Supporting Information for

Carbazole-modified thiazolo[3,2-*c*][1,3,5,2]oxadiazaborinines exhibiting aggregation-induced emission and mechanofluorochromism

Mykhaylo A. Potopnyk,* Mykola Kravets, Roman Luboradzki, Dmytro Volyniuk, Volodymyr Sashuk, and Juozas V. Grazulevicius*

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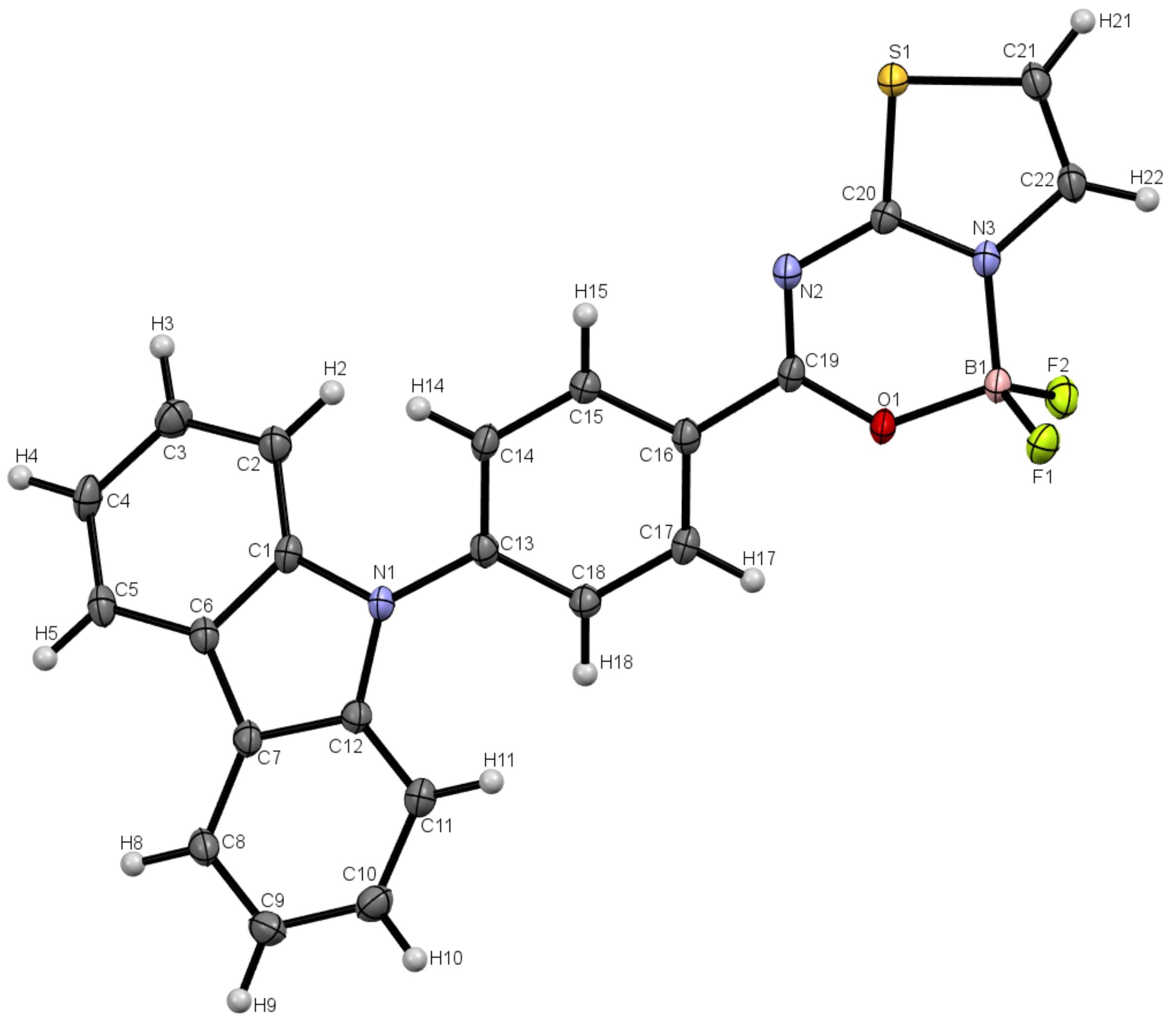

Figure S1. ORTEP diagram of complex **2**. The ellipsoid contour of probability level is 50%.

Table S1. Crystal data of complex 2.

Compound	**2**	
Empirical formula	$C_{22}H_{14}BF_2N_3OS$	
Moiety formula	$C_{22}H_{14}BF_2N_3OS$	
Formula weight	417.2389	
CCDC No.	CCDC 2013916	
Wavelength	1.54184	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.71398(13) Å	
	b = 15.00188(15) Å	β = 93.2060(9) °
	c = 9.01525(8) Å	
Volume	1851.86(3) Å^3	
Z	4	
Density Calc.	1.4965 g/cm^3	
Absorption coefficient	1.905 mm^{-1}	
F(000)	856	
Crystal	Yellow block	
Crystal size	0.3 × 0.2 × 0.06 mm	
Index ranges	-16 ≤ h ≤ 16, -18 ≤ k ≤ 18, -8 ≤ l ≤ 10	
Reflections collected (all / independent)	17802 / 3517 [R_{int} = 0.0658]	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Restraints / parameters	0 / 271	
Goodness-of-fit on F^2	1.0537	
Final R indices [$F^2 > 2\sigma(F^2)$]	R_1 = 0.0367, ωR_2 = 0.0994	
R indices (all data)	R_1 = 0.0370, ωR_2 = 0.0998	

Table S2. Selected geometrical parameters of compound 2 obtained from crystallography.

The B-N bond distance (Å)	1.559(2)
The B-O bond distance (Å)	1.483(2)
The B-F bond distances (Å)	1.371(2) 1.379(2)
The O-B-N angle (deg)	106.6(1)
The N-B-F angles (deg)	109.4(1) 111.2(1)
The angles O-B-F (deg)	109.3(1) 109.4(1)
The F-B-F angle (deg)	110.8(1)
The C1-N1-C13-C14 torsion angle (deg)	46.8(2)
The C12-N1-C13-C18 torsion angle (deg)	43.8(2)
The C15-C16-C19-N2 torsion angle (deg)	-1.0(2)
The C17-C16-C19-O1 torsion angle (deg)	0.4(2)

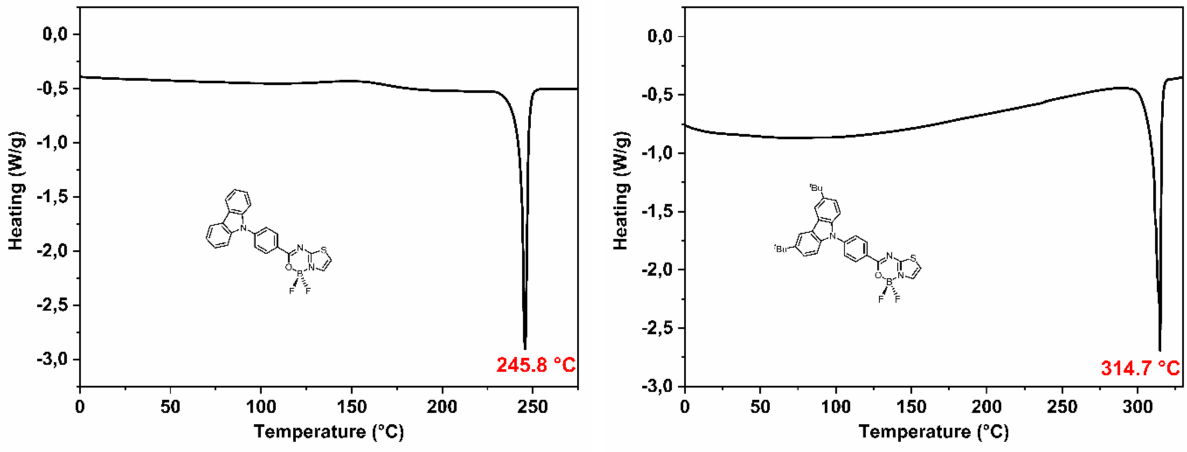

Figure S2. DSC thermograms of complexes **2** and **3**.

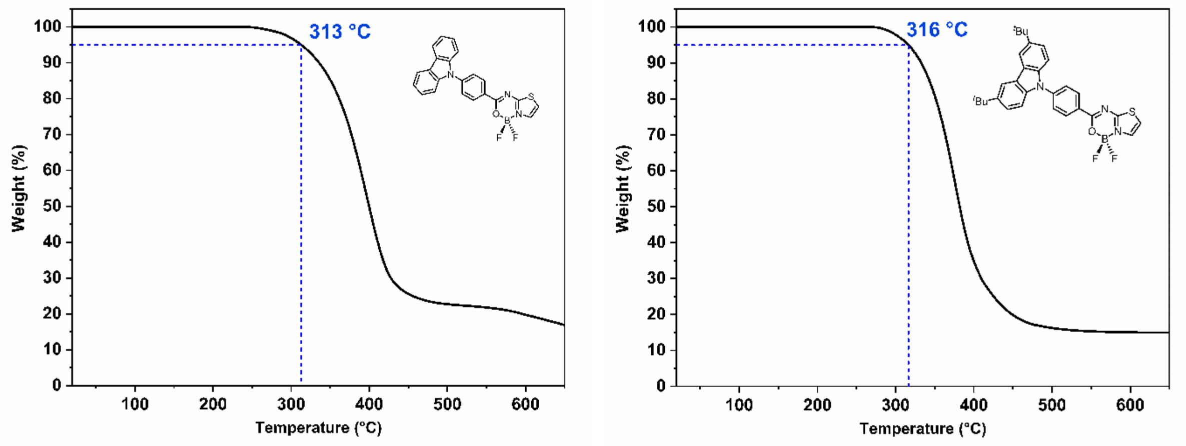

Figure S3. TGA curves of complexes **2** and **3**.

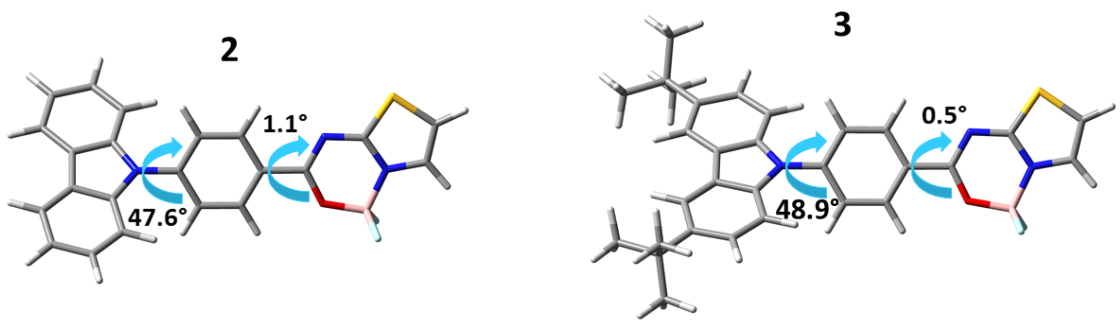

Figure S4. DFT-optimised structures of compounds **2** and **3**.

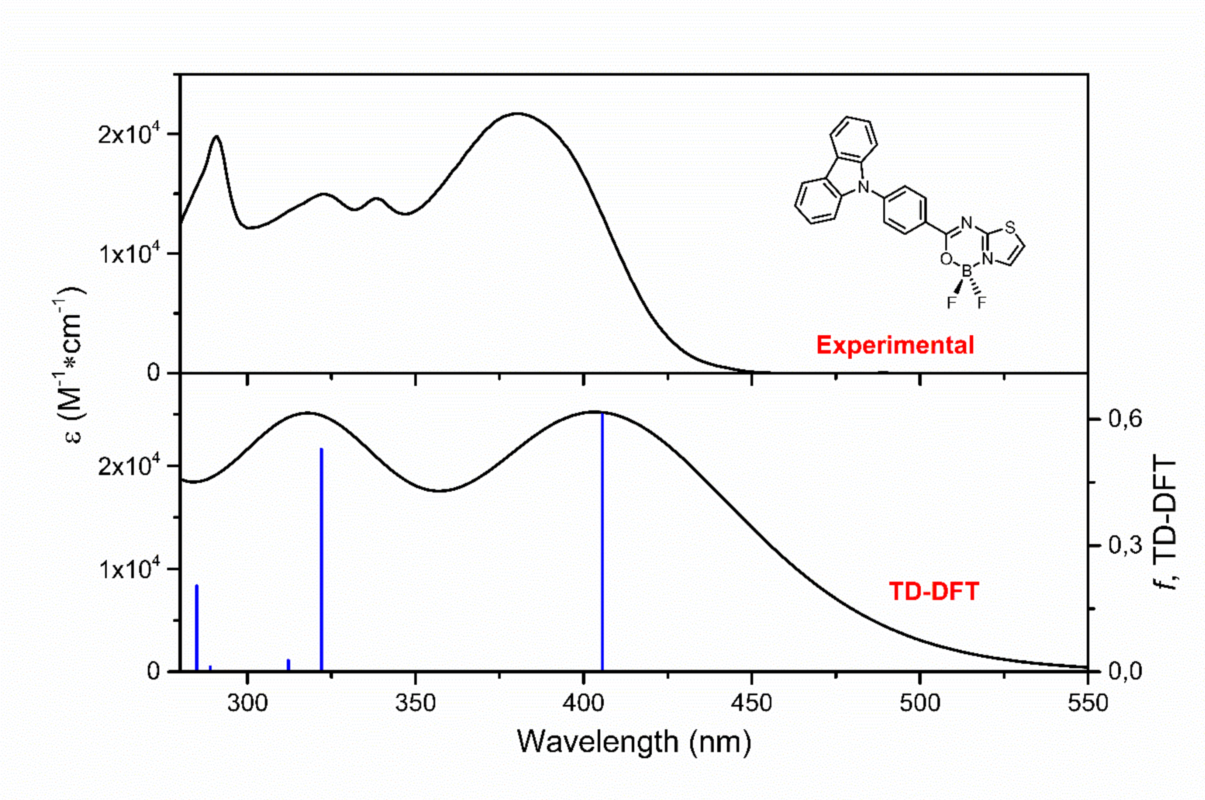

Figure S5. Experimental (top) and TD-DFT-predicted (bottom) absorption spectra of complex **2** in DCM.

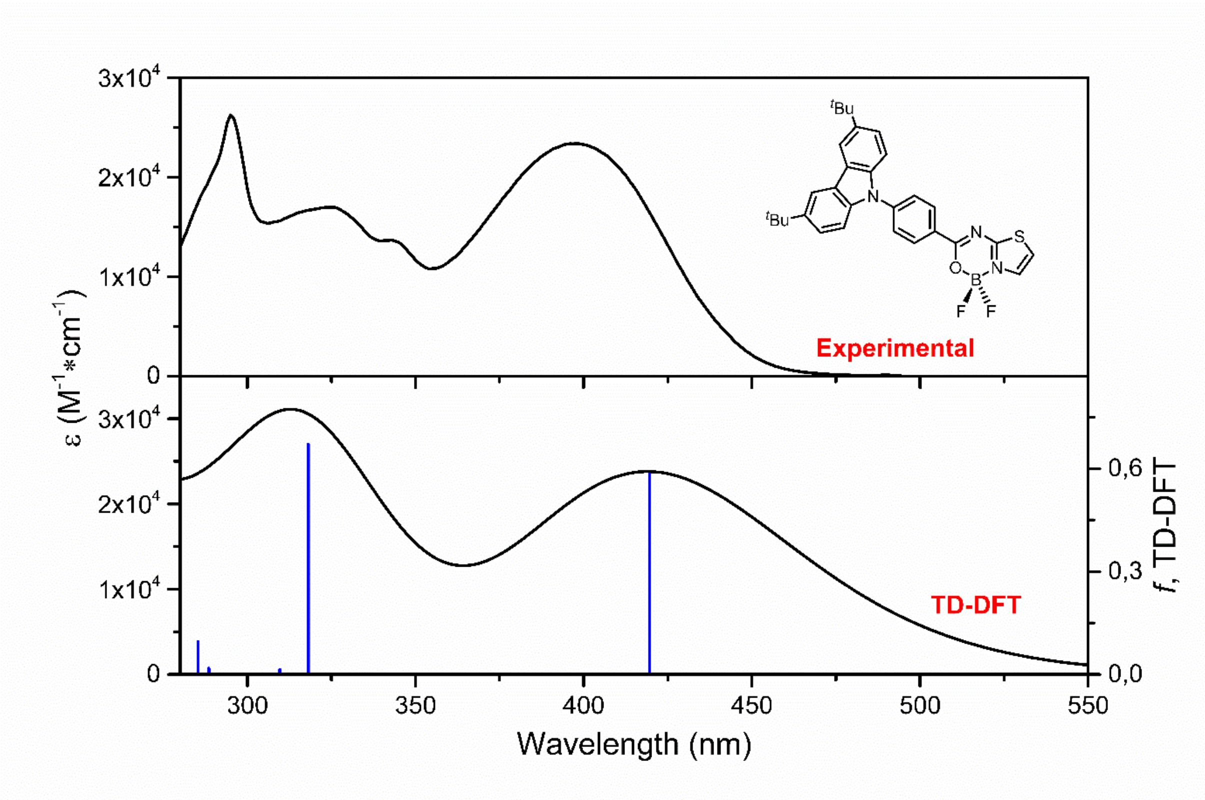

Figure S6. Experimental (top) and TD-DFT-predicted (bottom) absorption spectra of complex **3** in DCM.

