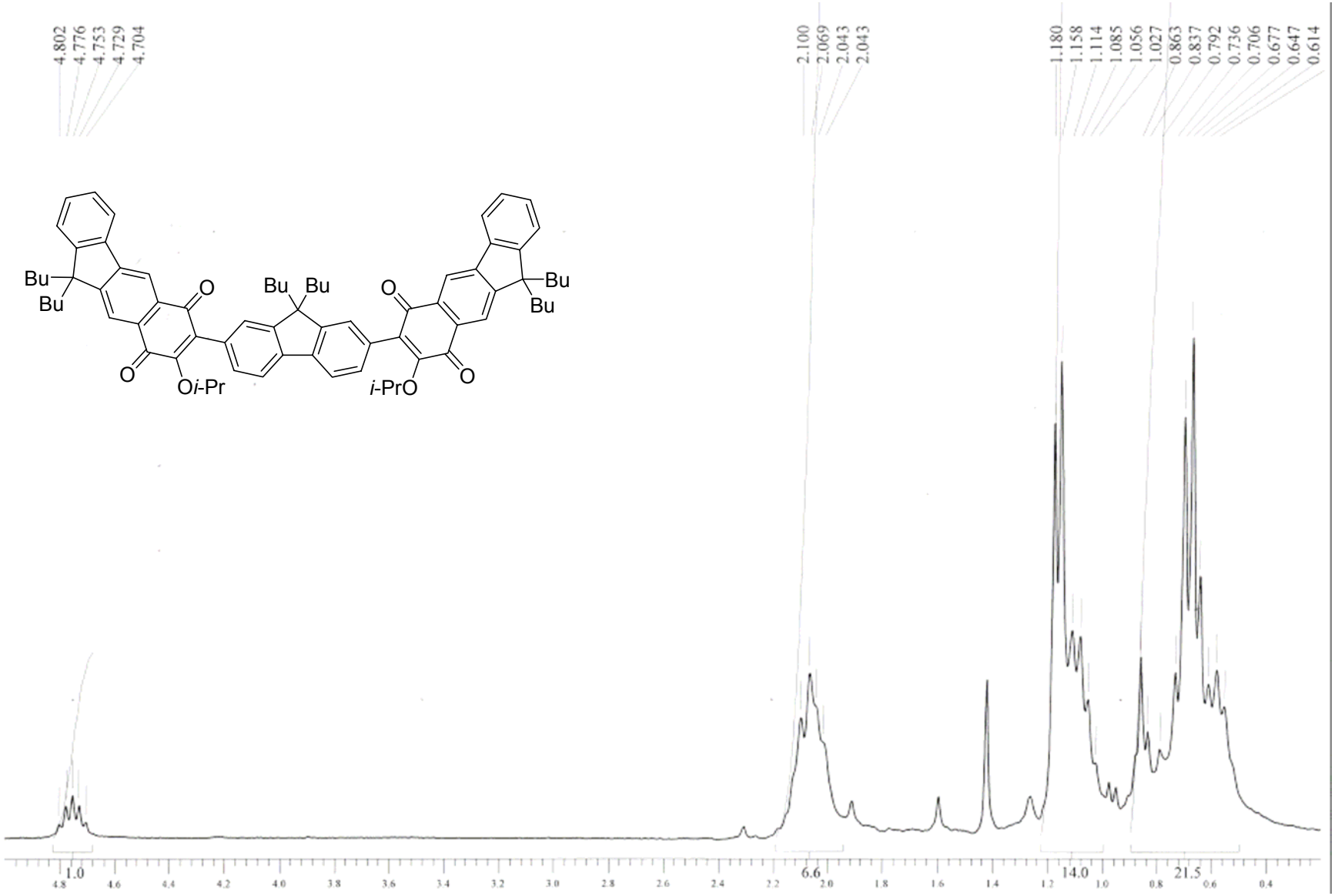


Figure S42. ^{1}H NMR spectrum of compound **Q5** (5.0–0.0 ppm).

