Benzimidazole-Branched Isomeric Dyes: Effect of Molecular Constitution on Photophysical, Electrochemical and Photovoltaic Properties

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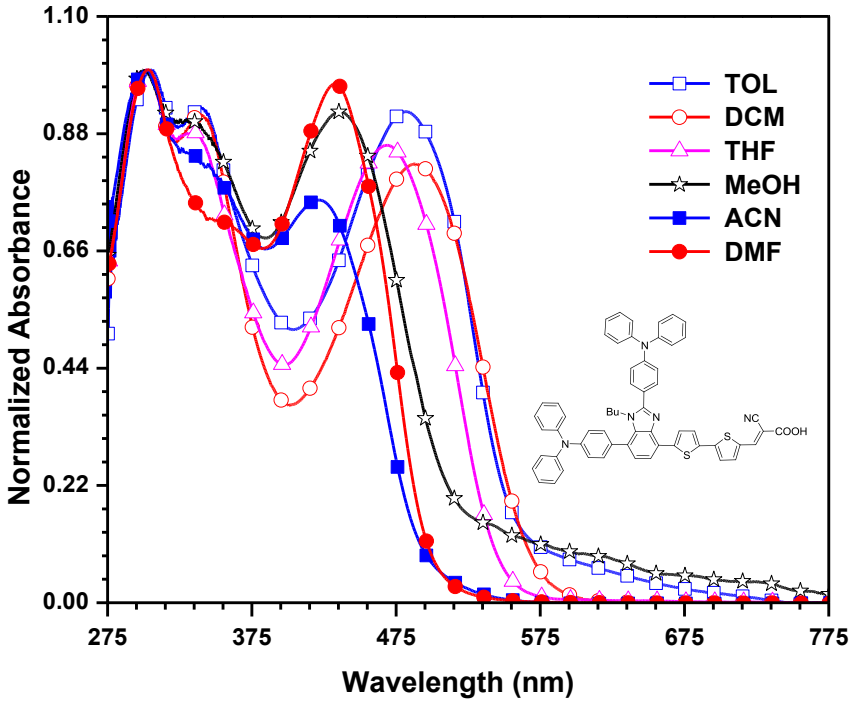

Figure S1. Absorption spectra of **7b** recorded in different solvents.

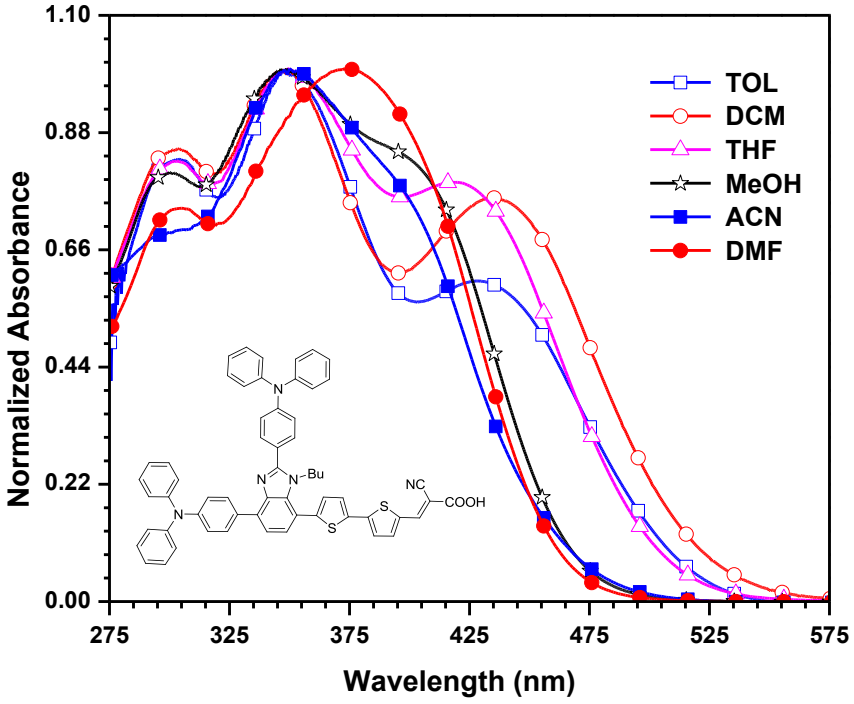

Figure S2. Absorption spectra of **7c** recorded in different solvents.

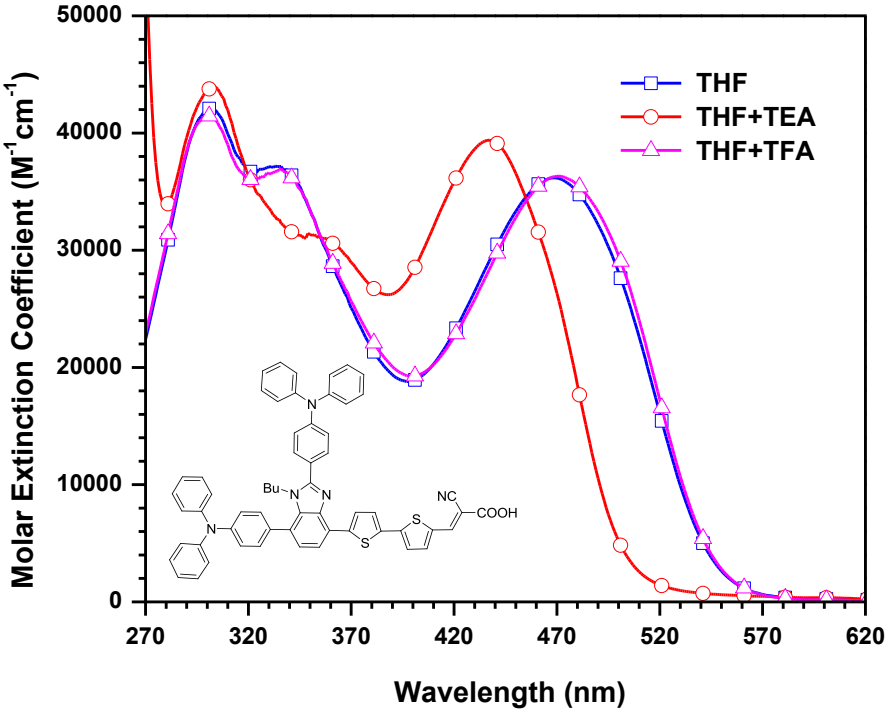

Figure S3. Absorption spectra of **7b** recorded in THF before and after addition of TFA or TEA.

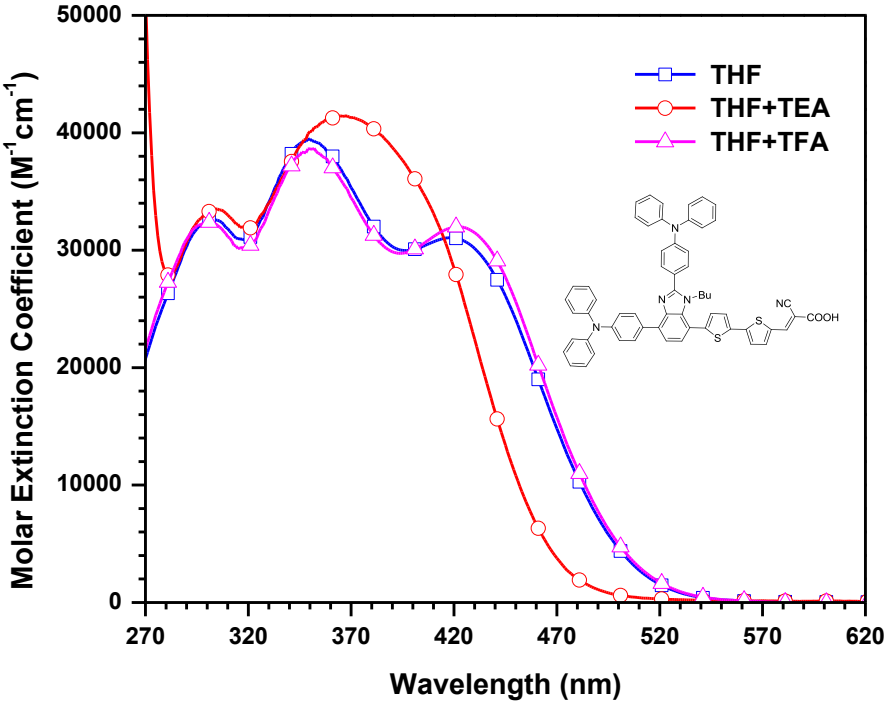

Figure S4. Absorption spectra of **7c** recorded in THF before and after addition of TFA or TEA.

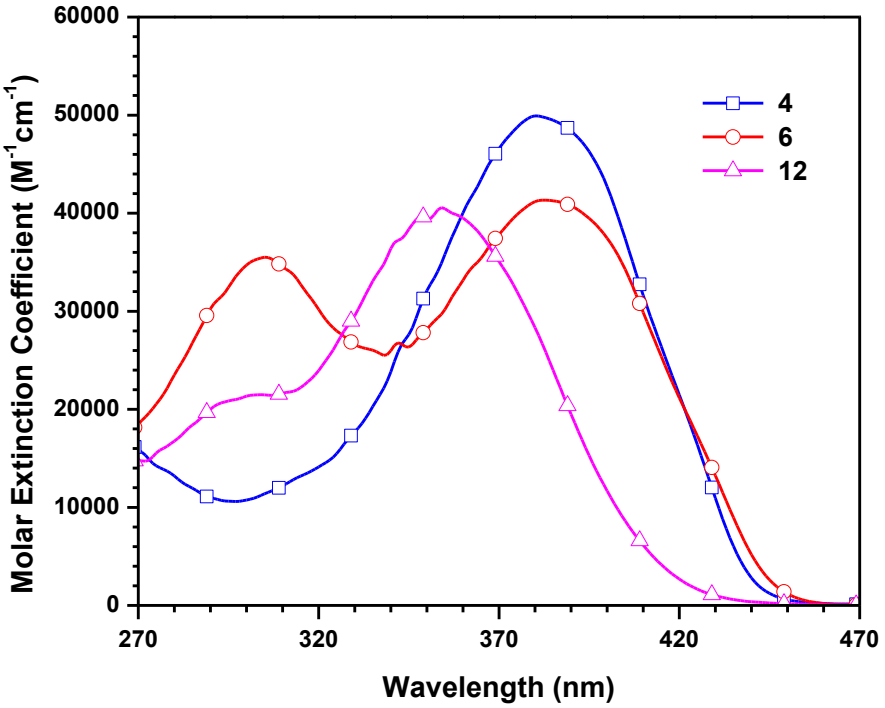

Figure S5. Absorption spectra of the intermediates **4**, **6** and **12** recorded in THF.

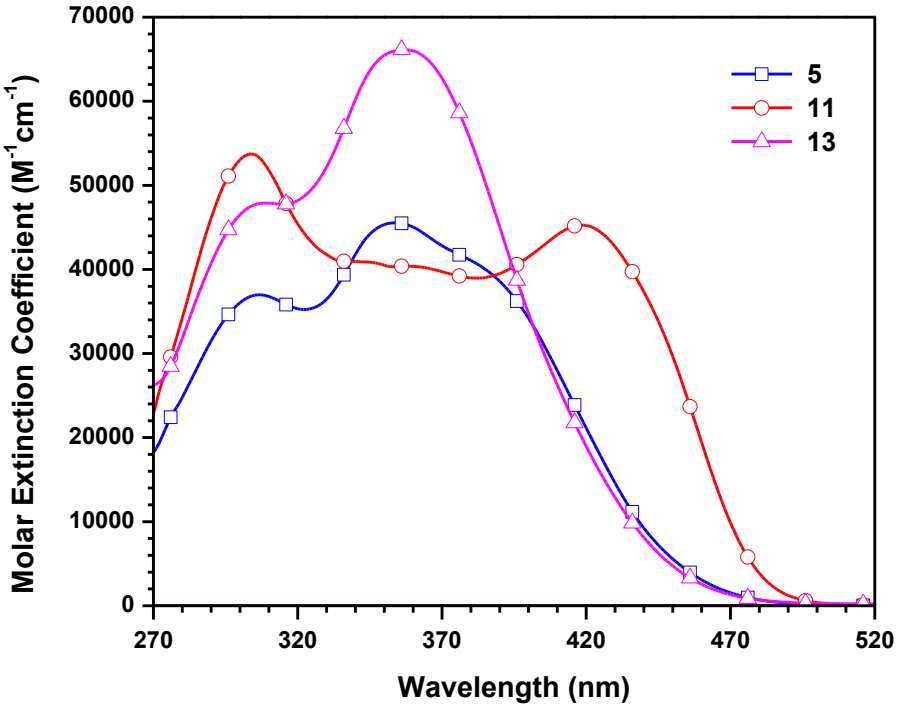

Figure S6. Absorption spectra of the intermediates **5**, **11** and **13** recorded in THF.

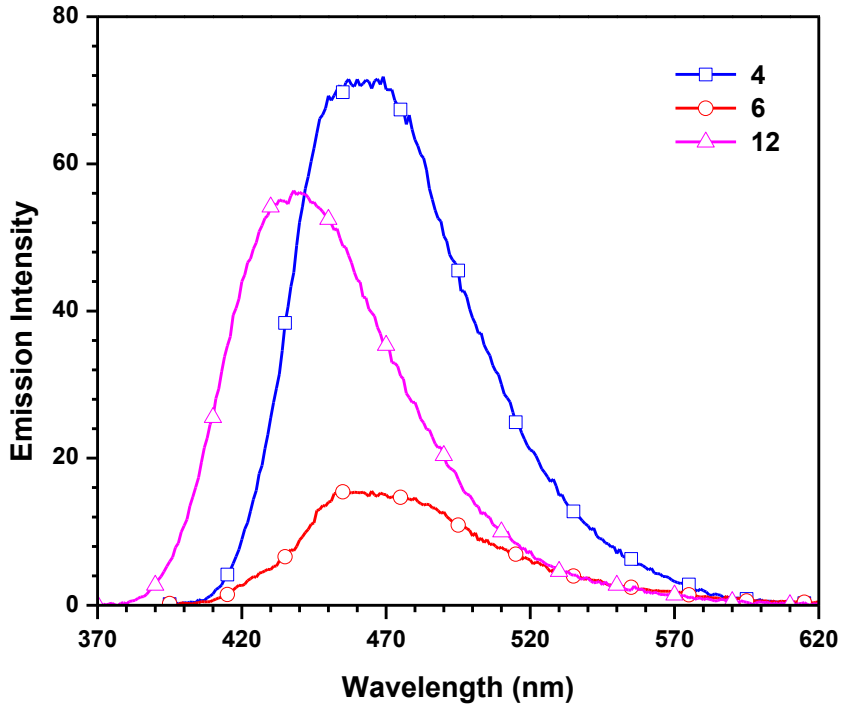

Figure S7. Emission spectra of the intermediates **4**, **6** and **12** recorded in THF.

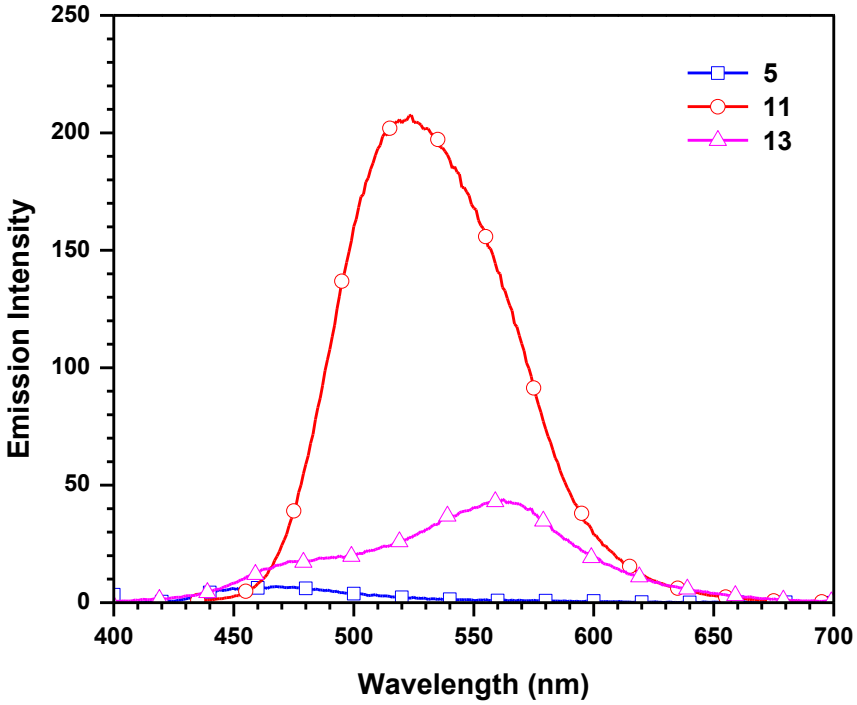

Figure S8. Emission spectra of the intermediates **5**, **11** and **13** recorded in THF.

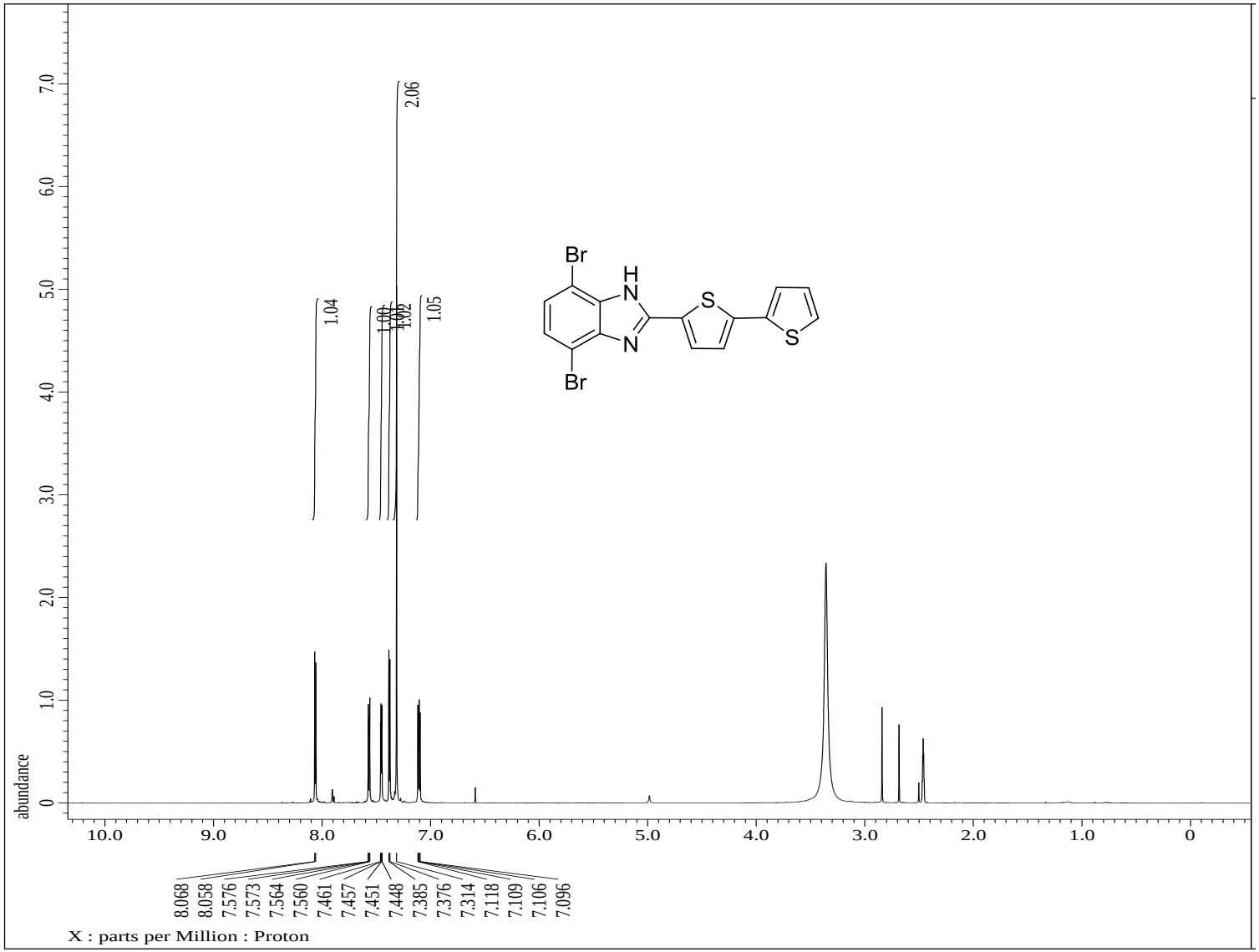

Figure S9. ^{13}C NMR spectra of **2** recorded in DMSO-d_6.

