Electronic Supplementary Information

4-Arylpyrazole-Decorated Dibenzofuran: Synthesis, Characterization, Optical Studies and Computational Analysis

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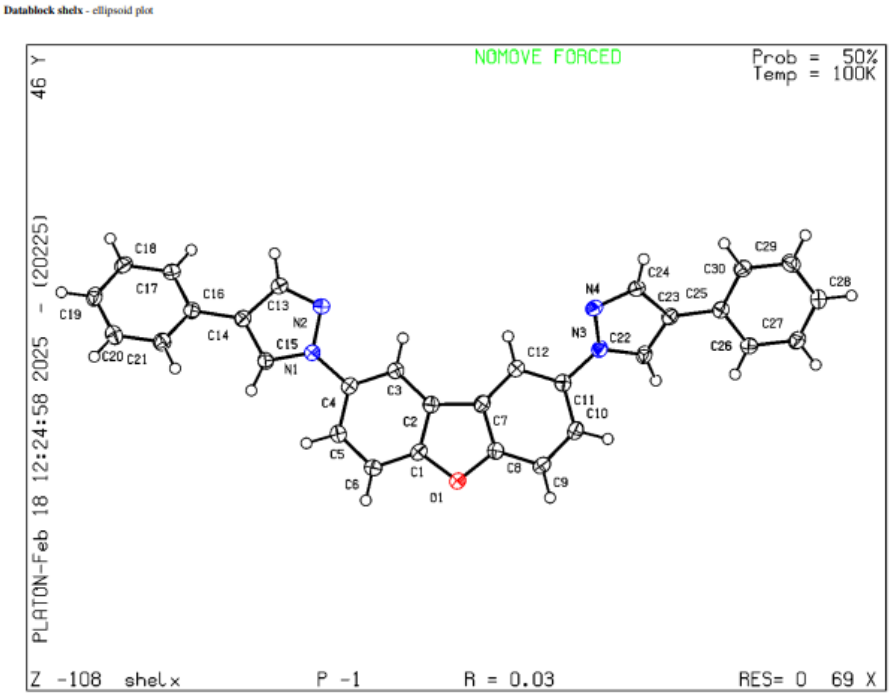
X-ray Crystallographic Analysis of 6a



Parameters	**6a** (CCDC no. 2474099)
Empirical formula	$C_{30}H_{20}N_4O_1$
Formula Weight	452.50
Temperature (K)	100(2)
Wavelength (Å)	1.54184
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	9.4030(1)
b (Å)	10.1164(1)
c (Å)	13.0455(1)
α (º)	83.04
β (º)	69.069(1)
γ (º)	69.003(1)
Volume (Å^3)	1082.06(2)
Z, Calculated Density (g/cm^3)	2, 1.389
Absorption coefficient (mm^{-1})	0.685
F (000)	472
Crystal size (mm)	0.14 x 0.12 x 0.09
θrange for data collection	3.628 to 74.751
Limiting indices	-11≤ h ≤ 11, -12≤ k ≤12, -15≤ l ≤16
No. of measured reflections	38993
No. of independent reflections	4211
R(int)	0.0142
Completeness to θ (%)	94.6
Data / restraints / parameters	4211 / 0 / 316

Goodness - of - fit on F^2	1.038
R_1, wR_2 [$I>2\sigma$ (I)]	0.0329, 0.0807
R_1, wR_2 (all data)	0.0333, 0.0809
Largest diff. peak and hole $eÅ^{-3}$	0.188, -0.243

Cyclic voltammograms

The cyclic voltammograms of **3a-b**, **6a-f** are shown in Fig. S1-S8. Highest occupied molecular orbital energy level (E_{HOMO}) of the compounds was calculated as following E_{HOMO} (eV) = - (E_{pa} (Oxid.) - $E_{Fc/Fc+}$ onset) - 4.80 eV, where E_{pa} (Oxid.) and $E_{Fc/Fc+}$ onset are onset oxidation potential of the compound and internal standard, respectively. Lowest unoccupied molecular orbital energy was obtained from $E(_{LUMO}) = E_g + E(_{HOMO})$; E_g is the band gap energy calculated from UV visible spectra.