Table S3. Calculated properties of the 12 lowest singlet excited states for complexes **2** and **3** determined through TD-DFT.

Comp.	Transition	Energy (eV)	Wavelength (nm)	Oscillator strength	Expansion coefficients for single-electron excitations*
2	$S_0 \rightarrow S_1$	3.0572	405.54	0.6111	0.69443 H→L
	$S_0 \rightarrow S_2$	3.5238	351.84	0.0004	0.70149 H-1→L
	$S_0 \rightarrow S_3$	3.8500	322.04	0.5292	0.69353 H-2→L
	$S_0 \rightarrow S_4$	3.9713	312.20	0.0273	-0.16514 H-1→L+4 / 0.67579 H-1→L+1
	$S_0 \rightarrow S_5$	4.2903	288.98	0.0114	-0.42420 H-4→L / -0.13168 H-3→L / 0.42610 H→L+2 / 0.30000 H→L+3
	$S_0 \rightarrow S_6$	4.3514	284.93	0.2045	-0.12580 H-3→L / 0.62966 H-1→L+1 / 0.24231 H→L+4
	$S_0 \rightarrow S_7$	4.5648	271.61	0.0184	0.28679 H-4→L / 0.48698 H-3→L / 0.38867 H→L+2
	$S_0 \rightarrow S_8$	4.6136	268.74	0.0379	-0.39828 H-4→L / 0.46634 H-3→L / -0.29601 H→L+2 / 0.11428 H→L+4
	$S_0 \rightarrow S_9$	4.7004	263.77	0.0061	0.60298 H-7→L / 0.11457 H→L+2 / -0.30321 H→L+3
	$S_0 \rightarrow S_{10}$	4.7112	263.17	0.0105	0.34658 H-7→L / 0.16048 H-4→L / -0.20179 H→L+2 / 0.52547 H→L+3 / -0.10902 H→L+5
	$S_0 \rightarrow S_{11}$	4.8783	254.15	0.1575	0.68039 H-5→L
	$S_0 \rightarrow S_{12}$	4.9281	251.59	0.1091	0.15092 H-3→L+1 / 0.56387 H-1→L+2 / 0.10475 H-1→L+5 / 0.13297 H-1→L+7 / -0.31095 H→L+4
3a	$S_0 \rightarrow S_1$	2.9549	419.58	0.5850	0.69692 H→L
	$S_0 \rightarrow S_2$	3.3697	367.94	0.0001	0.70231 H-1→L
	$S_0 \rightarrow S_3$	3.8970	318.15	0.6714	0.69001 H-2→L / 0.10825 H→L+1
	$S_0 \rightarrow S_4$	4.0044	309.62	0.0146	-0.10647 H-2→L / 0.16595 H-1→L+4 / 0.67087 H→L+1
	$S_0 \rightarrow S_5$	4.2970	288.53	0.0179	-0.38441 H-4→L / -0.25852 H-3→L / 0.14454 H-1→L+1 / 0.38523 H→L+2 / -0.30035 H→L+3
	$S_0 \rightarrow S_6$	4.3460	285.28	0.0963	0.16959 H-4→L / -0.40894 H-3→L / 0.46259 H-1→L+1 / -0.18103 H→L+2 / 0.13145 H→L+3 / -0.14605 H→L+4
	$S_0 \rightarrow S_7$	4.4358	279.51	0.1864	0.50503 H-3→L / 0.43721 H-1→L+1 / -0.17908 H→L+4
	$S_0 \rightarrow S_8$	4.5851	270.41	0.0385	0.48858 H-4→L / 0.47951 H→L+2
	$S_0 \rightarrow S_9$	4.6830	264.75	0.0267	-0.21343 H-4→L / 0.24046 H→L+2 / 0.60252 H→L+3 / -0.11382 H→L+5
	$S_0 \rightarrow S_{10}$	4.7262	262.33	0.0000	0.69340 H-7→L
	$S_0 \rightarrow S_{11}$	4.8840	253.86	0.1310	0.65223 H-5→L / -0.18076 H-1→L+2
	$S_0 \rightarrow S_{12}$	4.8974	253.16	0.0277	0.19508 H-5→L / -0.11108 H-3→L+1 / 0.61448 H-1→L+2 / -0.19157 H-1→L+3 / 0.12131 H→L+4

*H – HOMO, L – LUMO.

Optimized geometry for compound 2 obtained using the M06 method and def2tzvp basis set with the inclusion of DCM solvent effect through the conductor-like polarizable continuum model (CPCM).

Symbolic Z-matrix:

C	1.00004	-1.05748	0.69617
C	-0.38657	-1.09531	0.70556
C	-1.12816	-0.10358	0.04957
C	-0.45331	0.92322	-0.62583
C	0.9311	0.95654	-0.64918
C	1.66946	-0.03147	0.01701
H	1.57584	-1.81409	1.23532
H	-0.90924	-1.89103	1.2411
H	-1.03558	1.68724	-1.14584
H	1.45573	1.7431	-1.19789
C	-2.59464	-0.13129	0.06719
C	-4.59303	0.75652	-0.49935
O	-3.14071	-1.12919	0.69381
N	-3.261	0.82589	-0.53562
N	-5.31304	-0.19137	0.1059
S	-5.60443	1.93448	-1.26934
B	-4.59436	-1.3624	0.8782
F	-4.91488	-1.29811	2.20723
F	-4.95124	-2.56081	0.3228
C	3.92912	-1.04944	-0.30264
C	3.85515	1.14073	0.27183
C	3.62382	-2.35993	-0.67604
C	5.26764	-0.59643	-0.23593
C	3.46187	2.41825	0.67534
C	5.22072	0.80008	0.13302
C	4.68358	-3.21696	-0.95764
H	2.59018	-2.70722	-0.75276
C	6.3151	-1.47604	-0.52322
C	4.45979	3.35918	0.90955
H	2.40829	2.67546	0.81178
C	6.20541	1.76341	0.37145
C	6.01666	-2.78634	-0.87817
H	4.46797	-4.24927	-1.24829
H	7.35345	-1.13396	-0.47316
C	5.81792	3.04234	0.75352
H	4.17535	4.36756	1.22399
H	7.26464	1.50951	0.26508
H	6.82452	-3.48804	-1.10307
H	6.57585	3.80775	0.94164
N	3.07486	0.01317	0.00422
C	-7.01798	1.07901	-0.73106
H	-8.01767	1.43703	-0.97188
C	-6.67131	-0.01998	-0.01938
H	-7.34597	-0.74402	0.43964

Imaginary Frequency = 0

E(RM06) = -1708.84329592 a.u.

E(TD-HF/TD-DFT) = -1708.73094456 a.u.

Optimized geometry for compound 3 obtained using the M06 method and def2tzvp basis set with the inclusion of DCM solvent effect through the conductor-like polarizable continuum model (CPCM).

Symbolic Z-matrix:

C	-0.70799	-0.90475	0.87174
C	-2.09395	-0.9361	0.89468
C	-2.83752	-0.09151	0.05883
C	-2.16255	0.78194	-0.8059
C	-0.77776	0.80781	-0.84038
C	-0.03753	-0.03469	0.00134
H	-0.13264	-1.54203	1.54811
H	-2.61461	-1.60967	1.57893
H	-2.74583	1.43039	-1.46358
H	-0.25626	1.46849	-1.53767
C	-4.30334	-0.11644	0.08518
C	-6.30584	0.63374	-0.64191
O	-4.84513	-0.9621	0.9082
N	-4.97437	0.69358	-0.70158
N	-7.02046	-0.17285	0.14735
S	-7.32629	1.63717	-1.62039
B	-6.29696	-1.17394	1.12474
F	-6.6269	-0.86966	2.41761
F	-6.63664	-2.45873	0.79787
C	2.20964	-1.11879	-0.08927
C	2.16602	1.13936	0.03856
C	1.90636	-2.47587	-0.21411
C	3.5509	-0.68481	-0.06975
C	1.81203	2.48438	0.16007
C	3.52295	0.75687	0.01937
C	2.963	-3.37427	-0.29166
H	0.87373	-2.83208	-0.25848
C	4.59462	-1.61291	-0.14995
C	2.83421	3.4221	0.23752
H	0.76677	2.8023	0.20193
C	4.53073	1.72357	0.09933
C	4.31836	-2.97554	-0.25679
H	2.71892	-4.43725	-0.38722
H	5.62419	-1.24498	-0.13259
C	4.20388	3.07493	0.20485
H	2.54969	4.47525	0.33168
H	5.5734	1.3943	0.08276
N	1.36637	-0.00564	-0.02501
C	5.26102	4.17576	0.29366
C	5.10698	4.92456	1.62155
H	4.11806	5.40169	1.71843

H	5.23498	4.23808	2.4758
H	5.86856	5.71893	1.70698
C	5.08159	5.15535	-0.87043
H	5.84686	5.94923	-0.82342
H	5.1866	4.63952	-1.84012
H	4.09498	5.64633	-0.85479
C	6.67778	3.61352	0.22666
H	7.40834	4.43712	0.28424
H	6.88933	2.926	1.06267
H	6.86152	3.07258	-0.71688
C	5.4148	-4.03768	-0.34499
C	5.28821	-4.79281	-1.67225
H	5.38976	-4.10289	-2.52728
H	6.07905	-5.55807	-1.75724
H	4.31812	-5.30723	-1.7683
C	6.81031	-3.42462	-0.2781
H	6.97616	-2.88282	0.66826
H	7.57037	-4.22066	-0.34174
H	6.99438	-2.72457	-1.11026
C	5.27092	-5.02202	0.81996
H	5.35792	-4.50192	1.78915
H	4.30257	-5.54807	0.80536
H	6.0641	-5.78801	0.77326
C	-8.73411	0.90951	-0.90712
H	-9.73631	1.21481	-1.20374
C	-8.37986	-0.02581	0.00584
H	-9.0484	-0.6419	0.60889

Imaginary Frequency = 0

E(RM06) = -2021.31501870 a.u.

E(TD-HF/TD-DFT) = -2021.20642669 a.u.

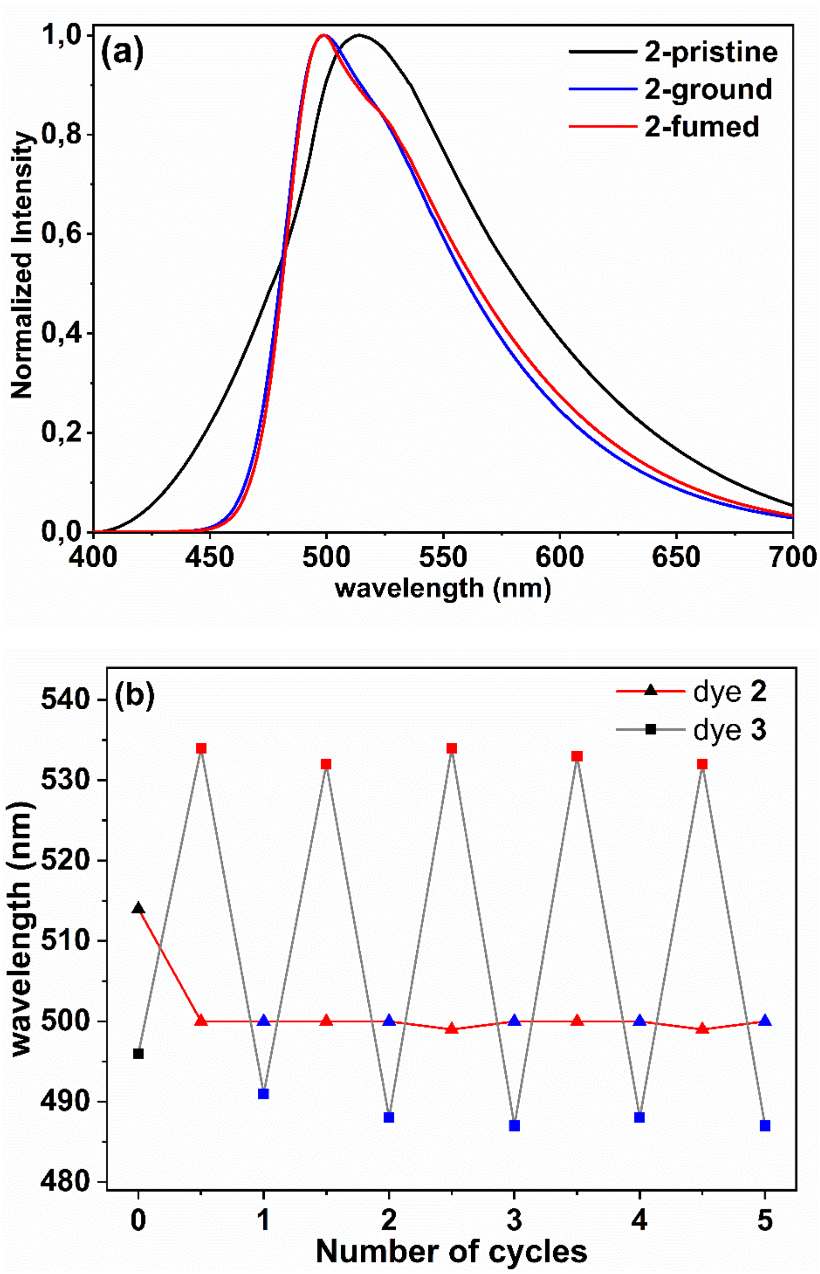

Figure S7. (a) Normalized emission spectra of dye **2** in different solid states (λ_{ex} = 374 nm). (b) Reversible switching of solid-state emission of dyes **2** and **3** by repeated grinding/DCM-fuming cycles.

Table S4. Fluorescence properties of complex **2** in the solid states.