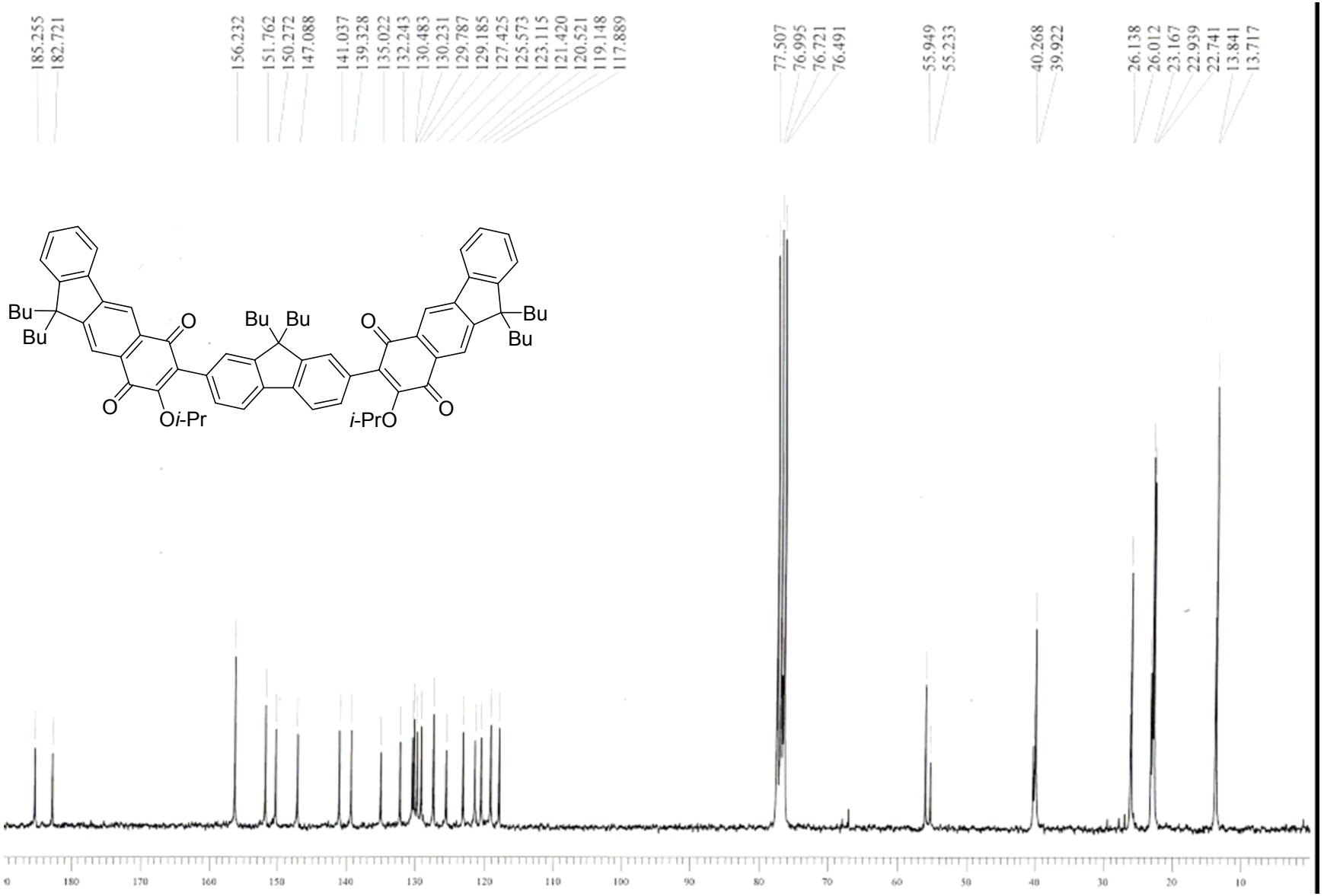


Figure S43. ^{13}C NMR spectrum of compound **Q5**.