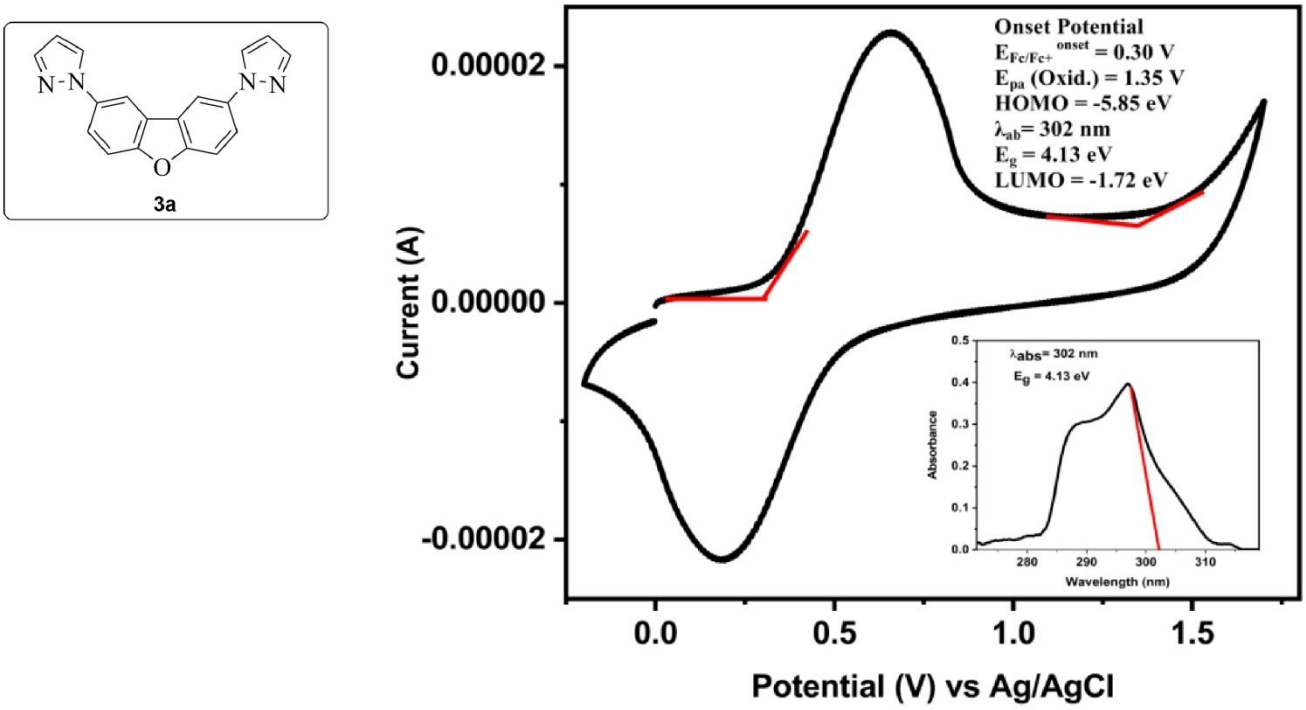


Figure S1. The cyclic voltammogram of **3a.**

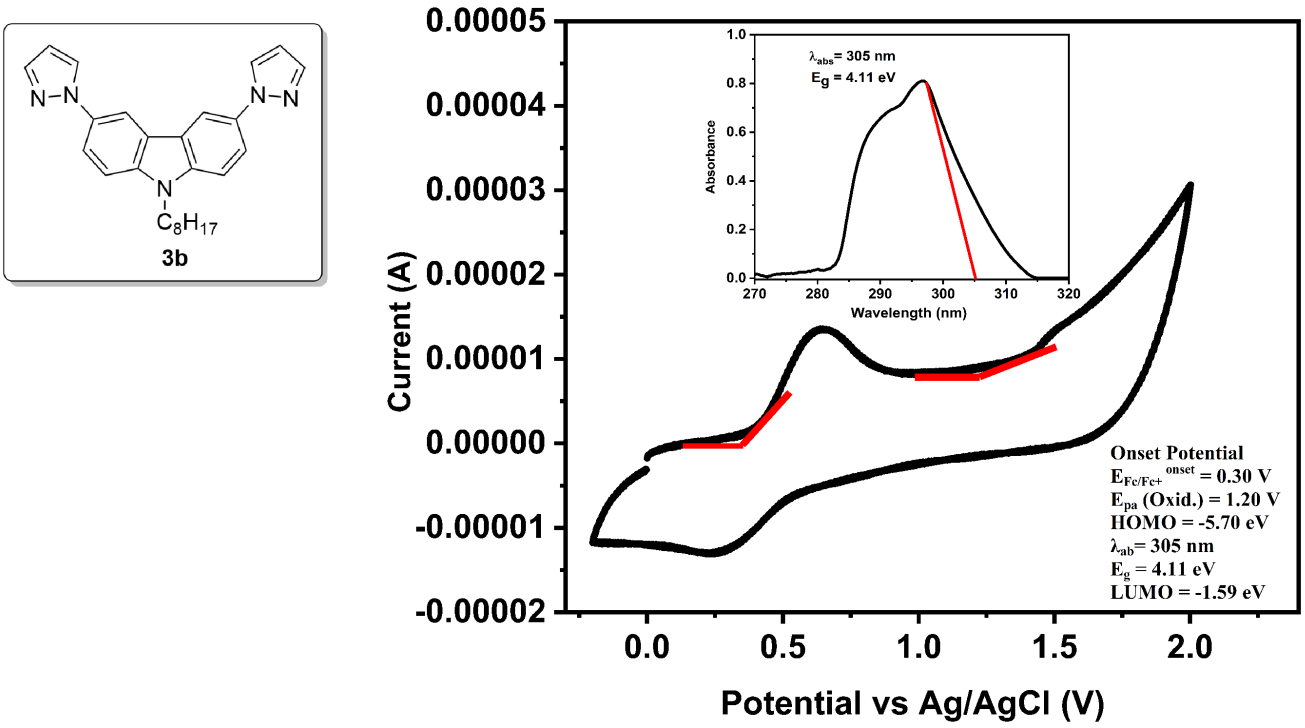


Figure S2. The cyclic voltammogram of **3b.**

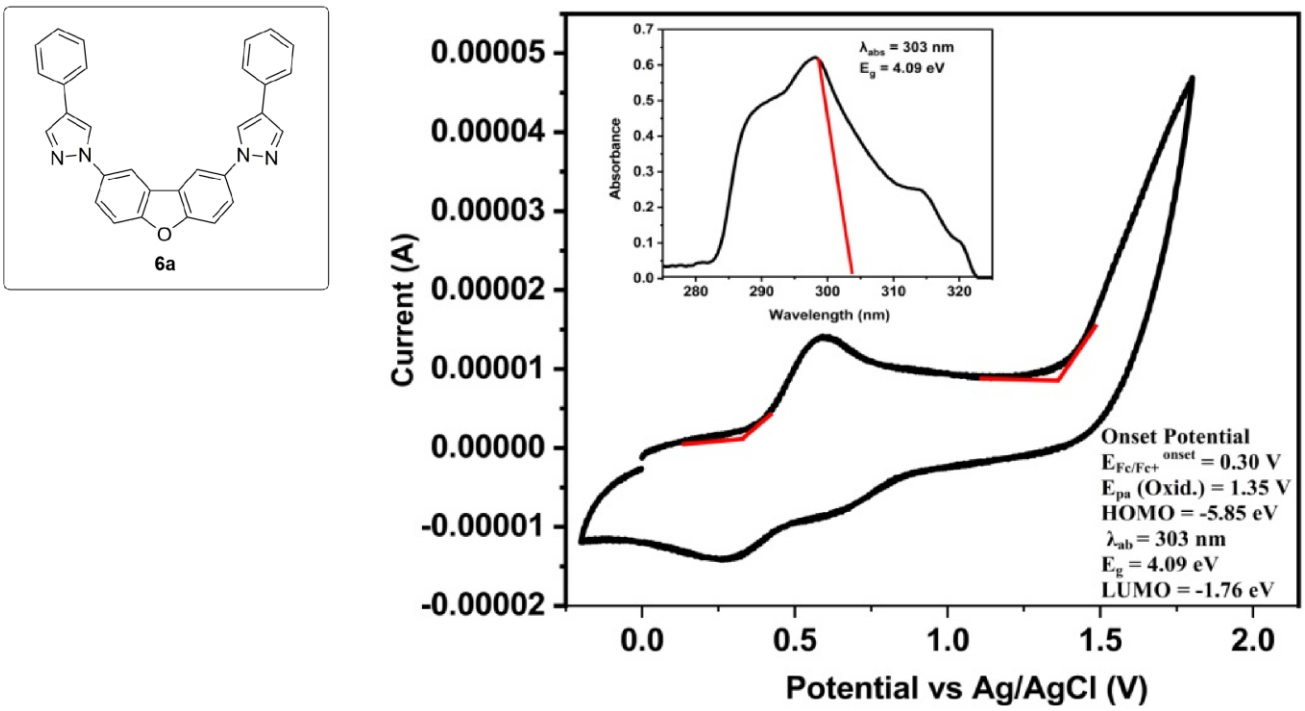


Figure S3. The cyclic voltammogram of **6a.**

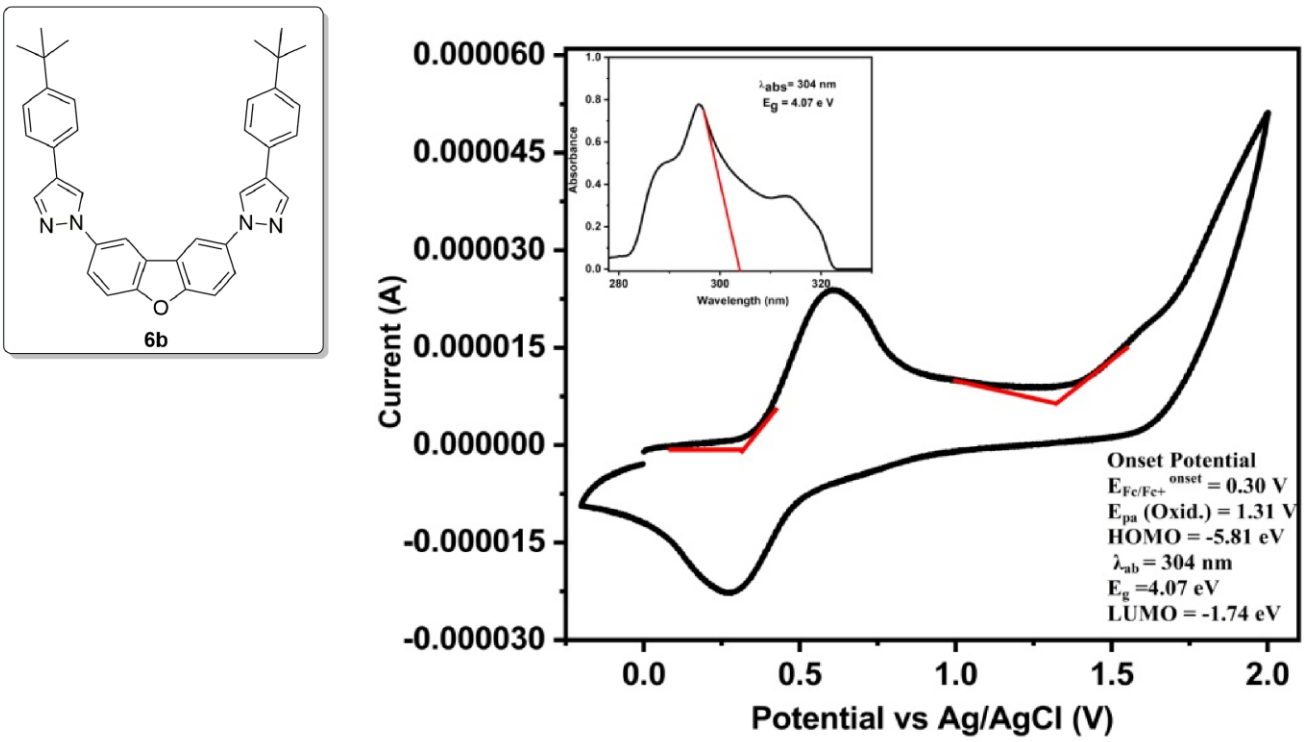


Figure S4. The cyclic voltammogram of **6b.**

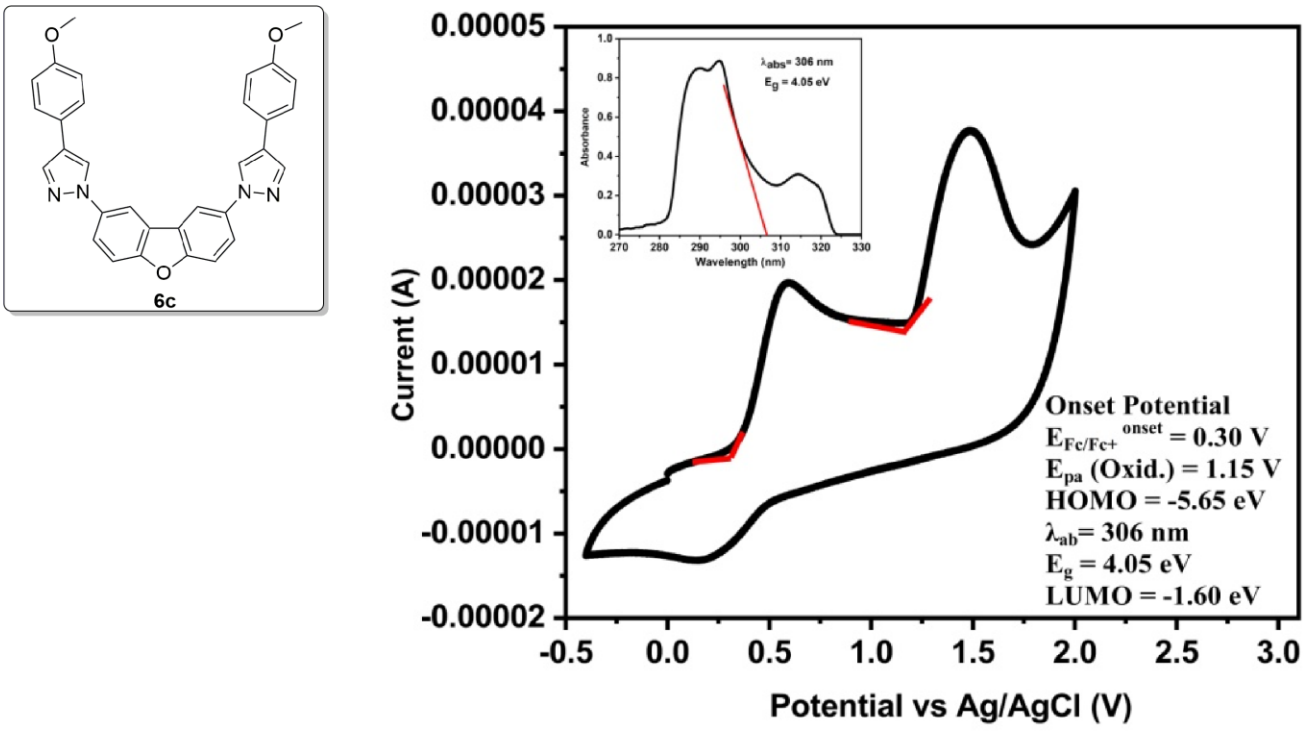


Figure S5. The cyclic voltammogram of **6c.**

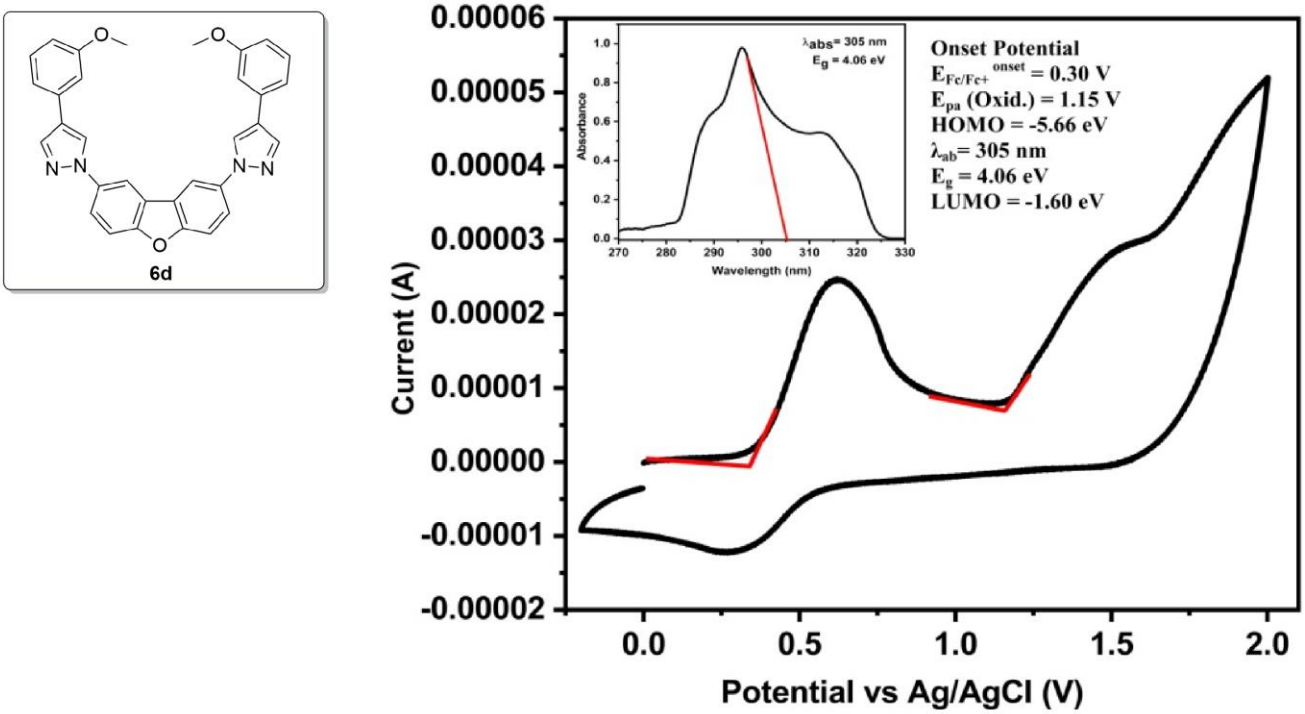


Figure S6. The cyclic voltammogram of **6d.**

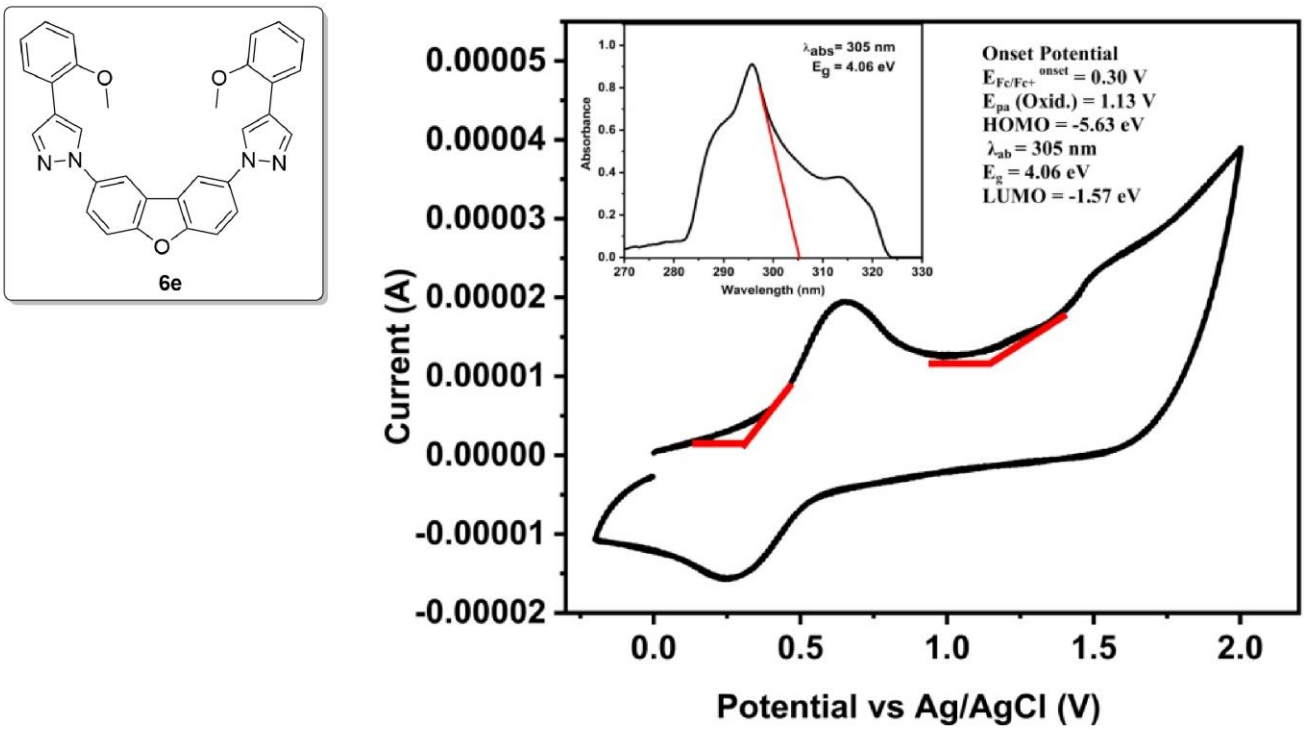


Figure S7. The cyclic voltammogram of **6e.**

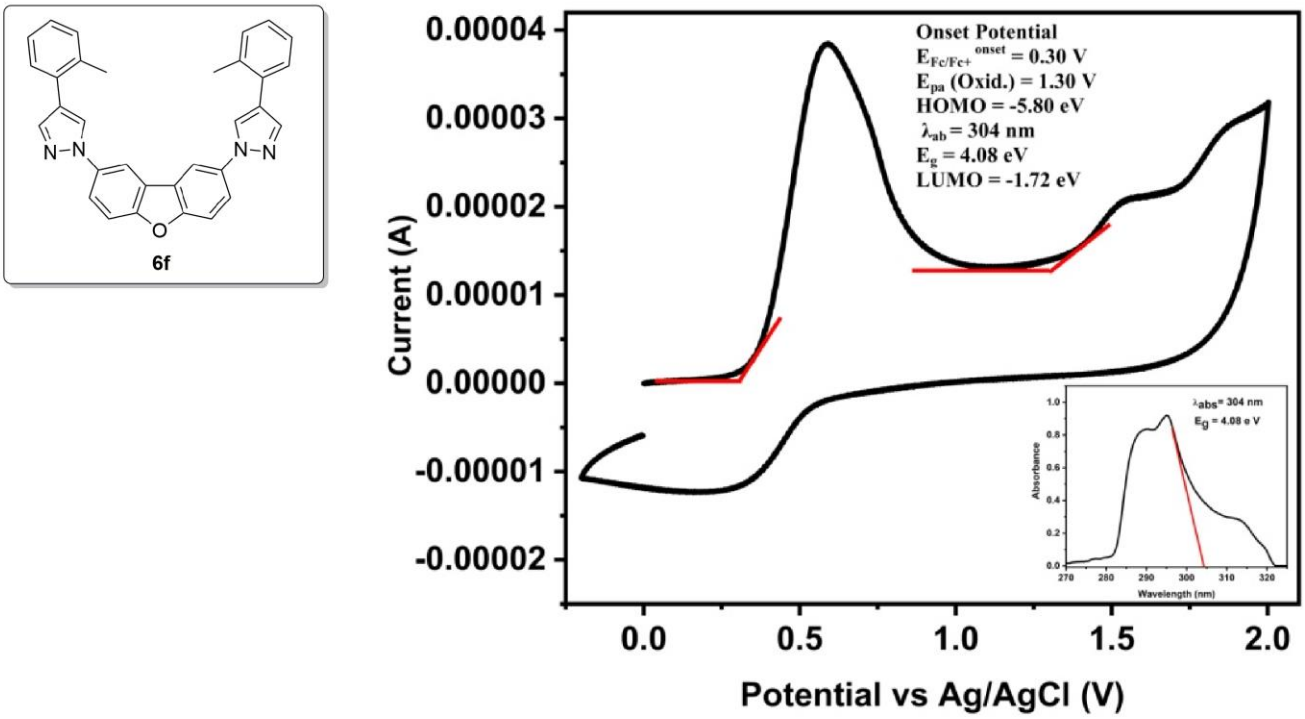


Figure S8. The cyclic voltammogram of **6f.**

Thermogravimetric (TG) Analysis

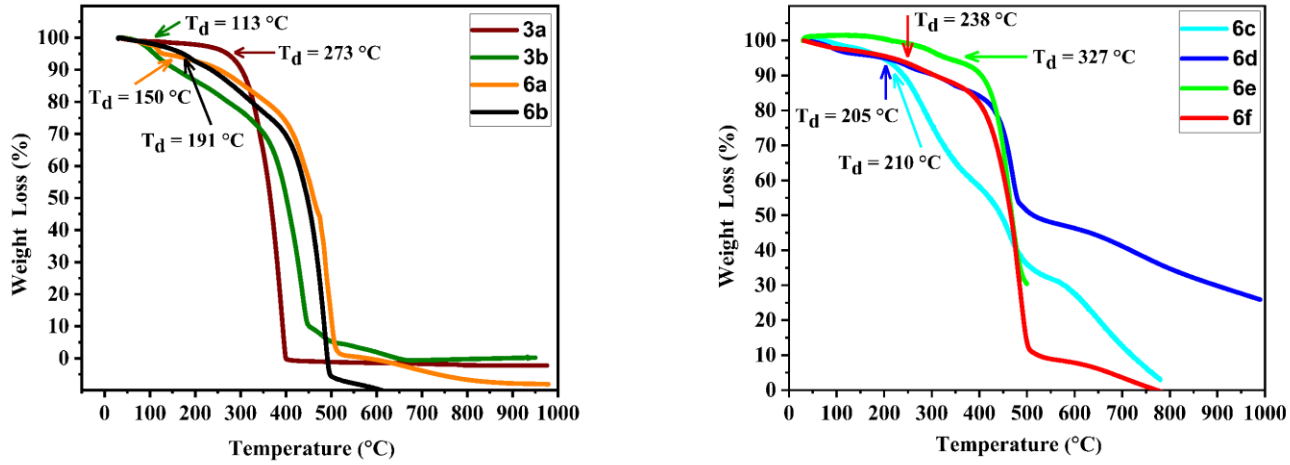


Figure S9. Left: TGA curves of **3a-b,** and **6a-b**; Right: TGA curves of **6c-f**.

Differential Scanning Calorimetry (DSC) Analysis

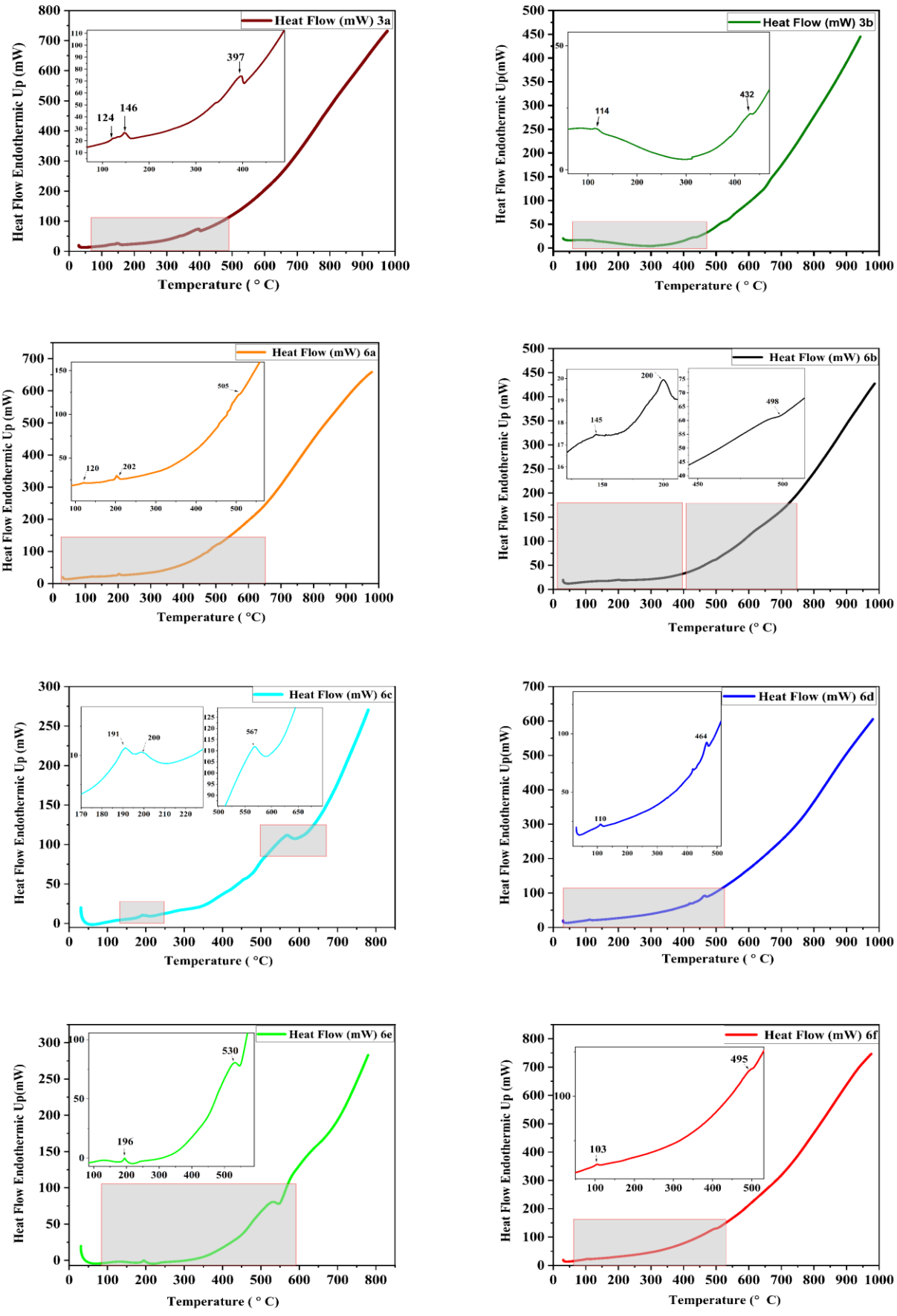


Figure S10. DSC curves of **3a-b** and **6a-f**.

Effect of solvation on absorption and emission spectrum

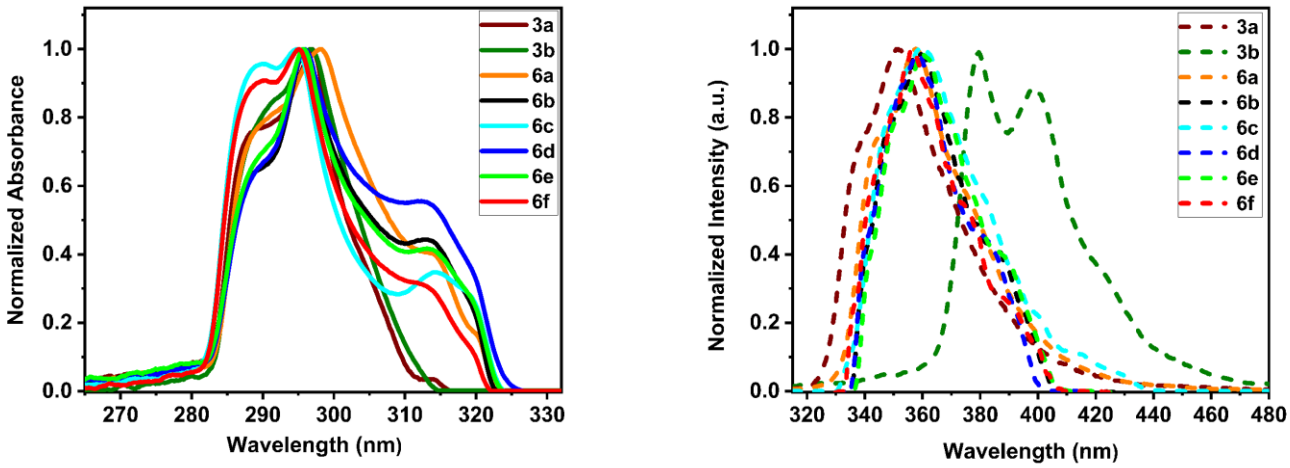


Figure S11. Normalized UV/Vis absorption (left) and emission (right) spectra of **3a-b**, and **6a-f** in toluene. The excitation wavelength was fixed at 295 nm. UV/Vis absorption and emission spectra were taken in toluene (concentration 1×10^{-5} M).

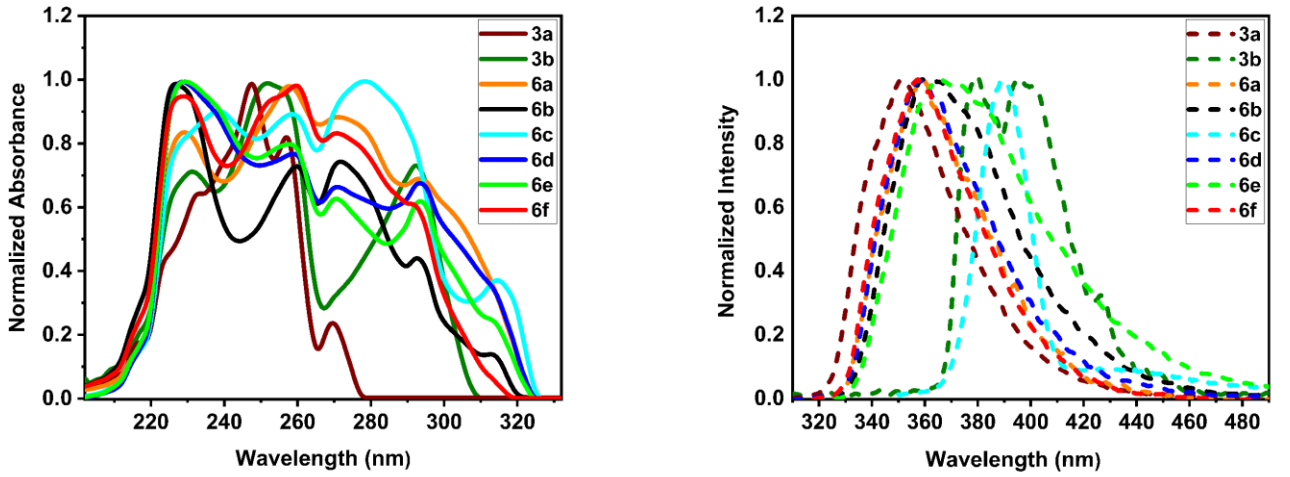


Figure S12. Normalized UV/Vis absorption (left) and emission (right) spectra of **3a-b**, **6a-f** in acetonitrile. The excitation wavelength was fixed at 295 nm. UV/Vis absorption and emission spectra were taken in acetonitrile (concentration 1×10^{-5} M).