State	λ_{em}, nm	$PLQY_{solid}$	τ, ns	α_1/α_2
pristine crystalline	514	0.26	0.99, 4.28	57.65/42.35
ground	500	0.24	0.94, 3.07	75.46/24.54
DCM-fumed	500	0.23	0.84, 3.07	74.57/25.43
film	514	0.24	2.30, 7.42	33.83/66.17

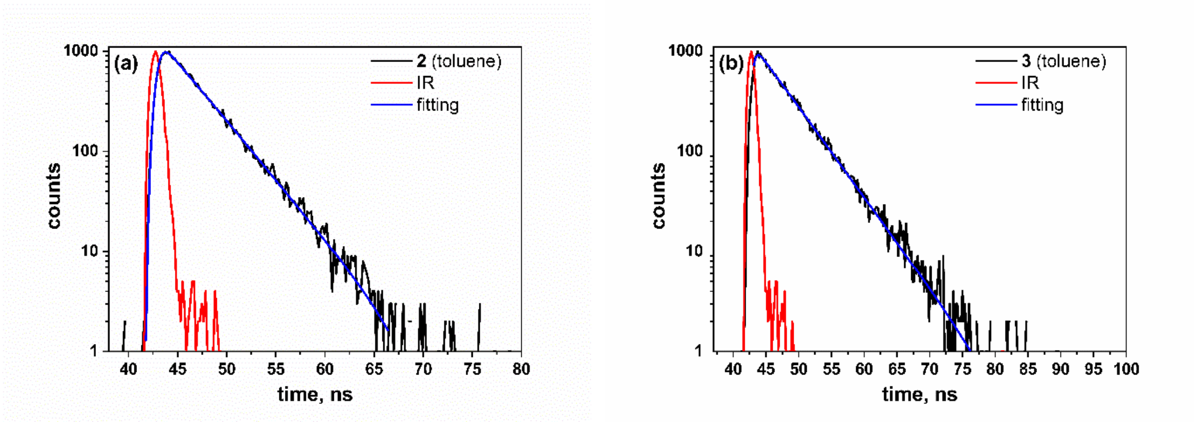

Figure S8. Fluorescence decay of complexes **2** and **3** in toluene solutions.

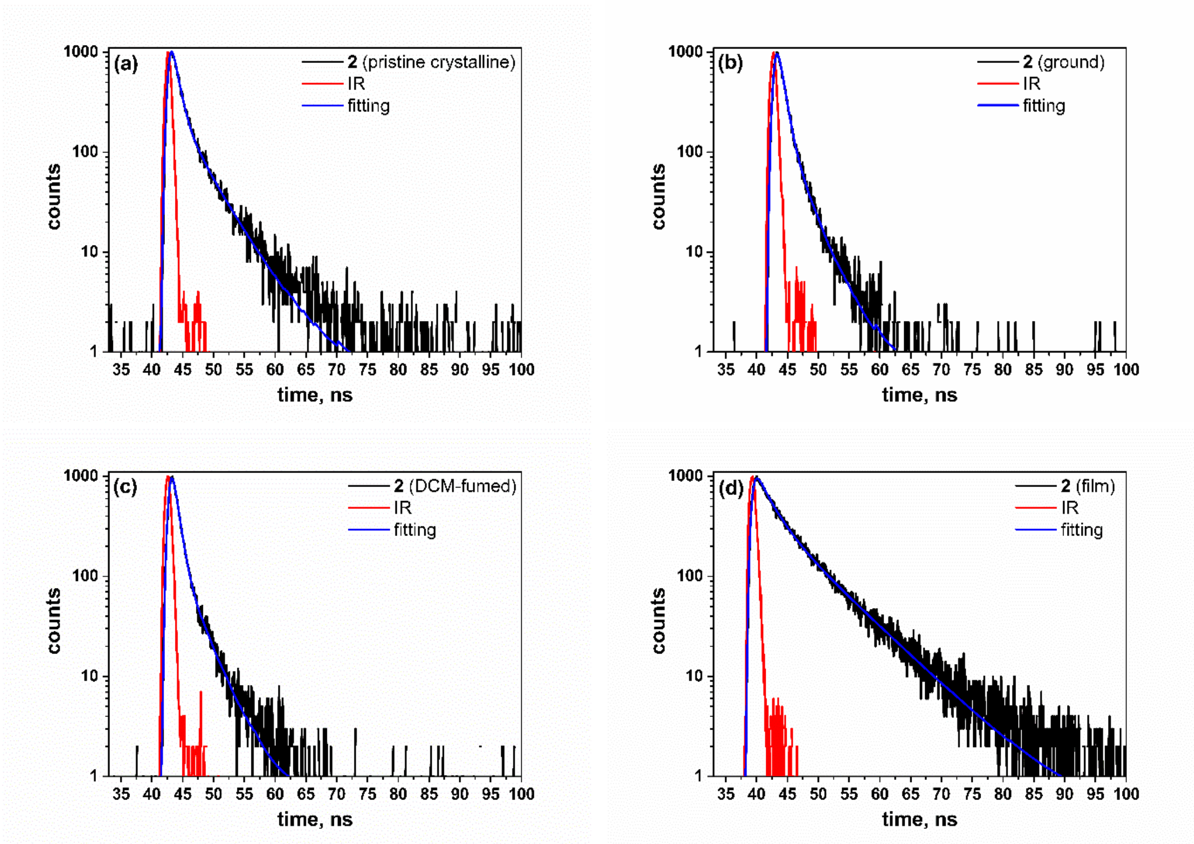

Figure S9. Fluorescence decay of complex **2** in the solid states: (a) pristine crystalline; (b) ground sample; (c) DCM-fumed sample; (d) film.

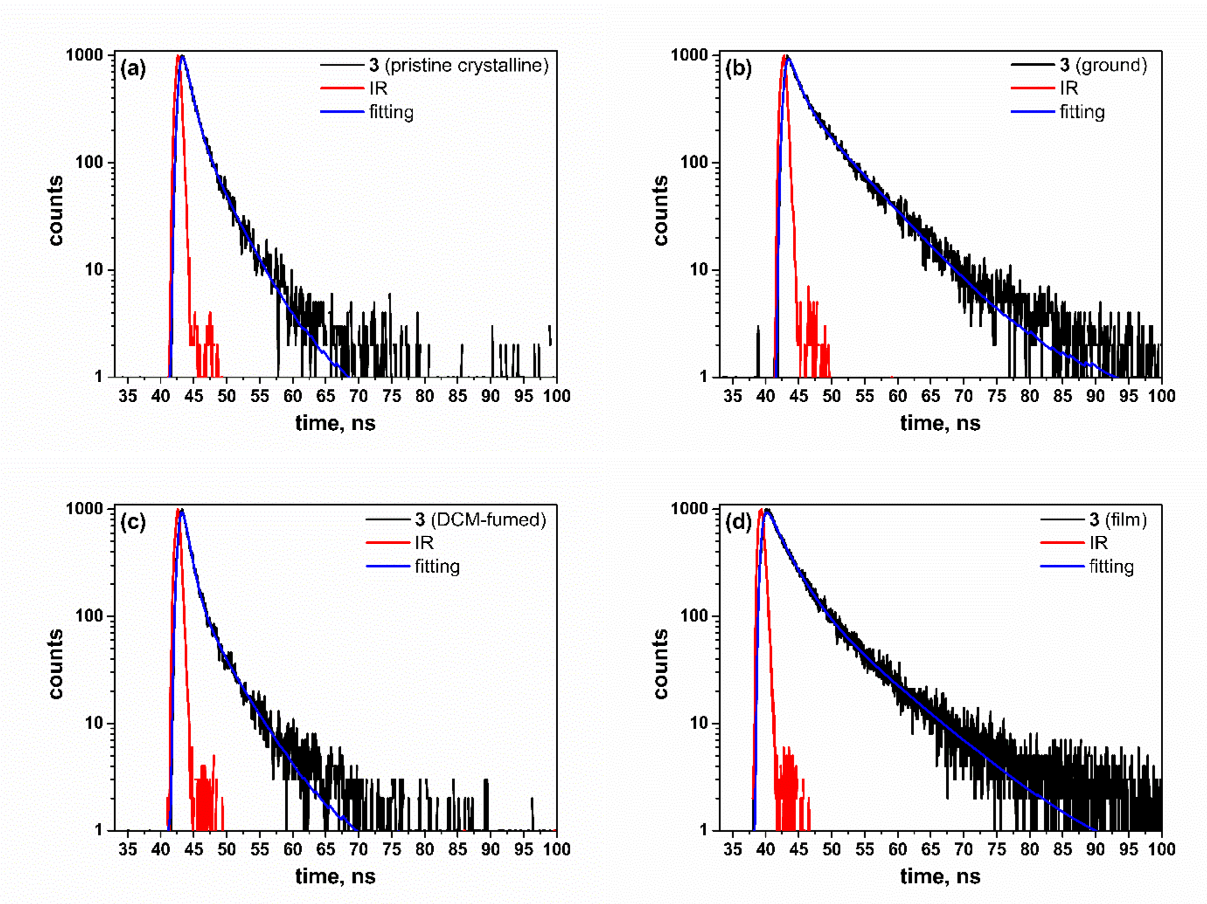

Figure S10. Fluorescence decay of complex **3** in the solid states: (a) pristine crystalline; (b) ground sample; (c) DCM-fumed sample; (d) film.

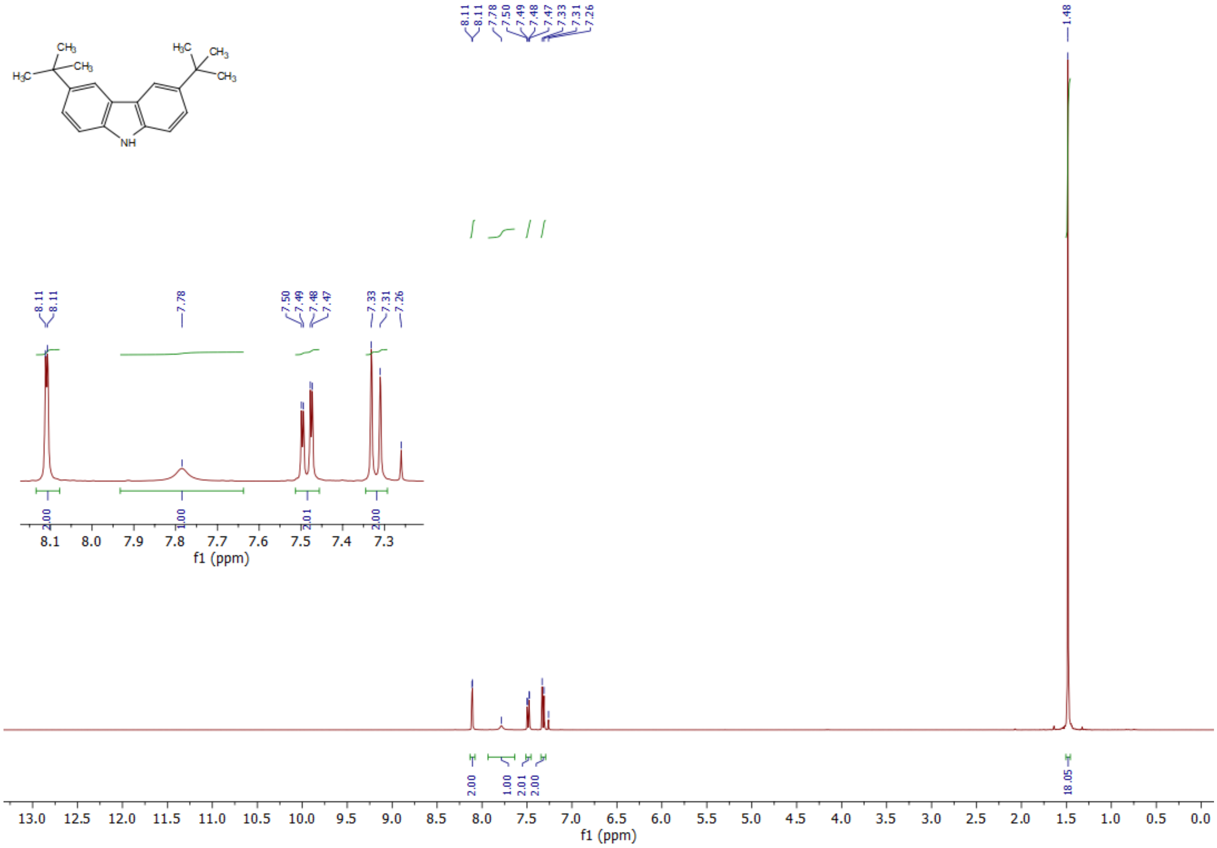

Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5**.

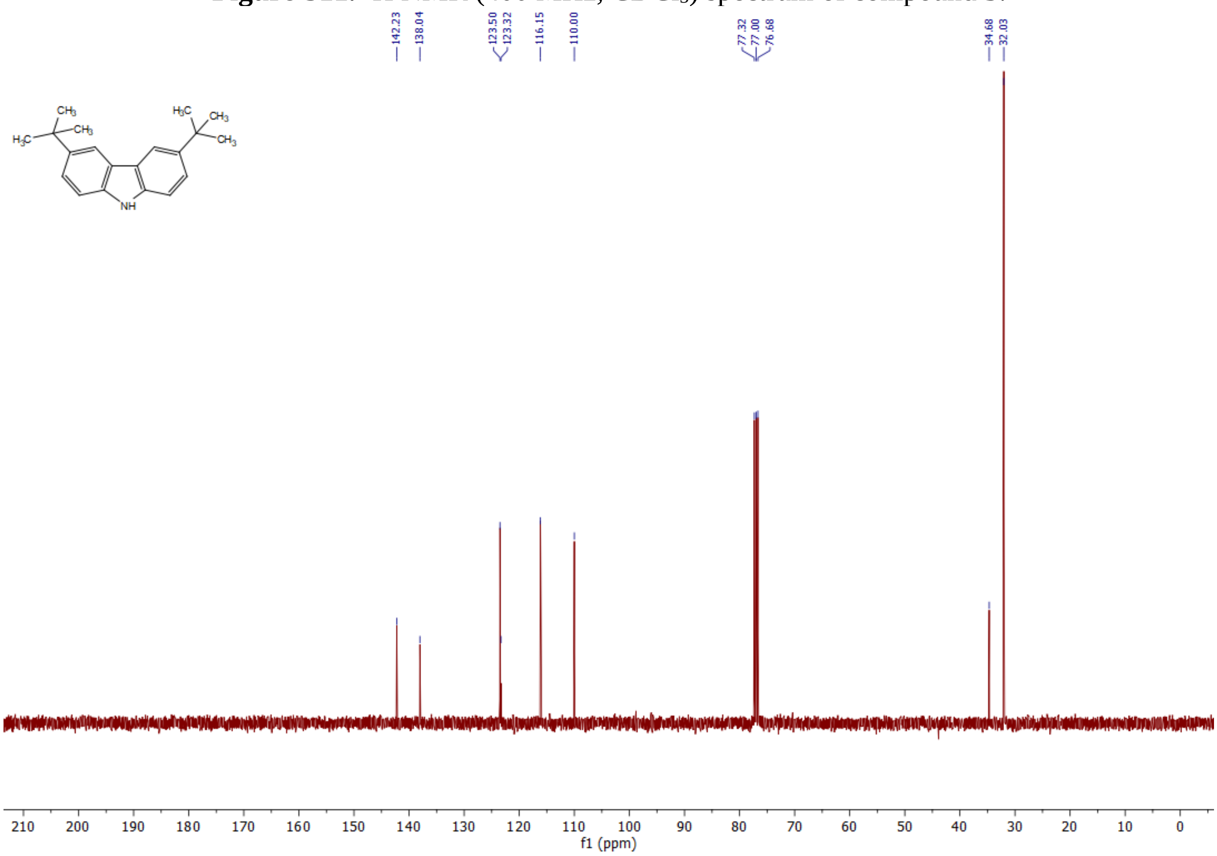

Figure S12. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5**.