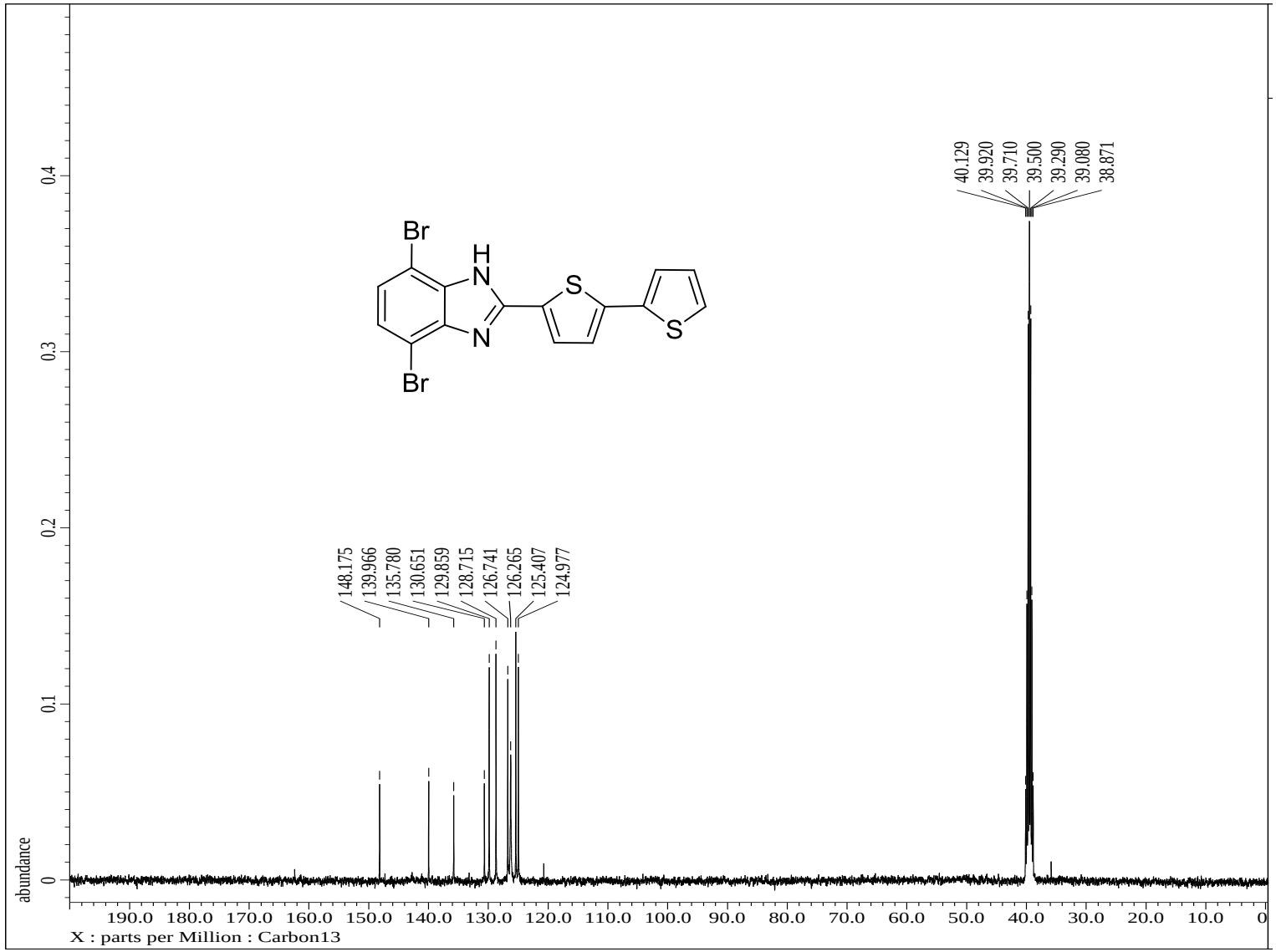

Figure S10. ^{13}C NMR spectra of **2** recorded in DMSO-d_6.

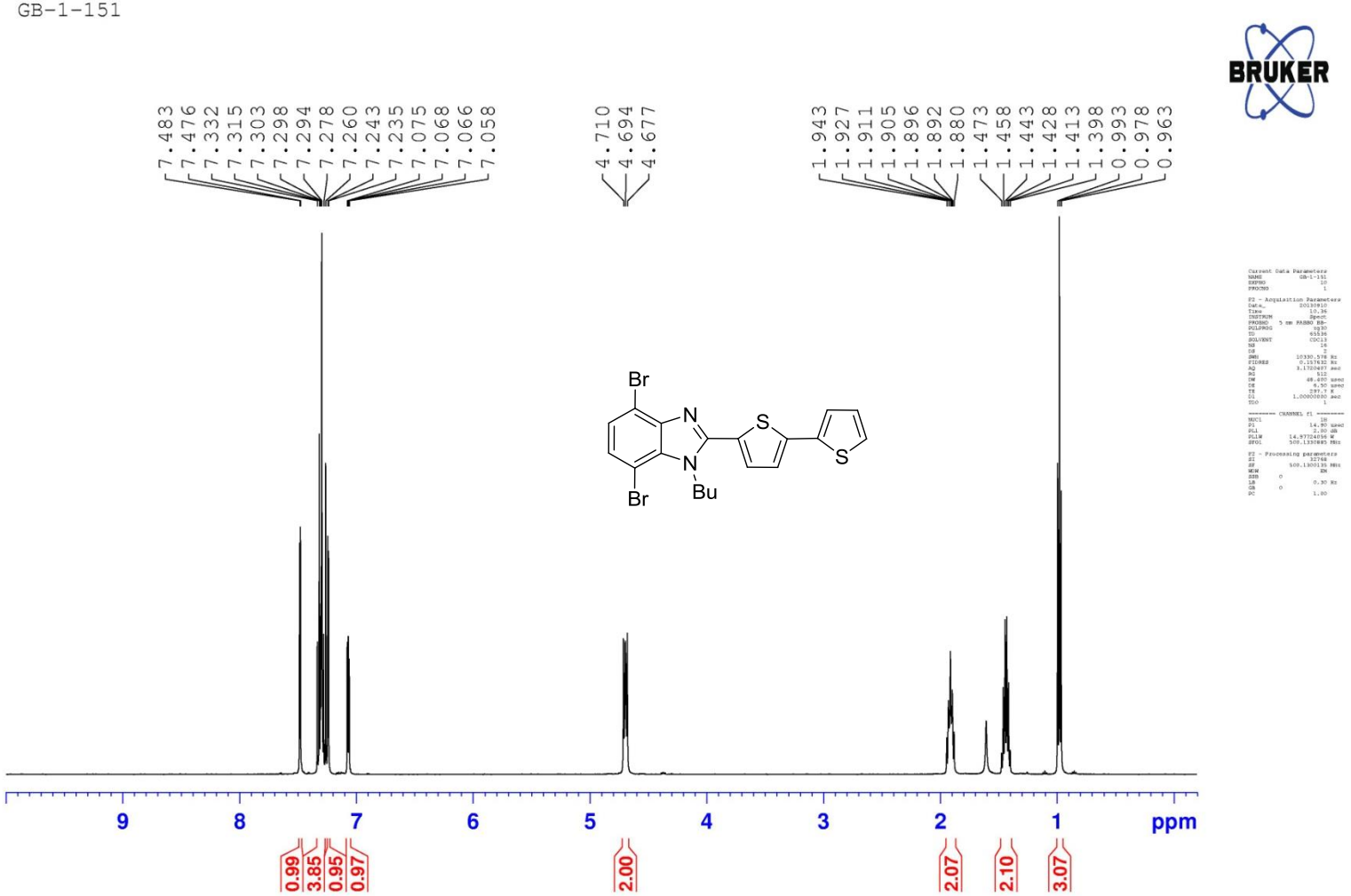

Figure S11. ^{1}H NMR spectra of **3** recorded in $CDCl_3$.

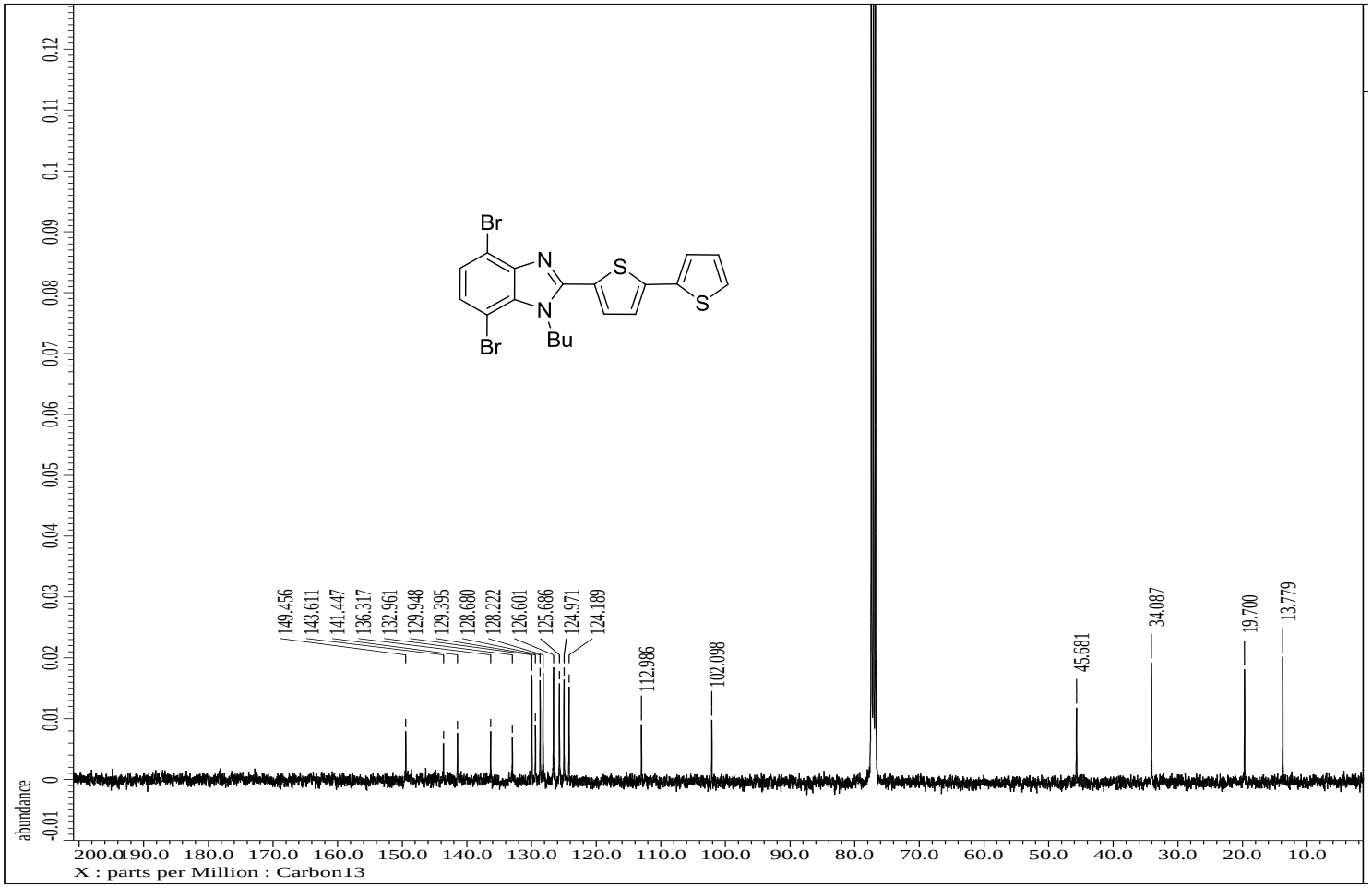

Figure S12. ^{13}C NMR spectra of **3** recorded in $CDCl_3$.

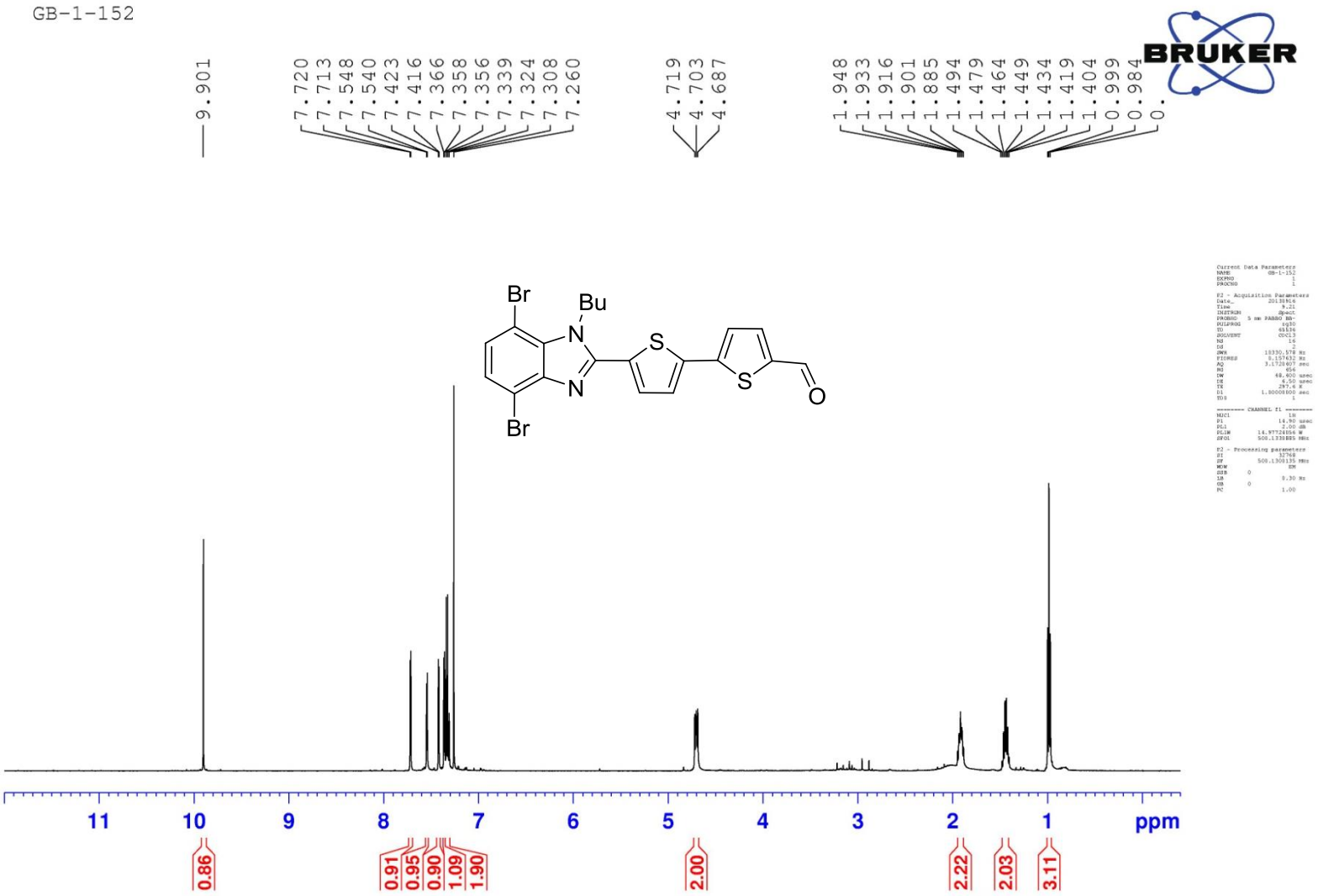

Figure S13. ^{1}H NMR spectra of **4** recorded in $CDCl_3$.

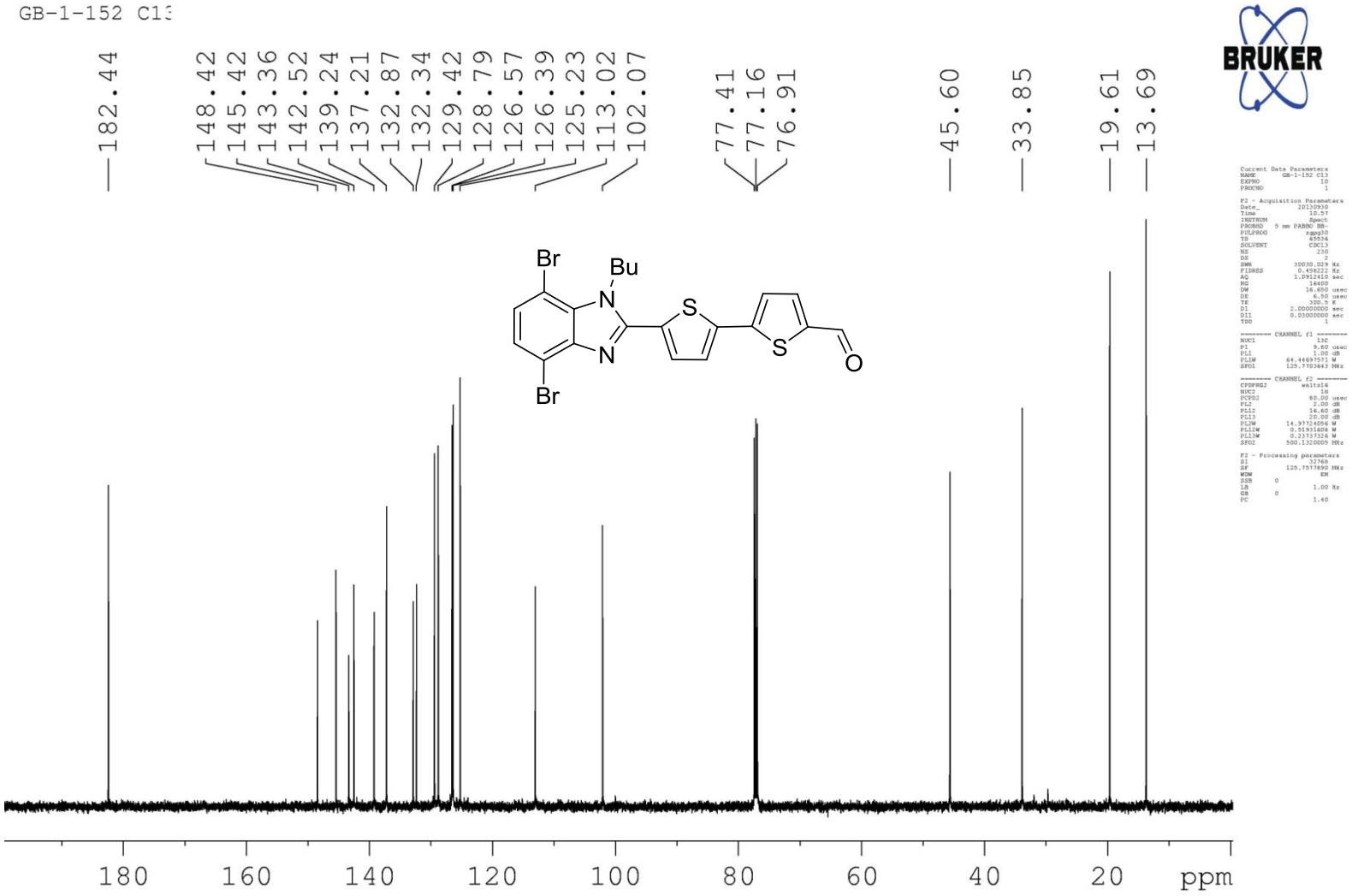

Figure S14. ^{13}C NMR spectra of **4** recorded in $CDCl_3$.