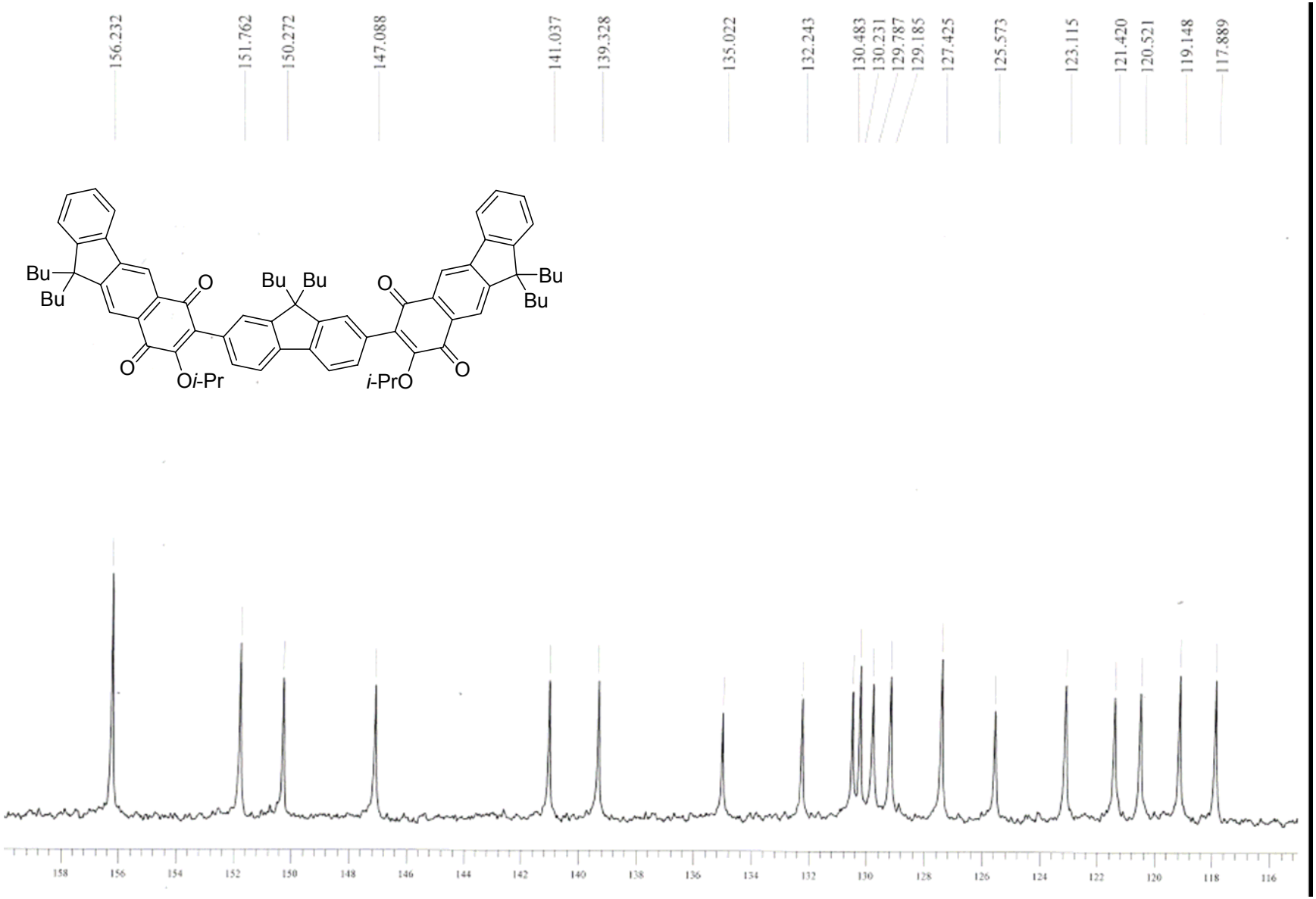


Figure S44. ^{13}C NMR spectrum of compound **Q5** (160–115 ppm).