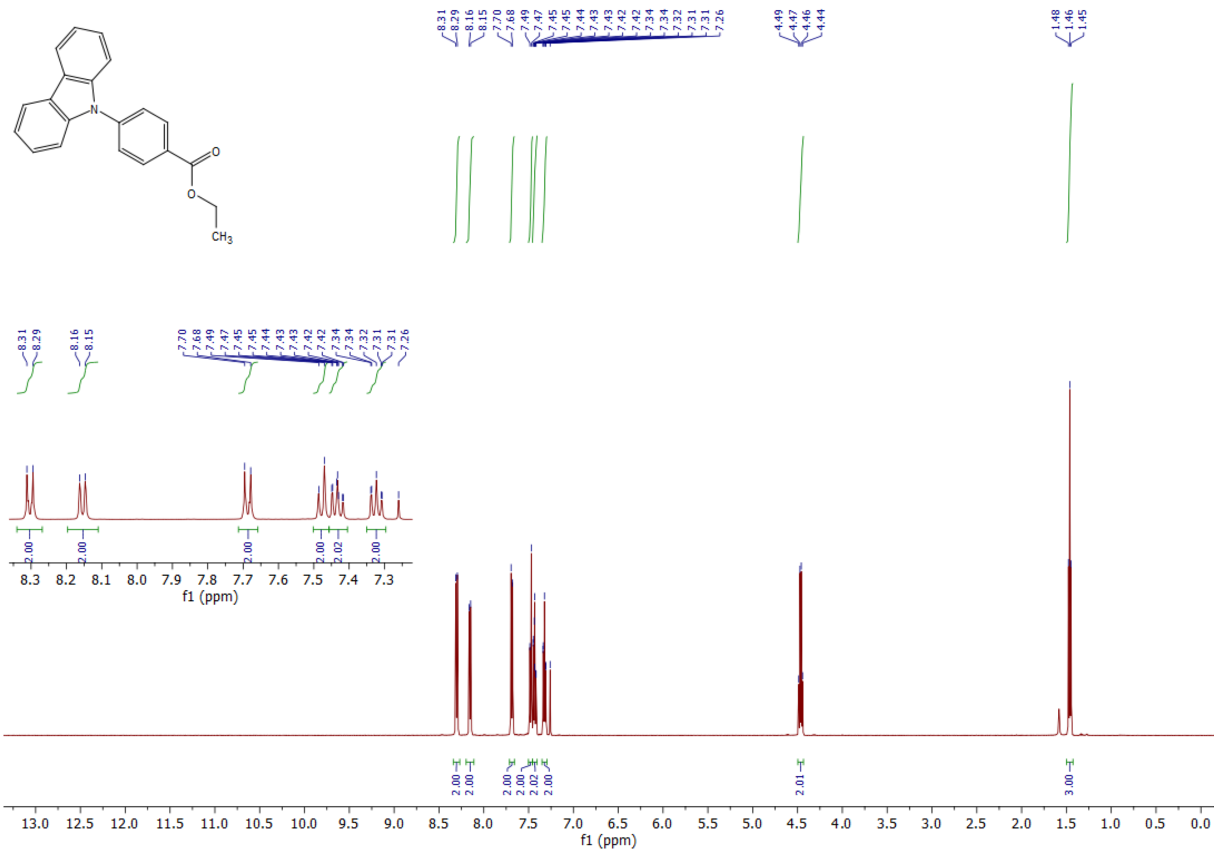

Figure S13. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **7**.

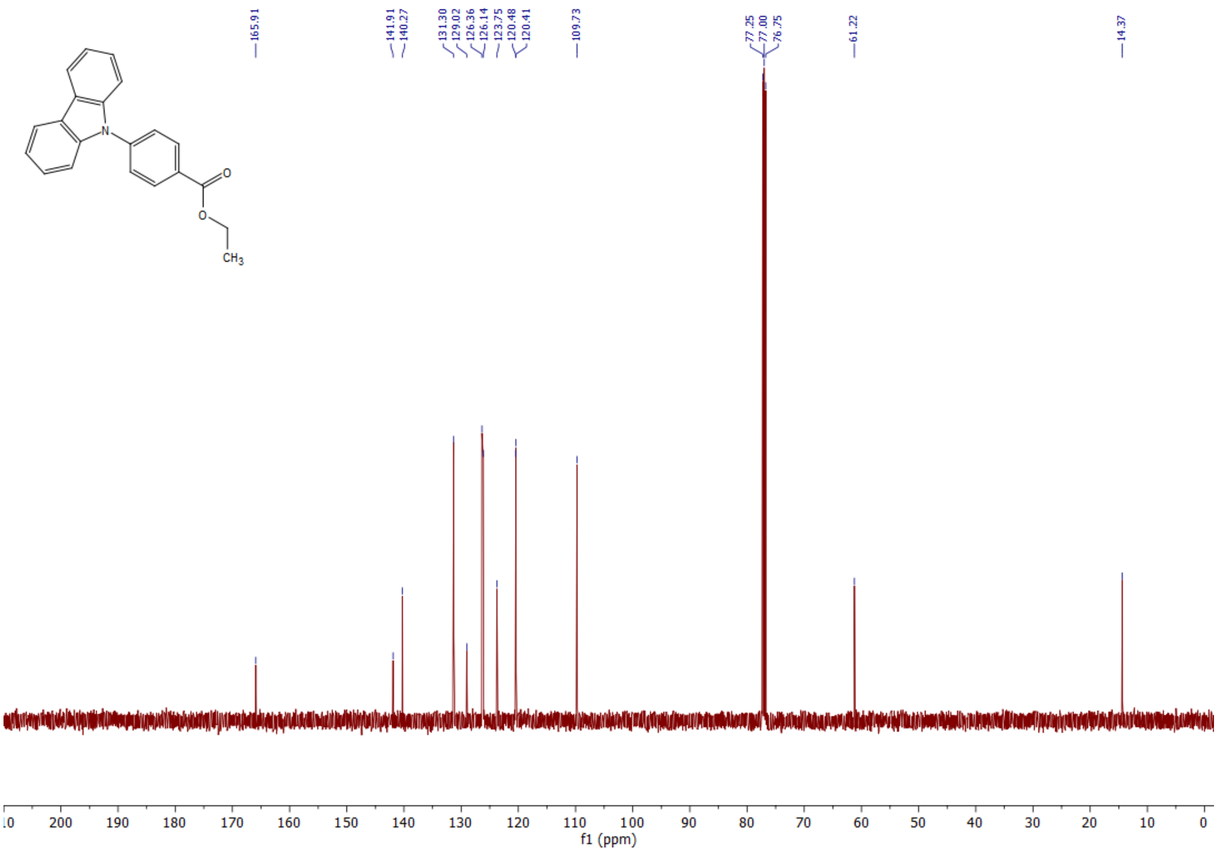

Figure S14. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **7**.

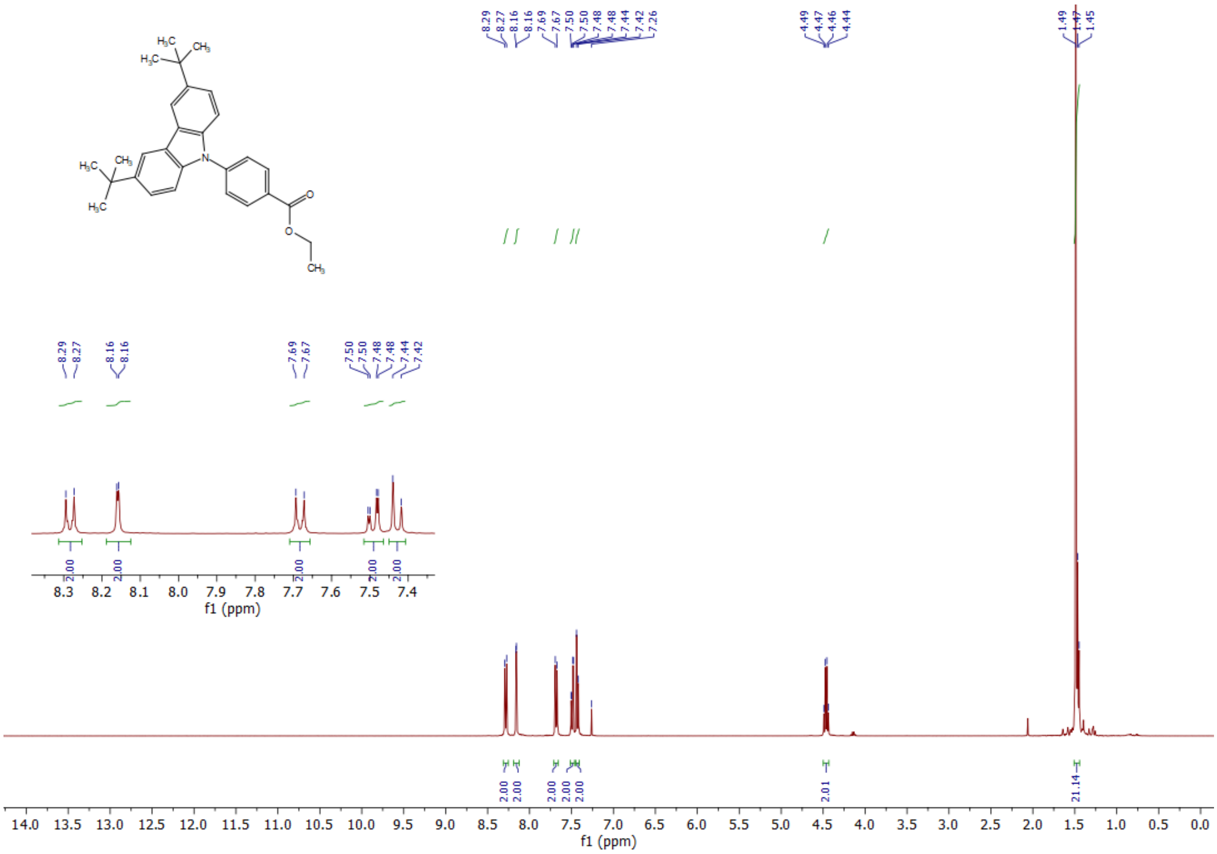

Figure S15. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **8**.

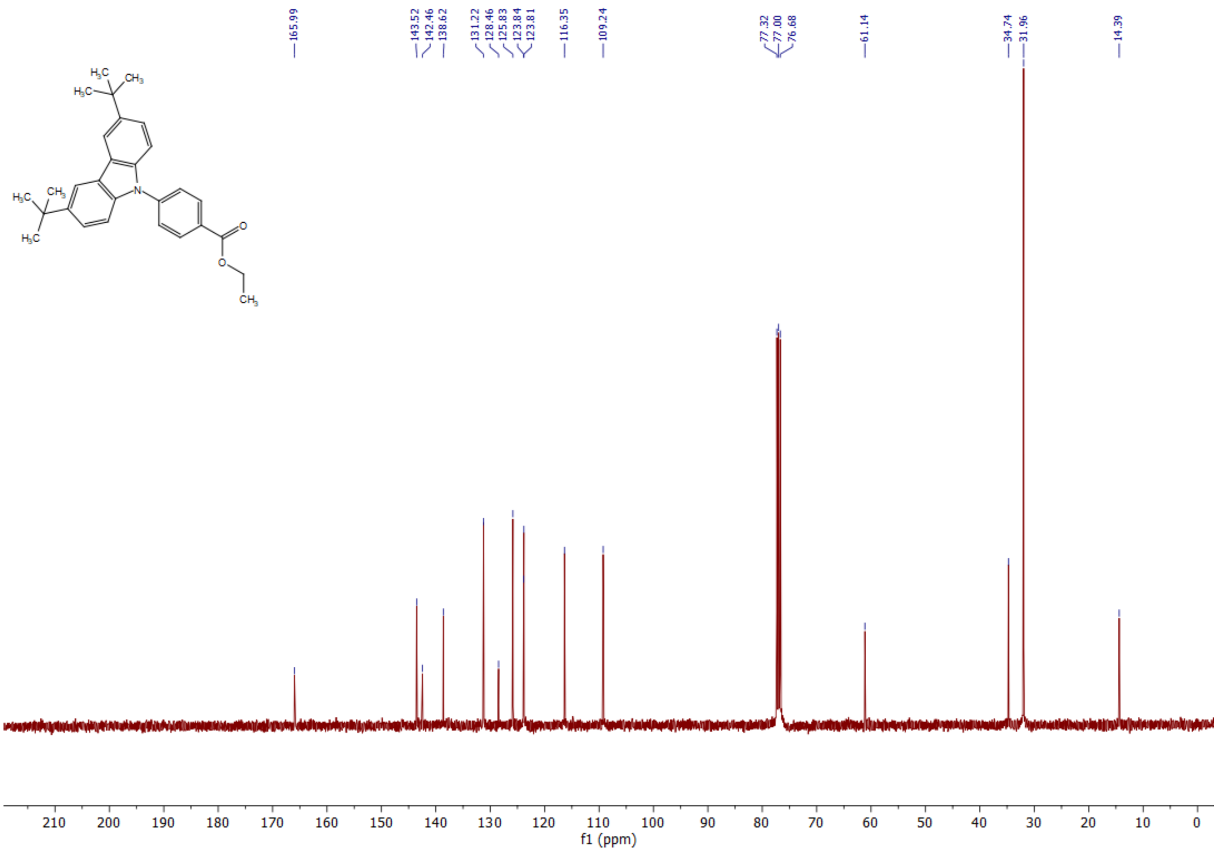

Figure S16. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8**.

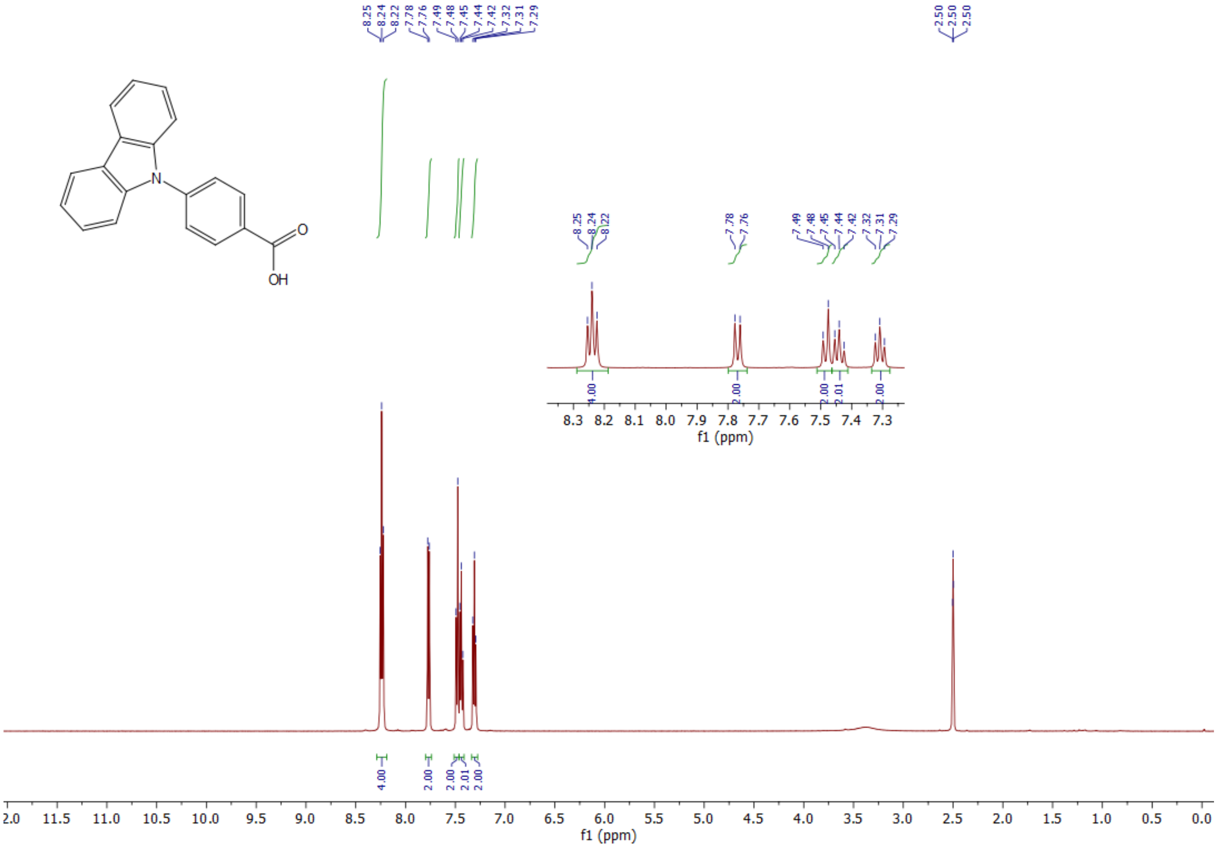

Figure S17. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **9**.