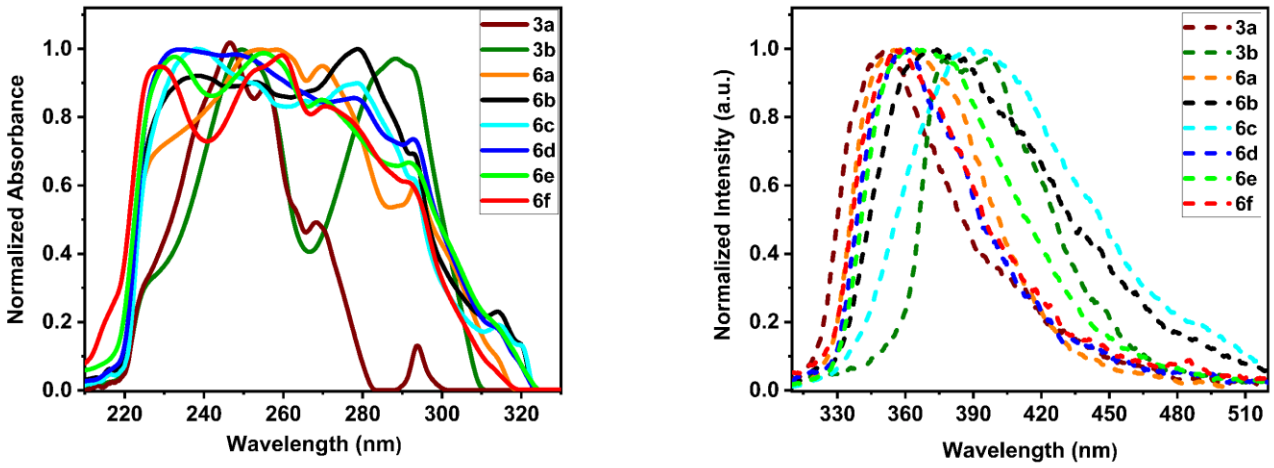


Figure S13. UV/Vis absorption (left) and emission (right) spectra of **3a-b**, **6a-f** in methanol. The excitation wavelength was fixed at 295 nm. UV/Vis absorption and emission spectra were taken in methanol (concentration 1×10^{-5} M).

Table S1. UV/Vis absorption and emission data of **3a, 3b, 6a-f** in toluene, in acetonitrile, and in methanol

Compound	**3a**			**3b**			**6a**			**6c**		
Solvent	Toluene	Acetonitrile	Methanol	Toluene	Acetonitrile	Methanol	Toluene	Acetonitrile	Methanol	Toluene	Acetonitrile	Methanol
λ_{max}(nm)[a]	287, 295	246, 256, 270	246, 256, 268, 293	295	230, 250, 294	250, 288	298, 314	228, 258, 272, 295	256, 270, 294	288, 294, 318	237, 268, 278, 314	238, 254, 265, 278, 314
ε ($M^{-1}cm^{-1}$)[b]	39,500	75,100	75,100	80,000	87,300	90,000	62,000	91,100	88,000	88,900	79,100	79,100
λ_{em}(nm)[c]	350	352	350	380, 399	380,396	378, 396	359	360	360	360	390	392
Stoke shift (nm)	55	82	57	85	86	90	45	65	66	42	76	78

Compound	**6b**			**6d**			**6e**			**6f**		
Solvent	Toluene	Acetonitrile	Methanol	Toluene	Acetonitrile	Methanol	Toluene	Acetonitrile	Methanol	Toluene	Acetonitrile	Methanol
λ_{max}(nm)[a]	296, 314	226, 259, 272, 292, 314	238, 253, 278, 314	296, 314	230, 258, 270, 294	232, 249, 278, 293, 314	296, 314	230, 258, 270, 293, 313	232, 254, 270, 292, 314	290, 295, 314	228, 259, 270, 292	233, 257, 270, 292
ε ($M^{-1}cm^{-1}$)[b]	78,000	62,800	92,700	98,000	80,600	82,430	90,900	70,000	70,000	90,000	88,000	88,000
λ_{em}(nm)[c]	358	362	374	358	360	360	360	368	368	356	357	358
Stoke shift (nm)	44	48	60	44	66	46	46	55	54	42	65	66

[a]Absorption maximum, [b] molar extinction co-efficient, [c]emission maxima in respective solvent following photo excitation at 295 nm.

Computational Studies:

Table S4. Vertical excitation energies ΔE (in eV and nm units), oscillator strength *f* (in dimensionless units) and electronic excitations for **3a** calculated at TD-B3LYP/6-31G(D,P) level of theory.

State	ΔE (eV)	ΔE (nm)	*f*	Transition	State	ΔE (eV)	ΔE (nm)	*f*	Transition
S_1	4.111	301.6	0.010	HOMO→LUMO	T_1	3.354	369.7	-	HOMO-1→LUMO
S_2	4.300	288.3	0.176	HOMO-1→LUMO	T_2	3.430	361.4	-	HOMO→LUMO
S_3	4.786	259.1	0.715	HOMO→LUMO+1	T_3	3.761	329.6	-	HOMO→LUMO+1
S_4	4.895	253.3	0.015	HOMO-1→LUMO+1	T_4	3.870	320.4	-	HOMO-1→LUMO+1
S_5	4.963	249.8	0.001	HOMO-3→LUMO	T_5	4.178	296.8	-	HOMO-2→LUMO

Table S5. Vertical excitation energies ΔE (in eV and nm units), oscillator strength *f* (in dimensionless units) and electronic excitations for **3b** calculated at TD-B3LYP/6-31G(D,P) level of theory.

State	ΔE (eV)	ΔE (nm)	*f*	Transition	State	ΔE (eV)	ΔE (nm)	*f*	Transition
S_1	3.761	329.7	0.021	HOMO→LUMO	T_1	3.075	403.2	-	HOMO→LUMO
S_2	4.142	299.3	0.009	HOMO→LUMO+1	T_2	3.318	373.7	-	HOMO-1→LUMO
S_3	4.546	272.7	1.045	HOMO→LUMO+1	T_3	3.58	346.3	-	HOMO→LUMO+1
S_4	4.713	263.1	0.012	HOMO→LUMO+2	T_4	3.81	324.9	-	HOMO→LUMO+2
S_5	5.022	246.9	0.082	HOMO-3→LUMO	T_5	4.14	298.8	-	HOMO-2→LUMO

Table S6. Vertical excitation energies ΔE (in eV and nm units), oscillator strength *f* (in dimensionless units) and electronic excitations for **6a** calculated at TD-B3LYP/6-31G(D,P) level of theory.

State	ΔE (eV)	ΔE (nm)	*f*	Transition	State	ΔE (eV)	ΔE (nm)	*f*	Transition
S_1	3.921	316.2	0.0006	HOMO→LUMO	T_1	3.328	372.6	-	HOMO-3→LUMO
S_2	3.986	311.0	0.209	HOMO-1→LUMO	T_2	3.358	369.2	-	HOMO→LUMO
S_3	4.351	285.0	0.821	HOMO→LUMO+1	T_3	3.490	355.3	-	HOMO→LUMO+1
S_4	4.429	280.0	0.010	HOMO-2→LUMO	T_4	3.542	350.0	-	HOMO-1→LUMO+1
S_5	4.542	273.0	0.191	HOMO-3→LUMO	T_5	3.760	329.8	-	HOMO-2→LUMO+1

Table S7. Vertical excitation energies ΔE (in eV and nm units), oscillator strength *f* (in dimensionless units) and electronic excitations for **6c** calculated at TD-B3LYP/6-31G(D,P) level of theory.

State	E (eV)	ΔE (nm)	*f*	Transition	State	E (eV)	ΔE (nm)	*f*	Transition
S_1	3.714	333.8	0.001	HOMO→LUMO	T_1	3.291	376.7	-	HOMO→LUMO
S_2	3.742	331.3	0.124	HOMO-1→LUMO	T_2	3.303	375.3	-	HOMO-3→LUMO
S_3	4.189	296.0	0.719	HOMO→LUMO+1	T_3	3.393	365.4	-	HOMO→LUMO+1
S_4	4.275	290.0	0.041	HOMO-1→LUMO+1	T_4	3.457	358.7	-	HOMO-1→LUMO+1
S_5	4.365	284.0	0.243	HOMO-1→LUMO+1	T_5	3.685	336.4	-	HOMO-1→LUMO

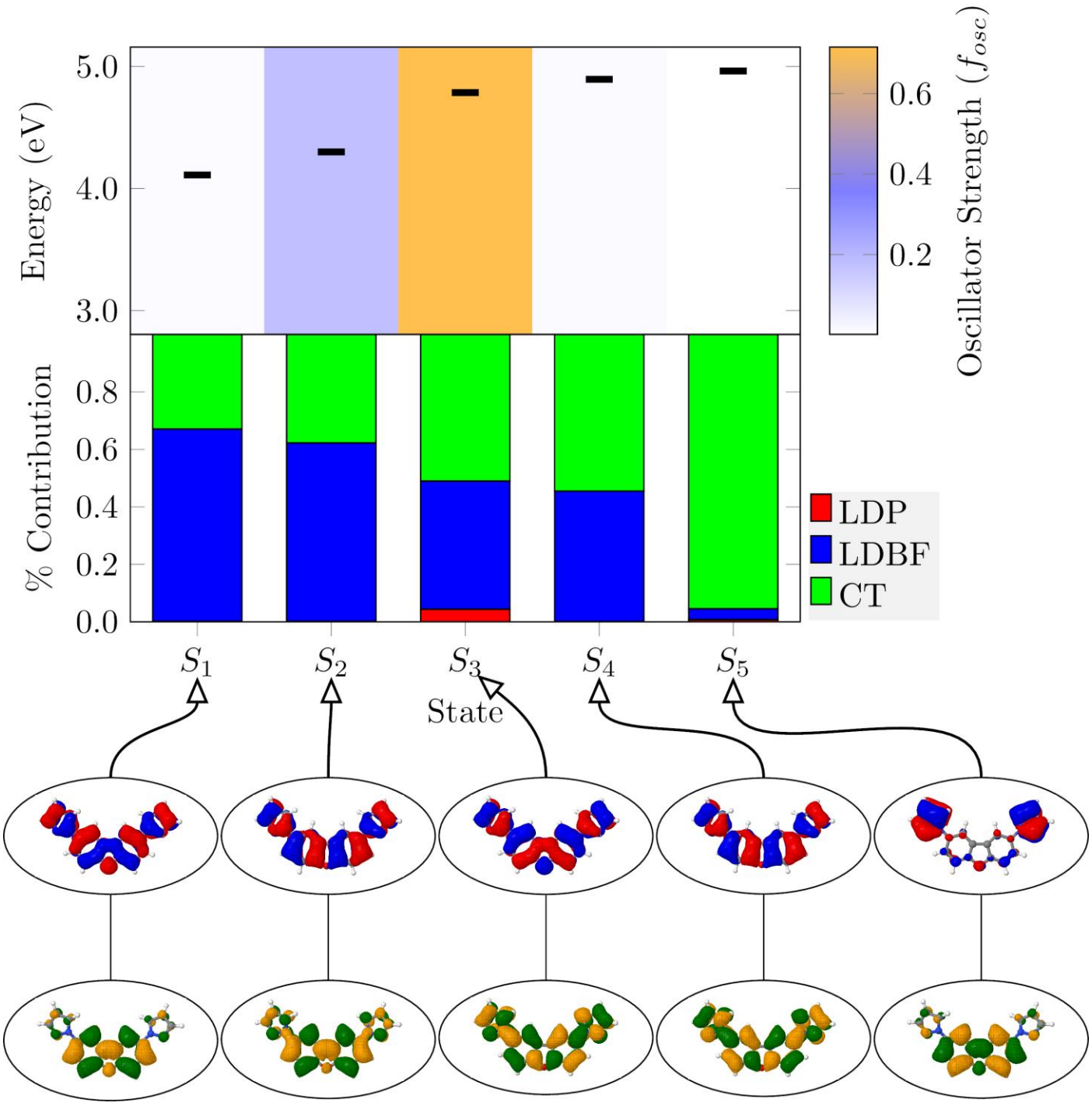


Figure S14. The characterization of first four excited states of the compound **3a**. LDP refer to local excitation in pyrazole units. LDBF is the local excitation in dibenzofuran unit. CT is the charge transfer from pyrazole to dibenzofuran unit.

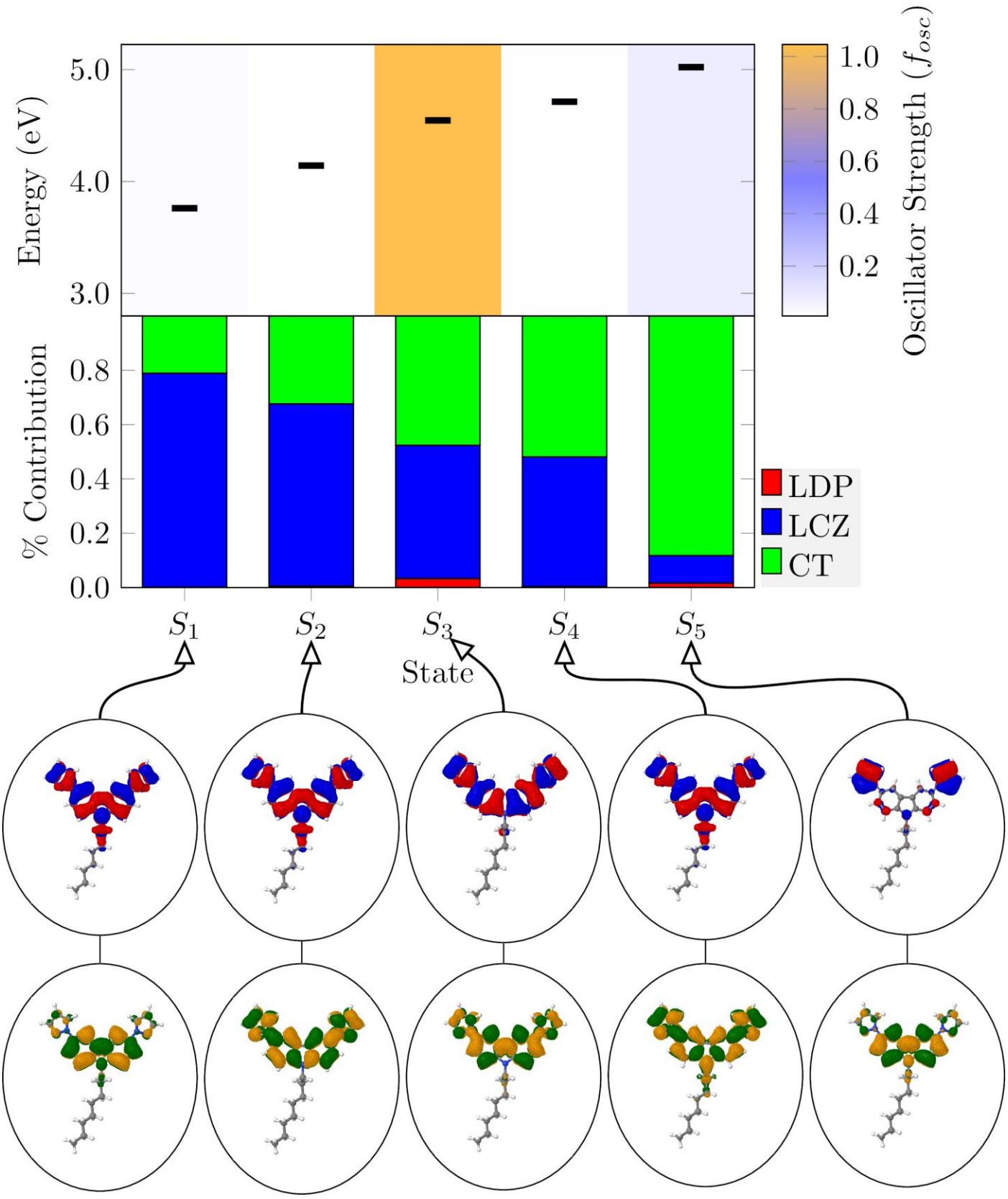


Figure S15. The characterization of first four singlet excited states of the compound **3b**. LDP refer to local excitation in pyrazole units. LCZ is the local excitation in carbazole unit. CT is the charge transfer from pyrazole to carbazole units.

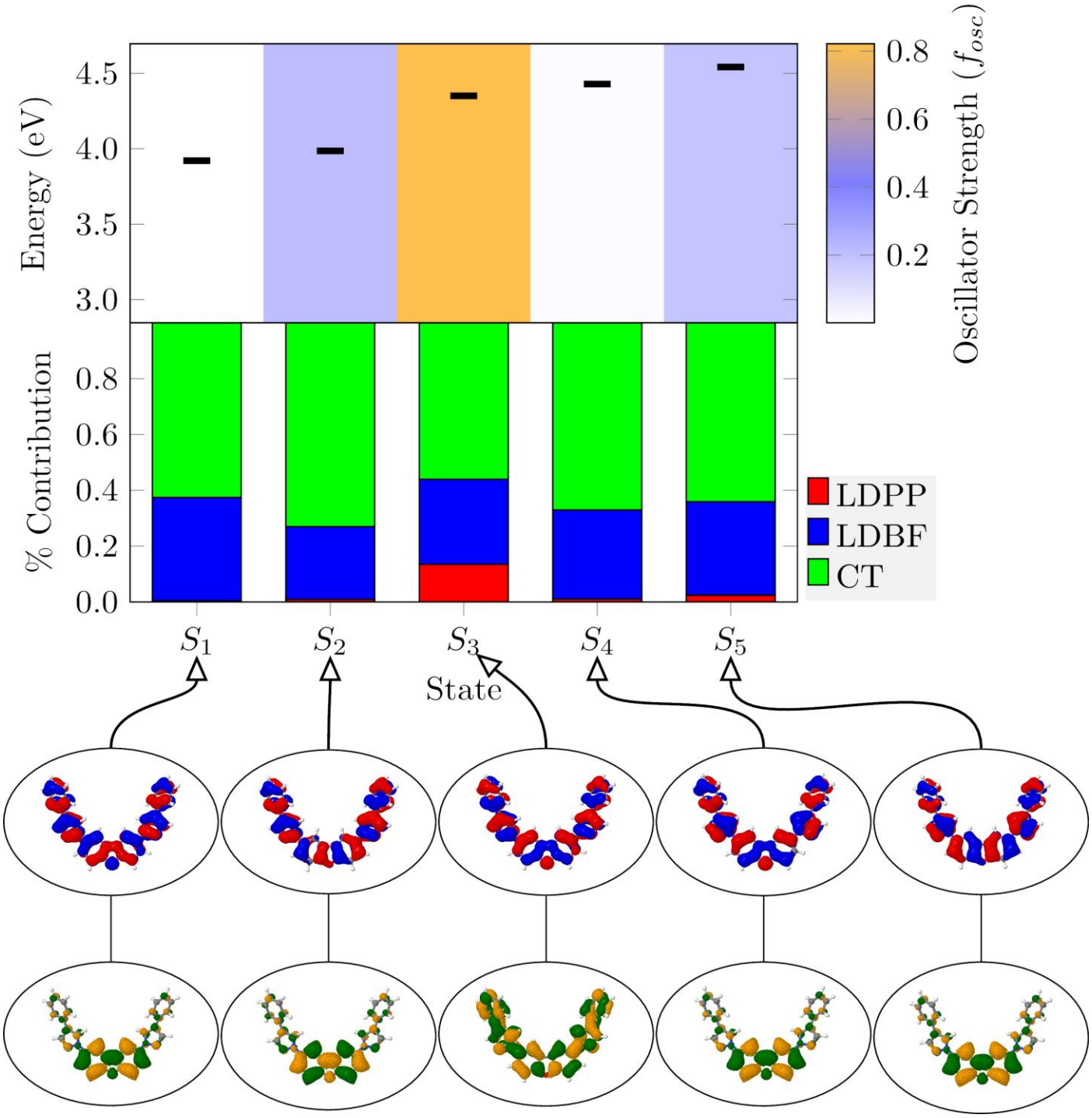


Figure S16. The characterization of first four excited states of the compound **6a**. LDPP refer to local excitation in 4-phenyl pyrazole units. LDBF is the local excitation in dibenzofuran unit. CT is the charge transfer from 4-phenyl pyrazole to dibenzofuran unit.