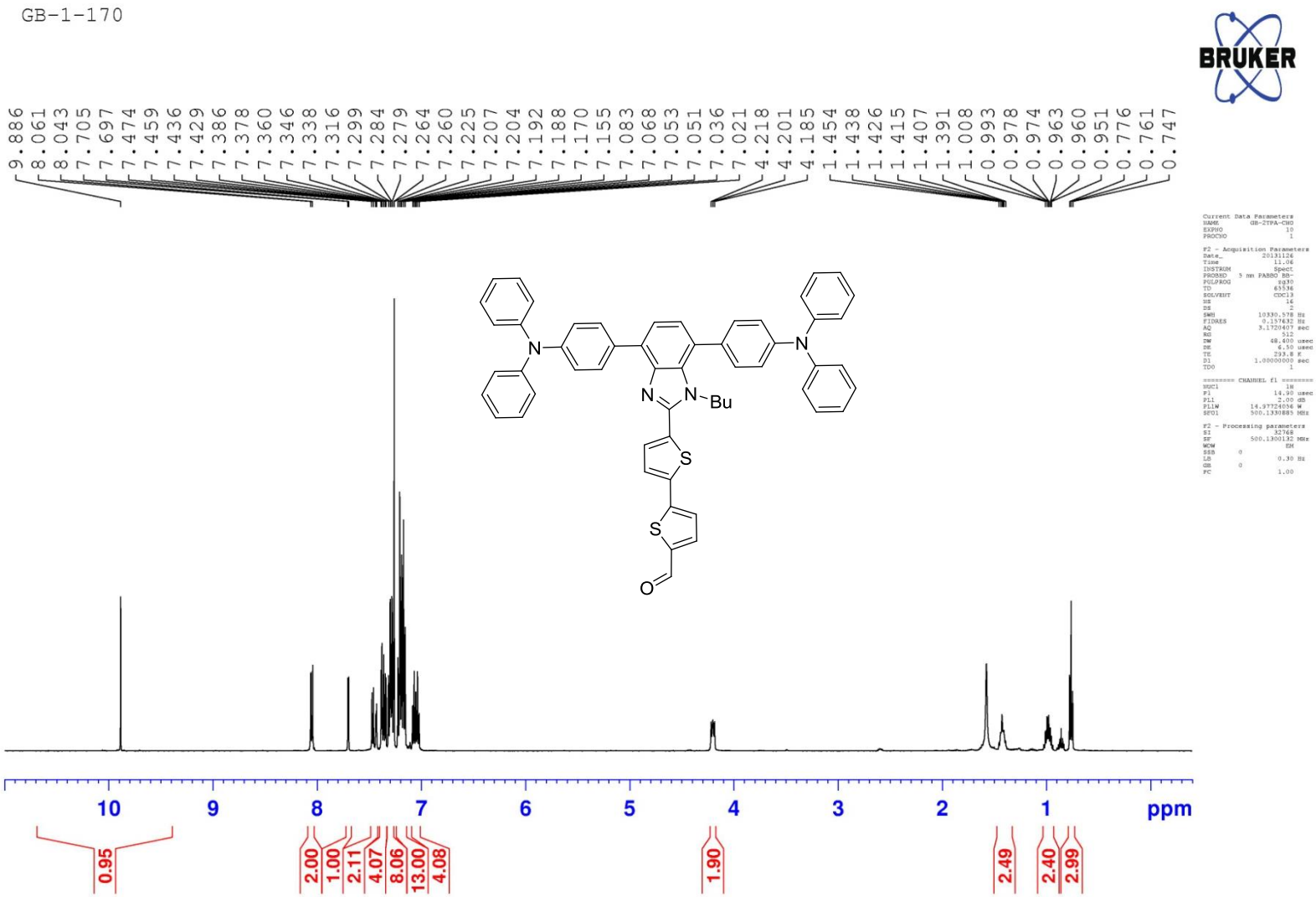

Figure S15.[1]H NMR spectra of **5** recorded in $CDCl_3$.

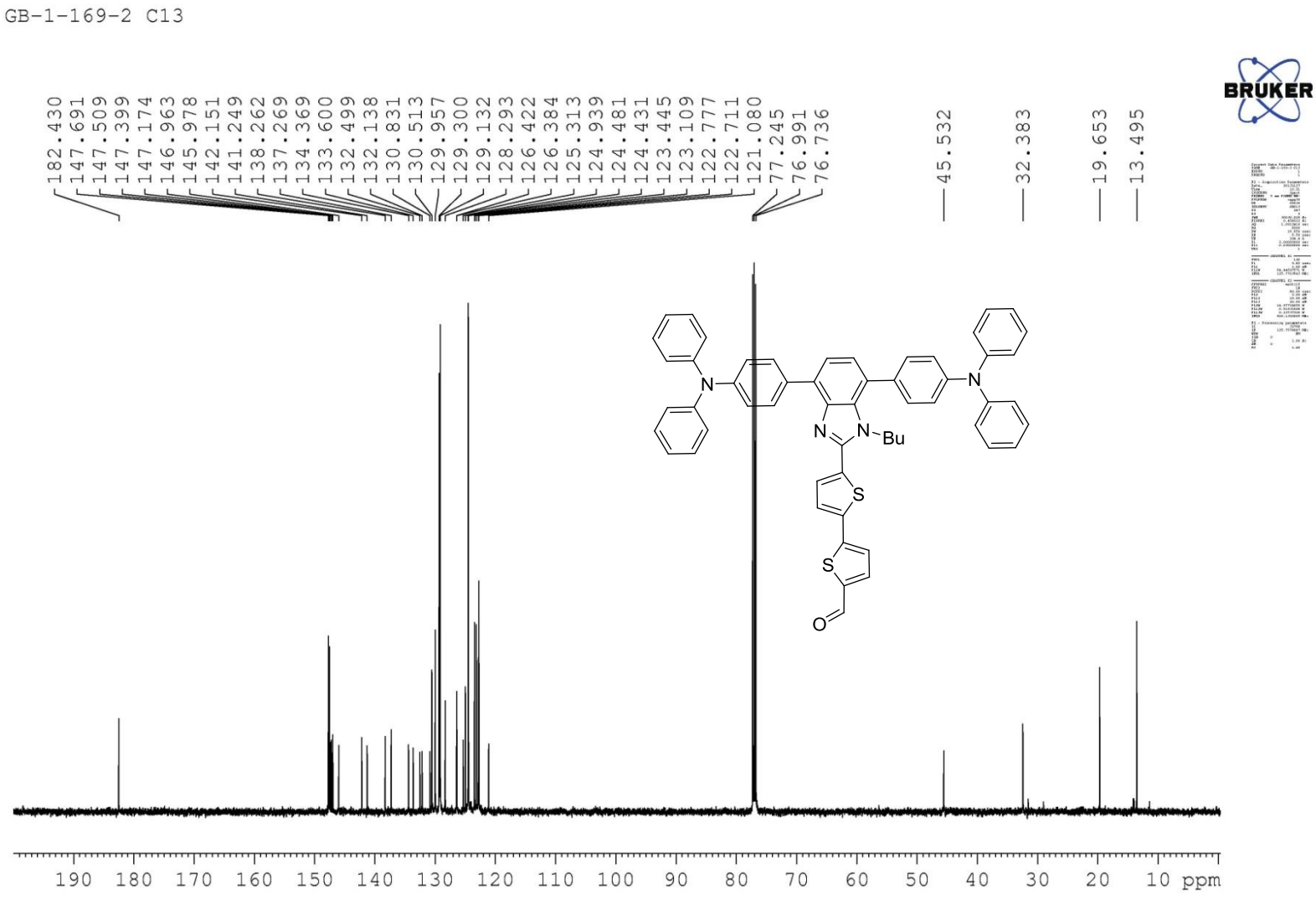

Figure S16.[13]C NMR spectra of **5** recorded in $CDCl_3$.

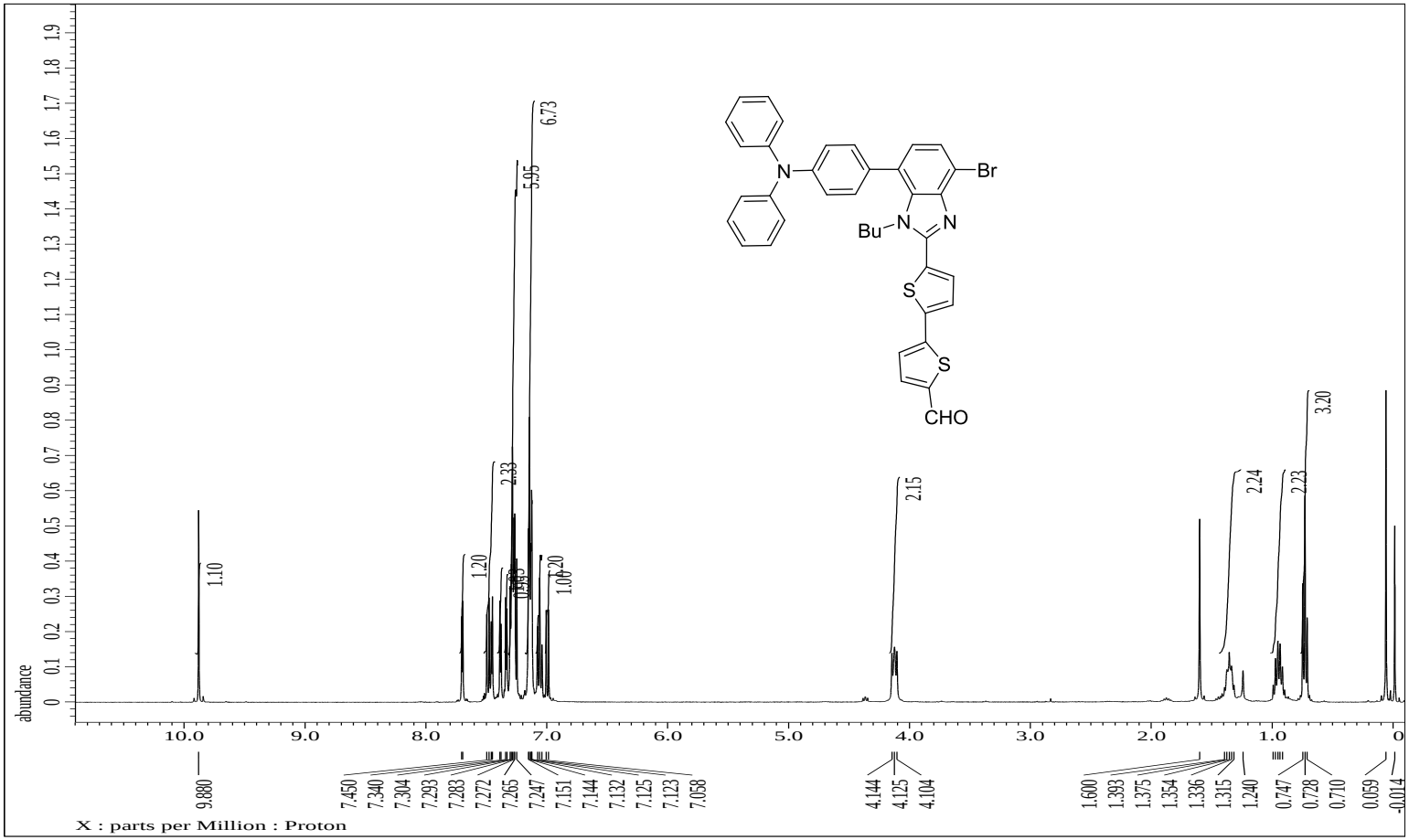

Figure S17. ^{1}H NMR spectra of **6** recorded in $CDCl_3$.

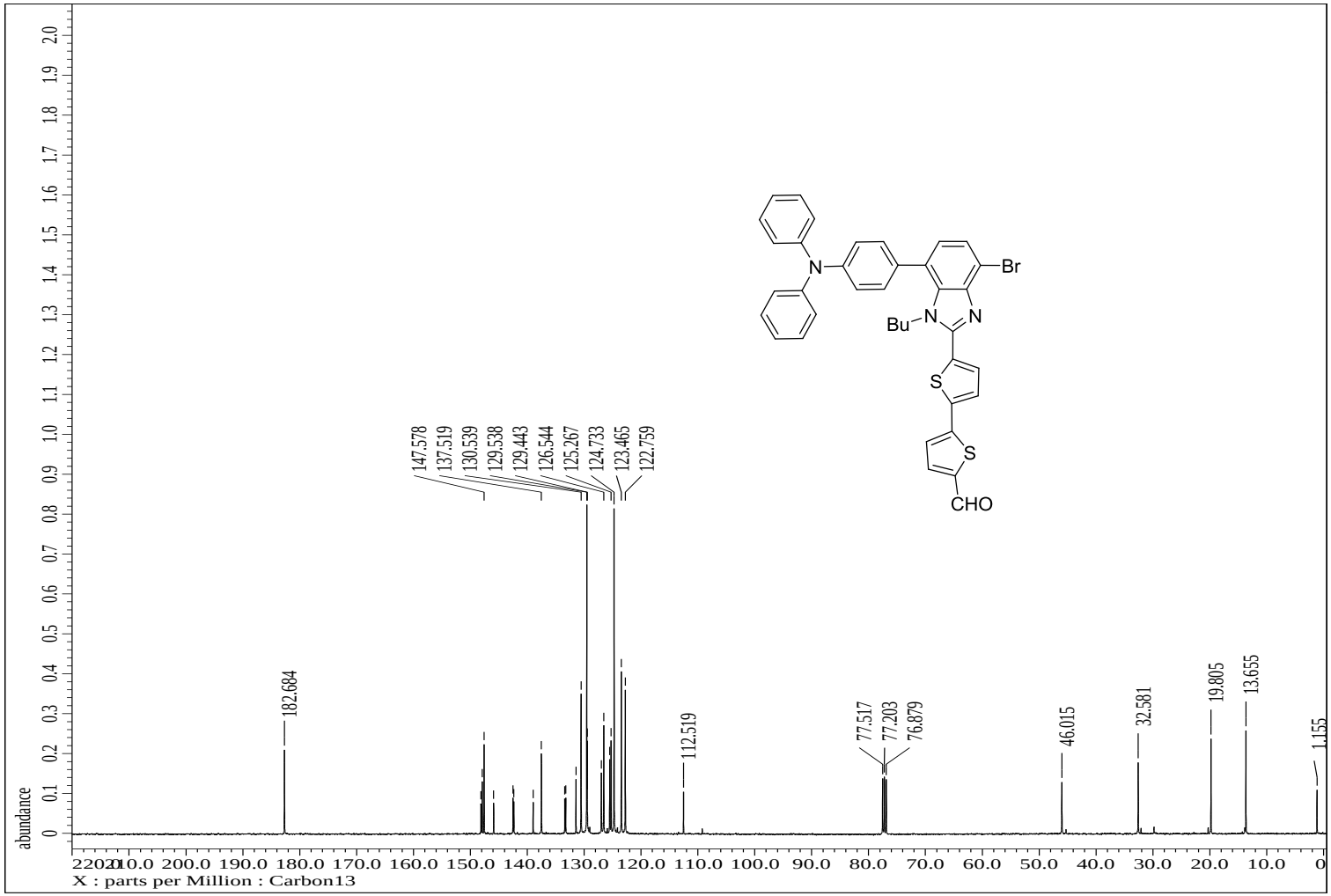

Figure S18. ^{13}C NMR spectra of **6** recorded in $CDCl_3$.

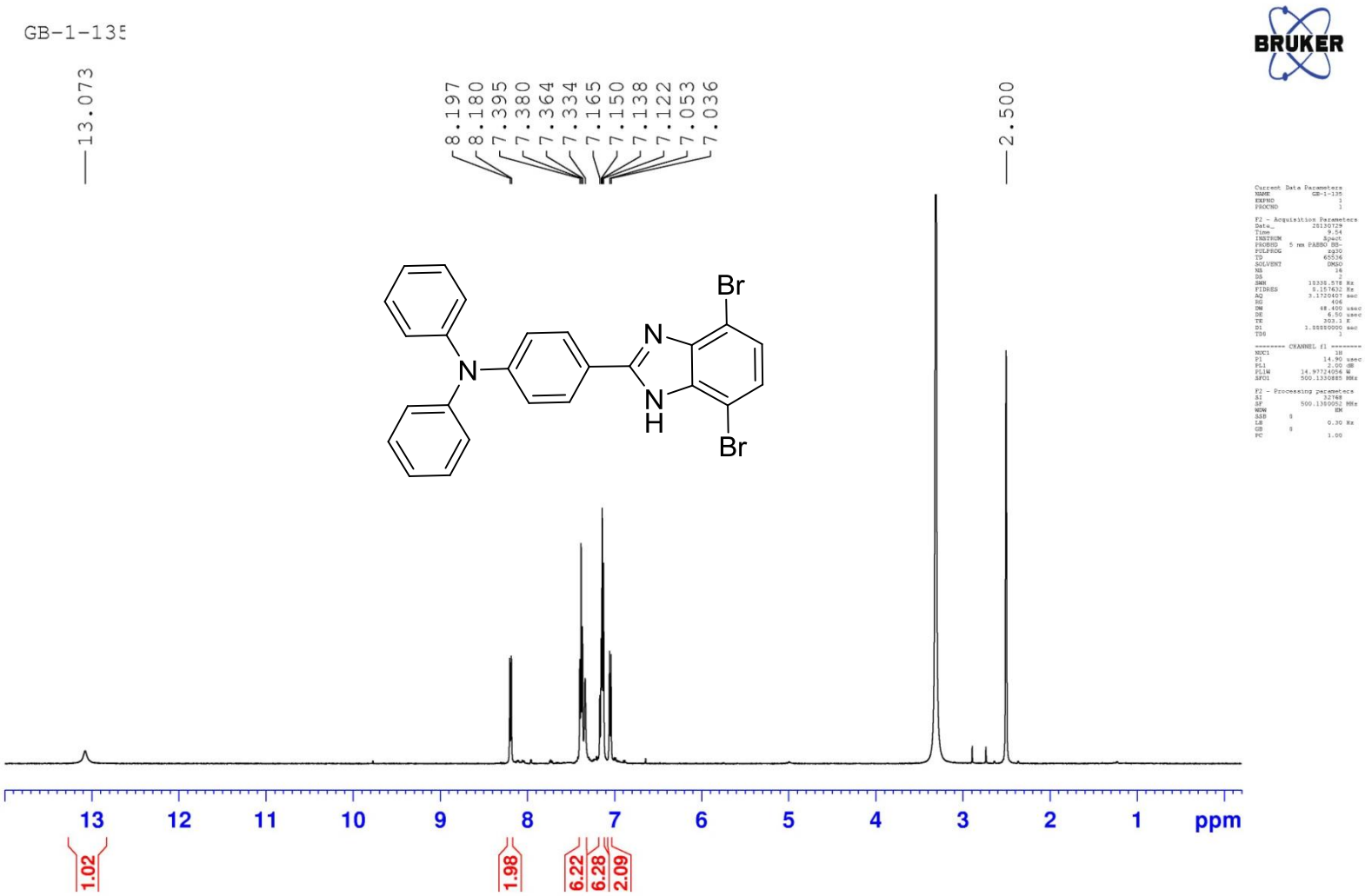

Figure S19. ^{1}H NMR spectra of **8** recorded in DMSO-d_6.