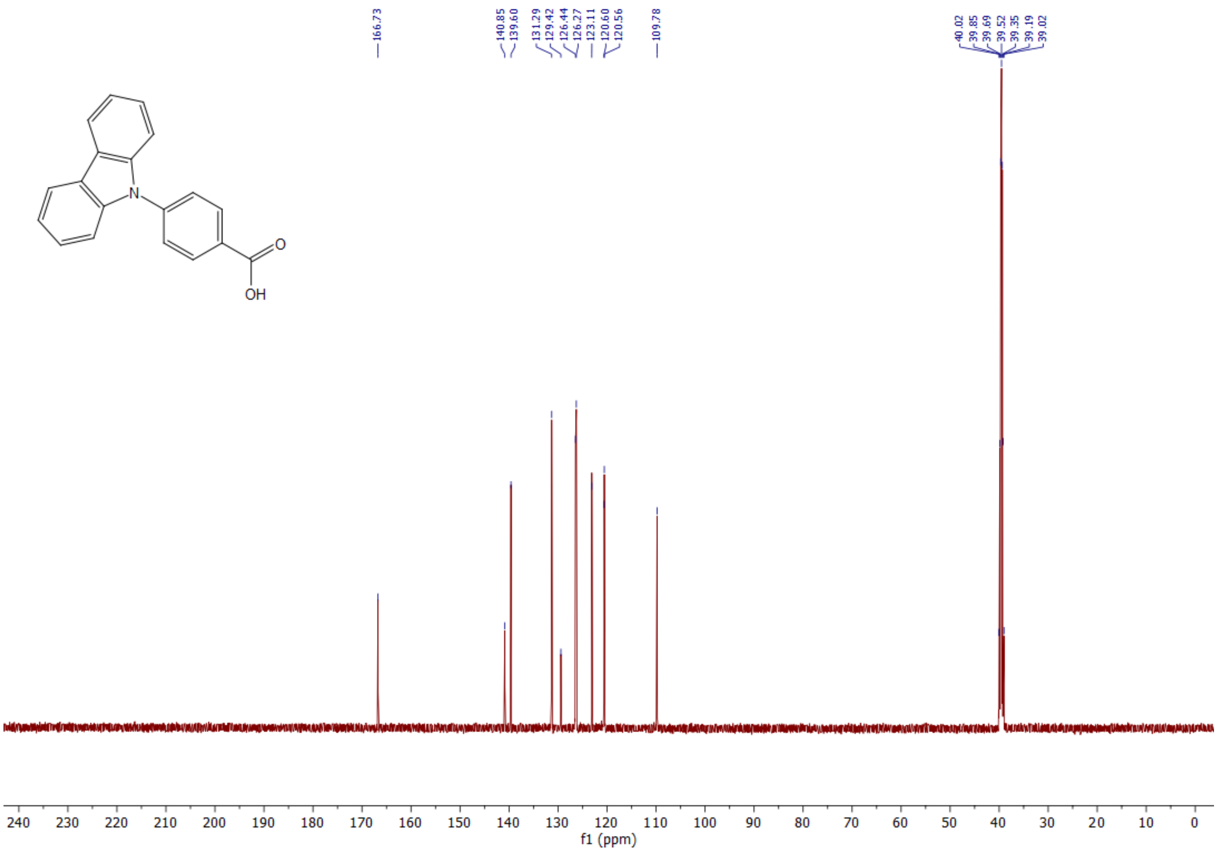

Figure S18. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **9**.

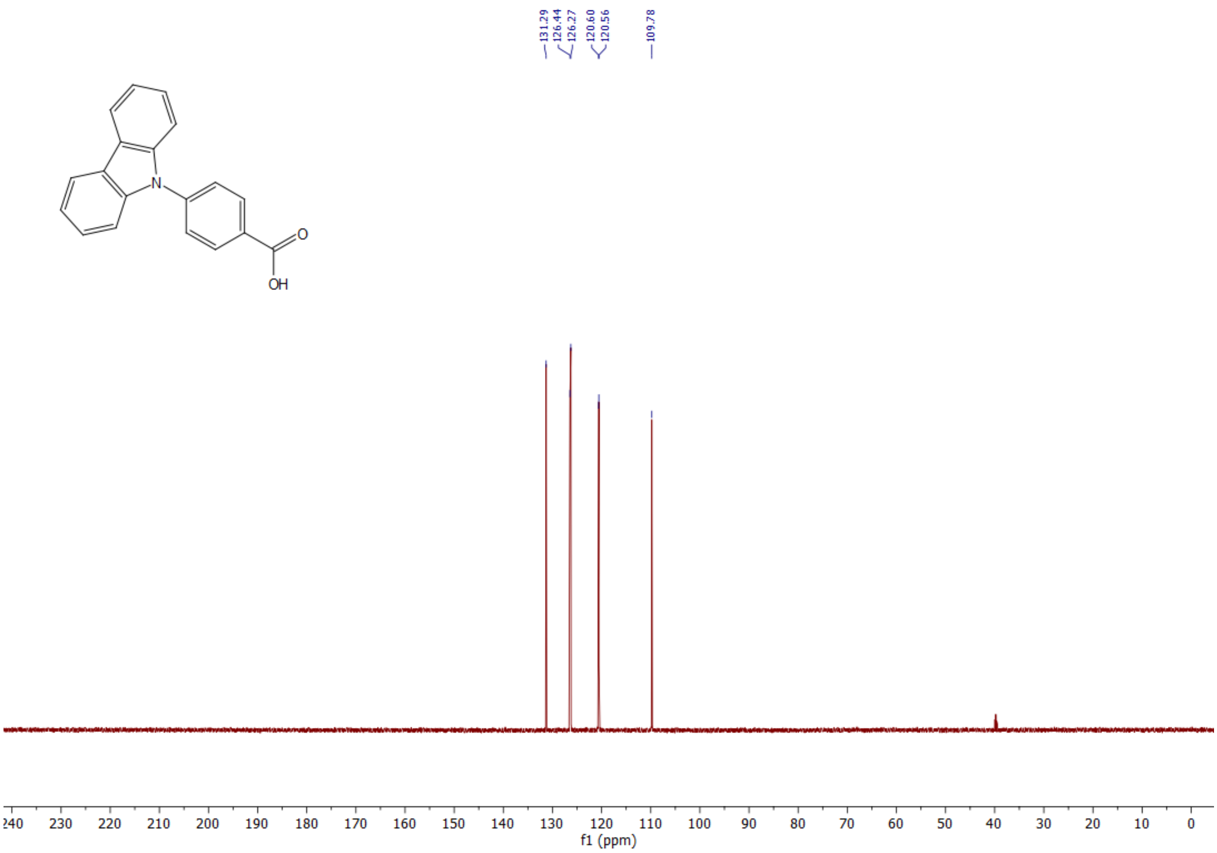

Figure S19. DEPT135 NMR (125 MHz, DMSO-d_6) spectrum of compound **9**.

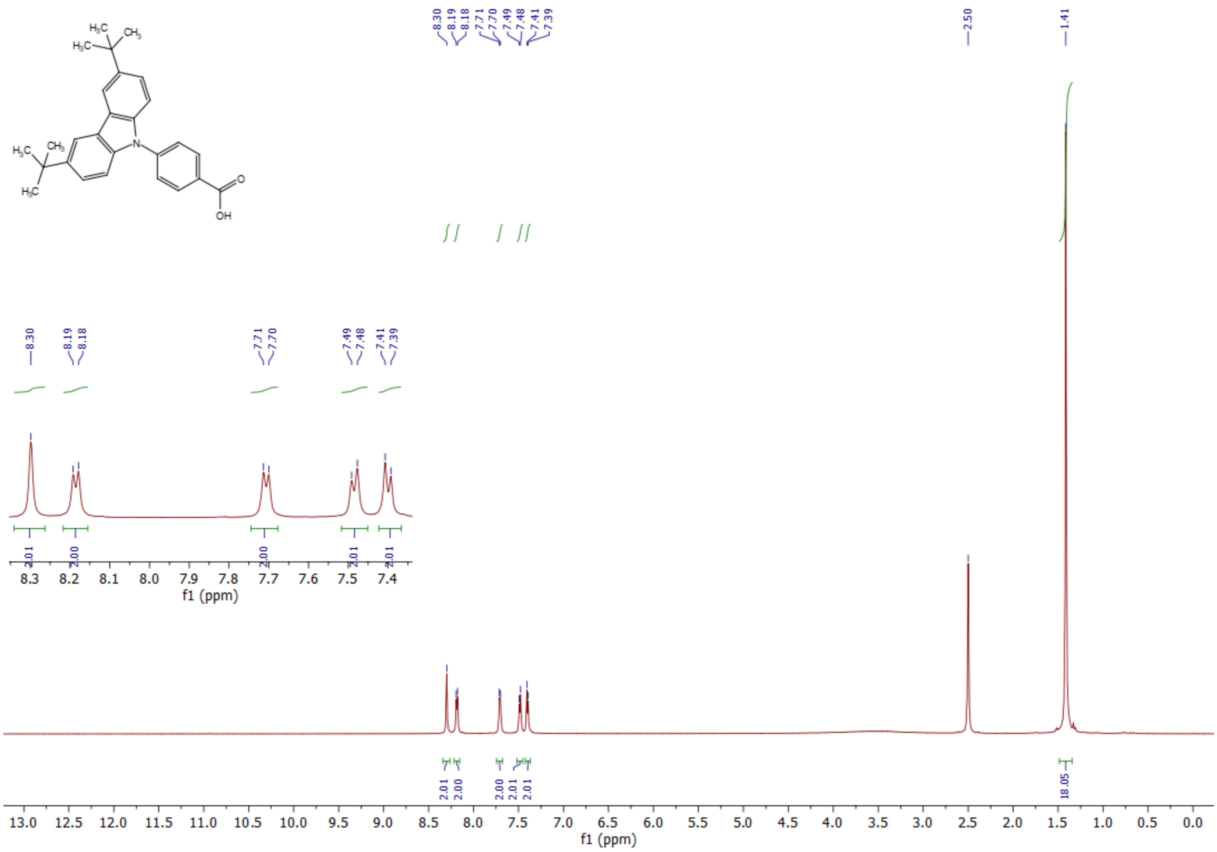

Figure S20. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound **10**.

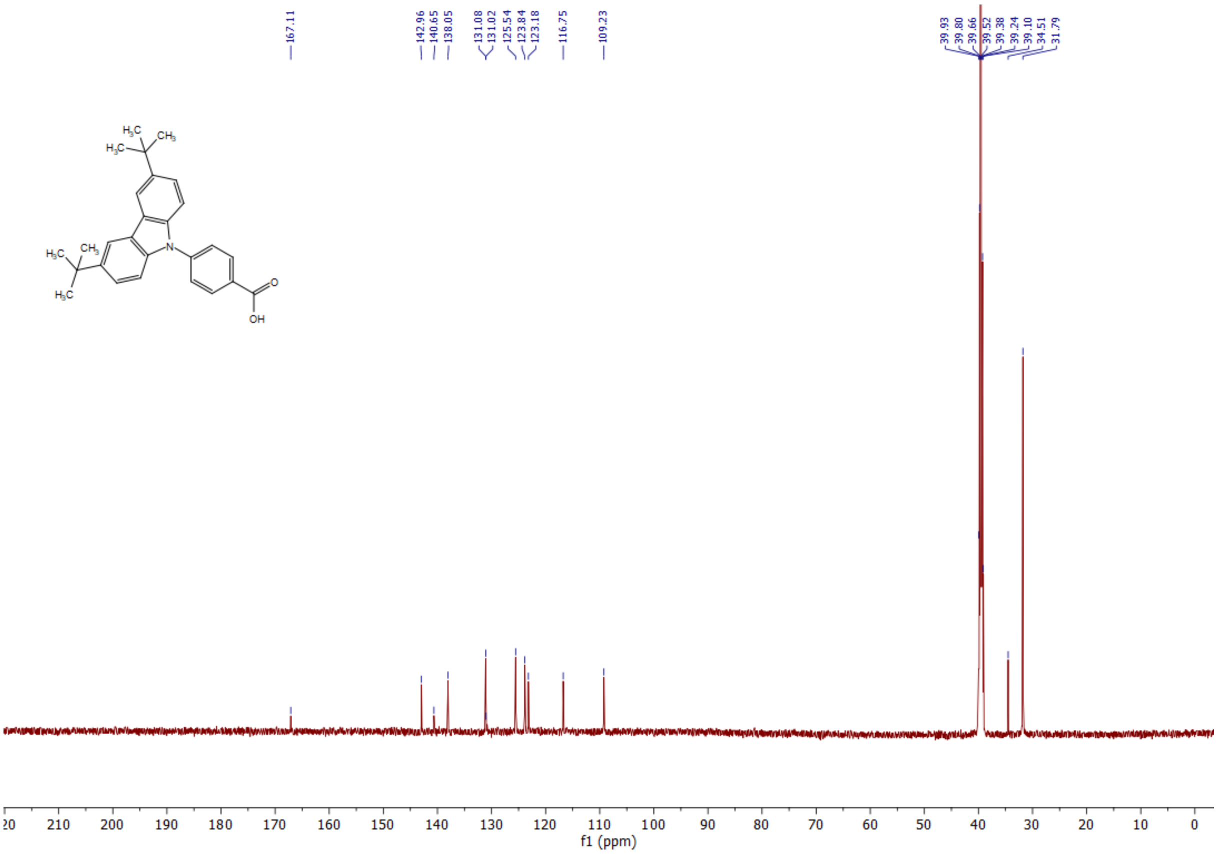

Figure S21. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound **10**.

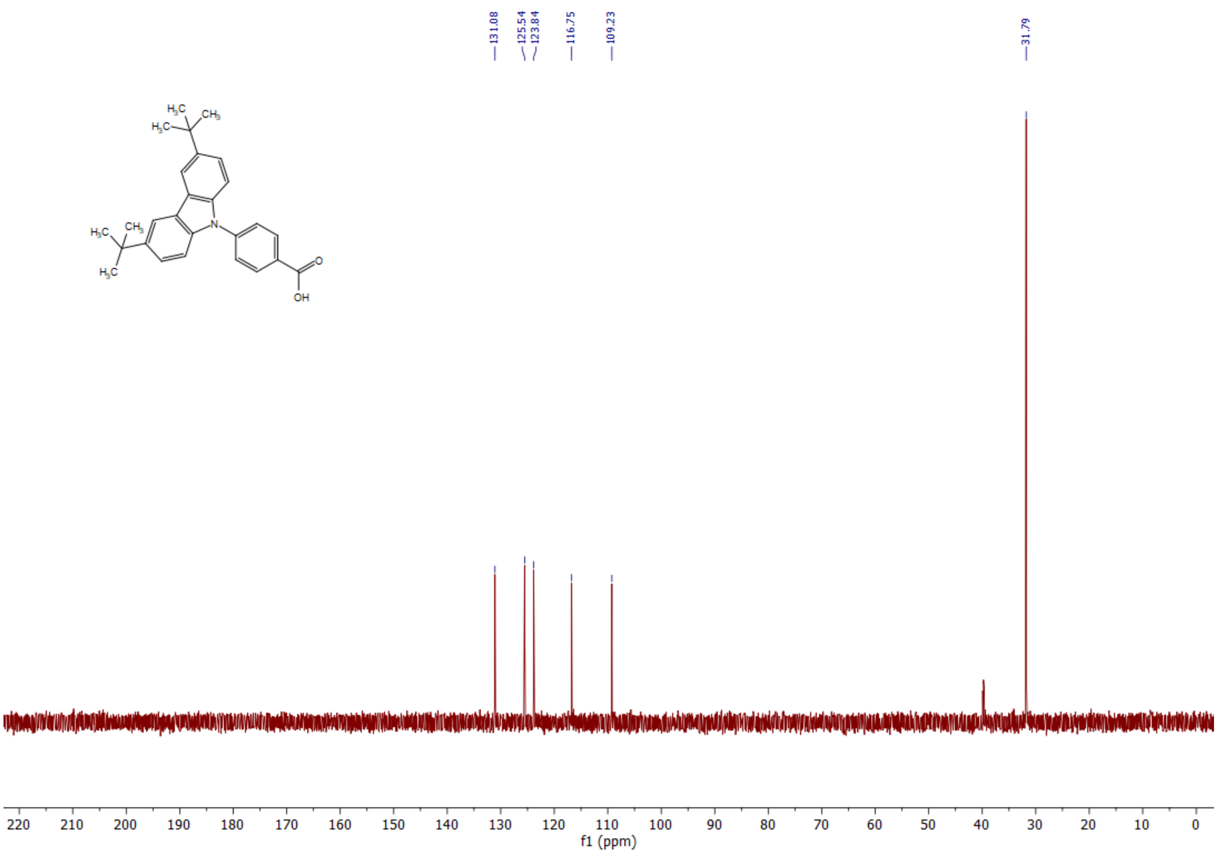

Figure S22. DEPT135 NMR (150 MHz, DMSO-d_6) spectrum of compound **10**.