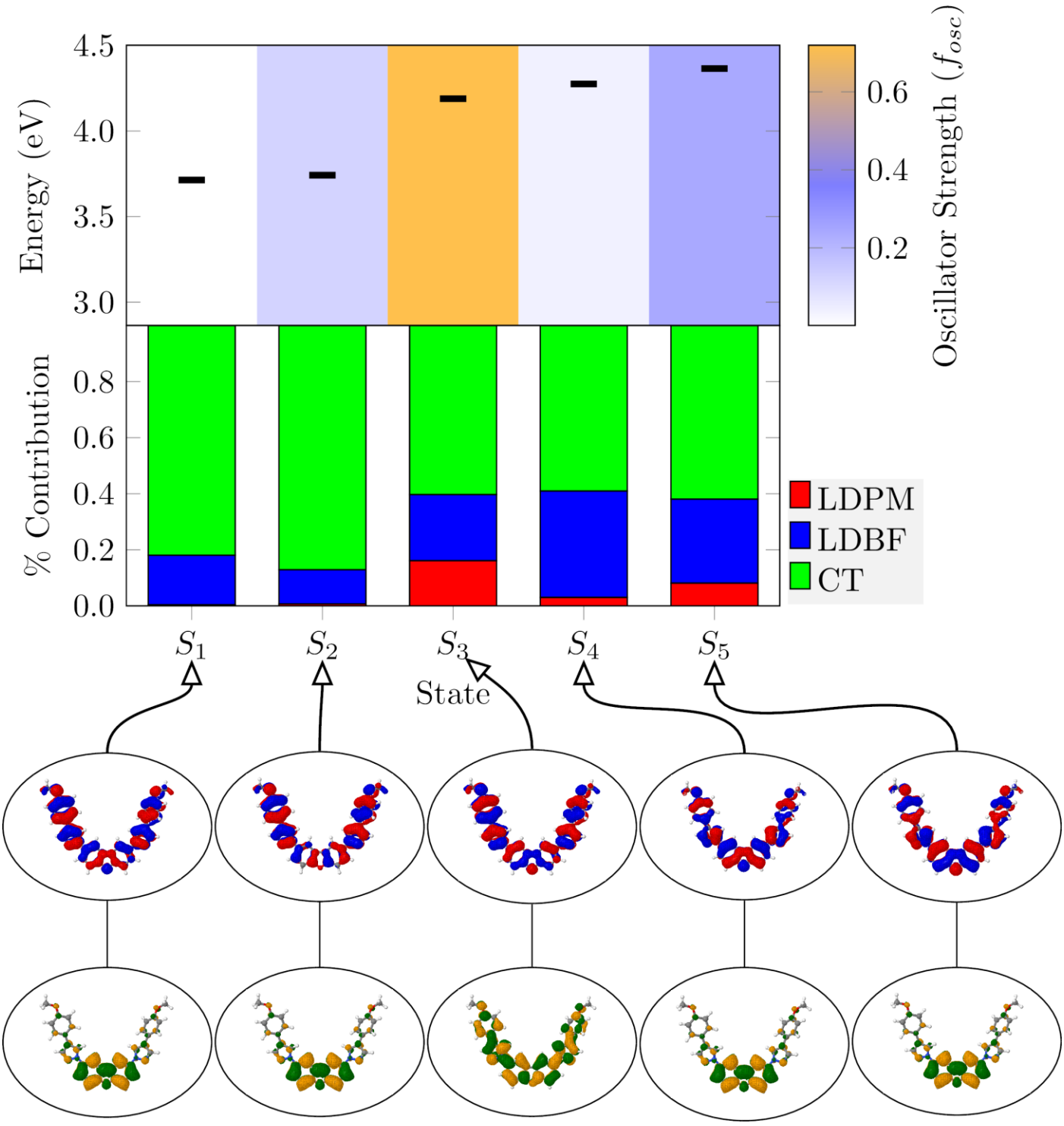


Figure S17. The characterization of first four excited states of the compound **6c**. LDPM refer to local excitation in 4-methoxyphenyl pyrazole units. LDBF is the local excitation in dibenzofuran unit. CT is the charge transfer from 4-methoxyphenyl pyrazole to dibenzofuran unit.

Optimized coordinates:

3a

C	-3.080861	2.515622	-0.009746
C	-4.423558	2.131018	-0.006262
C	-2.105381	1.513720	0.008032
C	-4.795196	0.772009	-0.014548
C	-2.500094	0.162906	0.003990
C	-3.831156	-0.232613	-0.015952
C	-0.653718	1.489219	0.008862
C	-0.304808	0.125884	0.016554
O	-1.416527	-0.684793	0.011530
C	0.354617	2.458107	0.023080
C	1.683721	2.028839	0.019953
C	2.009323	0.657951	0.031642
C	1.012287	-0.313915	0.036760
H	-2.801755	3.563213	-0.047046
H	-5.850358	0.528721	-0.026514
H	-4.107077	-1.281309	-0.023801
H	0.109810	3.514285	0.057383
H	1.253069	-1.371187	0.047377
H	3.055747	0.379534	0.043171
N	2.739712	2.979604	0.003763
N	3.963221	2.648941	0.493861
N	-5.446720	3.117032	0.006602
N	-6.676419	2.831748	-0.496085
C	2.713574	4.260176	-0.476422
C	3.972590	4.787668	-0.283056
C	4.704458	3.739190	0.321153
C	-5.380737	4.392699	0.495951
C	-7.381509	3.945498	-0.321444
C	-6.619378	4.964200	0.296176
H	5.738942	3.734892	0.638842
H	1.830946	4.676431	-0.937209
H	4.314210	5.776619	-0.550253
H	-8.412912	3.978696	-0.647362
H	-4.487900	4.774518	0.966875
H	-6.929533	5.962334	0.567504

3b

C	-5.393841	2.912420	-0.426529
C	-6.718085	3.332536	-0.544351
C	-5.137744	1.571024	-0.124334
C	-7.783426	2.423157	-0.388489
C	-6.216793	0.661304	0.035573
C	-7.543647	1.084009	-0.105655
C	-3.923433	0.807734	0.066632
C	-4.324141	-0.529280	0.330644
C	-2.563988	1.133719	0.023340
C	-1.625181	0.130895	0.262682
C	-2.030103	-1.194677	0.516068
C	-3.376773	-1.536987	0.544734
N	-5.712504	-0.601500	0.325568
N	-0.235010	0.432784	0.254743
N	0.672280	-0.529216	-0.054469
N	-7.016500	4.694331	-0.827353

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C	-8.140404	6.350701	-1.557462
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C	0.367224	1.625503	0.543516
C	1.854240	0.075030	0.039302
C	1.726742	1.433151	0.408874
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C	-6.760821	-2.551413	-0.839728
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H	-5.965388	-2.471586	1.183336
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H	-7.336041	-1.893753	-1.504225
H	-5.796006	-2.720317	-1.333172
C	-8.921841	-3.798004	-0.126658
H	-6.895384	-4.548993	-0.014167
H	-7.513875	-4.396048	-1.647303
C	-9.630477	-5.158218	-0.064082
H	-9.503861	-3.111759	-0.759100
H	-8.916299	-3.355171	0.878955
C	-11.053689	-5.087802	0.504760
H	-9.031385	-5.849912	0.545956
H	-9.662574	-5.595354	-1.072485
C	-11.756239	-6.451045	0.563589
H	-11.655491	-4.395642	-0.102115
H	-11.020679	-4.653739	1.514830
C	-13.173874	-6.378008	1.140956
H	-11.151443	-7.143140	1.165973
H	-11.792890	-6.881854	-0.446608
H	-13.164911	-5.987987	2.165500
H	-13.647624	-7.365108	1.165572
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H	-0.204715	2.489516	0.845240
H	-8.962869	6.869313	-2.032691
H	-5.330499	5.721728	-0.000068
H	-6.668542	7.931605	-0.928904

6a

C	-2.015078	3.434914	-0.090756
C	-3.364991	3.085174	-0.171850
C	-1.068251	2.407425	-0.032096
C	-1.496966	1.067752	-0.079055
C	-3.770685	1.736805	-0.223901
C	-2.834209	0.707462	-0.183598
C	0.379752	2.344153	0.052842
C	0.691968	0.971810	0.061916
C	1.410621	3.285270	0.139325
C	2.725569	2.819319	0.209608

C	3.014206	1.440027	0.221341
C	1.993501	0.495724	0.153199
O	-0.438211	0.191552	-0.019708
H	1.193476	4.347432	0.174170
H	4.050383	1.133078	0.290657
H	2.204726	-0.567833	0.162663
H	-1.708588	4.475430	-0.095927
H	-4.829172	1.521474	-0.301049
H	-3.135327	-0.333525	-0.223362
N	3.805987	3.740034	0.271093
N	4.981589	3.373728	0.846659
N	-4.362249	4.096689	-0.200344
N	-5.563387	3.855793	-0.788740
C	3.847974	5.022537	-0.196420
C	5.105391	5.530165	0.093627
C	5.756785	4.445509	0.745030
C	-4.295101	5.358108	0.317829
C	-5.503767	5.983289	0.050616
C	-6.244397	4.984989	-0.642518
H	-3.417490	5.710404	0.837382
H	-7.256292	5.046988	-1.021013
H	6.770154	4.406166	1.122794
H	3.004739	5.470694	-0.698861
C	-5.925384	7.343021	0.414794
C	5.644633	6.862166	-0.214597
C	6.672270	7.417302	0.568381
C	7.193068	8.677391	0.277476
C	6.694155	9.415007	-0.798269
C	5.670827	8.877686	-1.582753
C	5.156024	7.614100	-1.298036
C	-5.338787	8.022284	1.497799
C	-6.933440	8.000760	-0.312067
C	-7.341190	9.288471	0.032898
C	-5.740292	9.313064	1.836355
C	-6.745405	9.952790	1.107070
H	7.051423	6.863253	1.422436
H	7.985887	9.086925	0.897605
H	7.099147	10.397414	-1.023867
H	5.279579	9.439449	-2.426714
H	4.381506	7.194432	-1.934384
H	-4.576302	7.525624	2.091750
H	-5.274181	9.816856	2.678873
H	-7.061736	10.957055	1.374170
H	-7.388516	7.504894	-1.164818
H	-8.121352	9.776890	-0.544709

6c

C	1.197155	2.277214	-0.238279
C	-0.110429	1.805520	-0.380141
C	2.229441	1.340553	-0.120292
C	-0.388520	0.424711	-0.431901
C	1.926345	-0.032948	-0.171454
C	0.633989	-0.514532	-0.334120
C	3.671363	1.408901	0.040667
C	4.104183	0.070217	0.083739
O	3.055073	-0.809427	-0.048034
C	4.609290	2.438594	0.171777

C	5.954344	2.091803	0.320838
C	6.362946	0.743945	0.366190
C	5.435425	-0.287658	0.252849
N	6.945387	3.103447	0.429489
N	-1.193665	2.718964	-0.474519
N	-2.350770	2.342138	-1.078635
N	8.101271	2.854815	1.098333
C	6.917466	4.370310	-0.082944
C	8.794341	3.982736	1.006579
C	8.107289	4.988675	0.270727
C	-3.144872	3.400432	-0.980337
C	-1.263291	3.999260	0.000316
C	-2.522326	4.490687	-0.310178
C	8.566655	6.344881	-0.057643
C	-3.086484	5.813009	-0.009526
C	9.495391	7.009980	0.755022
C	8.103335	7.022301	-1.203136
C	8.544124	8.300058	-1.515453
C	9.955841	8.292503	0.449368
C	9.479431	8.946762	-0.692595
C	-2.263793	6.944171	0.160626
C	-4.470686	5.996129	0.117180
C	-2.798863	8.191255	0.449451
C	-5.025366	7.246390	0.397997
C	-4.187754	8.354762	0.569082
H	7.416650	0.531373	0.497441
H	5.738449	-1.328306	0.287044
H	4.299564	3.478201	0.182137
H	1.408399	3.341124	-0.240552
H	-1.418282	0.113490	-0.555161
H	0.430831	-1.578994	-0.373778
H	6.078956	4.727808	-0.660605
H	9.778121	4.039434	1.454112
H	10.673192	8.768470	1.107862
H	-4.135848	3.362849	-1.413788
H	-0.453896	4.439778	0.561731
H	-6.101318	7.339533	0.489490
H	-2.162363	9.061370	0.575710
H	8.190244	8.816627	-2.402066
H	7.402251	6.528569	-1.870590
H	9.858981	6.526499	1.657426
H	-1.187845	6.845616	0.044517
H	-5.134838	5.142753	0.012584
O	9.857689	10.196737	-1.091074
O	-4.616124	9.620669	0.849067
C	10.814883	10.889916	-0.306356
H	10.975747	11.848233	-0.803279
H	11.767447	10.346143	-0.254619
H	10.450597	11.070040	0.713815
C	-6.011233	9.843128	0.978300
H	-6.128491	10.905440	1.199399
H	-6.441390	9.254412	1.799331
H	-6.547801	9.607039	0.049753

Optimized S_1 coordinates of **6c**

C	1.218465	2.432575	-0.350509
C	-0.066127	1.921526	-0.558224

C	2.260969	1.483339	-0.127691
C	-0.403307	0.571856	-0.570221
C	1.904968	0.100144	-0.139080
C	0.635750	-0.384521	-0.354404
C	3.656160	1.535434	0.114441
C	4.082968	0.184482	0.247459
O	3.010756	-0.682283	0.087905
C	4.634606	2.558913	0.262844
C	5.956052	2.166883	0.507913
C	6.347664	0.830460	0.633021
C	5.376040	-0.198992	0.508193
N	6.962329	3.182893	0.615125
N	-1.141970	2.890594	-0.723877
N	-2.025294	2.818543	-1.784082
N	8.016028	3.039946	1.455027
C	7.020746	4.353423	-0.075383
C	8.737577	4.145024	1.287884
C	8.167203	5.026825	0.332762
C	-2.854315	3.822573	-1.620097
C	-1.408260	3.904624	0.081233
C	-2.539809	4.590715	-0.447059
C	8.676143	6.324991	-0.127794
C	-3.192089	5.737318	0.082360
C	9.539784	7.091049	0.668516
C	8.328643	6.851004	-1.388665
C	8.814317	8.076363	-1.824240
C	10.046520	8.320640	0.240000
C	9.682620	8.822057	-1.013964
C	-2.742107	6.369328	1.285886
C	-4.332179	6.301195	-0.569623
C	-3.383082	7.468733	1.794333
C	-4.983040	7.405872	-0.067647
C	-4.516728	8.006900	1.127552
H	7.387640	0.598179	0.818855
H	5.644657	-1.245048	0.602792
H	4.363365	3.608081	0.237884
H	1.422205	3.494685	-0.426722
H	-1.428017	0.258430	-0.720860
H	0.434096	-1.449099	-0.355412
H	6.262396	4.607894	-0.799662
H	9.658055	4.267013	1.844571
H	10.711596	8.874765	0.892676
H	-3.650687	3.978067	-2.335373
H	-0.812195	4.076719	0.963846
H	-5.844127	7.805714	-0.587939
H	-3.049315	7.952119	2.705322
H	8.547105	8.472433	-2.799208
H	7.681215	6.276809	-2.045713
H	9.815882	6.728548	1.654706
H	-1.879158	5.971474	1.806129
H	-4.696116	5.847440	-1.483833
O	10.114421	10.013385	-1.536477
O	-5.067653	9.073144	1.705511
C	11.018818	10.786037	-0.768267
H	11.245505	11.671636	-1.365344
H	11.950711	10.240884	-0.565507
H	10.578124	11.100945	0.187677

C	-6.215508	9.704143	1.116243
H	-6.457127	10.536364	1.775035
H	-7.058786	9.008539	1.072164
H	-5.979269	10.078783	0.115903

Optimized T_1 coordinates of **6c**

C	1.213024	2.222011	-0.172391
C	-0.082309	1.752719	-0.269253
C	2.275569	1.252574	-0.077650
C	-0.388898	0.358781	-0.302890
C	1.928962	-0.159613	-0.119115
C	0.655973	-0.620571	-0.232584
C	3.650829	1.317451	0.032988
C	4.129723	-0.055747	0.063378
O	3.068814	-0.935281	-0.031814
C	4.617146	2.382020	0.133334
C	5.951126	2.036840	0.225227
C	6.388334	0.678632	0.251982
C	5.440886	-0.394450	0.174911
N	6.948649	3.042174	0.281074
N	-1.169568	2.659687	-0.329280
N	-2.378761	2.251302	-0.804669
N	8.191011	2.752912	0.758568
C	6.841140	4.355100	-0.081964
C	8.852528	3.898593	0.698635
C	8.060292	4.961975	0.172712
C	-3.148678	3.326900	-0.742590
C	-1.187848	3.978643	0.029339
C	-2.460709	4.464075	-0.225137
C	8.448058	6.356984	-0.063178
C	-2.977999	5.819580	-0.008088
C	9.510054	6.944367	0.639742
C	7.768618	7.158823	-1.002966
C	8.127615	8.480280	-1.219614
C	9.888802	8.271202	0.427193
C	9.194127	9.050185	-0.505949
C	-2.116022	6.933753	0.046706
C	-4.351264	6.056766	0.149832
C	-2.602895	8.215347	0.254433
C	-4.857826	7.341973	0.351640
C	-3.981567	8.432564	0.407317
H	7.448044	0.479442	0.330490
H	5.765325	-1.427986	0.198599
H	4.290025	3.413650	0.169176
H	1.441406	3.280087	-0.201825
H	-1.424697	0.059999	-0.384279
H	0.430739	-1.679909	-0.264344
H	5.929244	4.753346	-0.497476
H	9.888219	3.930109	1.011117
H	10.713610	8.684232	0.996181
H	-4.172736	3.267082	-1.087609
H	-0.331174	4.453264	0.480857
H	-5.926501	7.476883	0.471447
H	-1.937005	9.071693	0.291022
H	7.605553	9.093820	-1.946988
H	6.957878	6.730817	-1.585991
H	10.045860	6.363070	1.384821

H	-1.048280	6.792493	-0.096464
H	-5.044576	5.220615	0.132775
O	9.471086	10.354533	-0.794167
O	-4.360502	9.729015	0.600463
C	10.551249	10.977982	-0.116860
H	10.597820	11.999097	-0.499055
H	11.503811	10.471835	-0.321747
H	10.387174	11.006561	0.968436
C	-5.743165	10.008855	0.755551
H	-5.818856	11.088942	0.892052
H	-6.162514	9.503982	1.635780
H	-6.318135	9.716444	-0.132946