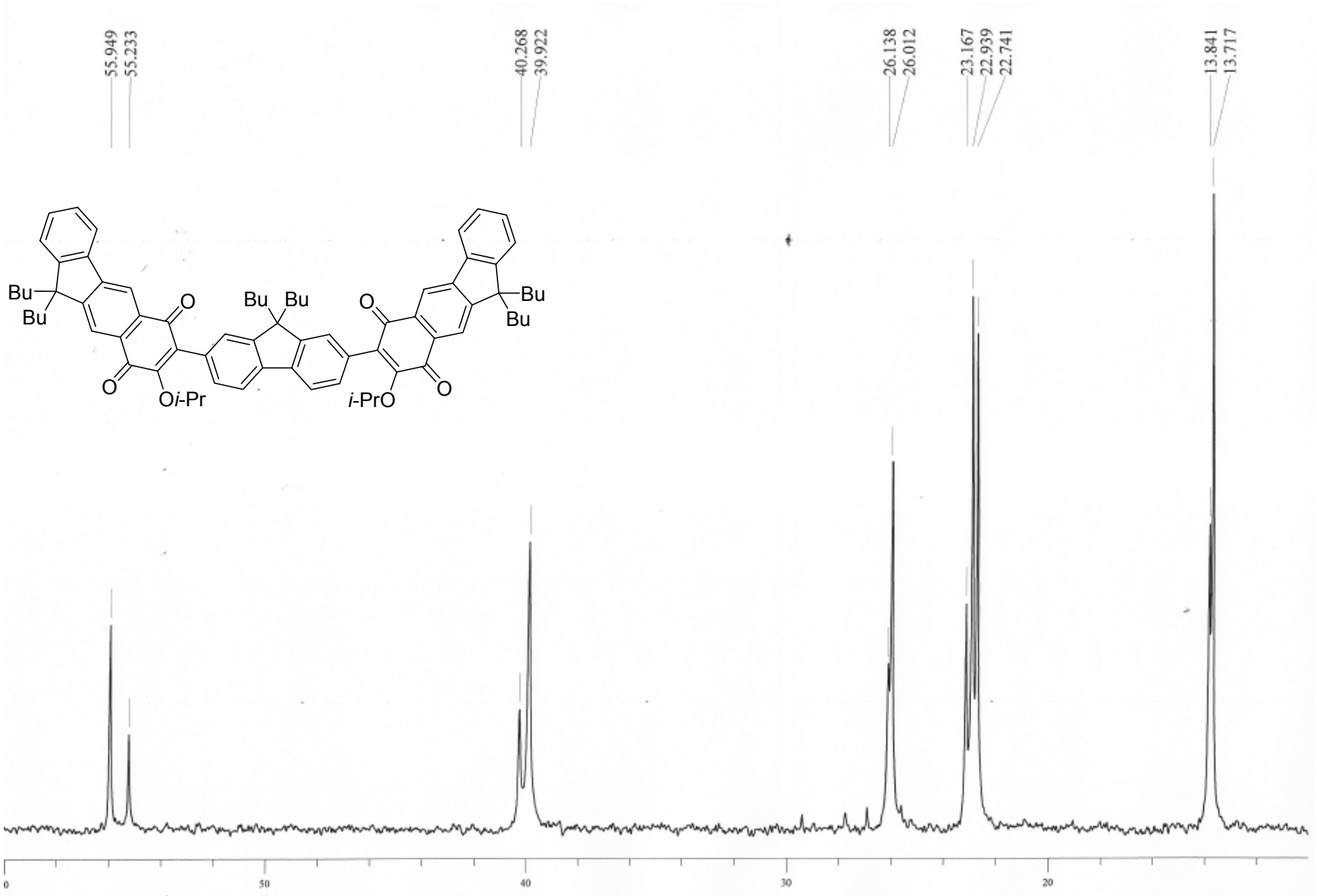


Figure S45. ^{13}C NMR spectrum of compound **Q5** (60–0.0 ppm).