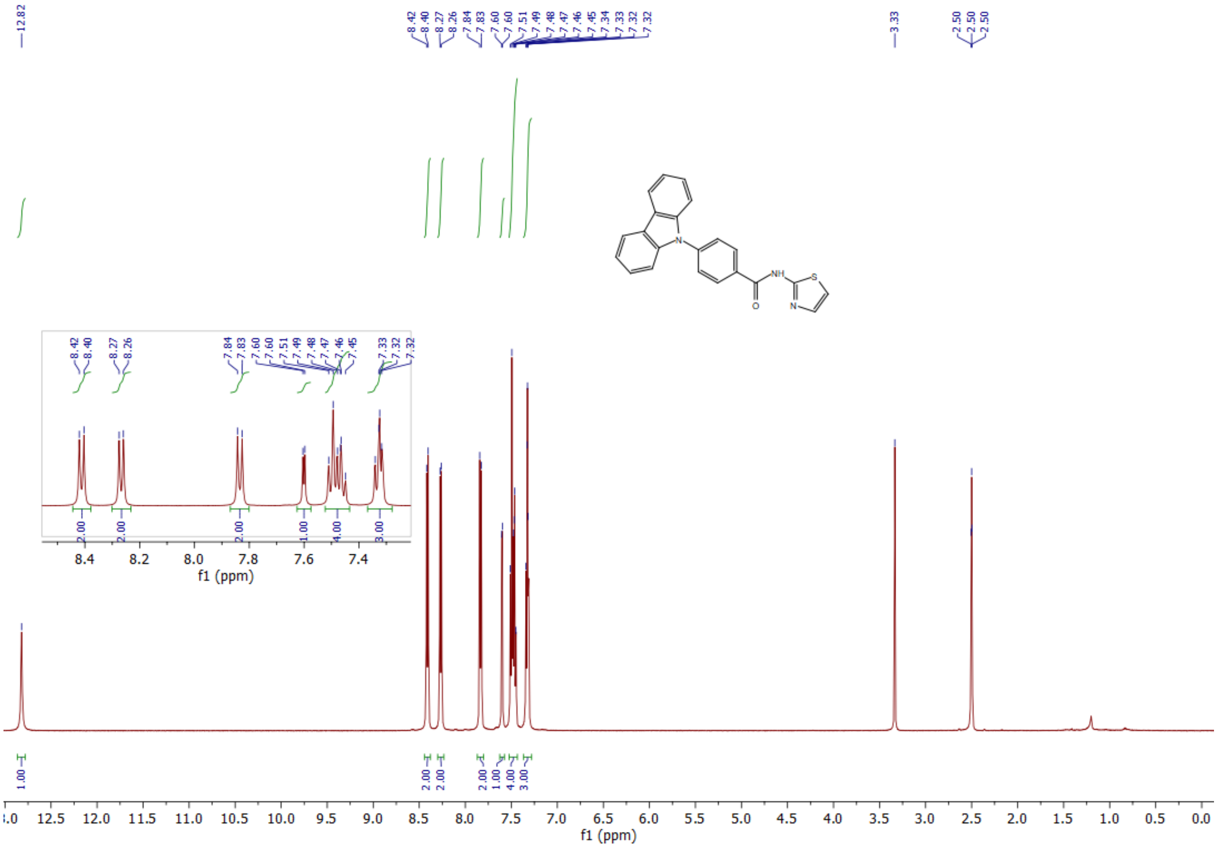

Figure S23. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **12**.

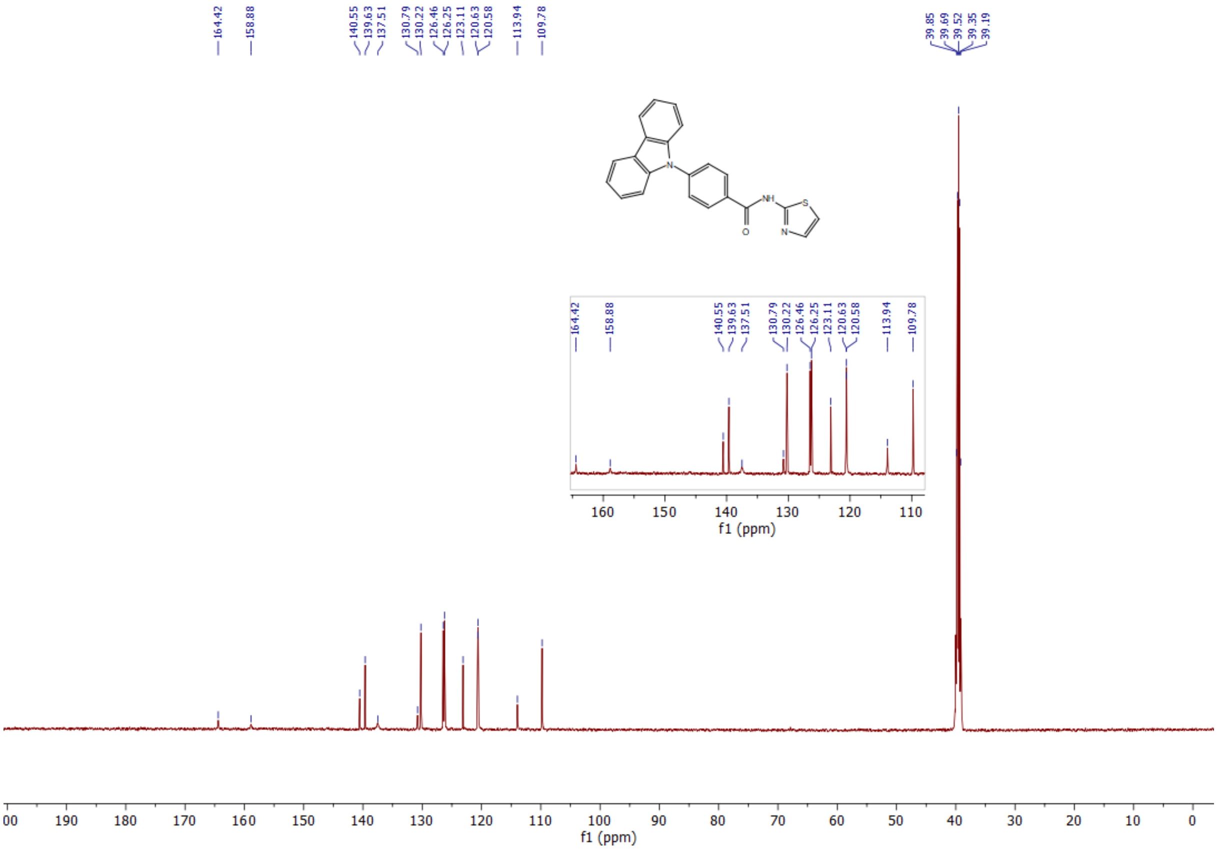

Figure S24. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **12**.

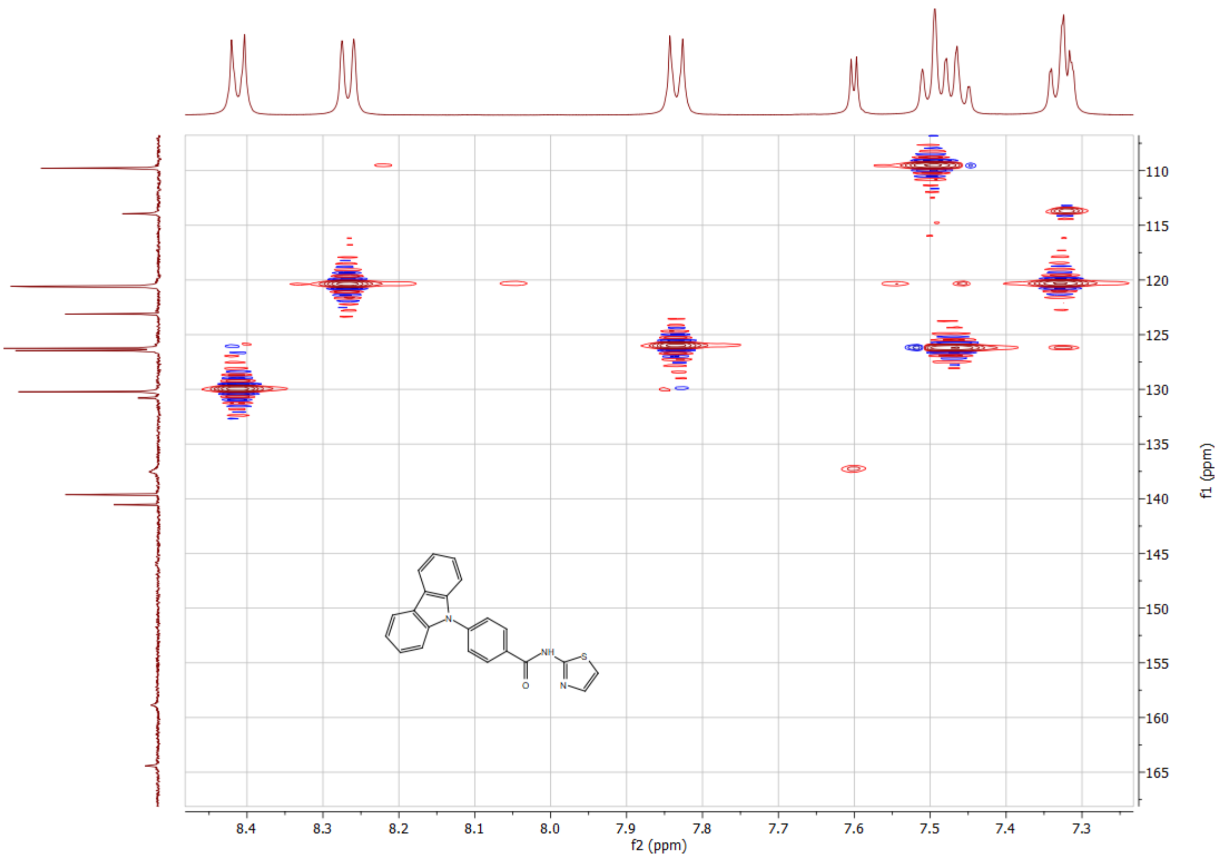

Figure S25. ^{1}H–^{13}C HSQC NMR (125 MHz, DMSO-d_6) spectrum of compound **12**.

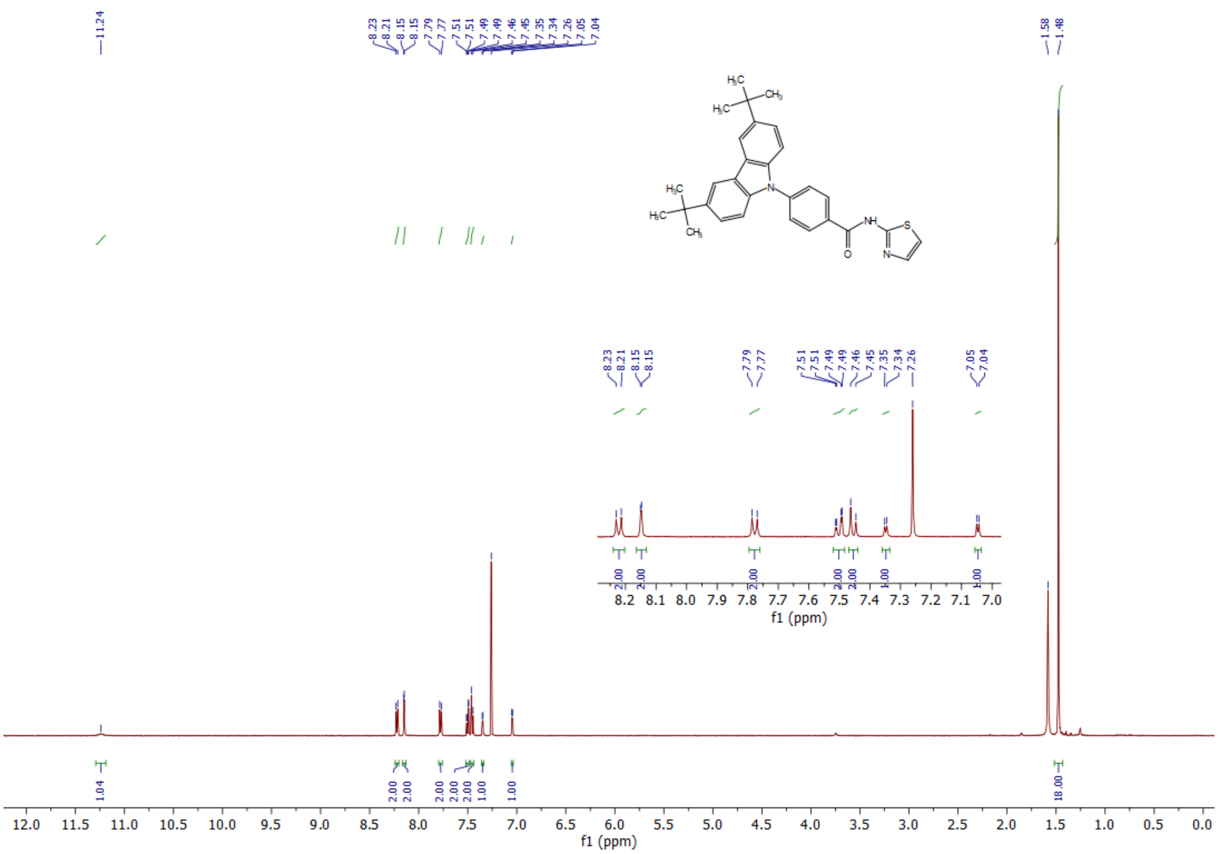

Figure S26. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **13**.

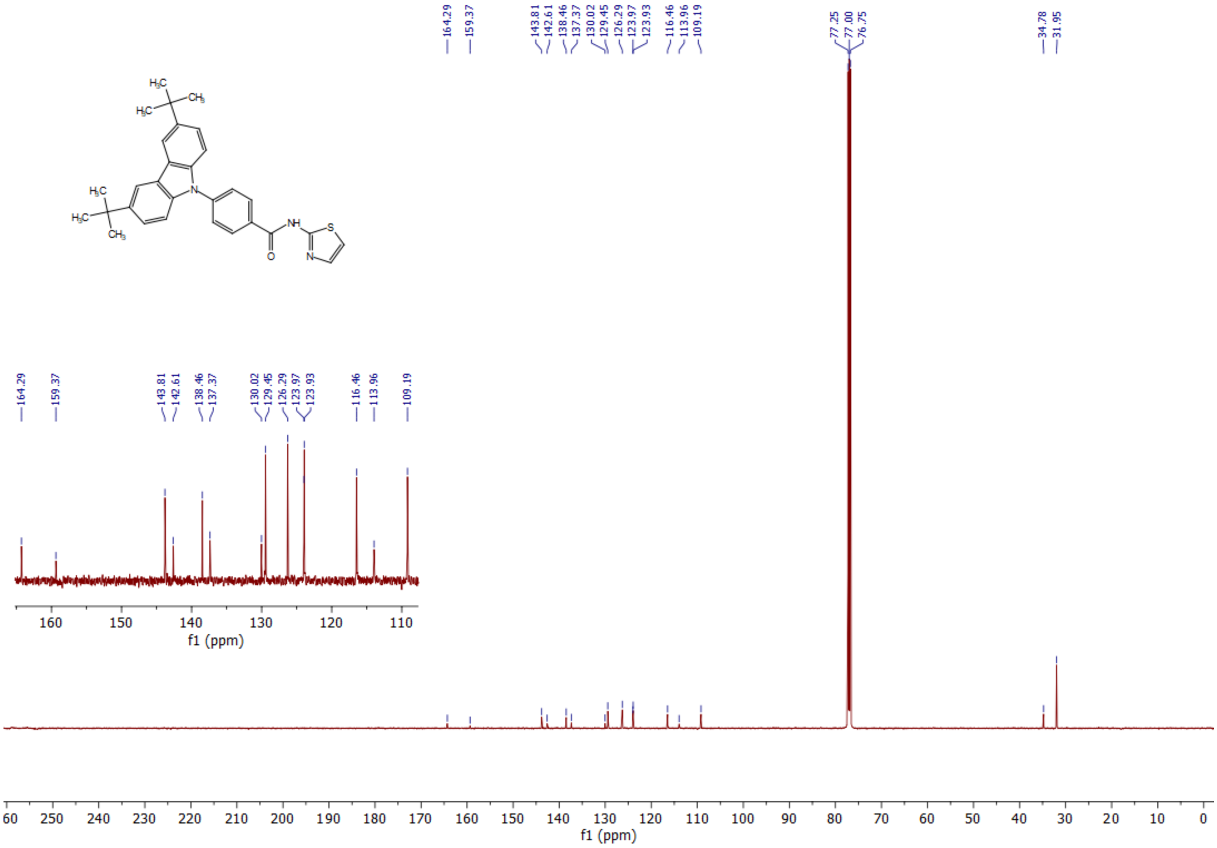

Figure S27. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **13**.