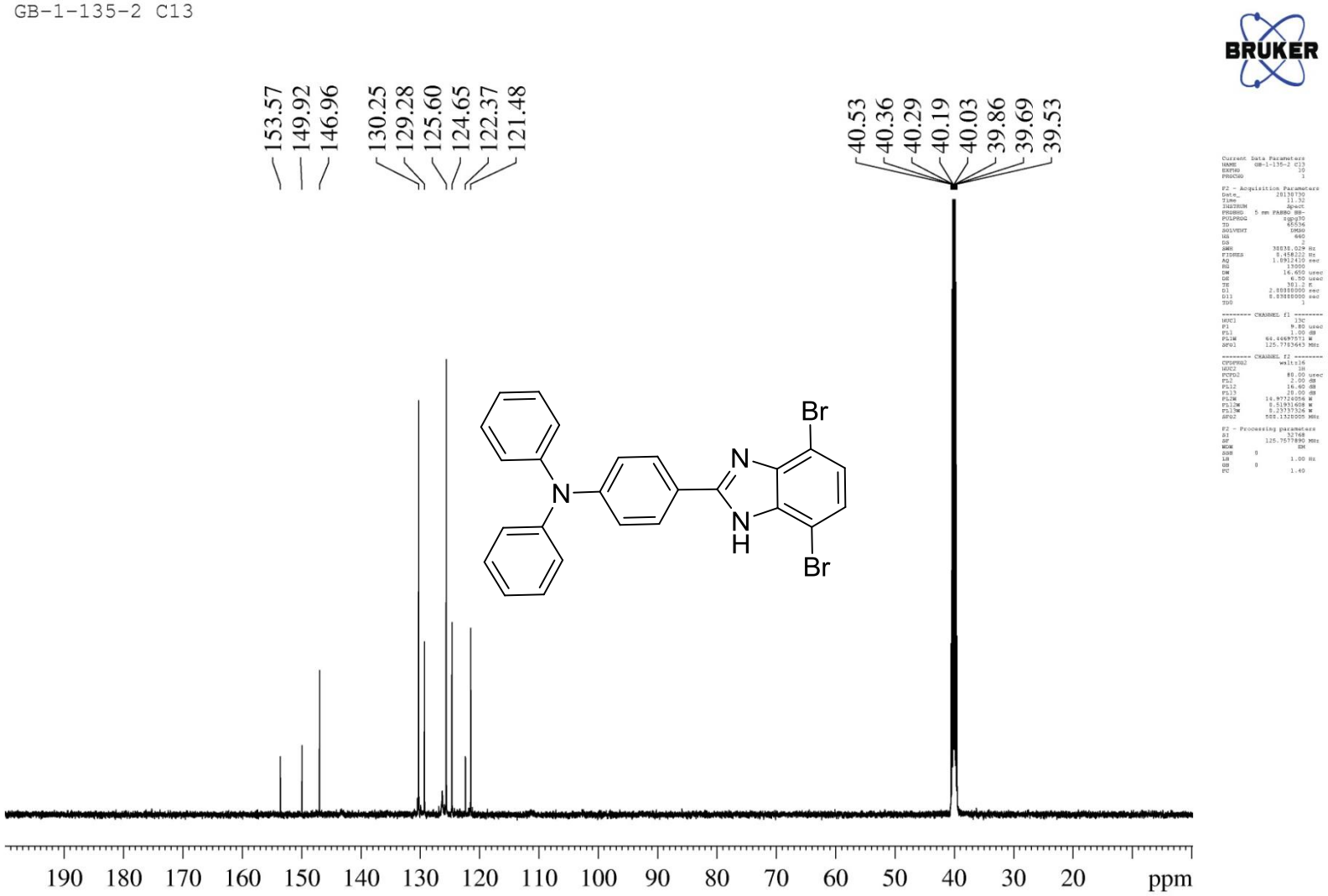

Figure S20. ^{13}C NMR spectra of **8** recorded in DMSO-d_6.

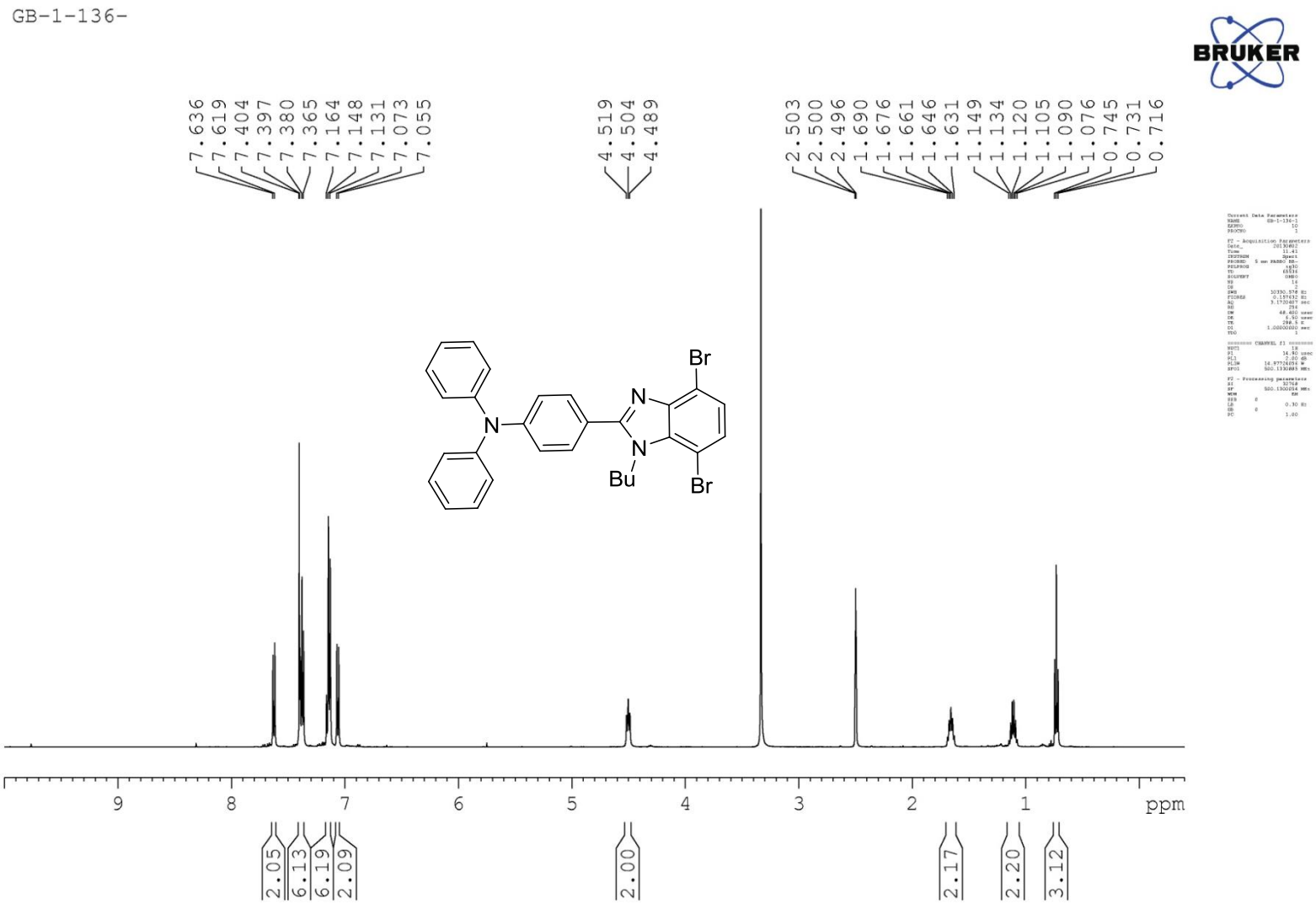

Figure S21. ^{1}H NMR spectra of **9** recorded in DMSO-d_6.

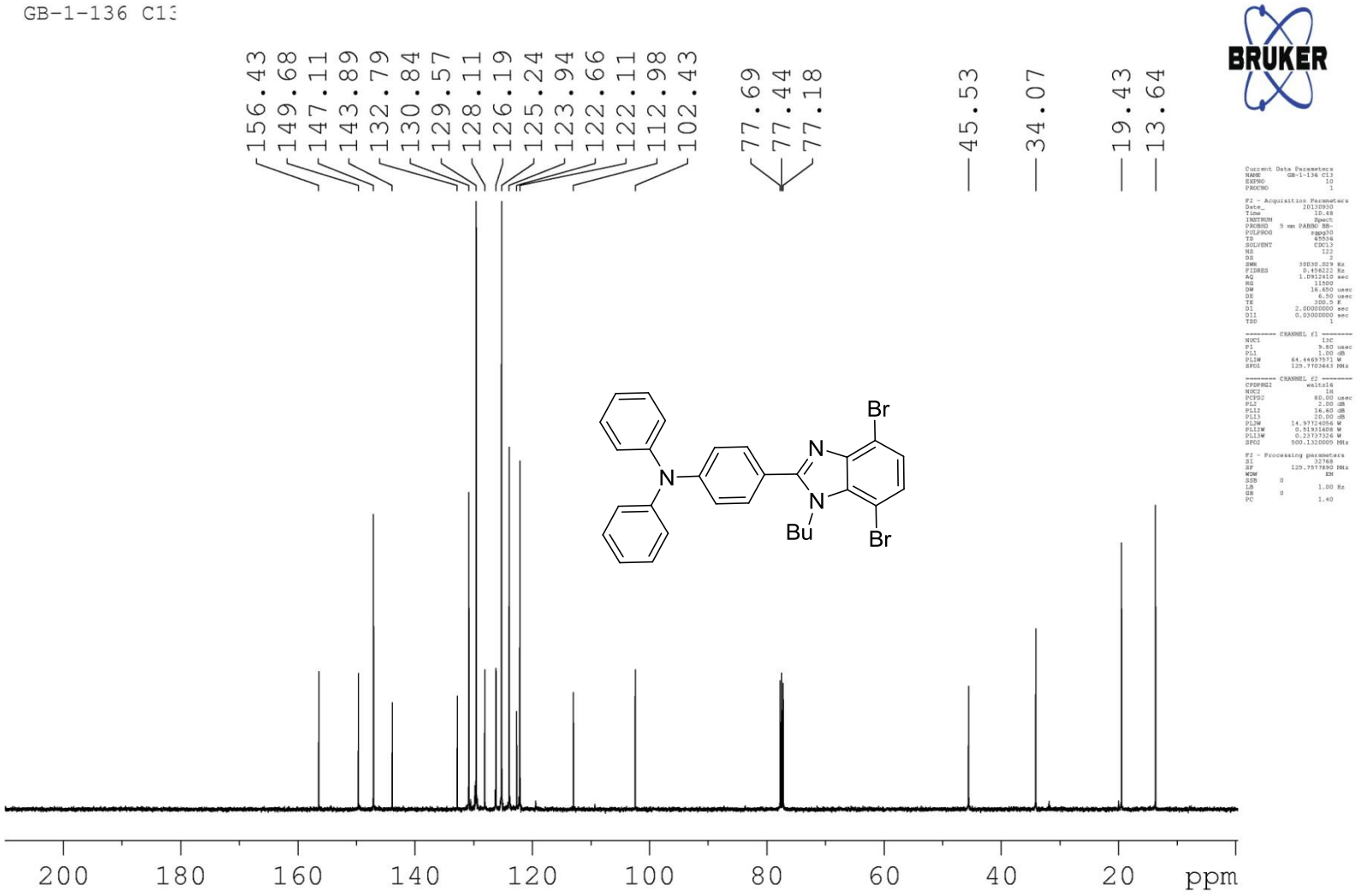

Figure S22. ^{13}C NMR spectra of **9** recorded in $CDCl_3$.

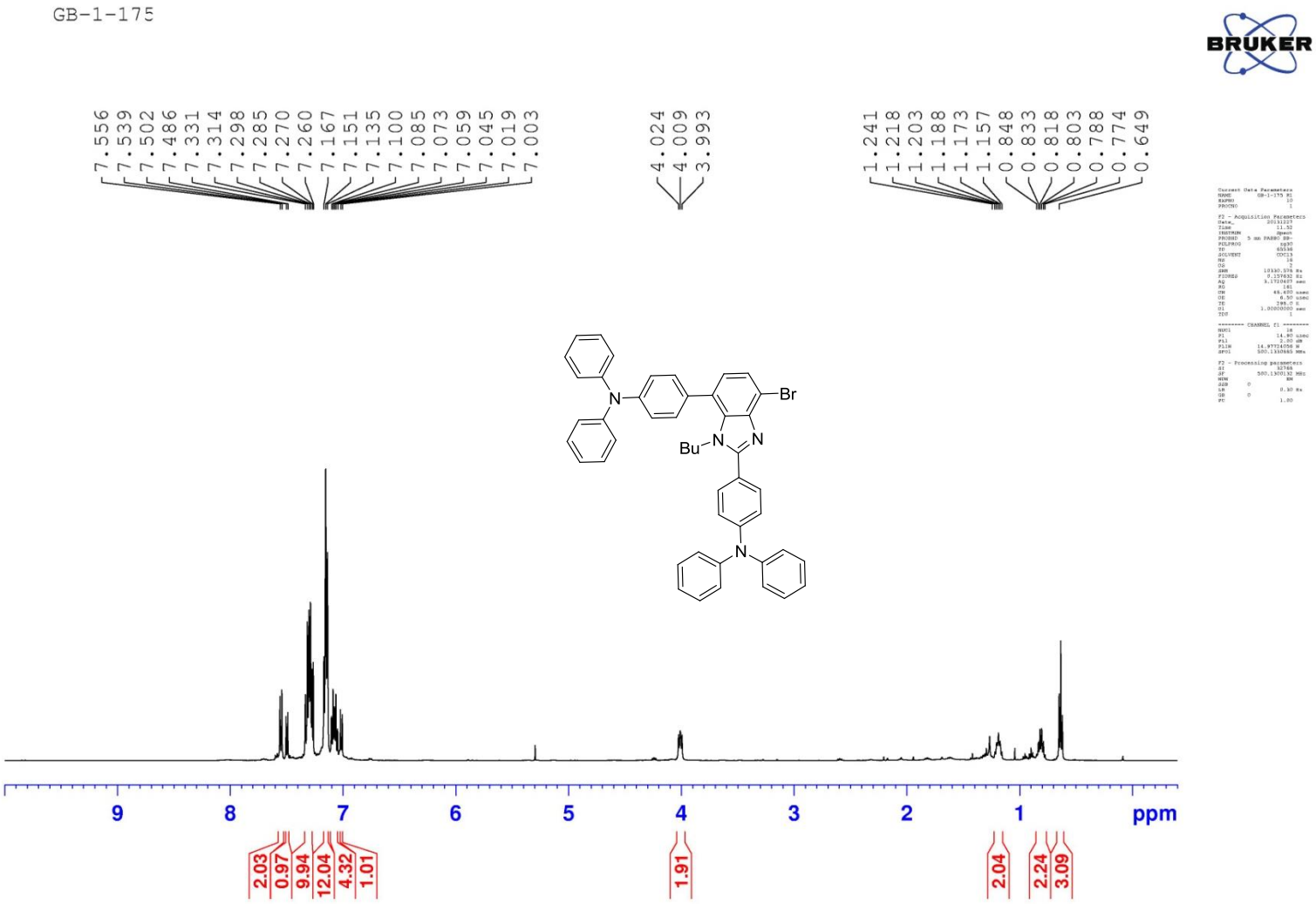

Figure S23. ^{1}H NMR spectra of **10** recorded in $CDCl_3$.

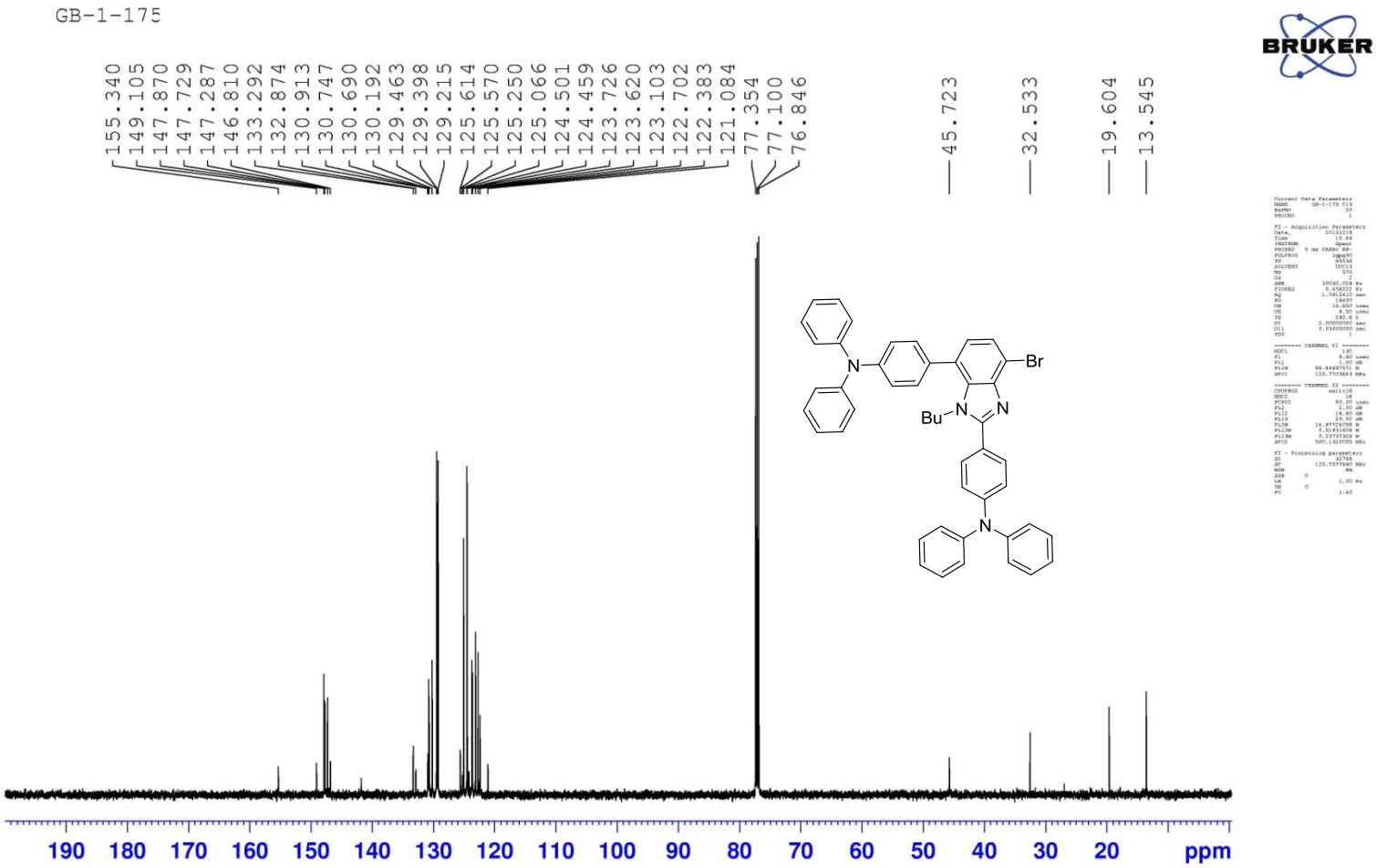

Figure S24. ^{13}C NMR spectra of **10** recorded in $CDCl_3$.