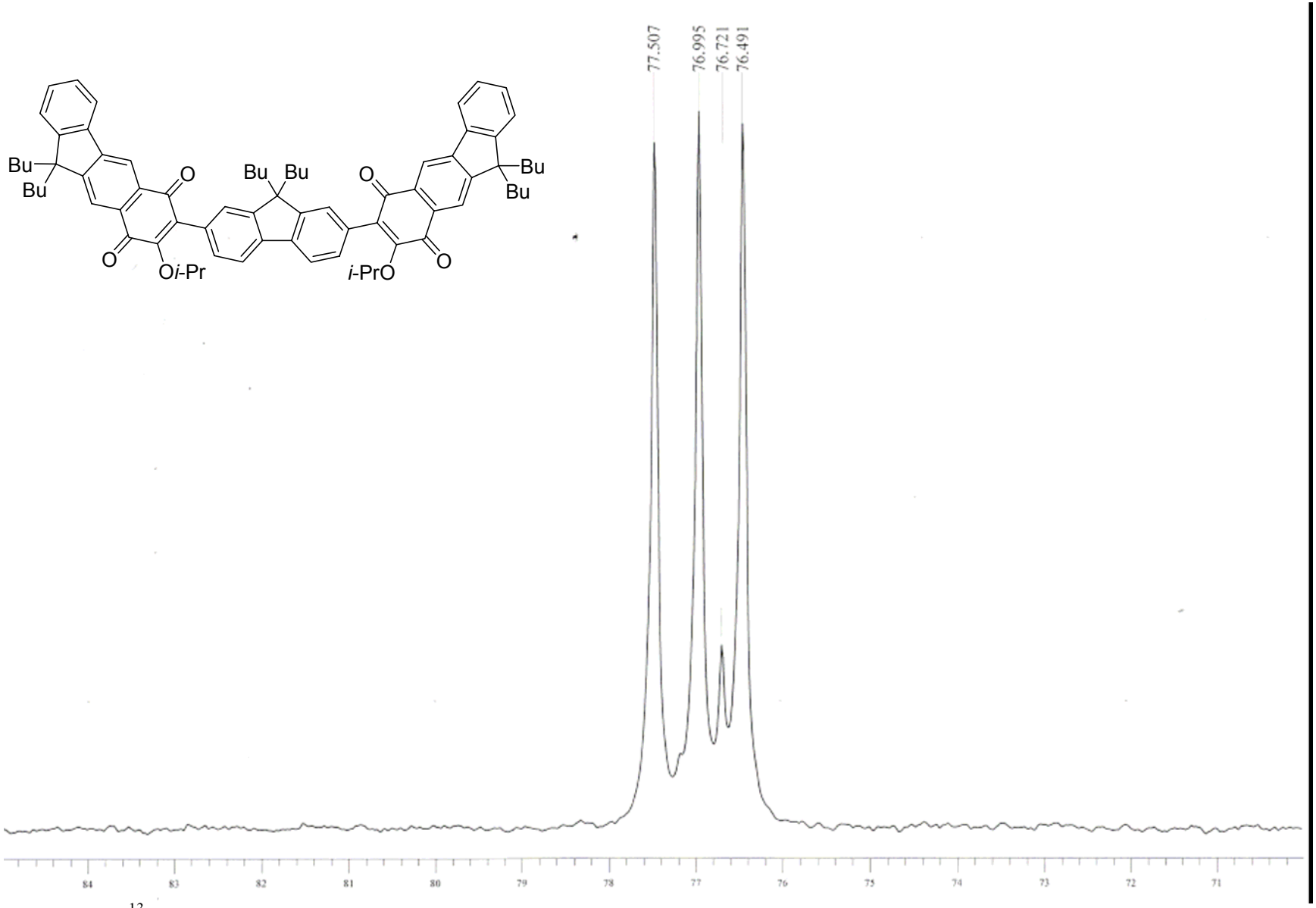


Figure S46. ^{13}C NMR spectrum of compound **Q5** (85–70 ppm).