Optimized T_4 coordinates of **6c**-

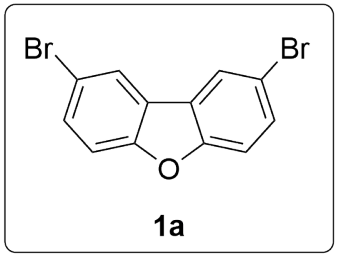
C	1.204344	2.207573	-0.162480
C	-0.111676	1.717810	-0.271037
C	2.252415	1.281060	-0.072281
C	-0.395262	0.337703	-0.315686
C	1.938354	-0.106116	-0.113711
C	0.654214	-0.597215	-0.240066
C	3.682876	1.354385	0.036864
C	4.137999	0.006707	0.064906
O	3.080456	-0.868816	-0.027625
C	4.629977	2.382888	0.136541
C	5.989822	2.030498	0.240005
C	6.414060	0.686633	0.269679
C	5.466183	-0.350546	0.185276
N	6.957817	3.056537	0.317017
N	-1.180843	2.638847	-0.337412
N	-2.391838	2.247503	-0.849012
N	8.206637	2.785223	0.815366
C	6.839213	4.367215	-0.052119
C	8.853551	3.933434	0.763417
C	8.058149	4.996515	0.226041
C	-3.157349	3.318919	-0.775681
C	-1.203557	3.945760	0.062014
C	-2.481828	4.447941	-0.209260
C	8.428883	6.380190	0.013294
C	-3.001781	5.776905	0.036555
C	9.738678	6.846977	0.278133
C	7.490757	7.332897	-0.471139
C	7.841192	8.653121	-0.674598
C	10.101738	8.172665	0.078494
C	9.152383	9.093368	-0.402618
C	-2.176478	6.812666	0.555252
C	-4.353833	6.104322	-0.225640
C	-2.671996	8.079201	0.795212
C	-4.862443	7.374994	0.010556
C	-4.023085	8.379533	0.527613
H	7.469562	0.471830	0.356906
H	5.767267	-1.391647	0.206850
H	4.319633	3.420626	0.171359
H	1.405683	3.272216	-0.186946
H	-1.423076	0.016517	-0.406749
H	0.461882	-1.663495	-0.272629
H	5.943748	4.739327	-0.521565
H	9.874189	3.976549	1.120590

H	11.117495	8.482546	0.295283
H	-4.175355	3.261337	-1.138258
H	-0.353901	4.399406	0.544799
H	-5.905175	7.577366	-0.205237
H	-2.037987	8.866585	1.190536
H	7.120854	9.376798	-1.042845
H	6.471652	7.023109	-0.681678
H	10.490159	6.154740	0.645144
H	-1.130284	6.611063	0.764390
H	-5.022272	5.344804	-0.619227
O	9.394400	10.412164	-0.635638
O	-4.411060	9.654965	0.801318
C	10.696045	10.919490	-0.375272
H	10.660809	11.980619	-0.626604
H	11.453397	10.425421	-0.997259
H	10.968528	10.806882	0.681947
C	-5.759952	10.023585	0.548433
H	-5.843361	11.073093	0.834773
H	-6.460065	9.428257	1.148446
H	-6.014707	9.917060	-0.513843

Optimized T_5 coordinates of **6c**-

C	1.209509	2.352798	-0.302418
C	-0.084798	1.859909	-0.496512
C	2.260109	1.407289	-0.133008
C	-0.373763	0.492773	-0.557976
C	1.942637	0.022836	-0.209804
C	0.672430	-0.459372	-0.425597
C	3.658524	1.478810	0.092332
C	4.119641	0.133798	0.142539
O	3.074451	-0.746808	-0.040945
C	4.604529	2.525589	0.281111
C	5.943115	2.167403	0.465941
C	6.374559	0.836983	0.499395
C	5.433906	-0.216655	0.348410
N	6.902777	3.214966	0.639698
N	-1.149260	2.803847	-0.648901
N	-2.121141	2.617982	-1.585509
N	7.880305	3.120311	1.583832
C	6.996638	4.359654	-0.079632
C	8.590550	4.230465	1.452229
C	8.092035	5.081430	0.418998
C	-2.944861	3.643380	-1.430946
C	-1.357235	3.922470	0.087664
C	-2.529169	4.528947	-0.389950
C	8.592470	6.370482	-0.014736
C	-3.162300	5.748688	0.069296
C	9.774465	6.925924	0.535463
C	7.921339	7.135970	-1.007190
C	8.398831	8.364188	-1.417992
C	10.263625	8.161021	0.131863
C	9.578561	8.896278	-0.853395
C	-2.555713	6.580726	1.049968
C	-4.417012	6.165862	-0.441156
C	-3.160991	7.741613	1.487144
C	-5.035023	7.332134	-0.010431
C	-4.411421	8.135527	0.962558

H	7.424775	0.623598	0.648284
H	5.742275	-1.254933	0.377437
H	4.297114	3.564080	0.324303
H	1.406991	3.418338	-0.324939
H	-1.395723	0.173270	-0.713230
H	0.474218	-1.523392	-0.475764
H	6.320163	4.555390	-0.897252
H	9.430645	4.397938	2.113092
H	11.172627	8.544623	0.580767
H	-3.804279	3.729748	-2.082512
H	-0.698928	4.177196	0.903816
H	-5.995934	7.609672	-0.428299
H	-2.693804	8.374326	2.235159
H	7.882488	8.945432	-2.175402
H	7.007757	6.753307	-1.452050
H	10.322175	6.373120	1.292179
H	-1.590259	6.304961	1.463281
H	-4.919357	5.557105	-1.186325
O	9.962190	10.111156	-1.324607
O	-4.919987	9.293524	1.457994
C	11.140759	10.707816	-0.796959
H	11.249770	11.662750	-1.312966
H	12.025543	10.088160	-0.989757
H	11.051883	10.886381	0.282050
C	-6.179264	9.748321	0.977795
H	-6.383872	10.678934	1.509003
H	-6.975998	9.025122	1.192737
H	-6.150450	9.945346	-0.101281



8.026
8.023
7.587
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7.260

BRUKER

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EXPNO 11
PROCNO 1

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Time 18.46 h
INSTRUM spect
PROBHD Z143956_0001 (
PULPROG zg30
TD 163840
SOLVENT CDCl3
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DS 0
SWH 20000.000 Hz
FIDRES 0.244141 Hz
AQ 4.0960002 sec
RG 456
DW 25.000 usec
DE 9.18 usec
TE 0 K
D1 40.00000000 sec
TD0 1
SFO1 500.2532516 MHz
NUC1 1H
P1 9.10 usec
PLW1 11.00000000 W

F2 - Processing parameters
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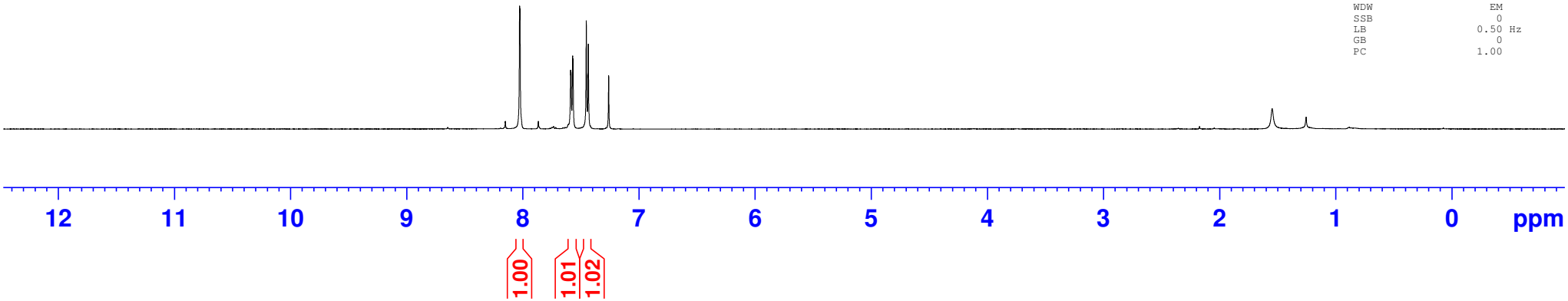
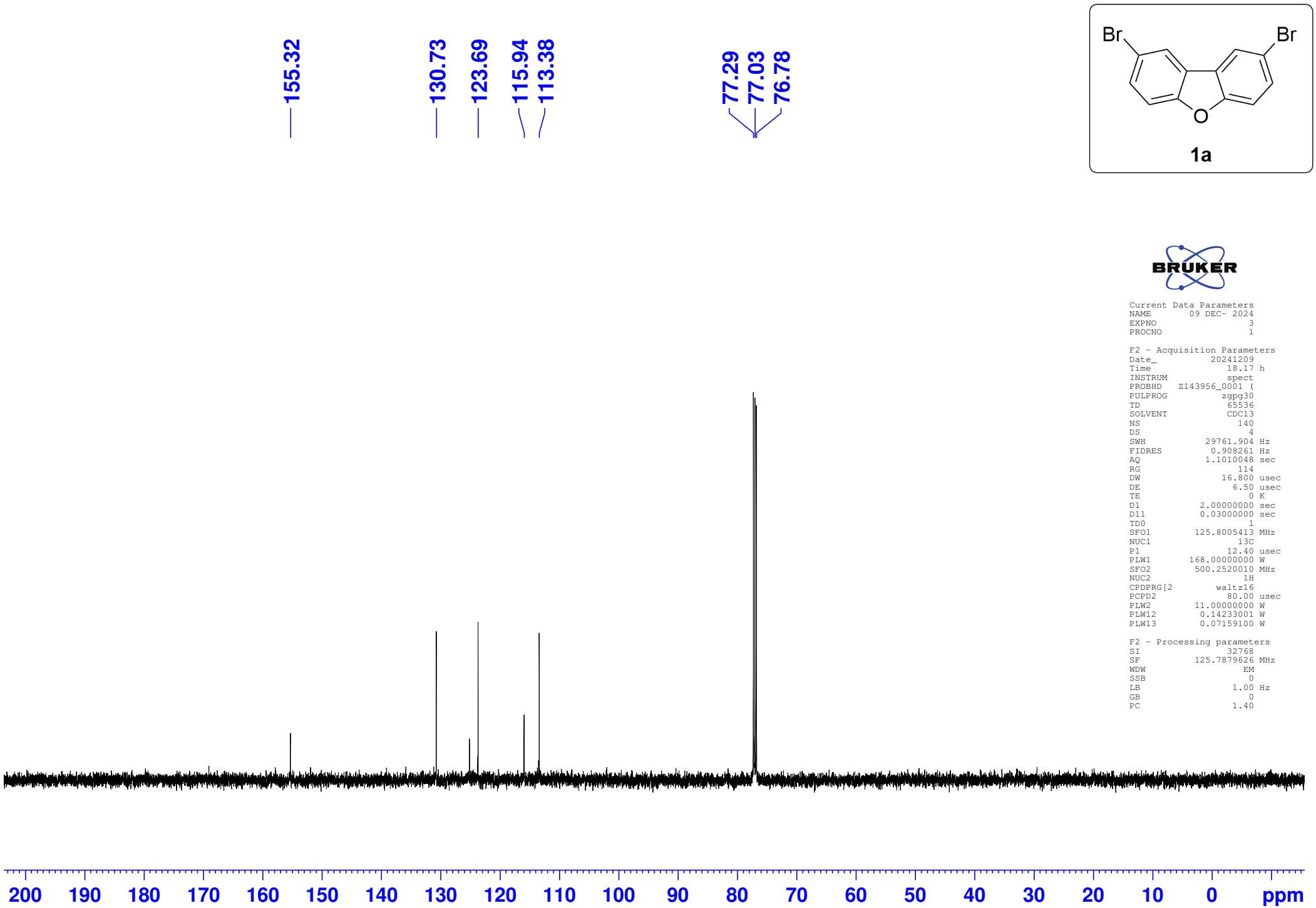
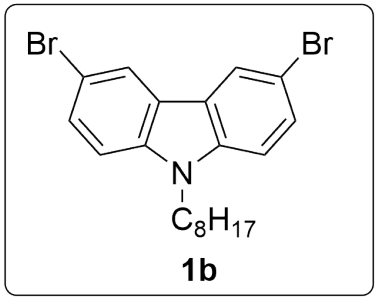
SF 500.2500140 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00




155.32
130.73
123.69
115.94
113.38
77.29
77.03
76.78
Br
Br
O
1a
BRUKER
Current Data Parameters
NAME 09 DEC- 2024
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20241209
Time 18.17 h
INSTRUM spect
PROBHD Z143956_0001 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 140
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 114
DW 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8005413 MHz
NUC1 13C
P1 12.40 usec
PLW1 168.00000000 W
SFO2 500.2520010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 11.00000000 W
PLW12 0.14233001 W
PLW13 0.07159100 W
F2 - Processing parameters
SI 32768
SF 125.7879626 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



1b

8.05 8.04 7.79 7.78 7.26

5.12 5.10 5.09

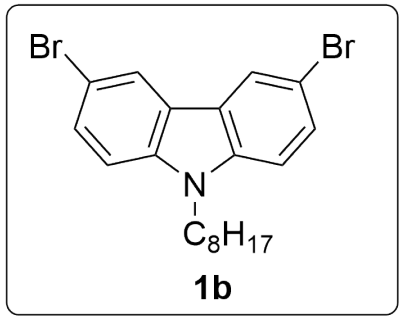
1.79 1.77 1.76 1.32 1.31 1.30 1.28 1.27 1.25 1.24 0.88 0.87 0.86