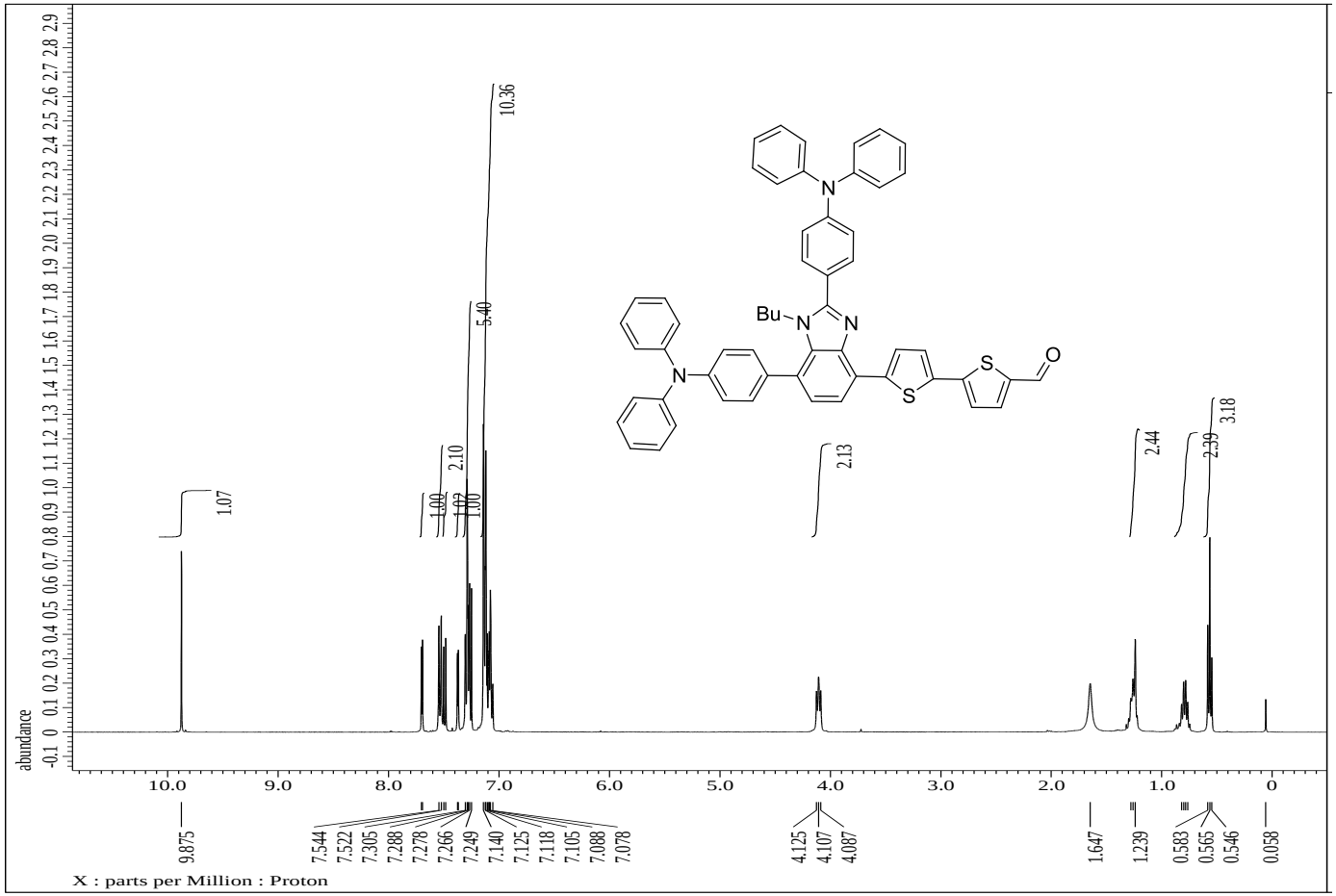

Figure S25. ^{1}H NMR spectra of **11** recorded in $CDCl_3$.

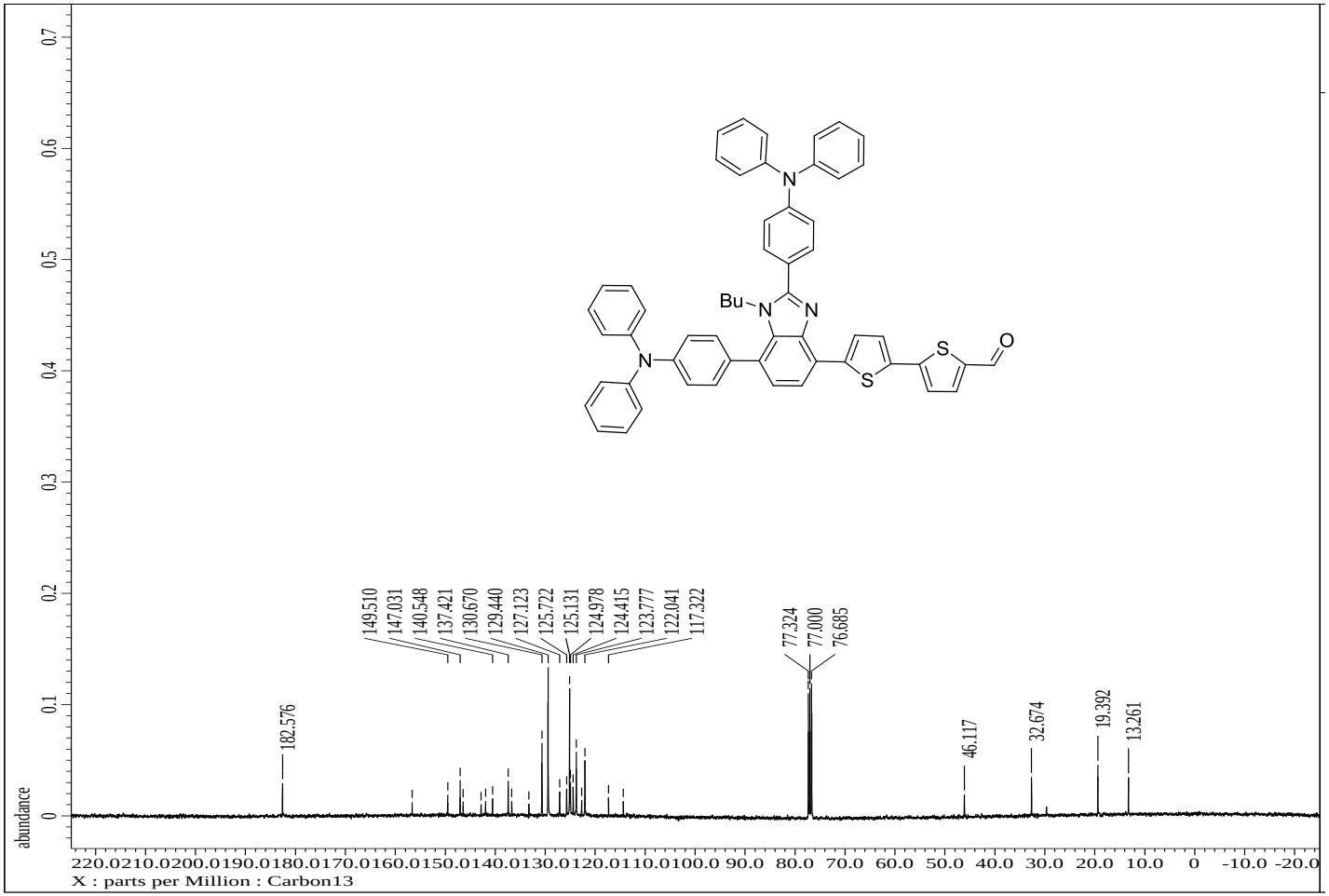

Figure S26. ^{13}C NMR spectra of **11** recorded in $CDCl_3$.

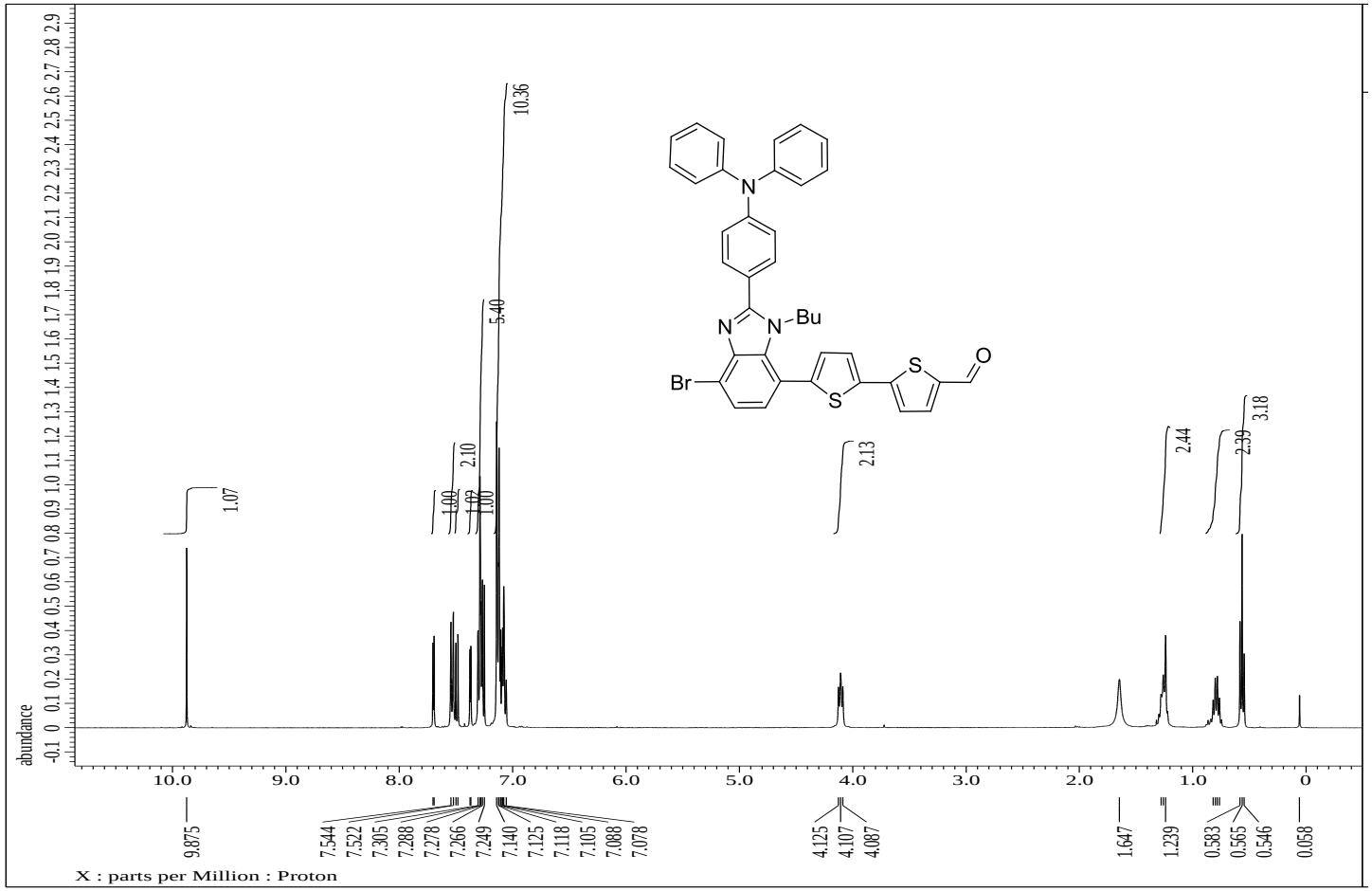

Figure S27. ^{1}H NMR spectra of **12** recorded in $CDCl_3$.

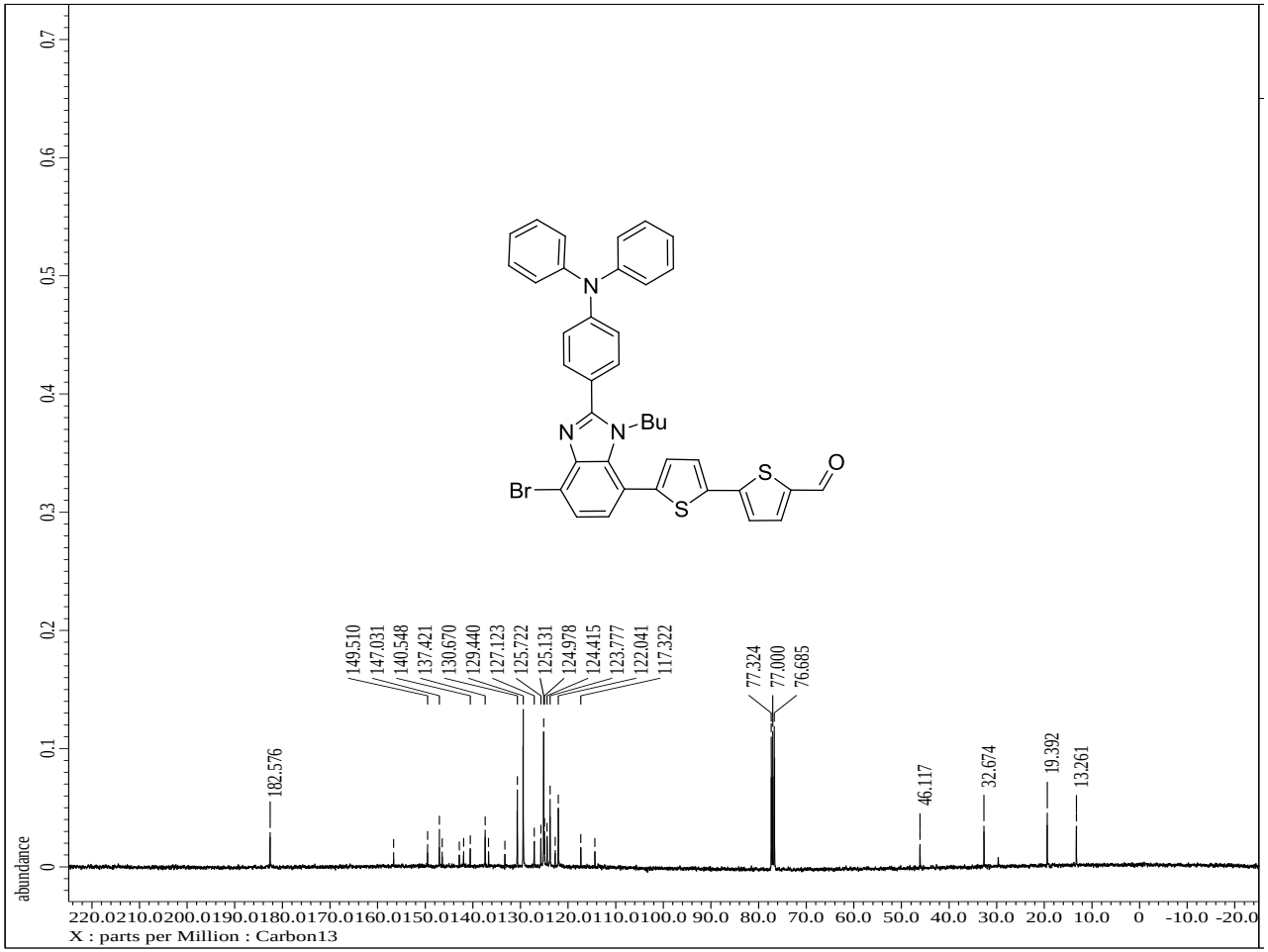

Figure S28. ^{13}C NMR spectra of **12** recorded in $CDCl_3$.

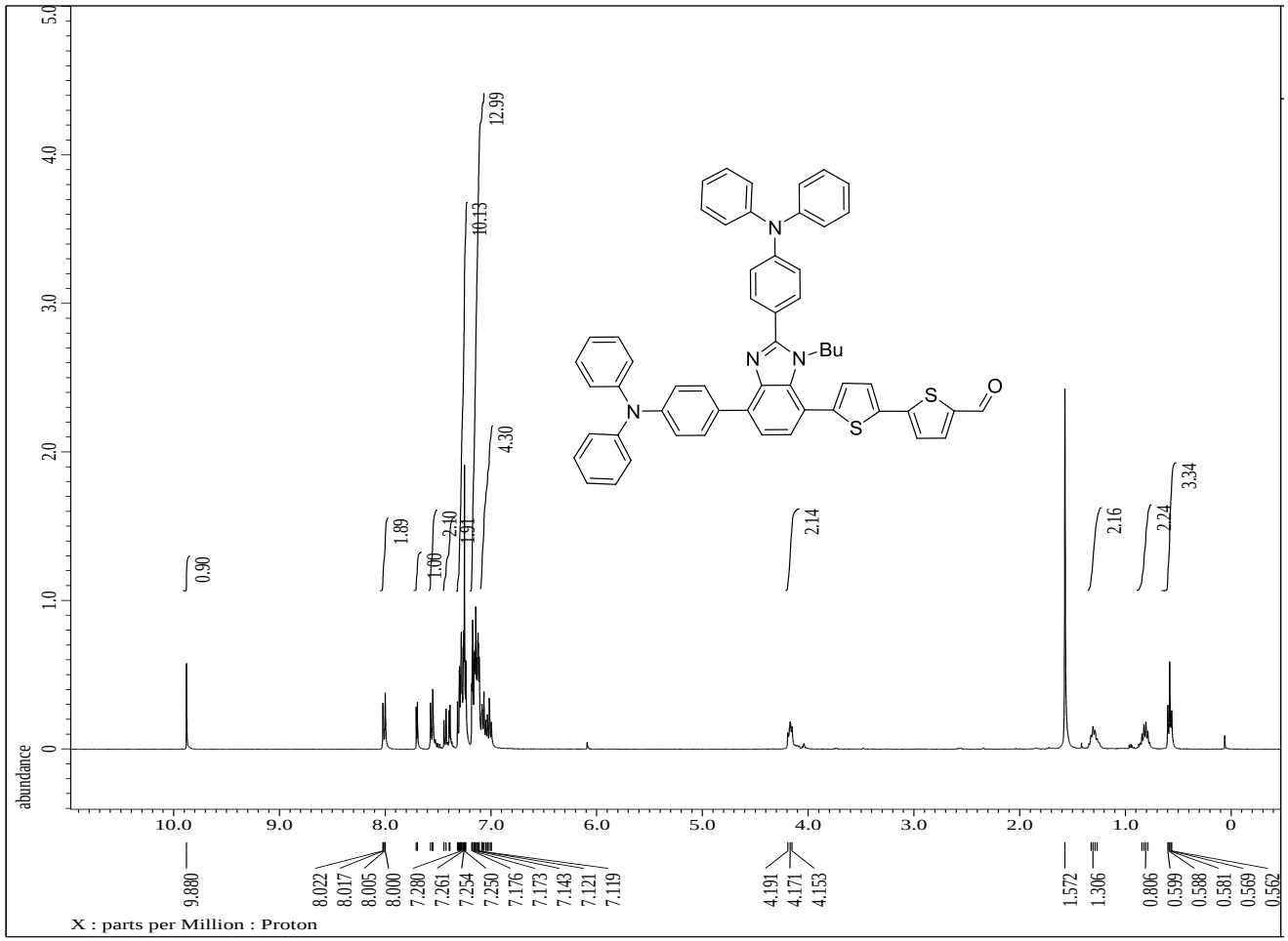

Figure S29. ^{1}H NMR spectra of **13** recorded in $CDCl_3$.