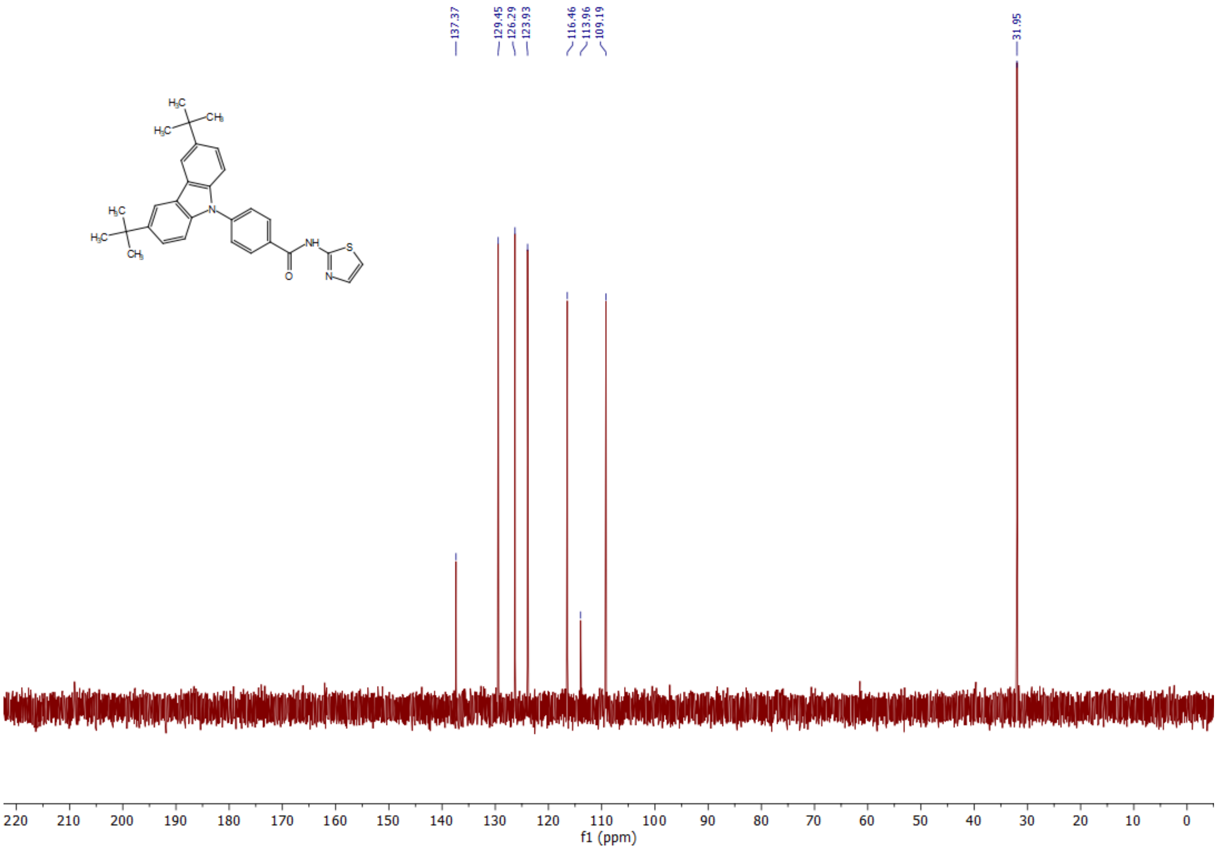

Figure S28. DEPT135 NMR (125 MHz, $CDCl_3$) spectrum of compound **13**.

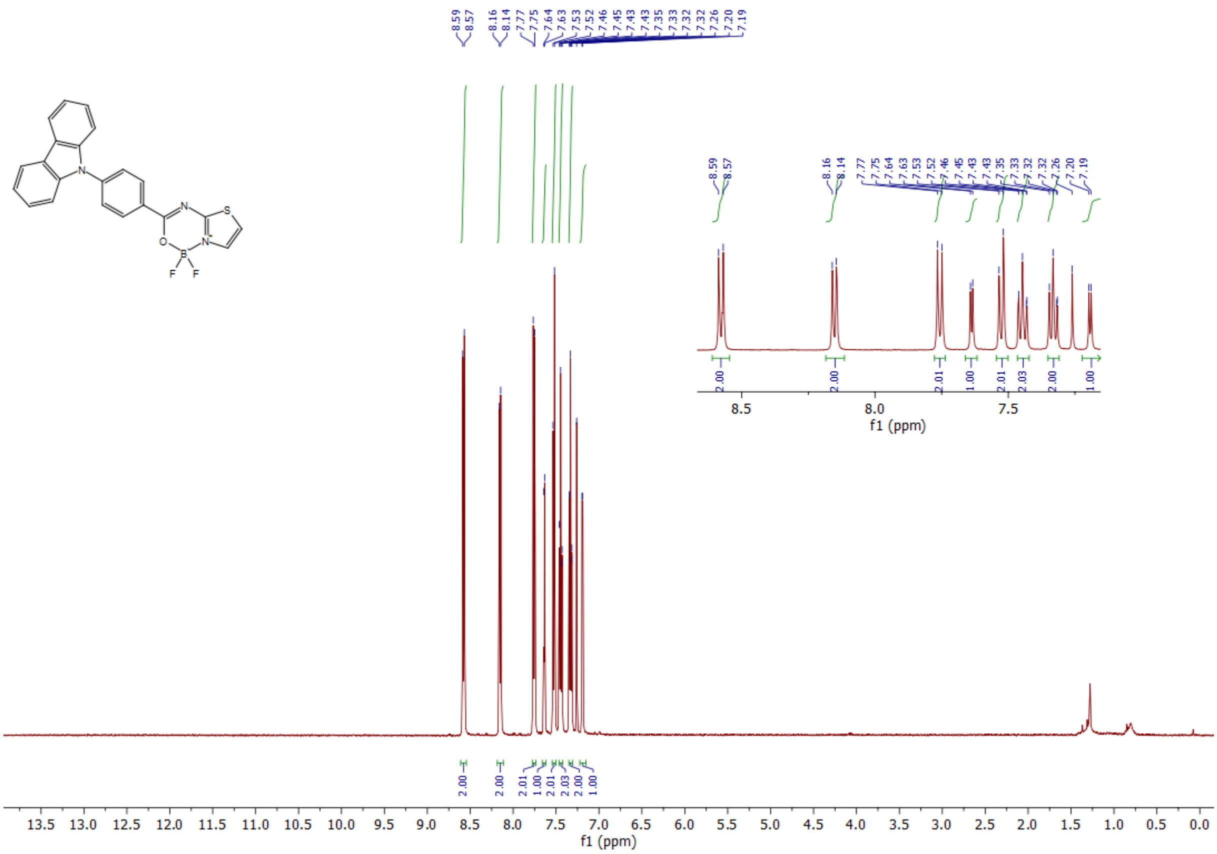

Figure S29. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **2**.

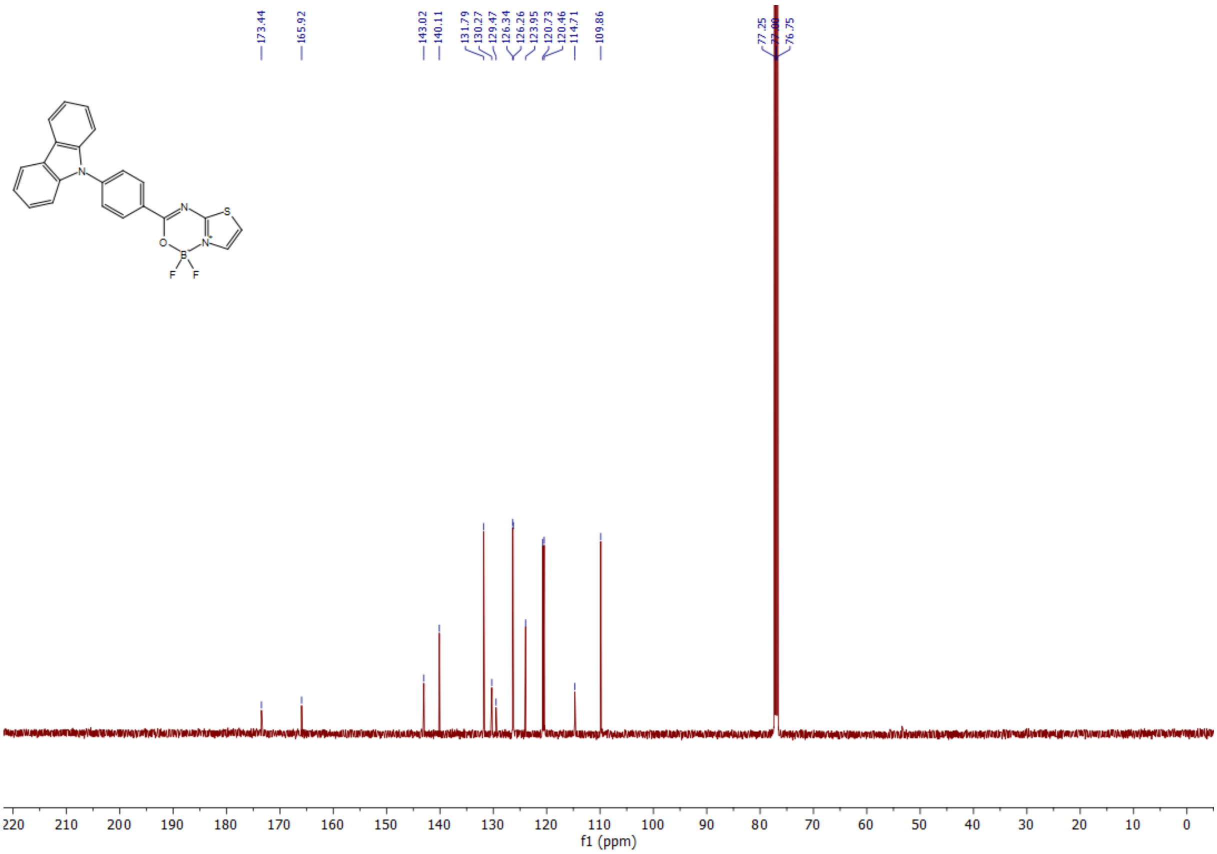

Figure S30. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **2**.

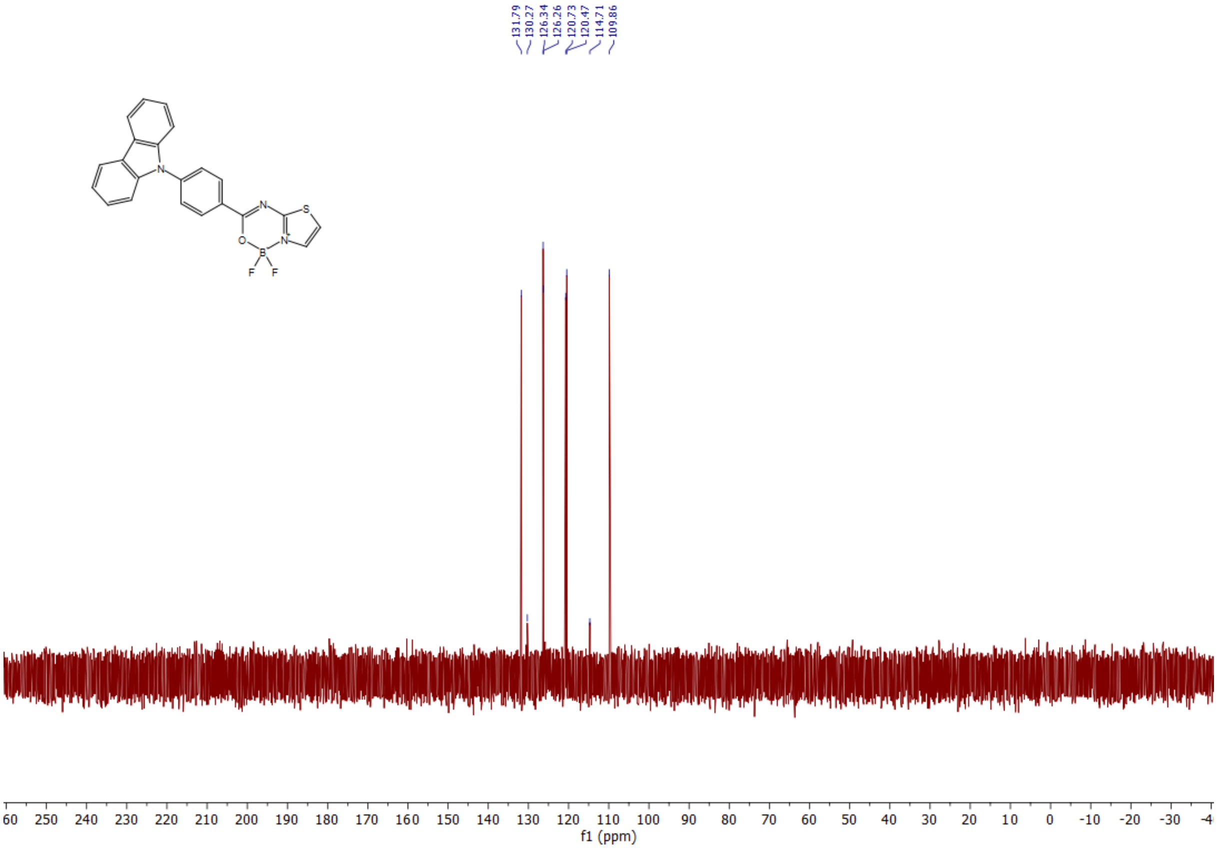

Figure S31. DEPT135 NMR (125 MHz, $CDCl_3$) spectrum of compound **2**.