BRUKER

```
Current Data Parameters
NAME        br2-carbazoleN-C8H17
EXPNO                          5
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20200215
Time                       18.12 h
INSTRUM                     spect
PROBHD    Z115265_0004 (
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                   10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                          456
DW                       50.000 usec
DE                        6.50 usec
TE                       300.6 K
D1                    1.00000000 sec
TD0                           1
SFO1                500.3030894 MHz
NUC1                        1H
P1                       15.10 usec
PLW1                15.13599968 W

F2 - Processing parameters
SI                        65536
SF                  500.3000135 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

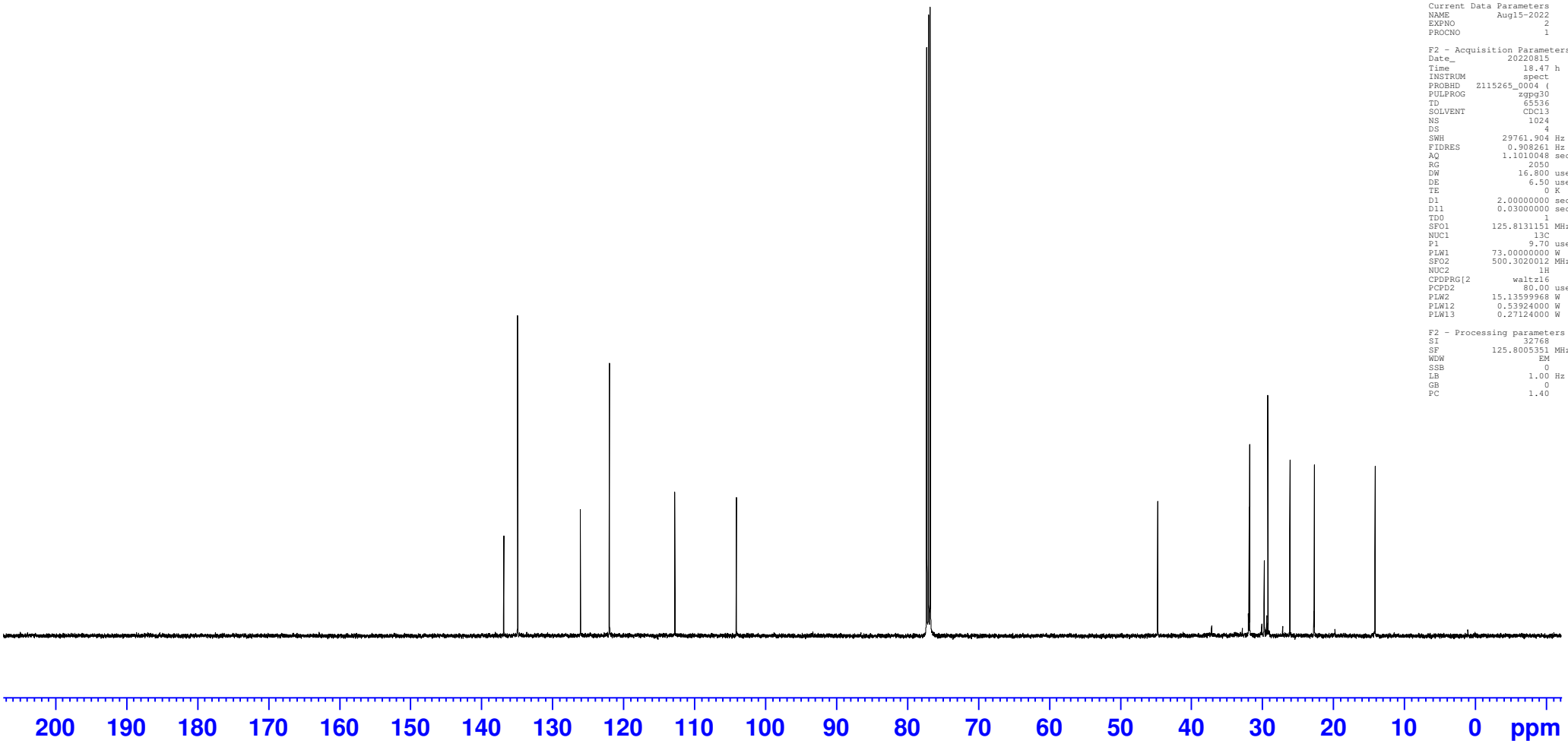
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.85 1.69 2.00 1.81 1.78 9.88 2.92



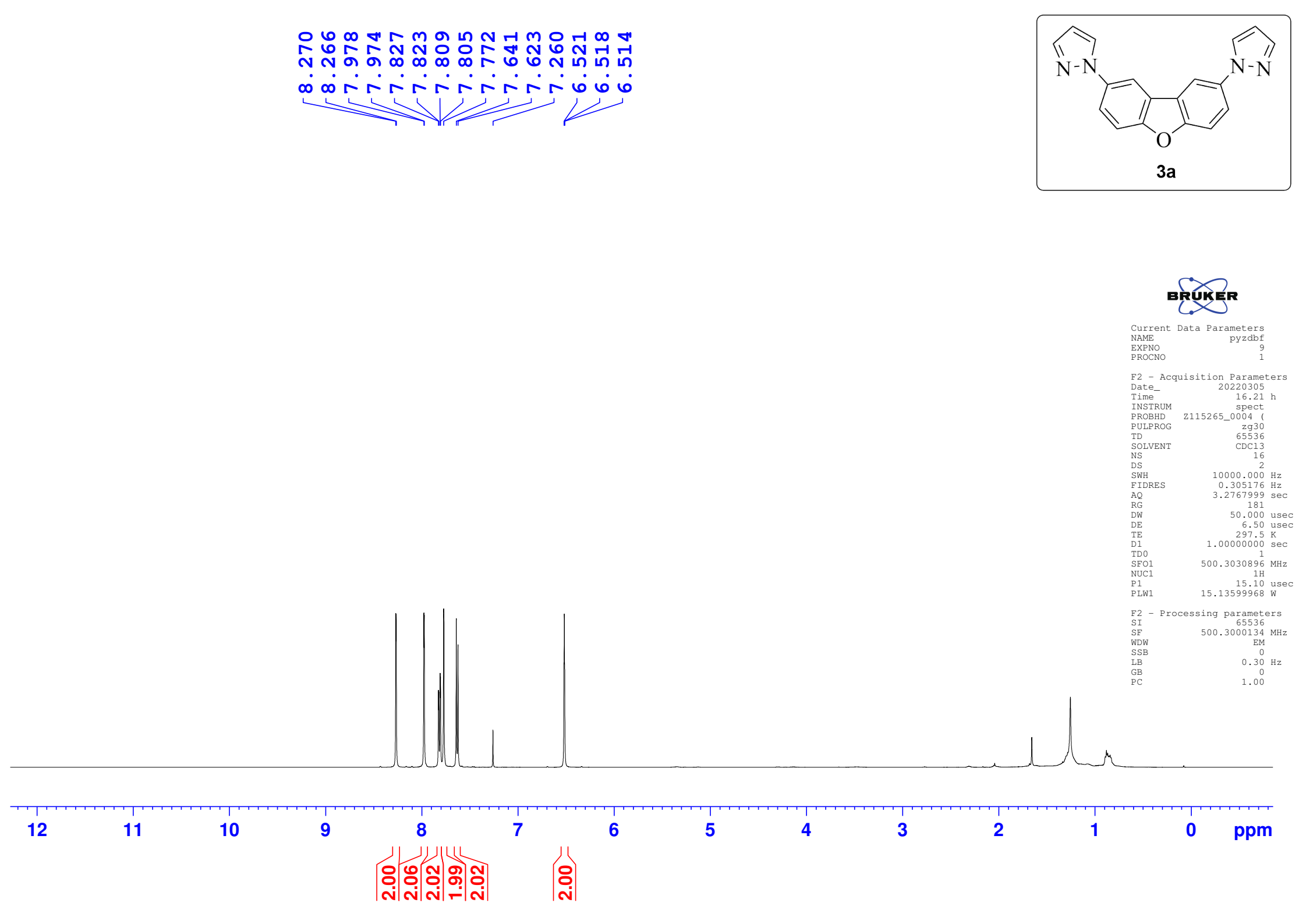
1b

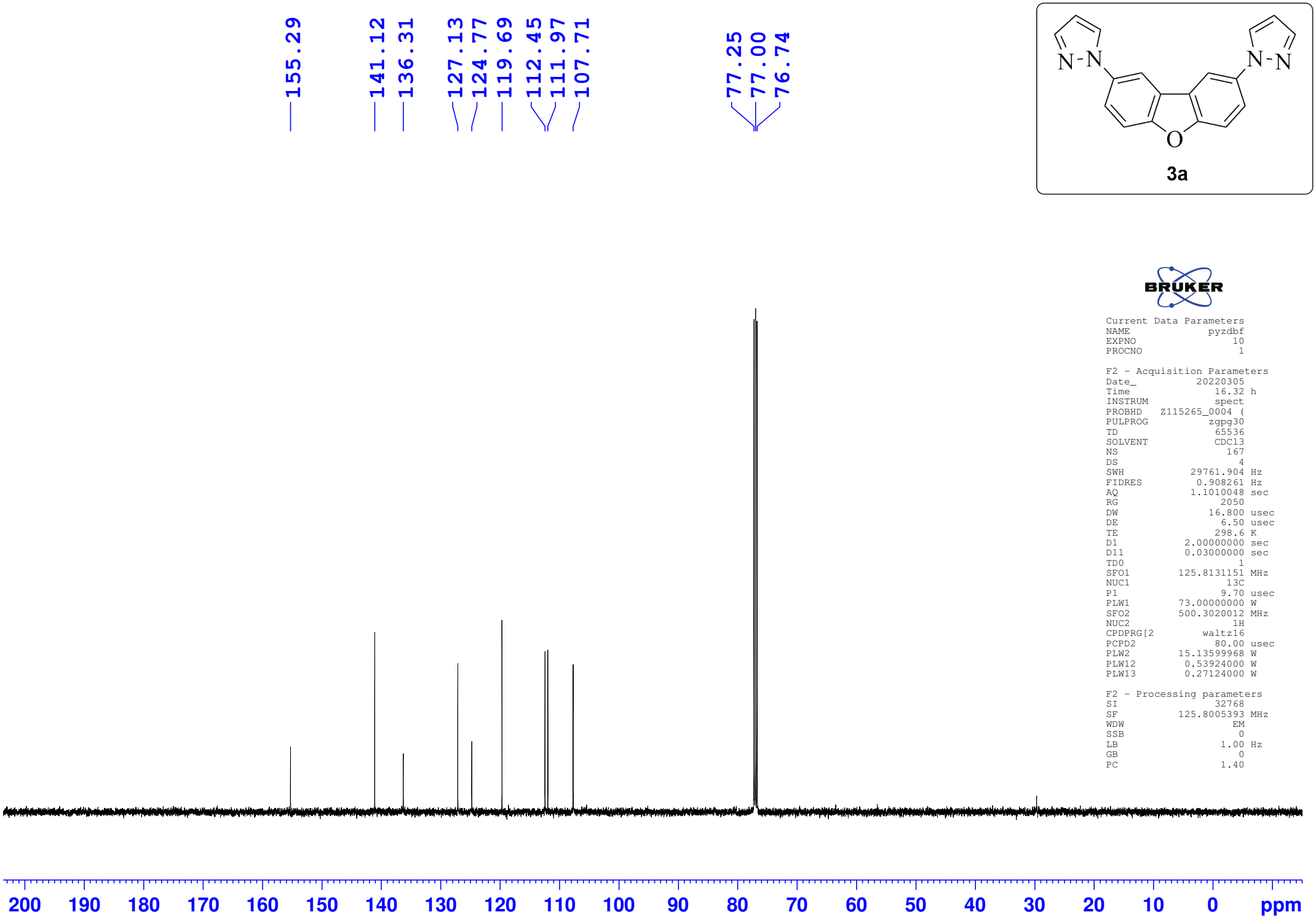
136.85
134.90
126.06
121.98
112.74
104.07
77.26
77.01
76.76
44.71
31.83
31.75
29.71
29.19
26.08
22.64
14.09

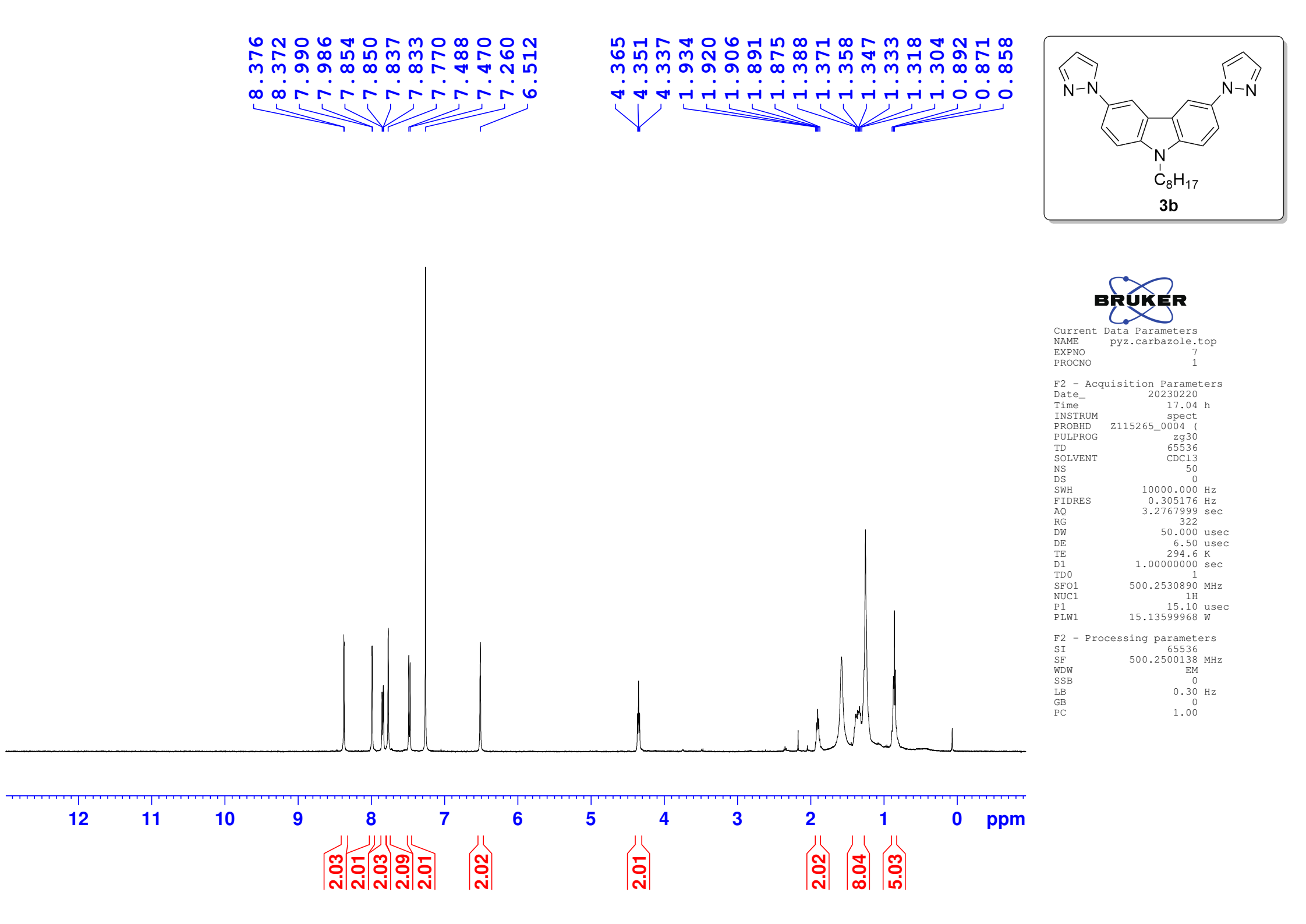


BRUKER

```
Current Data Parameters
NAME          Aug15-2022
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220815
Time              18.47 h
INSTRUM             spect
PROBHD   Z115265_0004 (
PULPROG           zppg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG                 2050
DW               16.800 usec
DE                6.50 usec
TE                   0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.8131151 MHz
NUC1               13C
P1                9.70 usec
PLW1        73.00000000 W
SFO2        500.3020012 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2        15.13599968 W
PLW12        0.53924000 W
PLW13        0.27124000 W

F2 - Processing parameters
SI                32768
SF          125.8005351 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


8.270
8.266
7.978
7.974
7.827
7.823
7.809
7.805
7.772
7.641
7.623
7.260
6.521
6.518
6.514
N-N
N-N
O
3a
BRUKER
Current Data Parameters
NAME pyzdbf
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220305
Time 16.21 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
F2 - Processing parameters
SI 65536
SF 500.3000134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.06
2.02
1.99
2.02
2.00


155.29
141.12
136.31
127.13
124.77
119.69
112.45
111.97
107.71
77.25
77.00
76.74
N-N
N-N
O
3a
BRUKER
Current Data Parameters
NAME pyzdbf
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220305
Time 16.32 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 167
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8131151 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.27124000 W
F2 - Processing parameters
SI 32768
SF 125.8005393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

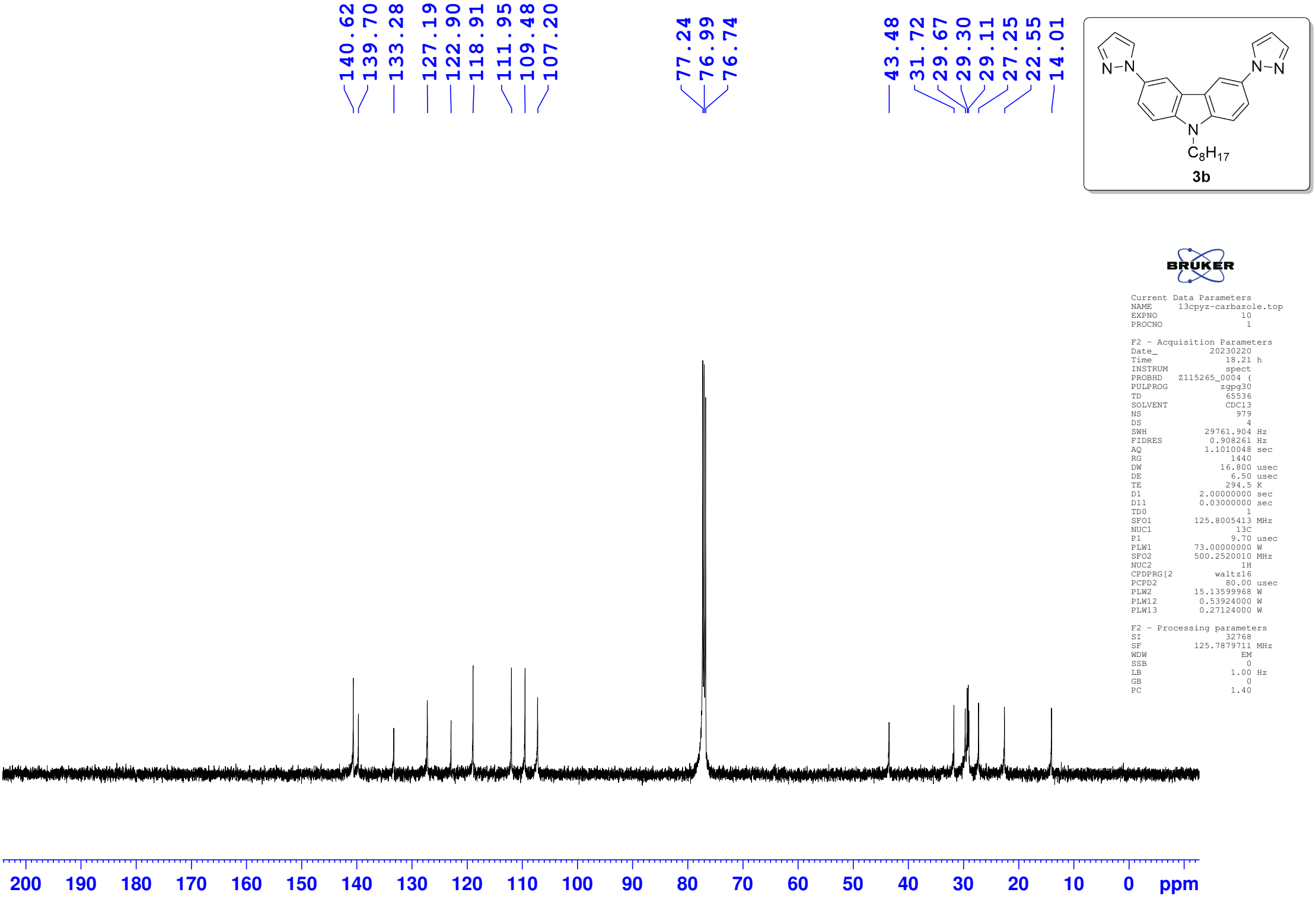


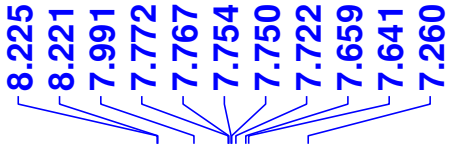
BRUKER

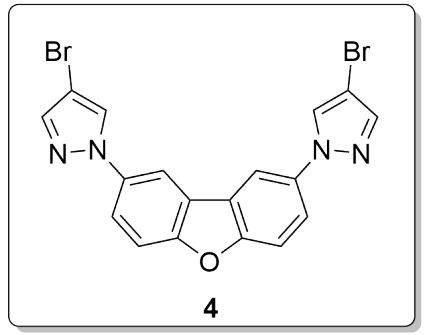
Current Data Parameters
NAME pyz.carbazole.top
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230220
Time 17.04 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 50
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 322
DW 50.000 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

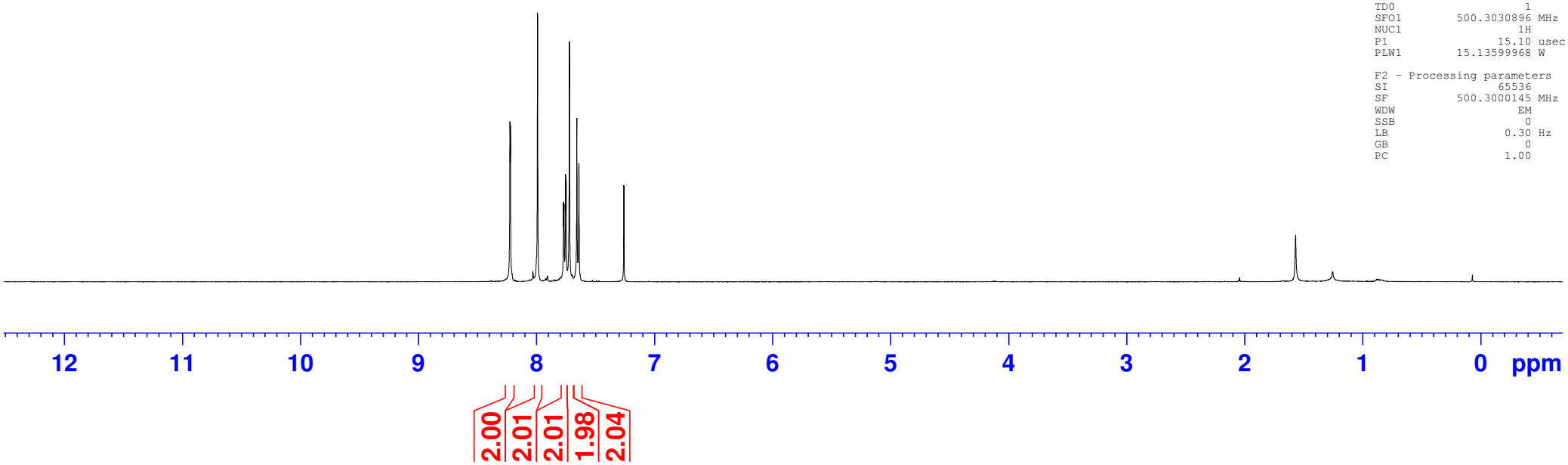

140.62
139.70
133.28
127.19
122.90
118.91
111.95
109.48
107.20
77.24
76.99
76.74
43.48
31.72
29.67
29.30
29.11
27.25
22.55
14.01
N
N
N
N
C_8H_{17}
3b
BRUKER
Current Data Parameters
NAME 13cpyz-carbazole.top
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230220
Time 18.21 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 979
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 1440
DW 16.800 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
SFO2 500.2520010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.27124000 W
F2 - Processing parameters
SI 32768
SF 125.7879711 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