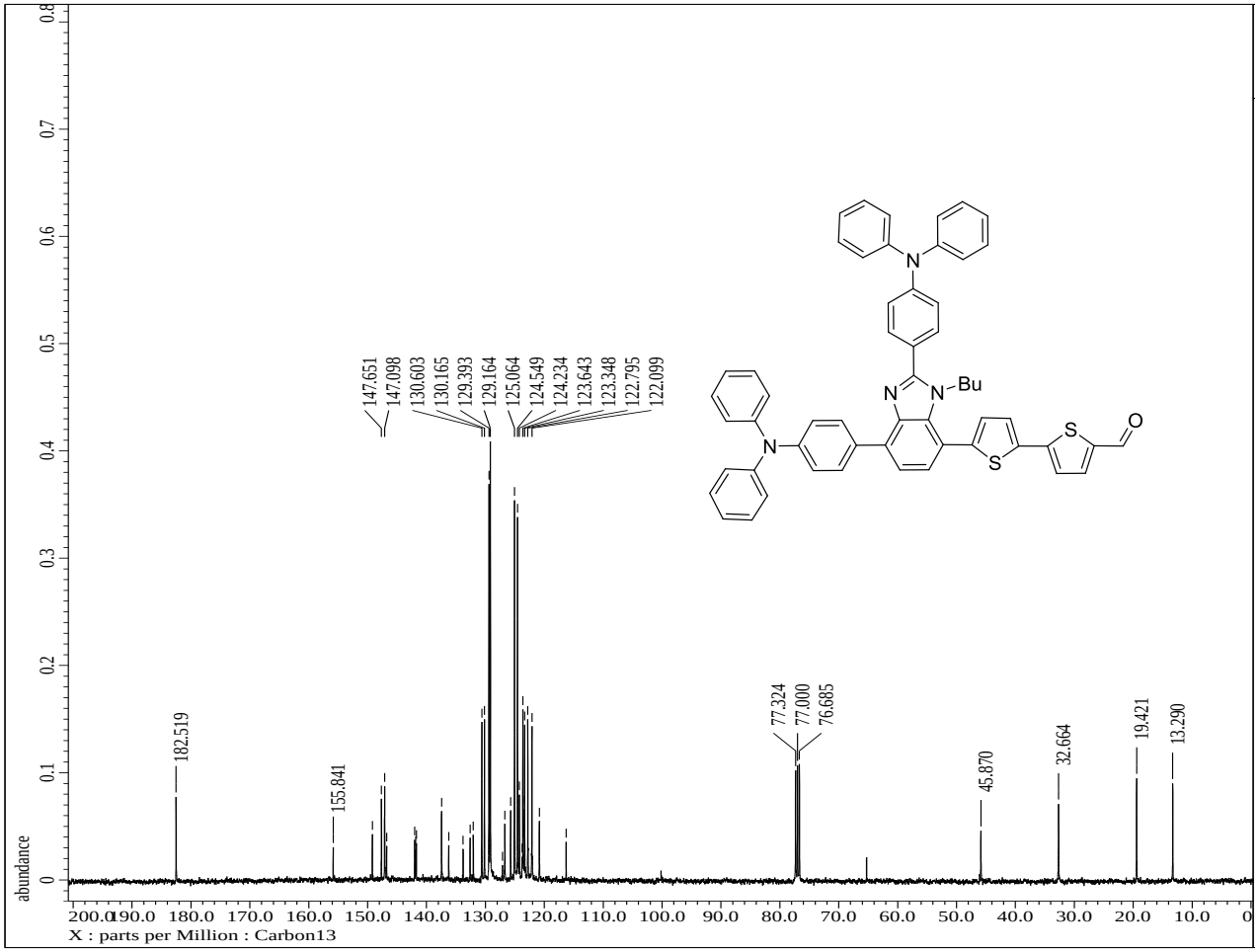

Figure S30. ^{13}C NMR spectra of **13** recorded in $CDCl_3$.

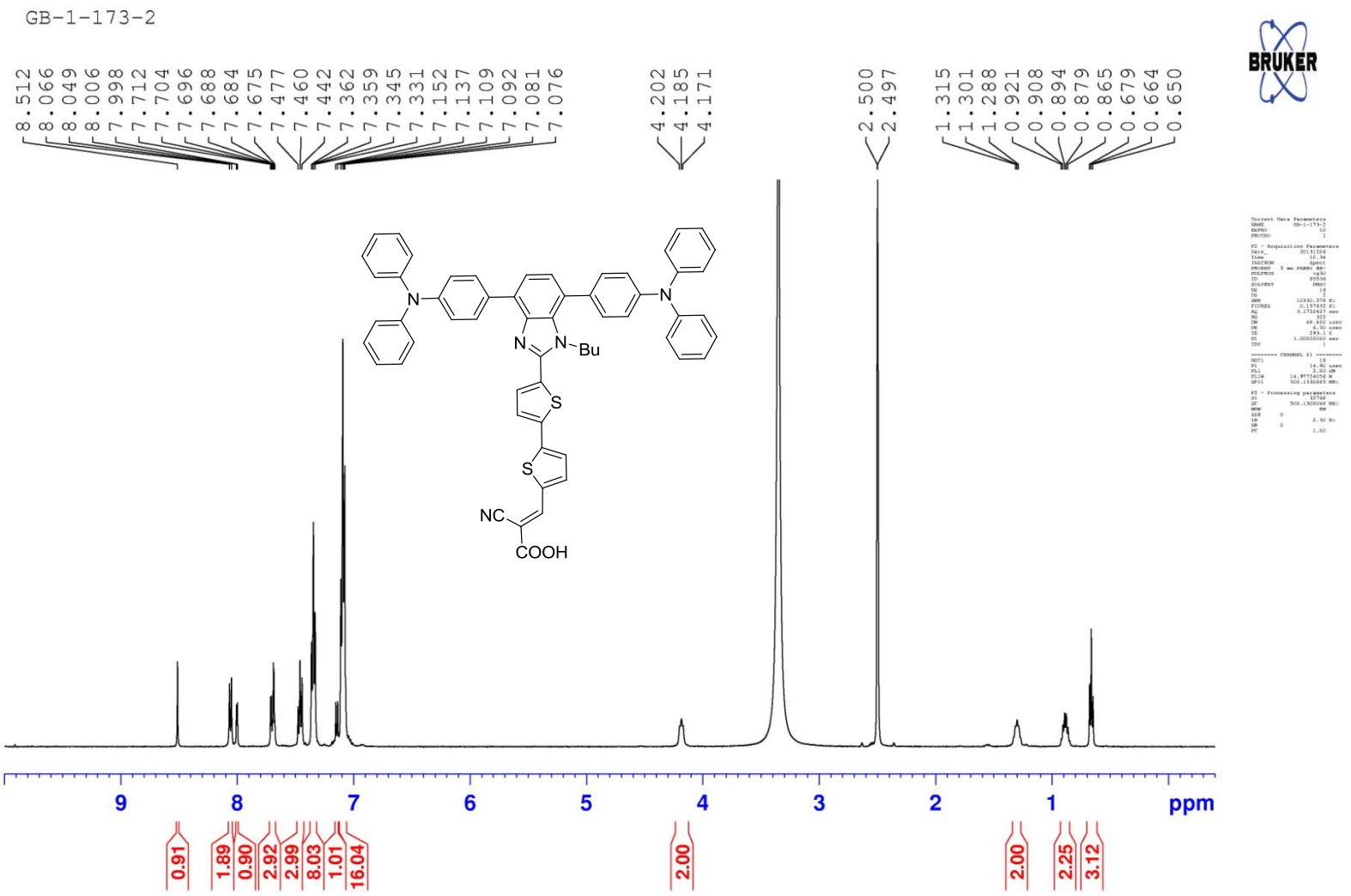

Figure S31. ^{1}H NMR spectra of **7a** recorded in DMSO-d_6.

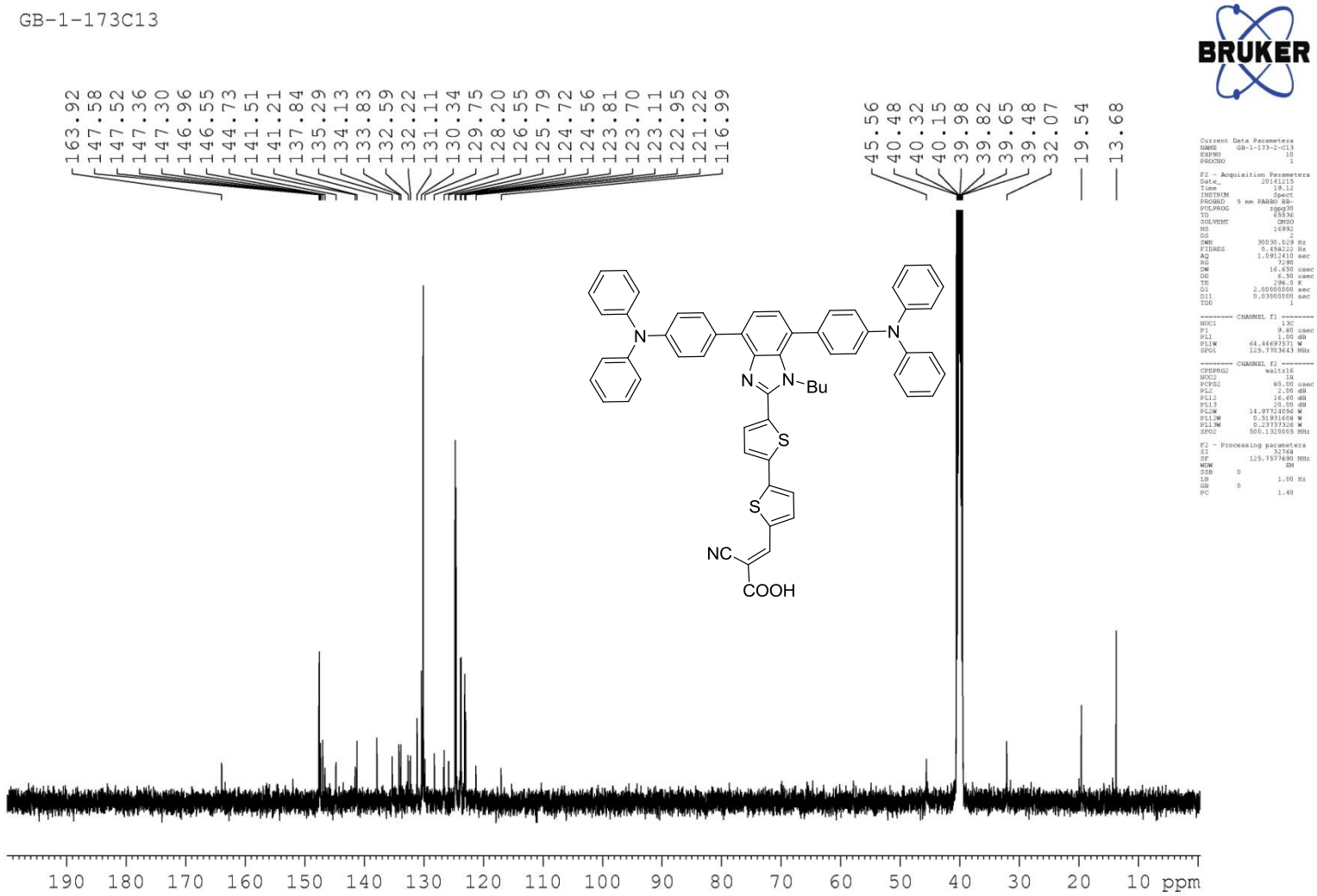

Figure S32. ^{13}C NMR spectra of **7a** recorded in DMSO-d_6.

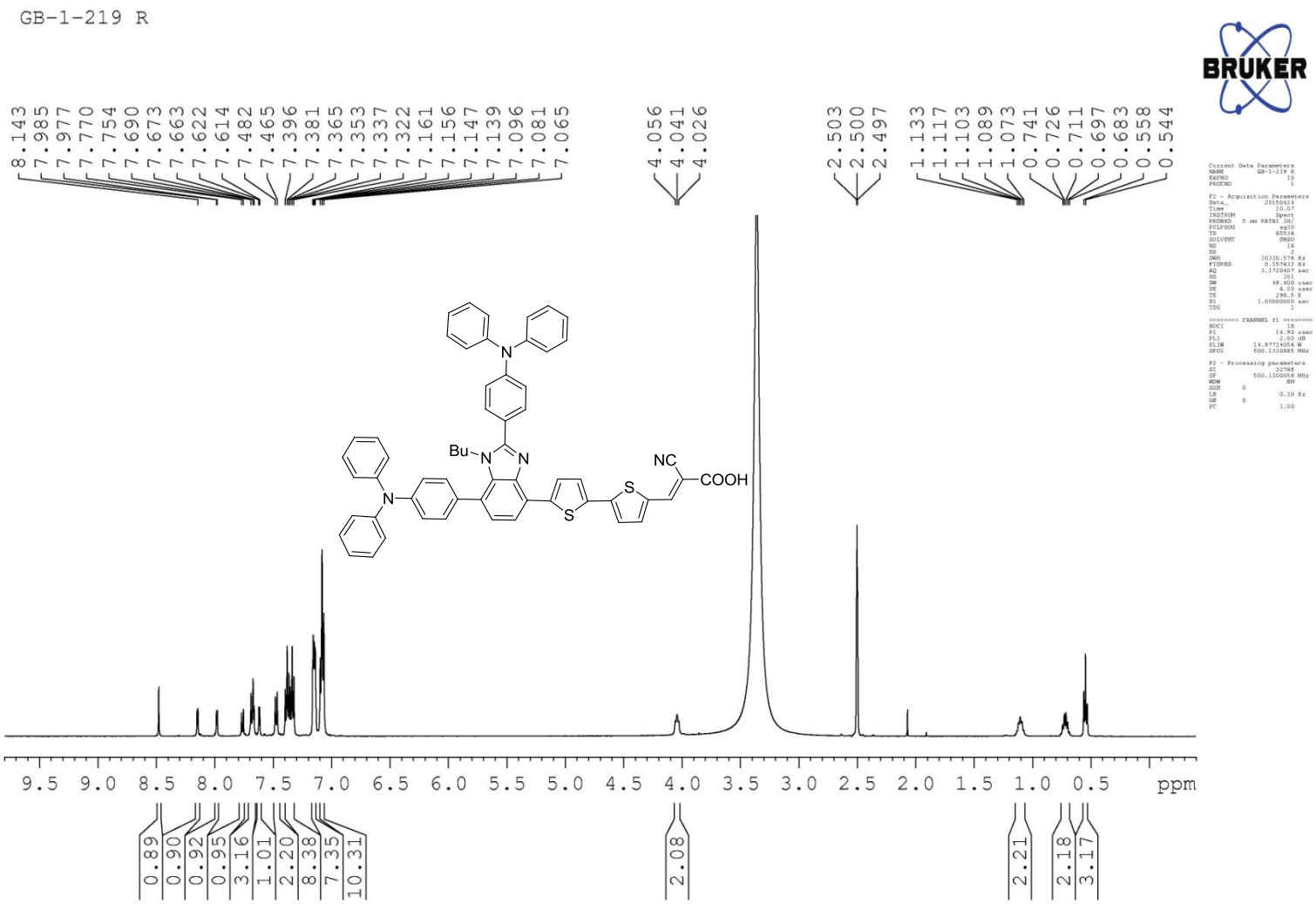

Figure S33. ^{1}H NMR spectra of **7b** recorded in DMSO-d_6.

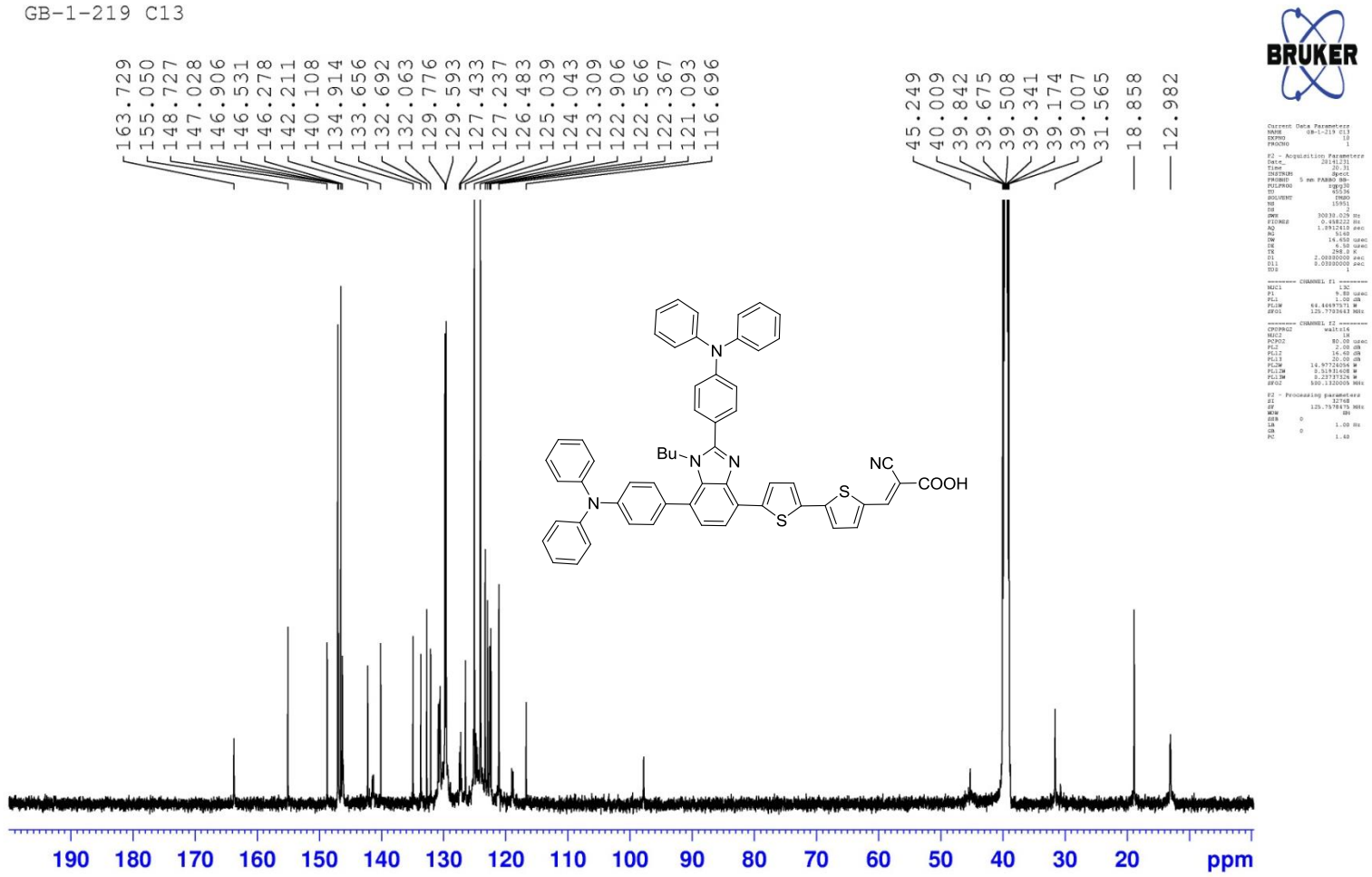

Figure S34. ^{13}C NMR spectra of **7b** recorded in DMSO-d_6.