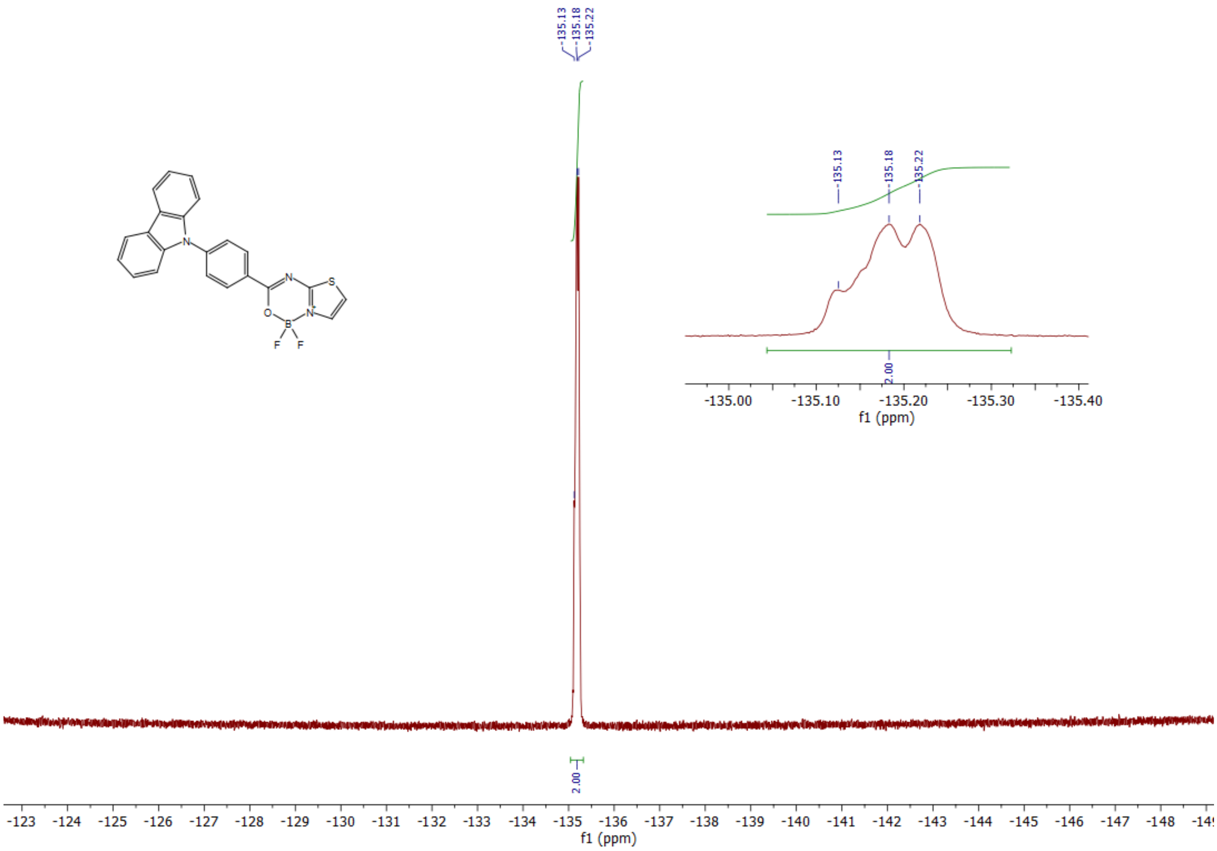

Figure S32. ^{19}F NMR (470 MHz, $CDCl_3$) spectrum of compound **2**.

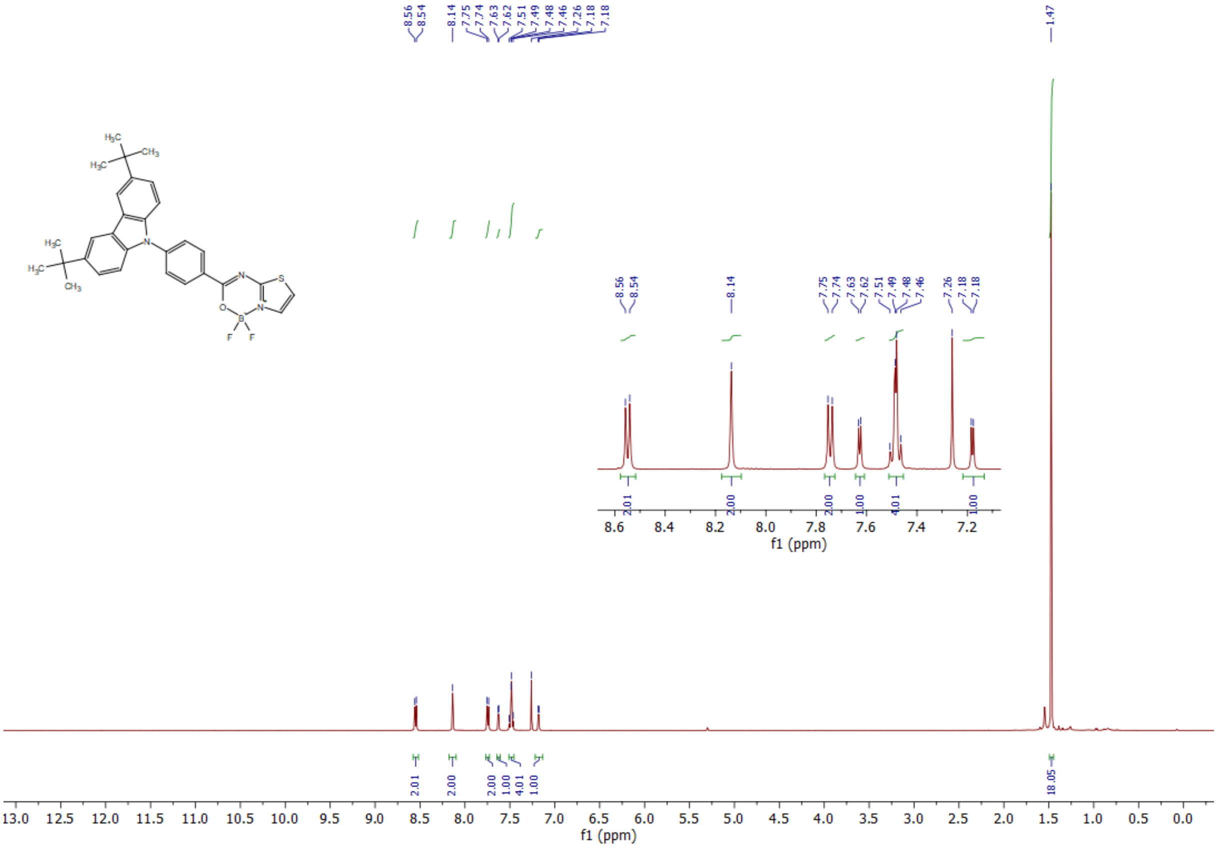

Figure S33. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **3**.

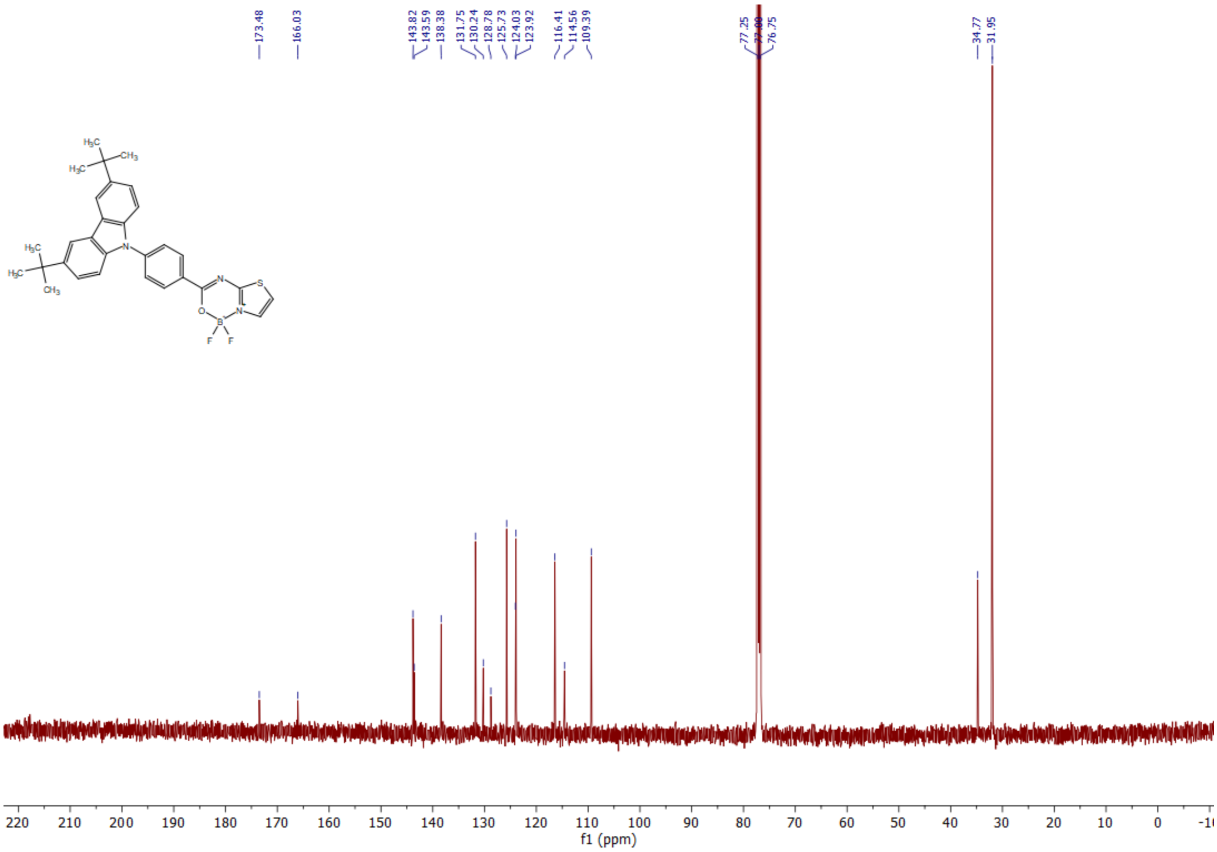

Figure S34. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **3**.

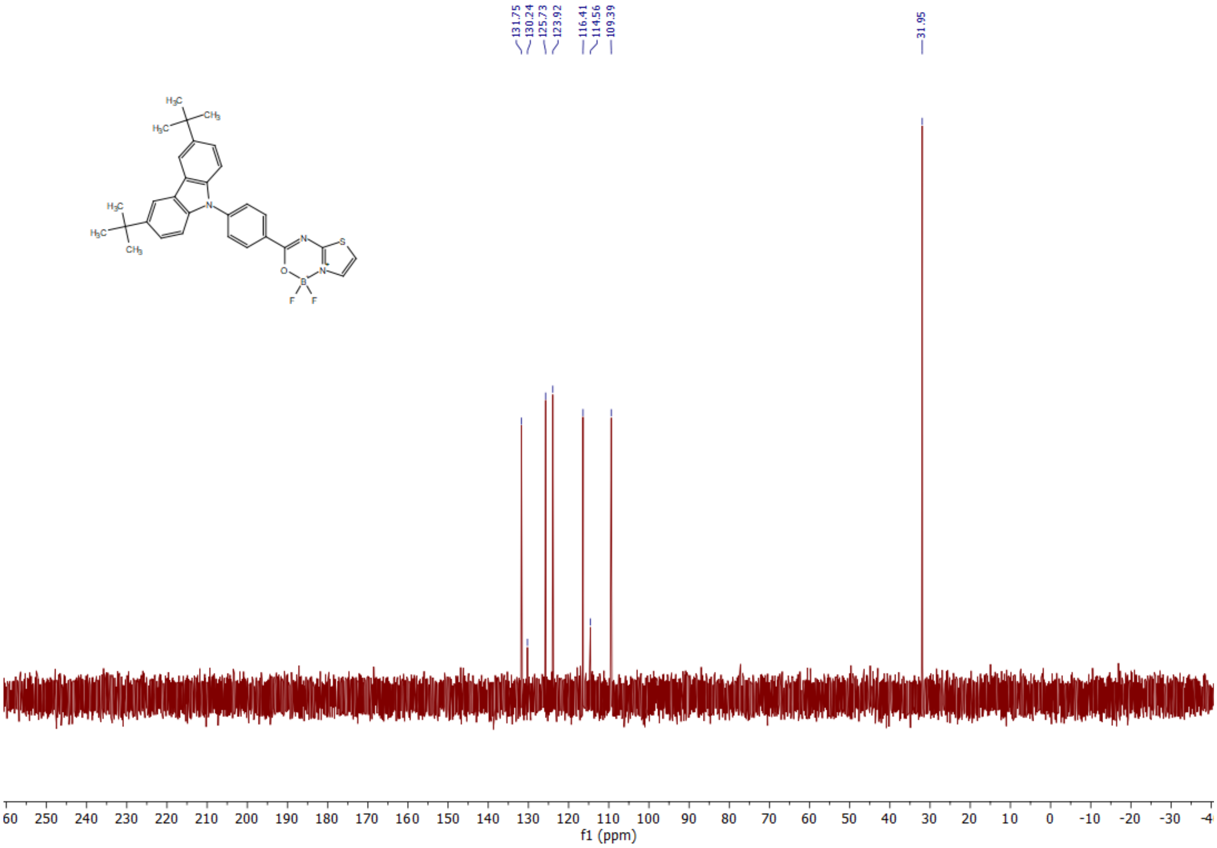

Figure S35. DEPT135 NMR (125 MHz, $CDCl_3$) spectrum of compound **3**.

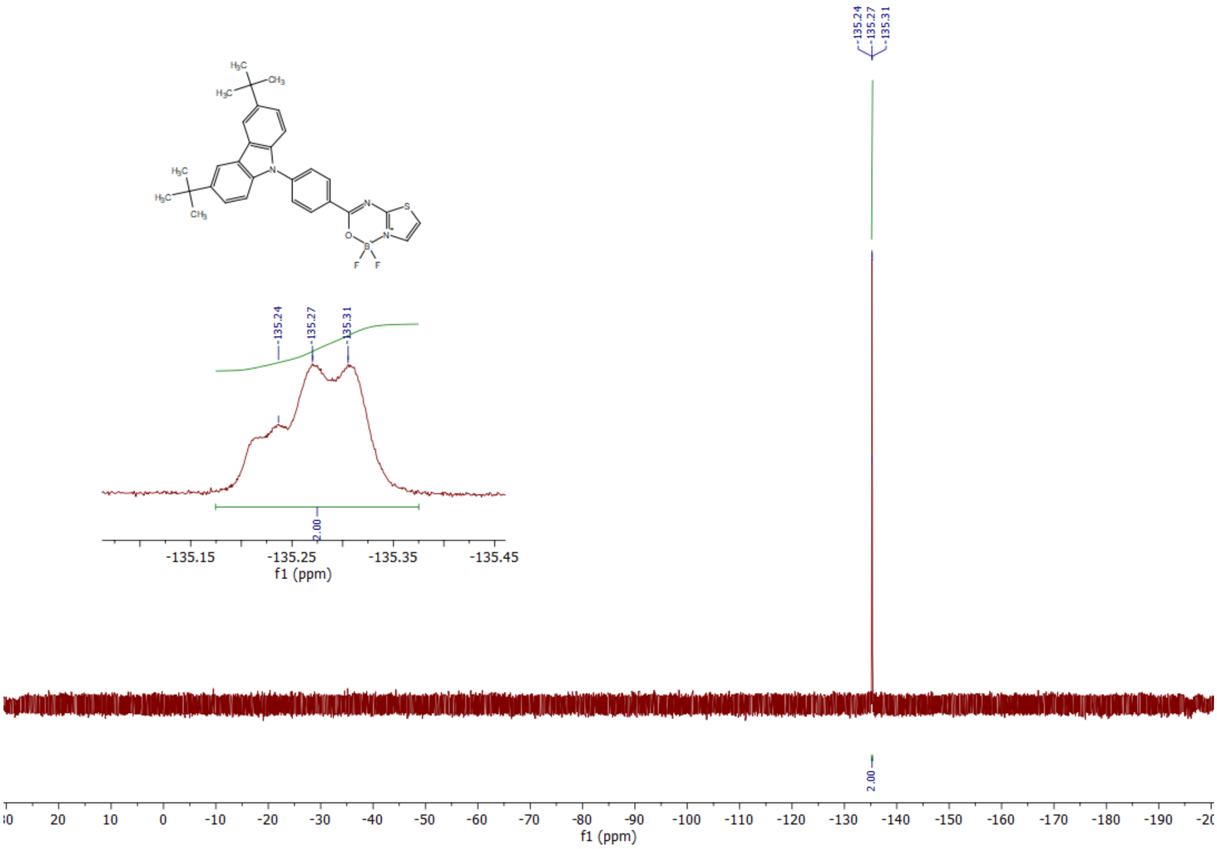

Figure S36. ^{19}F NMR (470 MHz, $CDCl_3$) spectrum of compound **3**.