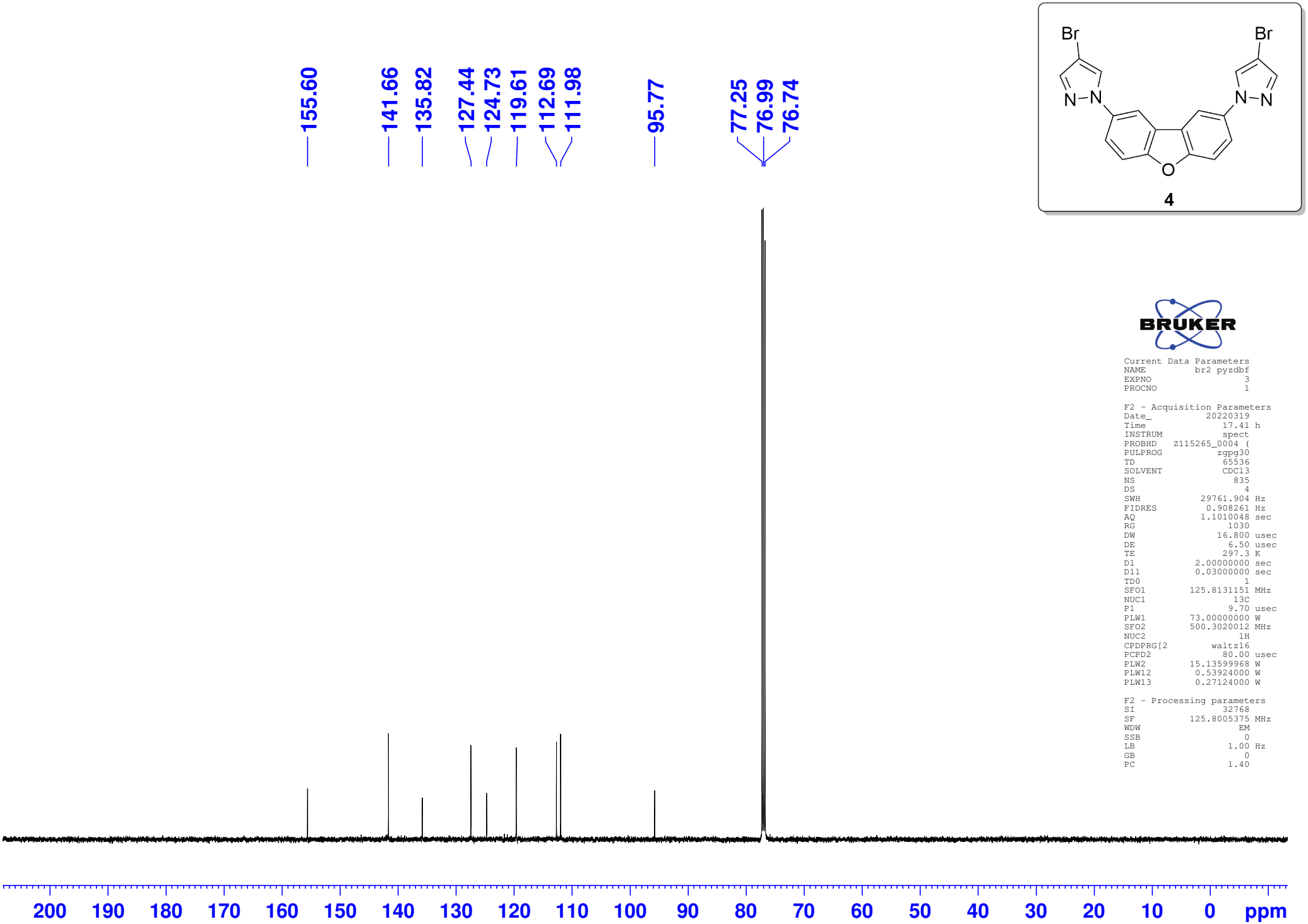




BRUKER

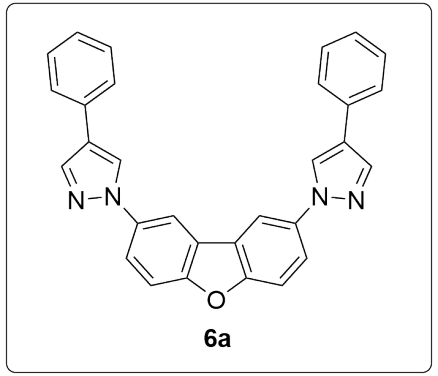
```
Current Data Parameters
NAME          br2 pyzdbf
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220319
Time               16.54 h
INSTRUM             spect
PROBHD    Z115265_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ              3.2767999 sec
RG                   322
DW                50.000 usec
DE                 6.50 usec
TE                297.0 K
D1             1.00000000 sec
TD0                    1
SFO1         500.3030896 MHz
NUC1                  1H
P1                15.10 usec
PLW1         15.13599968 W

F2 - Processing parameters
SI                 65536
SF           500.3000145 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





BRUKER

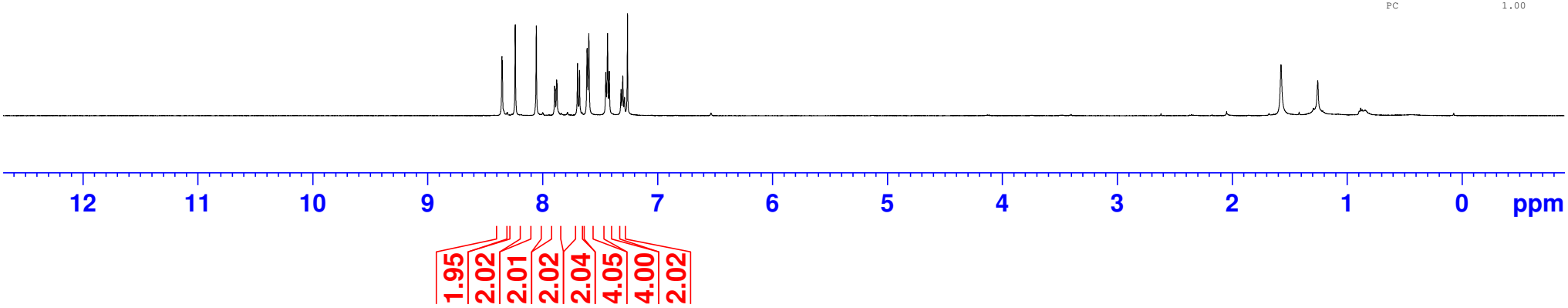
```
Current Data Parameters
NAME          br2 pyzdbf
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220319
Time              17.41 h
INSTRUM             spect
PROBHD   Z115265_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  835
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG                 1030
DW               16.800 usec
DE                6.50 usec
TE               297.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.8131151 MHz
NUC1                13C
P1                 9.70 usec
PLW1         73.00000000 W
SFO2        500.3020012 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2         15.13599968 W
PLW12         0.53924000 W
PLW13         0.27124000 W

F2 - Processing parameters
SI                32768
SF          125.8005375 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



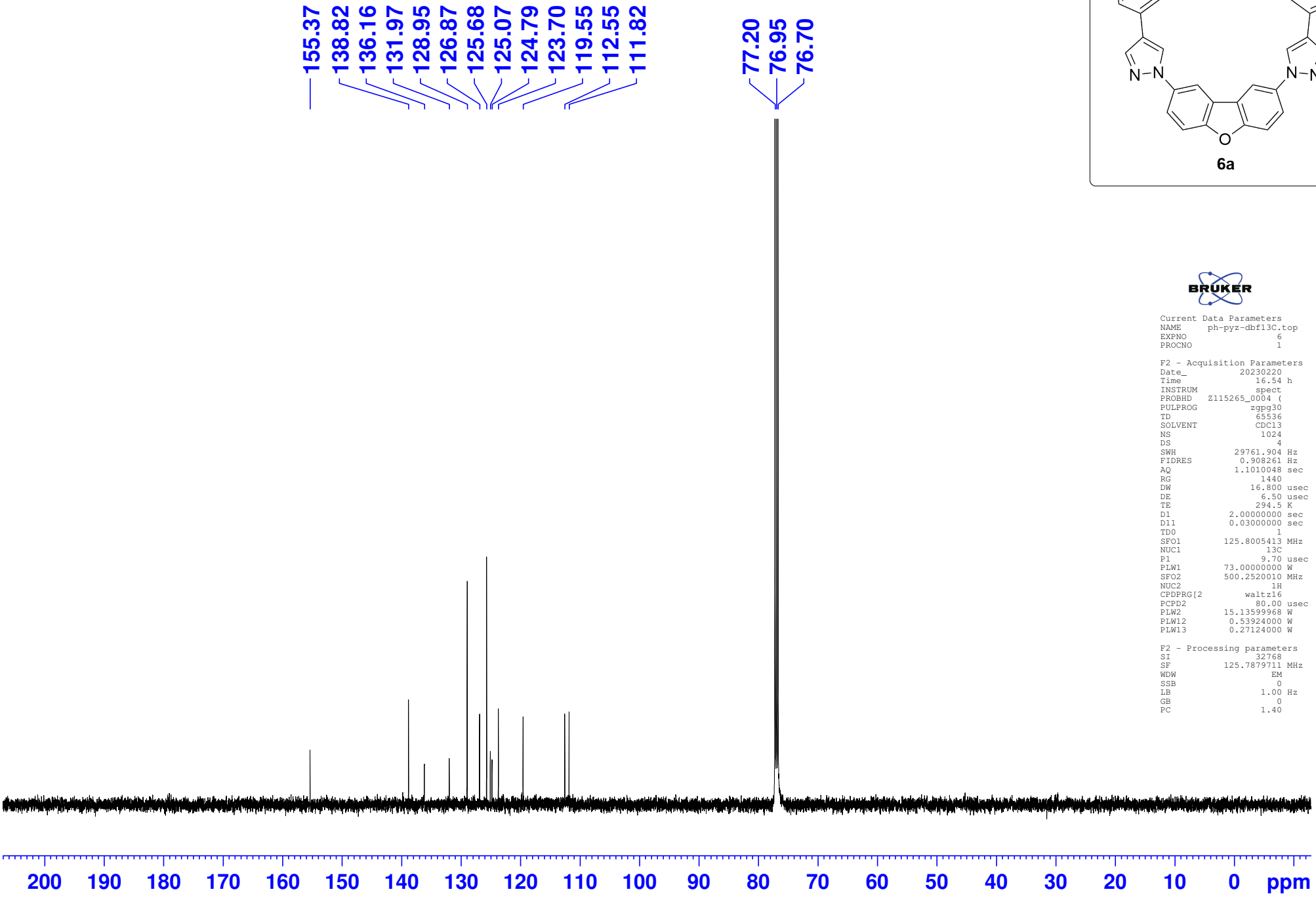
8.353 8.349 8.237 8.054 7.894 7.890 7.877 7.872 7.695 7.677 7.611 7.596 7.449 7.434 7.418 7.316 7.301 7.286 7.260

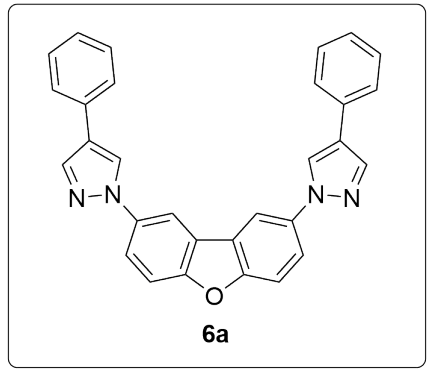
BRUKER

```
Current Data Parameters
NAME      ph-pyz-dbf.top
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230220
Time              15.57 h
INSTRUM             spect
PROBHD   Z115265_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                   287
DW                50.000 usec
DE                 6.50 usec
TE                294.4 K
D1           1.00000000 sec
TD0                    1
SFO1        500.2530890 MHz
NUC1                  1H
P1                15.10 usec
PLW1        15.13599968 W

F2 - Processing parameters
SI                 65536
SF          500.2500131 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



1.95 2.02 2.01 2.02 2.04 4.05 4.00 2.02

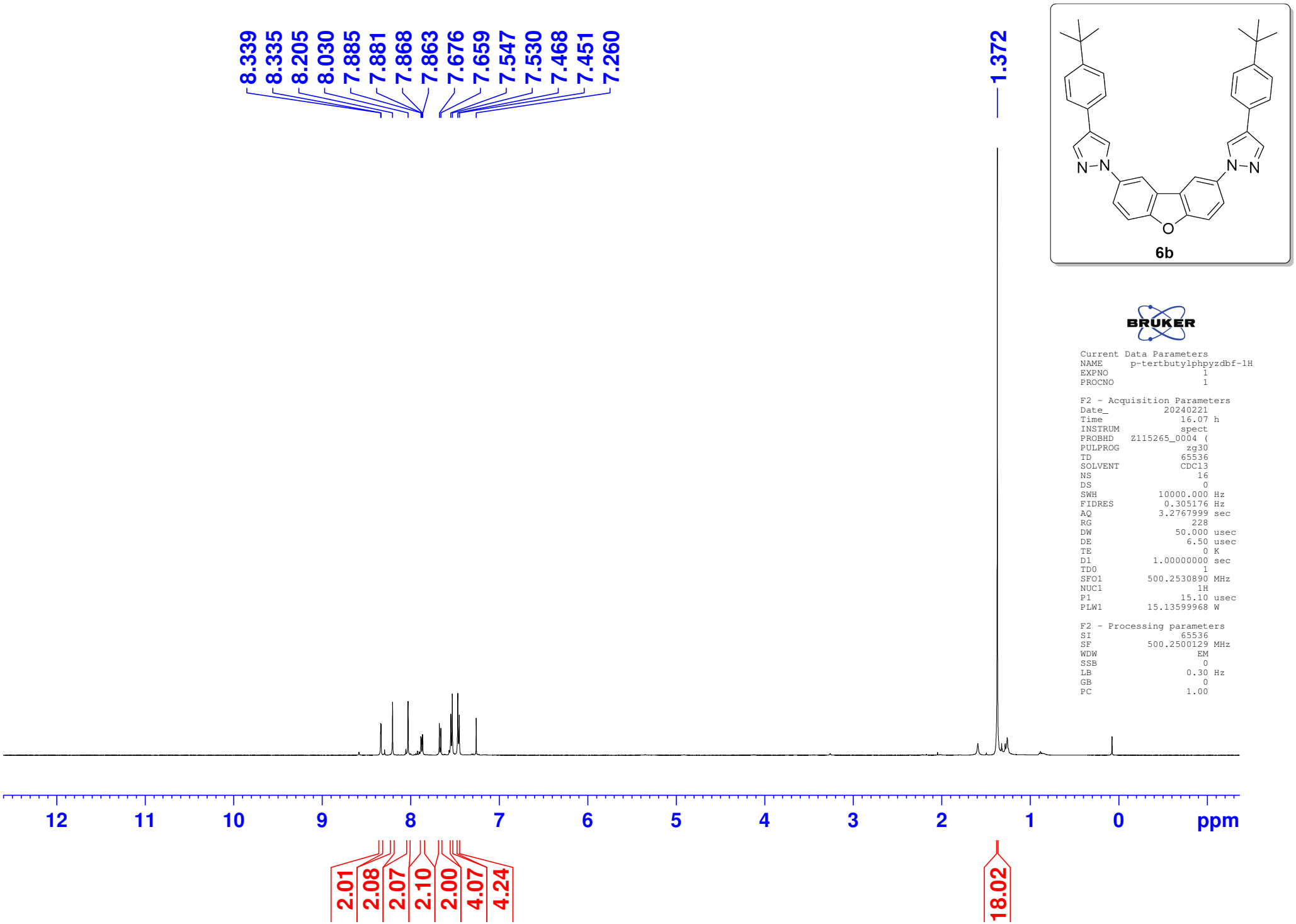


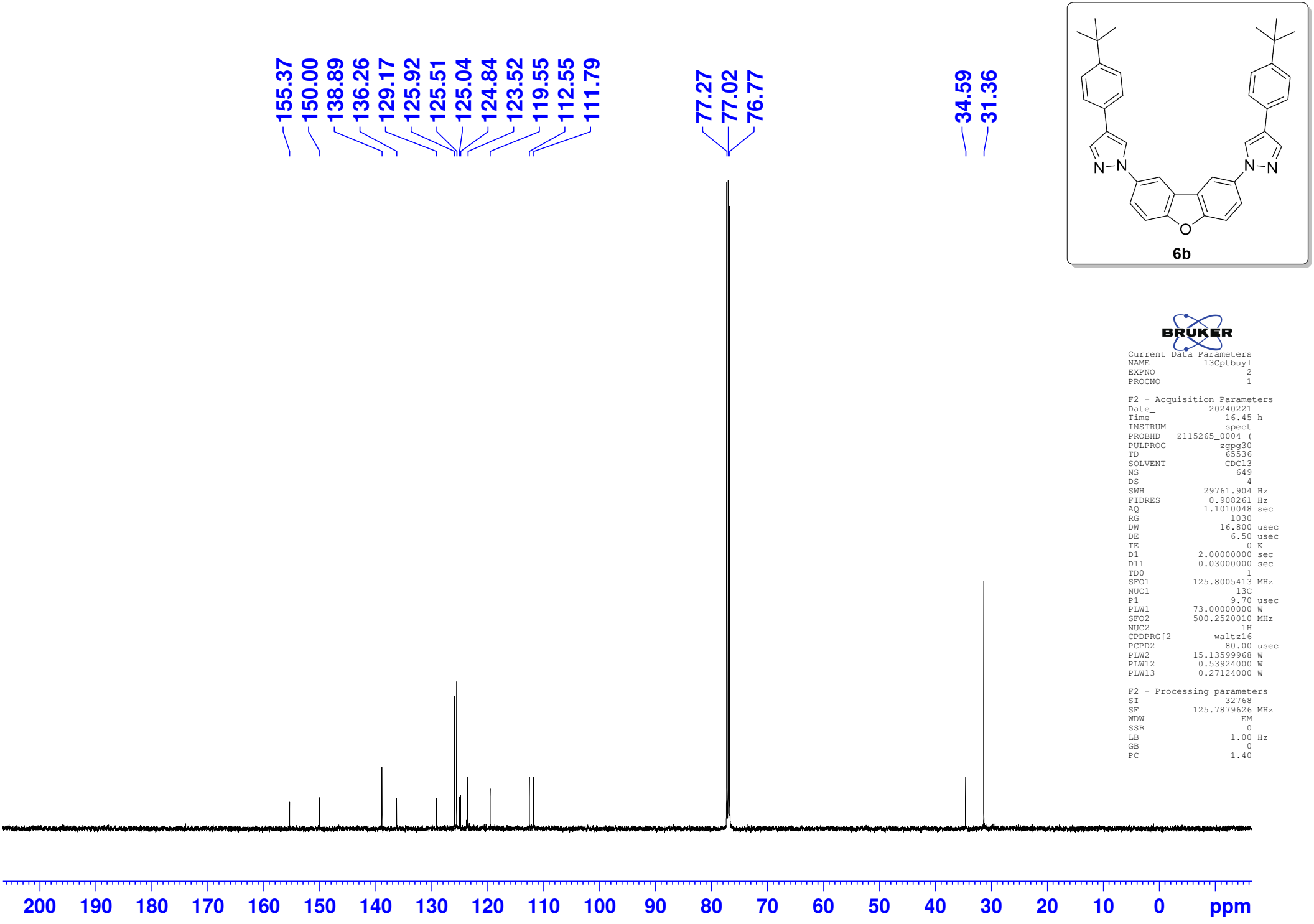


6a

BRUKER

```
Current Data Parameters
NAME      ph-pyz-dbf13C.top
EXPNO                     6
PROCNO                    1

F2 - Acquisition Parameters
Date_           20230220
Time              16.54 h
INSTRUM             spect
PROBHD   Z115265_0004 (
PULPROG           zgpg30
TD                65536
SOLVENT             CDC13
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG                 1440
DW               16.800 usec
DE                6.50 usec
TE                294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.8005413 MHz
NUC1               13C
P1                9.70 usec
PLW1        73.00000000 W
SFO2        500.2520010 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.13599968 W
PLW12        0.53924000 W
PLW13        0.27124000 W

F2 - Processing parameters
SI                32768
SF          125.7879711 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