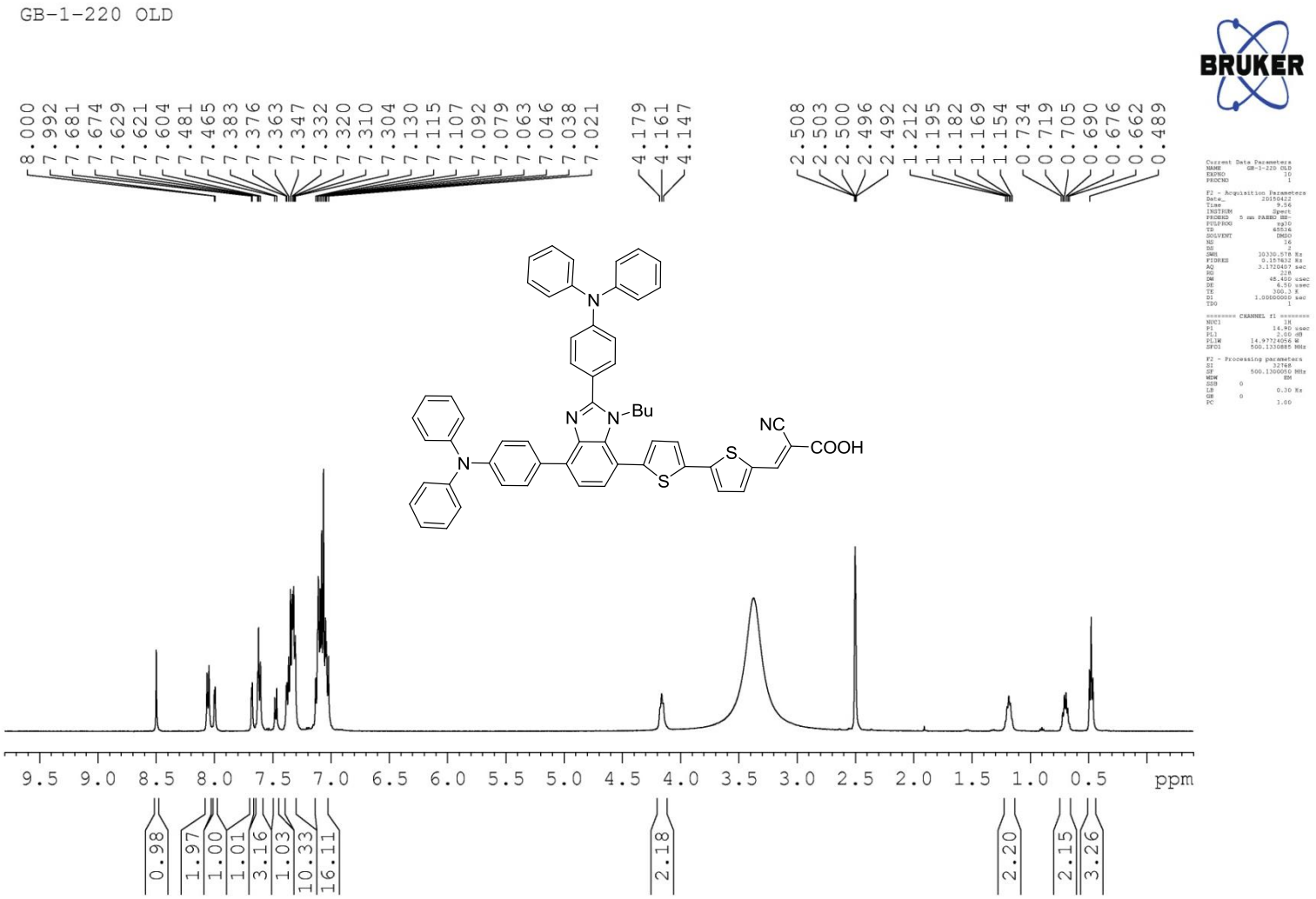

Figure S35. ^{1}H NMR spectra of **7c** recorded in DMSO-d_6.

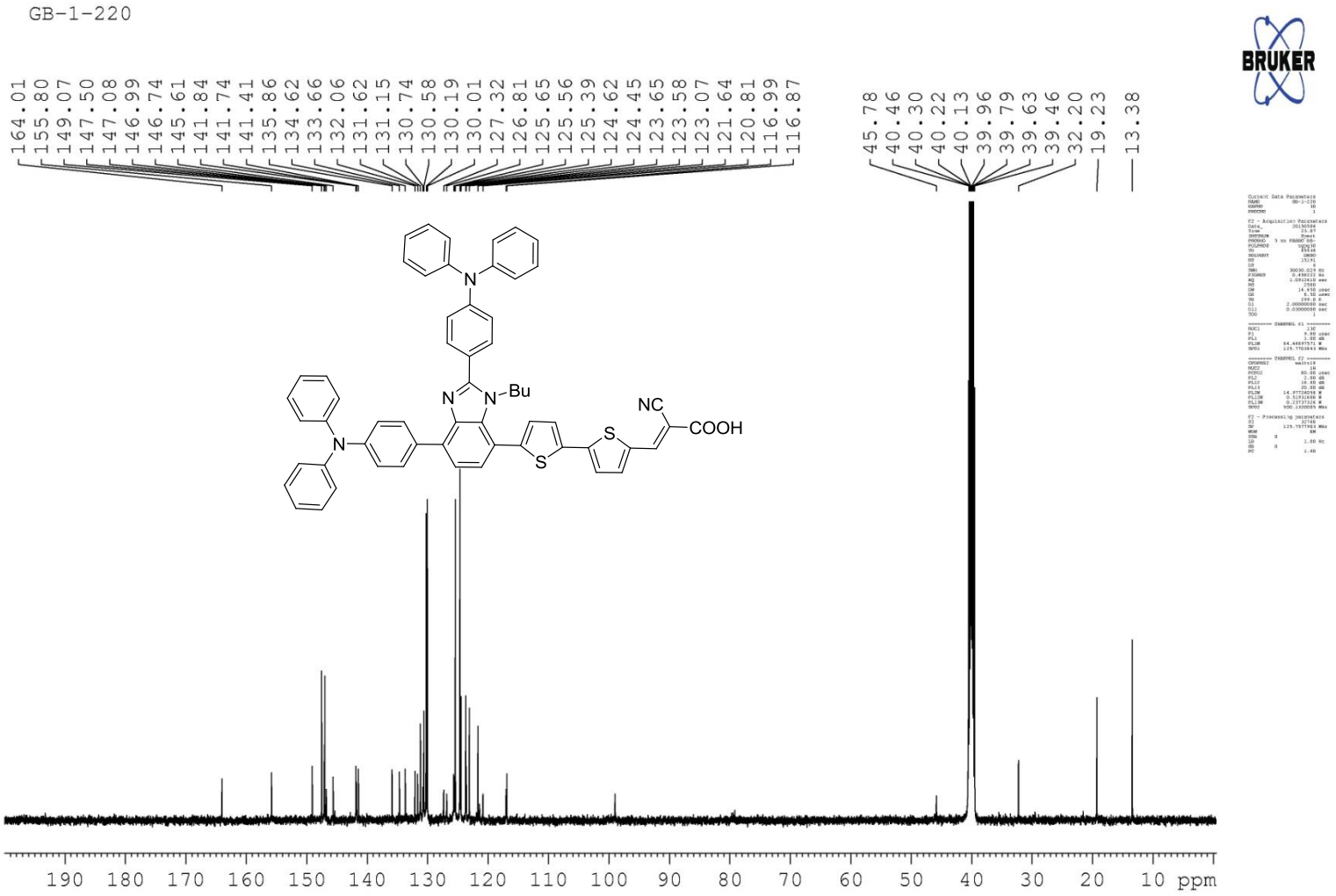

Figure S36. ^{13}C NMR spectra of **7c** recorded in DMSO-d_6.

Computational Methods. All the computations were performed with the Gaussian 09 program package. The ground-state geometries were fully optimized without any symmetry constraints at the DFT level with Becke's three parameters hybrid functional and Lee, Yang and Parr's correlational functional (B3LYP) using 6-31G(D, P) basis set on all atoms. The default parameters for the convergence criteria were used. Vibrational analyses on the optimized structures were performed to confirm the structure. No negative frequency vibrations were observed for the optimized geometries. The excitation energies and oscillator strengths for the lowest 10 singlet transitions for the optimized geometry in the ground state were obtained by TD-DFT calculations using the same basis set.

X-ray Crystal Structure Determination. Crystals of the compounds **6** suitable for X-ray data collection were grown from dichloromethane/hexane mixture. X-ray data of **6** was collected on a CCD diffractometer using Mo Kα (λ=0.71073). The data were corrected for Lorentz and polarization effects. A total of 29055 reflections were measured out of which 8174 were independent and 2383 were observed [I>2 σ(I)] for maximum theta 28.341° at room temperature. The structures were solved by direct methods using SHELXS-97 and refined by full-matrix least squares refinement methods based on F^2, using SHELXL-2014/7. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were fixed geometrically with their U_{iso} values 1.2 times of the phenylene and methylene carbons and 1.5 times of the methyl carbons. All calculations were performed using Bruker SHELXTL package. A final refinement of 410 parameters gave R_1 = 0.0534, wR_2 = 0.1326 for the observed data and R_1 = 0.2493, wR_2 = 0.2249 for all data.

Table S1. Crystal data and structure refinement for **6**.

Empirical formula	C38 H30 Br N3 O S2	
Formula weight	688.68	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.0416(5) Å	a= 99.687(3)°.
	b = 12.3341(6) Å	b= 97.512(3)°.
	c = 14.3639(7) Å	g = 104.946(3)°.
Volume	1665.77(14) $Å^3$	
Z	2	
Density (calculated)	1.373 Mg/m^3	
Absorption coefficient	1.394 mm^{-1}	
F(000)	708	
Crystal size	0.12 x 0.09 x 0.07 mm^3	
Theta range for data collection	1.463 to 28.341°.	
Index ranges	-13<=h<=13, -16<=k<=12, -19<=l<=19	
Reflections collected	29055	
Independent reflections	8174 [R(int) = 0.1032]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8174 / 0 / 410	
Goodness-of-fit on F^2	0.877	
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1326	
R indices (all data)	R1 = 0.2493, wR2 = 0.2249	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.324 and -0.330 $e.Å^{-3}$	

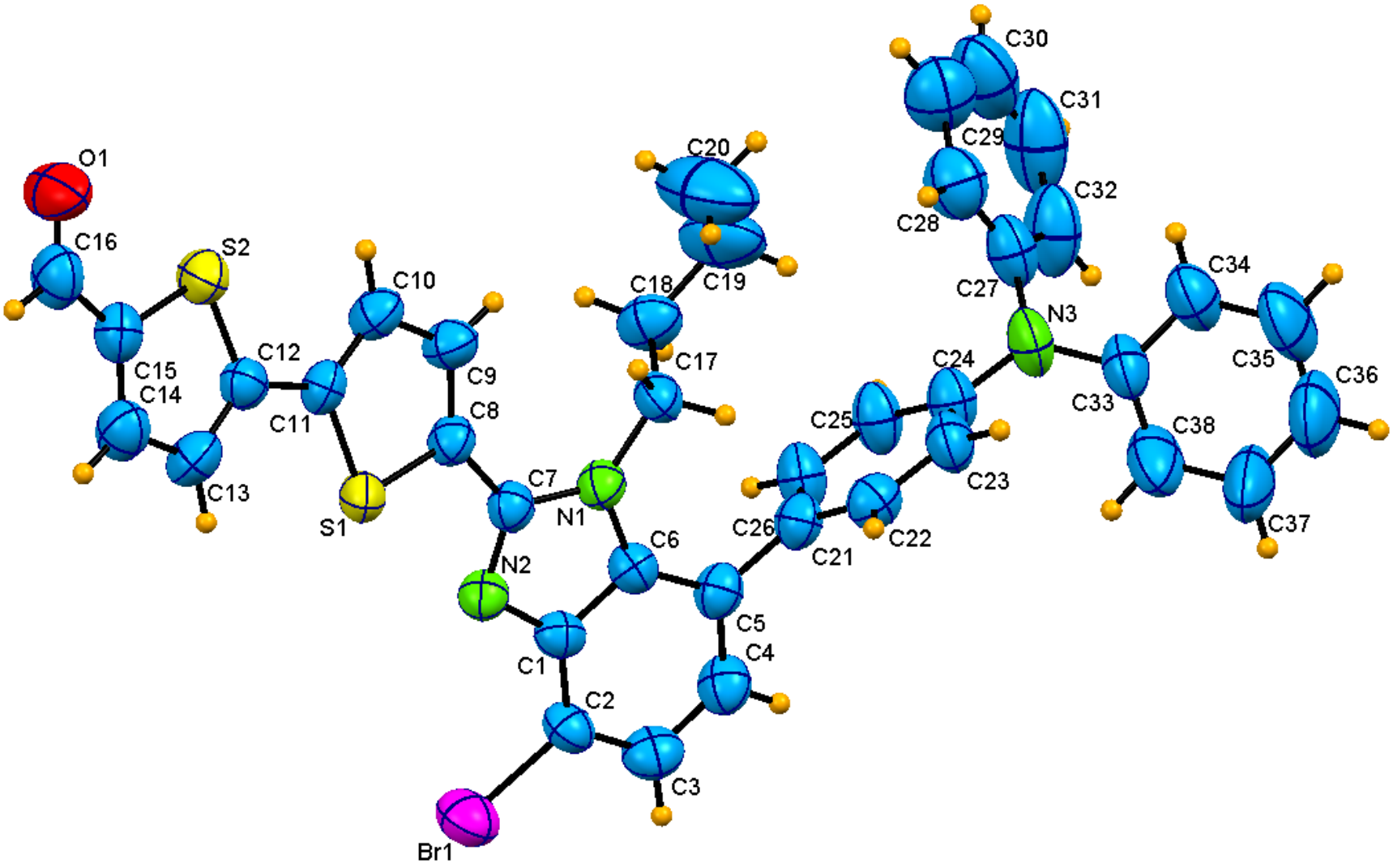

Figure S37. Molecular structure of **6** (40% thermal ellipsoids).

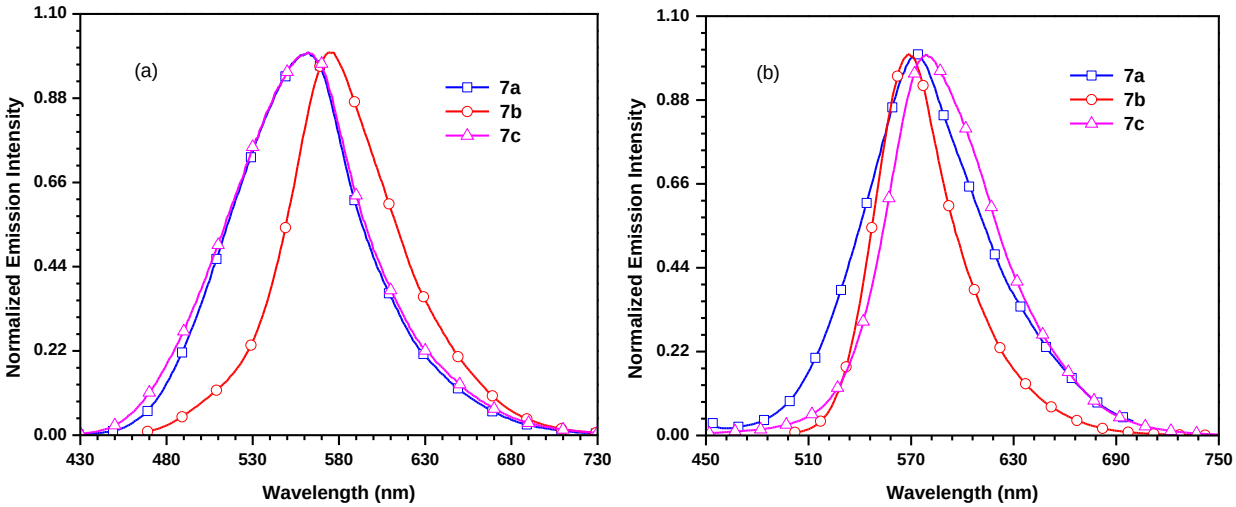

Figure S38. Emission spectra of the dyes recorded in (a) THF and (b) toluene.

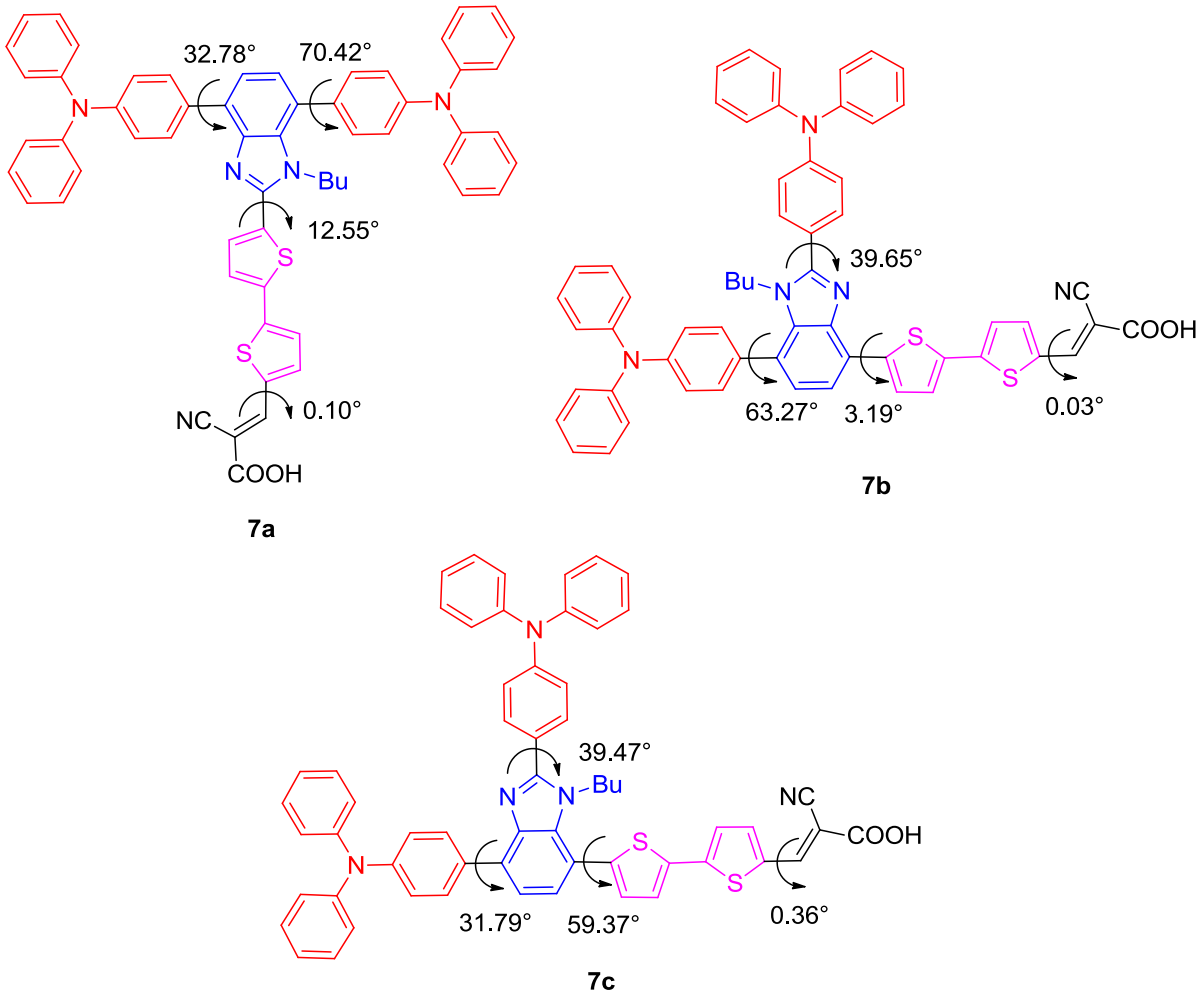

Figure S39. Calculated interplanar angles between various aromatic segments in the dyes.

Table S1. Cartesian coordinates for the optimized structure of **7a**.

Total Energy: -3495.97535867 hartrees

At. No.	X	Y	Z
6	0.334352	0.298817	-0.0765742
7	1.102609	-0.777009	-0.096339
7	-1.020005	-0.012184	-0.067714
6	0.250673	-1.851807	-0.079954
6	-1.100368	-1.405536	-0.072385
6	0.582845	-3.230604	-0.063396
6	-2.188191	-2.305266	-0.066237
6	-0.505009	-4.106533	-0.018144
6	-1.833379	-3.657903	-0.021700
1	-0.321521	-5.174994	0.038060
1	-2.633931	-4.392329	-0.003970
6	-2.141171	0.916935	0.085991
6	-2.523984	1.168740	1.550744
1	-2.992850	0.504906	-0.455315
1	-1.878444	1.850925	-0.417611
6	-3.715099	2.126135	1.680381
1	-2.769743	0.207601	2.019179
1	-1.659088	1.572865	2.093114
6	-4.111068	2.388467	3.136835
1	-3.474538	3.079337	1.188075
1	-4.573870	1.706693	1.137486
1	-4.963449	3.074022	3.199856
1	-4.393494	1.457619	3.642824
1	-3.281550	2.833646	3.699270
6	-3.636210	-1.947341	-0.124377
6	-4.479532	-2.178554	0.973289
6	-4.223565	-1.453149	-1.301346
6	-5.843692	-1.903477	0.913267
1	-4.054798	-2.565908	1.895713
6	-5.588409	-1.191608	-1.378563
1	-3.603987	-1.300176	-2.181647
6	-6.422223	-1.408220	-0.267452
1	-6.468517	-2.075366	1.783618
1	-6.018339	-0.829814	-2.306827
7	-7.811758	-1.142535	-0.339483
6	-8.740098	-2.001304	0.316302
6	-8.294253	-0.028161	-1.081969
6	-9.811325	-1.461631	1.045183
6	-8.601534	-3.396062	0.238519

6	-9.414995	-0.162281	-1.916812
6	-7.663873	1.222647	-0.985431
6	-10.726384	-2.302987	1.675443
1	-9.920795	-0.383758	1.111601
6	-9.510865	-4.229324	0.887603
1	-7.780396	-3.819851	-0.331035
6	-9.894716	0.933933	-2.631261
1	-9.904926	-1.127242	-1.999587
6	-8.139575	2.308774	-1.717660
1	-6.803435	1.337264	-0.333291
6	-10.580224	-3.690013	1.605826
1	-11.550556	-1.869117	2.235571
1	-9.389233	-5.307063	0.817561
6	-9.259050	2.174065	-2.541475
1	-10.763560	0.811853	-3.272667
1	-7.639584	3.269947	-1.630408
1	-11.291217	-4.342555	2.104380
1	-9.631646	3.024462	-3.105217
6	1.973993	-3.732722	-0.090310
6	2.279547	-4.953675	-0.720359
6	3.035260	-3.042772	0.524811
6	3.571037	-5.465914	-0.735493
1	1.498023	-5.495140	-1.245893
6	4.326686	-3.557231	0.529640
1	2.838991	-2.097586	1.015871
6	4.618543	-4.777523	-0.101608
1	3.777606	-6.398947	-1.249898
1	5.120682	-3.013654	1.031825
7	5.937837	-5.298842	-0.105968
6	6.153006	-6.693788	0.064979
6	7.048707	-4.428717	-0.286834
6	7.102278	-7.370947	-0.717747
6	5.420652	-7.416527	1.021017
6	8.207922	-4.583026	0.490340
6	7.003670	-3.404303	-1.246157
6	7.316304	-8.736361	-0.539091
1	7.668111	-6.821161	-1.463133
6	5.629037	-8.785183	1.179582
1	4.690860	-6.899105	1.635640
6	9.298386	-3.735968	0.301948
1	8.246537	-5.368300	1.238615
6	8.092384	-2.550834	-1.414553
1	6.113169	-3.283153	-1.854665
6	6.579714	-9.454143	0.405638
1	8.055140	-9.243451	-1.154325
1	5.053125	-9.327666	1.924981

6	9.247792	-2.712595	-0.646922
1	10.187524	-3.869627	0.912724
1	8.040221	-1.763154	-2.161728
1	6.744633	-10.519748	0.537201
1	10.096861	-2.049439	-0.785679
6	0.950663	1.618573	-0.102399
6	2.299226	1.808753	-0.353181
16	0.180631	3.156907	0.231899
6	2.707766	3.154628	-0.290663
1	2.951759	0.973839	-0.573815
6	1.684557	4.035705	0.014773
1	3.728280	3.476251	-0.470459
6	1.729764	5.468173	0.150220
6	0.685861	6.342685	0.434767
16	3.237148	6.334777	-0.044669
6	1.090509	7.683356	0.493671
1	-0.335642	6.014481	0.592061
6	2.449157	7.879953	0.257852
1	0.418565	8.509568	0.702497
6	3.075910	9.159156	0.266900
6	4.381182	9.519620	0.054994
1	2.395036	9.979495	0.477890
6	5.410148	8.574684	-0.235385
6	4.819396	10.933950	0.112564
7	6.228850	7.780617	-0.471108
8	5.958122	11.311396	-0.066197
8	3.800796	11.792944	0.391400
1	4.206666	12.678986	0.402701

Table S2. Cartesian coordinates for the optimized structure of **7b**.

Total Energy: -3495.98141070 hartrees

At. No.	X	Y	Z
6	-0.116307	0.553529	0.080237
7	0.785825	-0.408937	0.019363
7	-1.415587	0.059590	0.095439
6	0.083670	-1.585948	0.011476
6	-1.312828	-1.333085	0.040713
6	0.615660	-2.895592	0.010449
6	-2.255864	-2.382906	0.029811
6	-0.331370	-3.930015	0.050071
6	-1.704375	-3.674246	0.055827
1	-0.002994	-4.963687	0.065124
1	-2.390407	-4.516400	0.049355
6	-2.644042	0.854753	0.148342
6	-3.303709	0.885772	1.533353
1	-3.346961	0.452377	-0.583696
1	-2.384967	1.864973	-0.176267
6	-4.541079	1.792148	1.556522
1	-3.587203	-0.133890	1.818719
1	-2.575579	1.226652	2.281818
6	-5.245116	1.802887	2.917234
1	-4.249959	2.816968	1.284599
1	-5.245348	1.459196	0.781199
1	-6.119890	2.462668	2.908314
1	-5.586370	0.797856	3.192264
1	-4.571915	2.152956	3.709144
6	0.268566	1.974767	0.077142
6	-0.338300	2.966249	0.866468
6	1.362863	2.356387	-0.721131
6	0.111605	4.281826	0.845751
1	-1.139438	2.708275	1.550695
6	1.808000	3.669767	-0.758686
1	1.852313	1.601746	-1.327701
6	1.186597	4.661801	0.023580
1	-0.361038	5.020747	1.483909
1	2.638862	3.938138	-1.402425
7	1.635116	5.999999	-0.009754
6	0.710863	7.075693	0.129499
6	3.020128	6.294028	-0.176645
6	1.004810	8.156591	0.974657
6	-0.497094	7.075735	-0.585409
6	3.426689	7.294592	-1.072283

6	3.991703	5.597760	0.558735
6	0.107408	9.216129	1.096666
1	1.937287	8.160104	1.530243
6	-1.396469	8.130924	-0.443426
1	-0.722783	6.248111	-1.250613
6	4.779536	7.594257	-1.222388
1	2.678187	7.832644	-1.645430
6	5.343504	5.891977	0.388791
1	3.681871	4.829195	1.260028
6	-1.099420	9.208250	0.394219
1	0.349505	10.045997	1.755312
1	-2.327210	8.116997	-1.004521
6	5.745764	6.893108	-0.497919
1	5.078731	8.371979	-1.920036
1	6.084172	5.344403	0.965622
1	-1.799151	10.032754	0.496580
1	6.799701	7.124797	-0.622067
6	-3.738232	-2.254572	-0.039875
6	-4.549332	-2.779025	0.980416
6	-4.383727	-1.712663	-1.164299
6	-5.938374	-2.739447	0.899791
1	-4.080107	-3.207674	1.862047
6	-5.771783	-1.683772	-1.263572
1	-3.787566	-1.351186	-1.998500
6	-6.574442	-2.194004	-0.228507
1	-6.538499	-3.135217	1.712648
1	-6.241242	-1.281768	-2.155462
7	-7.986734	-2.170282	-0.325615
6	-8.758757	-3.264535	0.159608
6	-8.646022	-1.067553	-0.938804
6	-9.931222	-3.031825	0.895337
6	-8.365219	-4.587308	-0.097228
6	-9.686780	-1.281665	-1.855902
6	-8.270883	0.249294	-0.629069
6	-10.694988	-4.102645	1.356161
1	-10.238001	-2.010913	1.100026
6	-9.125669	-5.651867	0.383381
1	-7.464815	-4.773658	-0.674070
6	-10.338721	-0.199182	-2.443884
1	-9.978958	-2.297615	-2.101952
6	-8.916197	1.325416	-1.235451
1	-7.477587	0.420868	0.092060
6	-10.296007	-5.417783	1.108430
1	-11.600421	-3.905446	1.924078
1	-8.807399	-6.670055	0.175493
6	-9.955650	1.109540	-2.142837

1	-11.142549	-0.382715	-3.151943
1	-8.613953	2.338711	-0.983849
1	-10.890004	-6.249903	1.475304
1	-10.461761	1.950551	-2.608019
6	2.048549	-3.168981	-0.020812
6	2.660436	-4.412991	-0.083973
16	3.265217	-1.903897	0.027244
6	4.066445	-4.365374	-0.090058
1	2.106229	-5.342838	-0.130114
6	4.571151	-3.076688	-0.032813
1	4.692905	-5.250298	-0.137208
6	5.946211	-2.655959	-0.023364
6	6.450709	-1.358595	0.033342
16	7.245928	-3.827558	-0.086541
6	7.849806	-1.309688	0.025861
1	5.815306	-0.481266	0.079031
6	8.467115	-2.558529	-0.036164
1	8.423295	-0.388925	0.064524
6	9.876663	-2.741196	-0.054233
6	10.637034	-3.882825	-0.112704
1	10.438803	-1.811882	-0.014500
6	10.071111	-5.191106	-0.170240
6	12.115406	-3.833782	-0.119926
7	9.584135	-6.248262	-0.216410
8	12.841670	-4.805071	-0.169818
8	12.606298	-2.563428	-0.063812
1	13.575432	-2.664794	-0.074717

Table S3. Cartesian coordinates for the optimized structure of **7c**.

Total Energy: -3495.97736545 hartrees

At. No.	X	Y	Z
6	0.690349	0.810167	-0.117194
7	1.540734	-0.194897	-0.143868
7	-0.635406	0.390223	-0.195827
6	0.777995	-1.337836	-0.222123
6	-0.603466	-1.001425	-0.277246
6	1.226176	-2.680327	-0.232943
6	-1.602554	-1.997962	-0.385846
6	0.219583	-3.652664	-0.288233
6	-1.135352	-3.322438	-0.363075
1	0.493680	-4.702430	-0.259452
1	-1.866272	-4.122533	-0.435023
6	-1.815295	1.256762	-0.205158
6	-2.573027	1.289687	1.128598
1	-2.484710	0.921833	-0.999127
1	-1.474226	2.258231	-0.476006
6	-3.792157	2.219748	1.073335
1	-2.895287	0.274087	1.386876
1	-1.892935	1.609212	1.929943
6	-4.567158	2.264016	2.394096
1	-3.466914	3.235143	0.804798
1	-4.461798	1.888854	0.267728
1	-5.432711	2.931747	2.323461
1	-4.934741	1.268417	2.669379
1	-3.934038	2.623081	3.214641
6	1.149799	2.209216	-0.066313
6	0.554002	3.217781	0.709332
6	2.307373	2.543687	-0.793008
6	1.075123	4.506884	0.741568
1	-0.298440	2.992225	1.341330
6	2.824123	3.831151	-0.778579
1	2.790244	1.772291	-1.383555
6	2.213395	4.841696	-0.012045
1	0.607346	5.259445	1.367322
1	3.703973	4.064527	-1.368545
7	2.732787	6.155132	0.005981
6	1.856859	7.274732	0.106238
6	4.137919	6.378430	-0.078382
6	2.154650	8.331053	0.980703
6	0.692731	7.342106	-0.675103
6	4.645142	7.382822	-0.916959

6	5.030940	5.606776	0.681363
6	1.305003	9.432756	1.065376
1	3.052913	8.282516	1.588138
6	-0.160278	8.439322	-0.570617
1	0.463697	6.532969	-1.361496
6	6.018106	7.612185	-0.986281
1	3.958840	7.979147	-1.509844
6	6.403646	5.830529	0.590827
1	4.644168	4.834191	1.338391
6	0.141289	9.492281	0.295860
1	1.549716	10.242767	1.747402
1	-1.057503	8.476931	-1.182858
6	6.905726	6.835883	-0.238336
1	6.394970	8.394125	-1.640286
1	7.081997	5.223524	1.184540
1	-0.521827	10.349480	0.369193
1	7.975730	7.012415	-0.300352
6	2.654932	-3.060562	-0.187126
6	3.102485	-4.234225	-0.822635
6	3.614204	-2.296481	0.504097
6	4.432736	-4.632269	-0.771286
1	2.404089	-4.827778	-1.405590
6	4.942643	-2.698608	0.576507
1	3.308336	-1.380978	0.994805
6	5.376588	-3.872698	-0.060537
1	4.750309	-5.529852	-1.292203
1	5.655689	-2.100261	1.134678
7	6.735249	-4.276345	0.003837
6	7.064653	-5.650845	0.157589
6	7.771522	-3.306726	-0.093260
6	8.120336	-6.218239	-0.574576
6	6.340838	-6.462324	1.046612
6	8.895626	-3.377811	0.745439
6	7.687303	-2.264836	-1.030973
6	8.445484	-7.563549	-0.412140
1	8.681027	-5.599250	-1.267667
6	6.661939	-7.810852	1.188363
1	5.529331	-6.028921	1.622412
6	9.913752	-2.432271	0.638202
1	8.964449	-4.176523	1.477120
6	8.701935	-1.313700	-1.118183
1	6.824192	-2.206233	-1.686251
6	7.717565	-8.370252	0.465118
1	9.265404	-7.985526	-0.987628
1	6.090835	-8.423373	1.881332
6	9.823336	-1.392434	-0.289567

1	10.776516	-2.503069	1.295594
1	8.619546	-0.514162	-1.849903
1	7.969669	-9.420201	0.583769
1	10.615852	-0.653346	-0.365454
6	-3.050134	-1.773231	-0.546836
6	-3.741422	-1.140537	-1.558783
16	-4.175792	-2.473321	0.601221
6	-5.150202	-1.203688	-1.421678
1	-3.243870	-0.686864	-2.408943
6	-5.567331	-1.899568	-0.302604
1	-5.840527	-0.778396	-2.142998
6	-6.912066	-2.165938	0.145846
6	-7.331548	-3.047170	1.135429
16	-8.271390	-1.325890	-0.564439
6	-8.723095	-3.054968	1.311811
1	-6.647623	-3.673448	1.697433
6	-9.409543	-2.184365	0.469130
1	-9.237935	-3.683129	2.031644
6	-10.826187	-2.032557	0.473614
6	-11.645126	-1.233071	-0.280185
1	-11.331814	-2.660512	1.202390
6	-11.153972	-0.344007	-1.282510
6	-13.116365	-1.235809	-0.103405
7	-10.724054	0.372969	-2.093372
8	-13.889006	-0.551039	-0.740066
8	-13.531795	-2.098985	0.863630
1	-14.502365	-2.012922	0.886616

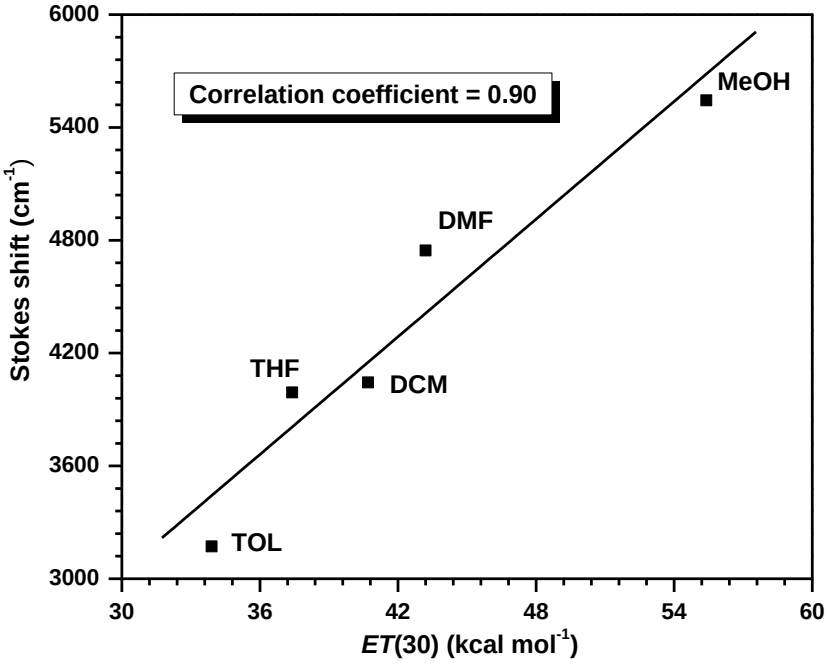

Figure S40. Correlation between Stokes shift and ET(30) parameter for dye **7b**.