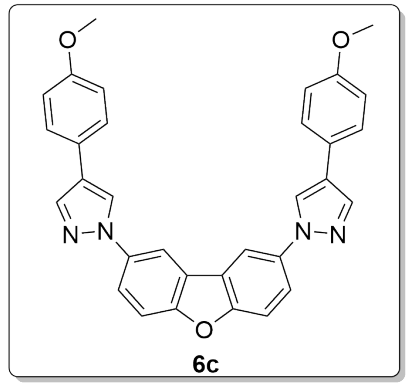

8.339
8.335
8.205
8.030
7.885
7.881
7.868
7.863
7.676
7.659
7.547
7.530
7.468
7.451
7.260
1.372
6b
BRUKER
Current Data Parameters
NAME p-tertbutylphpyzdbf-1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240221
Time 16.07 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 228
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
F2 - Processing parameters
SI 65536
SF 500.2500129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.08
2.07
2.10
2.00
4.07
4.24
18.02



6b

BRUKER

```
Current Data Parameters
NAME                 13Cptbuyl
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20240221
Time                   16.45 h
INSTRUM                spect
PROBHD    Z115265_0004 (
PULPROG              zgpg30
TD                        65536
SOLVENT                  CDCl3
NS                         649
DS                           4
SWH                29761.904 Hz
FIDRES              0.908261 Hz
AQ                  1.1010048 sec
RG                        1030
DW                     16.800 usec
DE                      6.50 usec
TE                         0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1
SFO1            125.8005413 MHz
NUC1                       13C
P1                      9.70 usec
PLW1            73.00000000 W
SFO2            500.2520010 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  80.00 usec
PLW2            15.13599968 W
PLW12            0.53924000 W
PLW13            0.27124000 W

F2 - Processing parameters
SI                       32768
SF              125.7879626 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                        1.40
```



6c

8.266
8.262
8.109
7.962
7.826
7.822
7.808
7.804
7.620
7.602
7.499
7.482
7.260
6.960
6.943

3.841

BRUKER

Current Data Parameters
NAME 1H-p-och3phpyzdbf
EXPNO 1
PROCNO 1

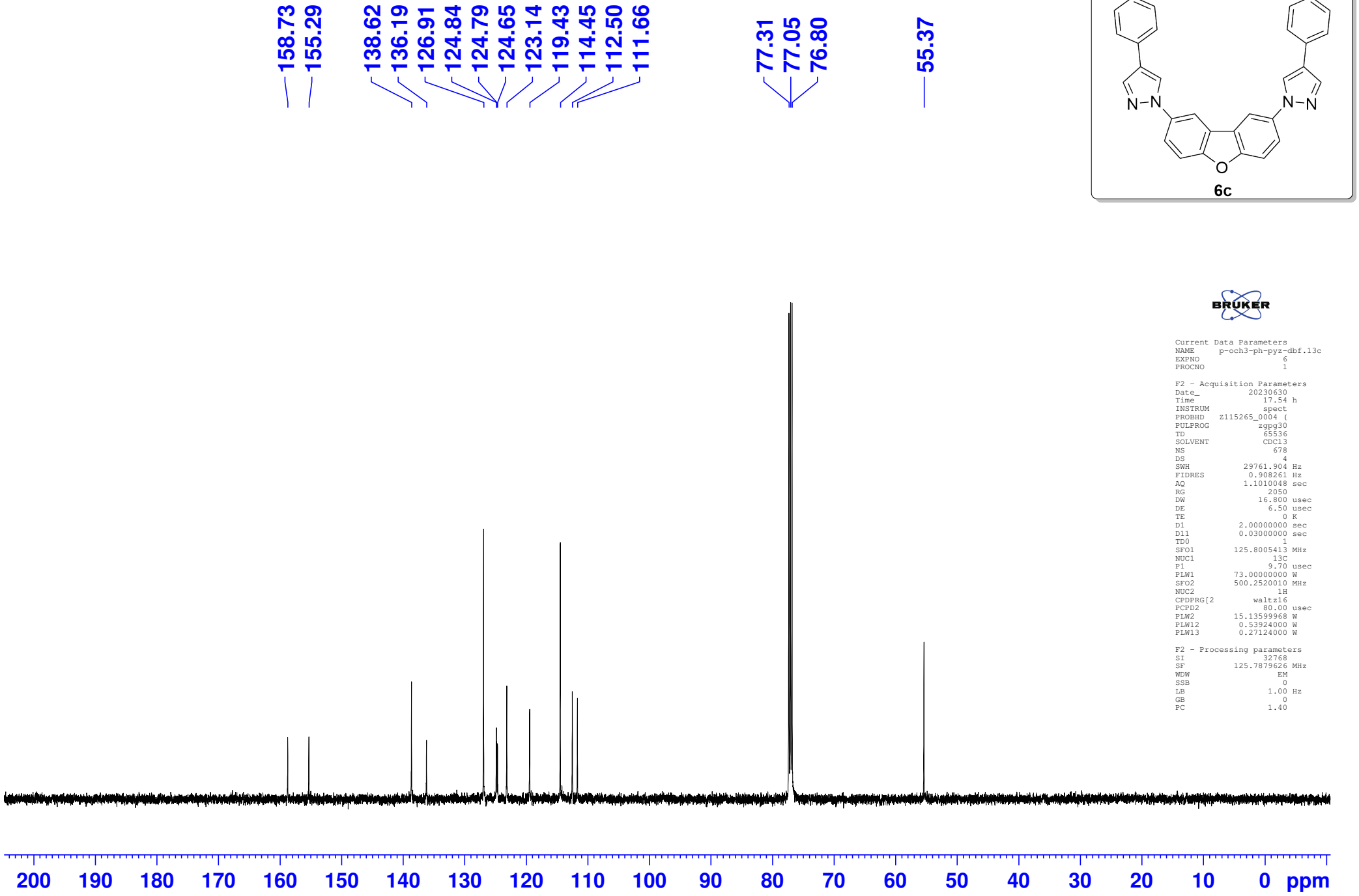
F2 - Acquisition Parameters
Date_ 20230630
Time 16.38 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

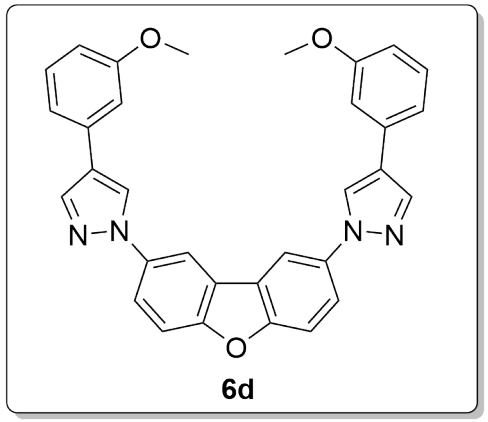
F2 - Processing parameters
SI 65536
SF 500.2500135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

2.03 2.01 2.05 2.05 2.05 4.02 4.00

6.00


158.73
155.29
138.62
136.19
126.91
124.84
124.79
124.65
123.14
119.43
114.45
112.50
111.66
77.31
77.05
76.80
55.37
O
O
N–N
N–N
O
6c
BRUKER
Current Data Parameters
NAME p-och3-ph-pyz-dbf.13c
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230630
Time 17.54 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 678
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
SFO2 500.2520010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.27124000 W
F2 - Processing parameters
SI 32768
SF 125.7879626 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



6d

8.269 8.265 8.173 8.016 7.831 7.827 7.813 7.809 7.622 7.604 7.346 7.330 7.314 7.260 7.176 7.161 7.111 6.849 6.845 6.832 6.828

3.873

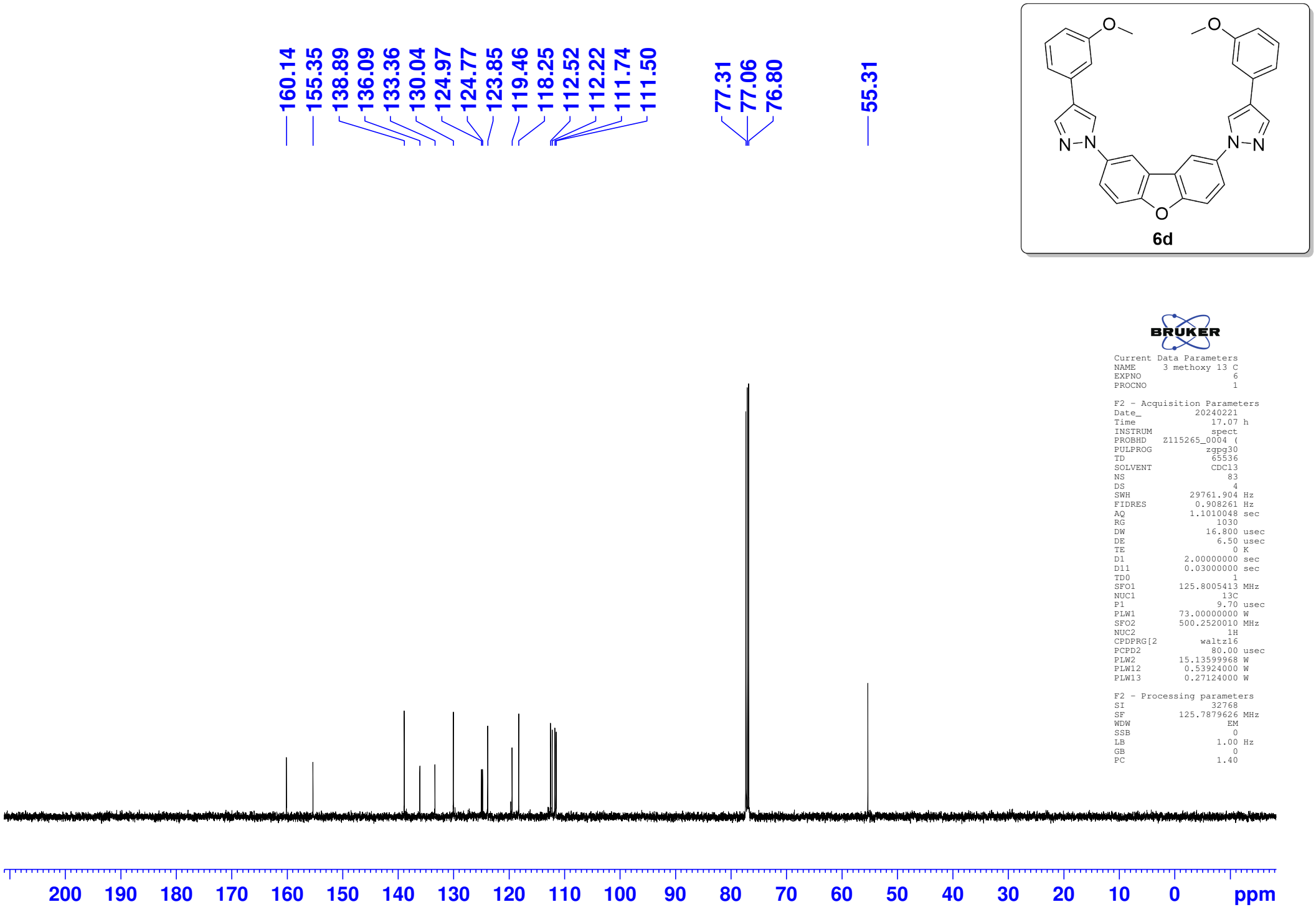
BRUKER

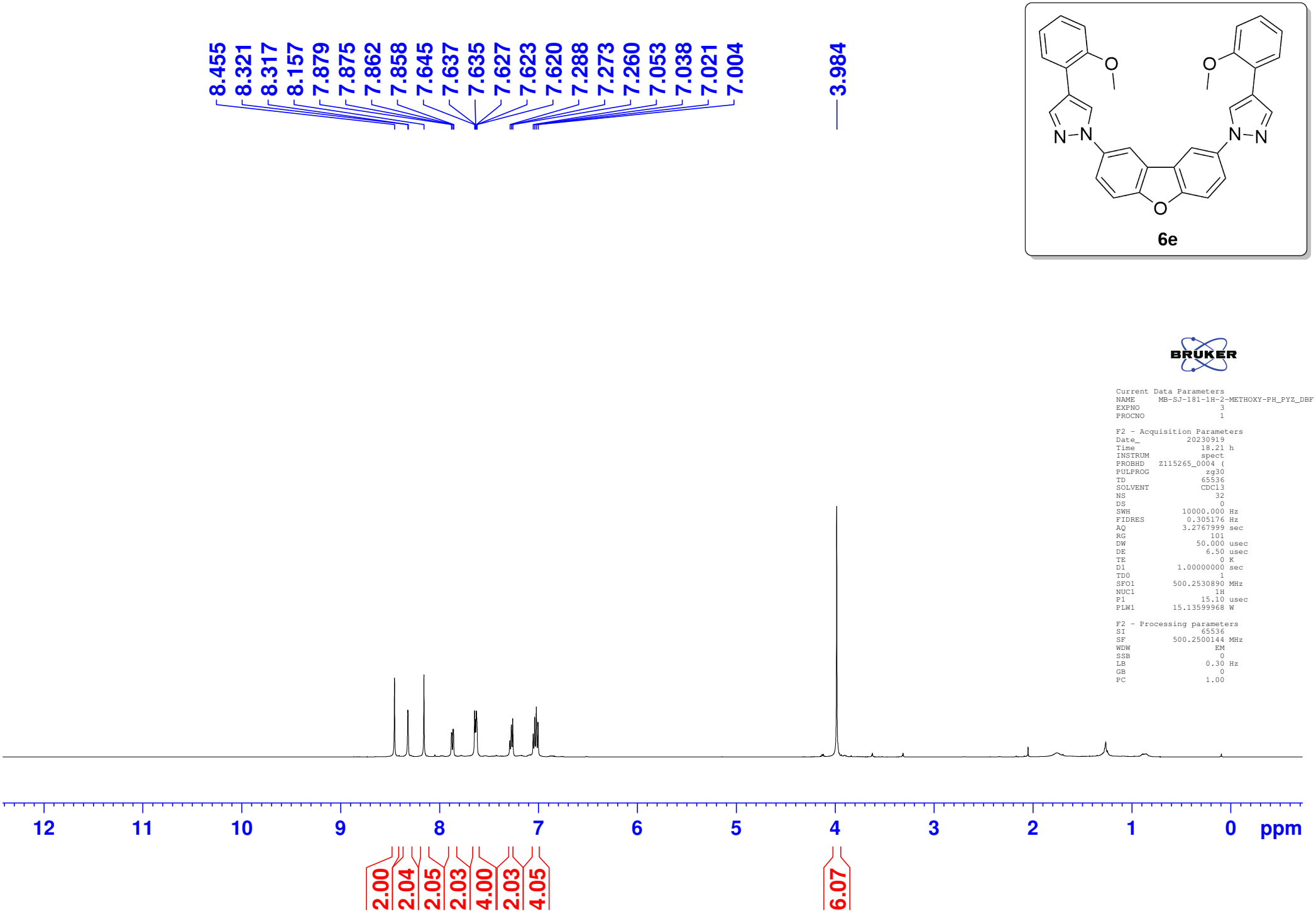
```
Current Data Parameters
NAME                  3methoxy
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20240221
Time                     16.51 h
INSTRUM                  spect
PROBHD    Z115265_0004 (
PULPROG                  zg30
TD                      65536
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                10000.000 Hz
FIDRES                 0.305176 Hz
AQ                 3.2767999 sec
RG                         128
DW                      50.000 usec
DE                       6.50 usec
TE                          0 K
D1                 1.00000000 sec
TD0                          1
SFO1               500.2530890 MHz
NUC1                        1H
P1                      15.10 usec
PLW1               15.13599968 W

F2 - Processing parameters
SI                      65536
SF                 500.2500139 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

2.00 2.06 2.07 2.03 2.10 2.13 2.04 2.05 2.09

6.03


160.14
155.35
138.89
136.09
133.36
130.04
124.97
124.77
123.85
119.46
118.25
112.52
112.22
111.74
111.50
77.31
77.06
76.80
55.31
6d
BRUKER
Current Data Parameters
NAME 3 methoxy 13 C
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240221
Time 17.07 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 83
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
SFO2 500.2520010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.27124000 W
F2 - Processing parameters
SI 32768
SF 125.7879626 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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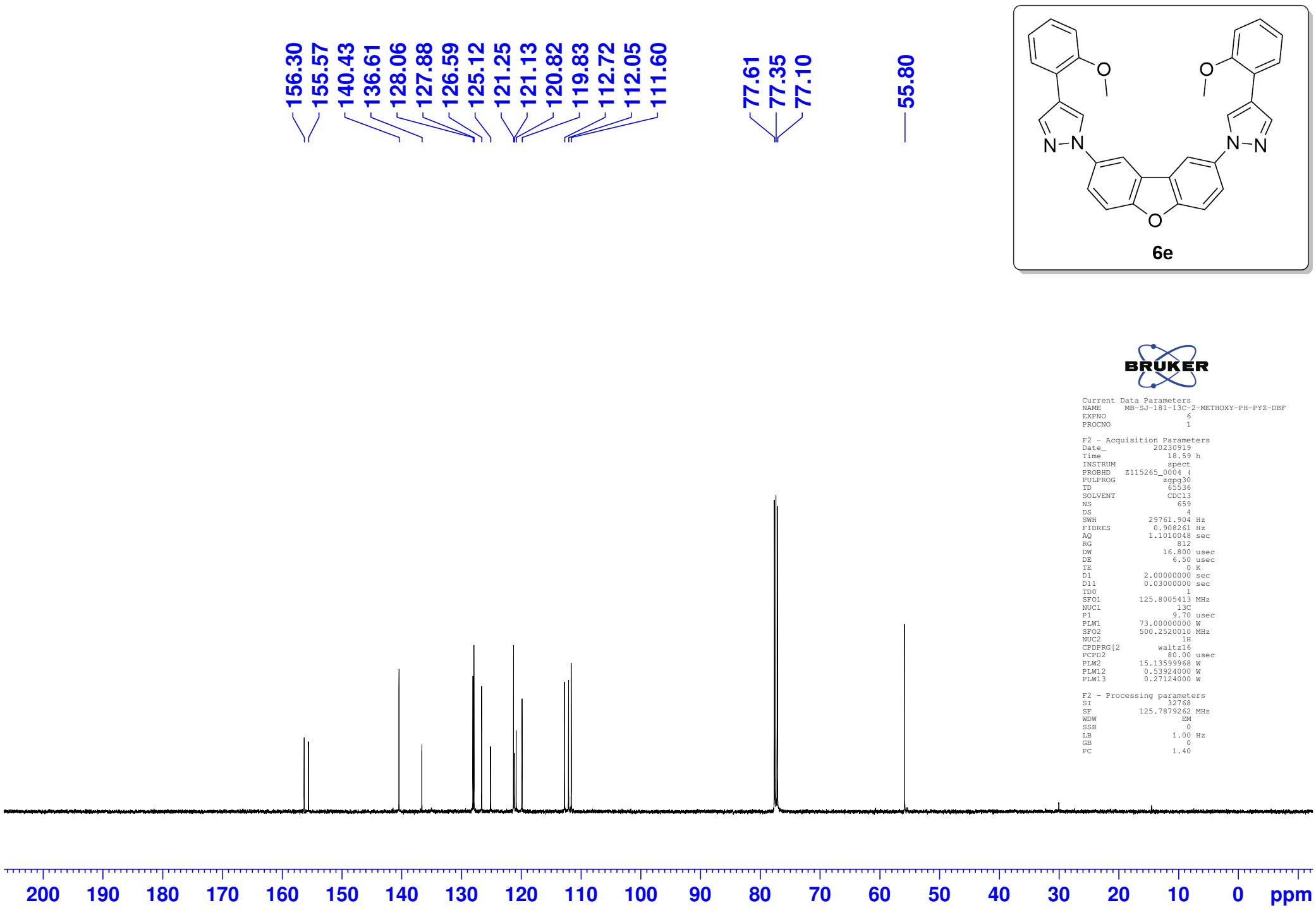
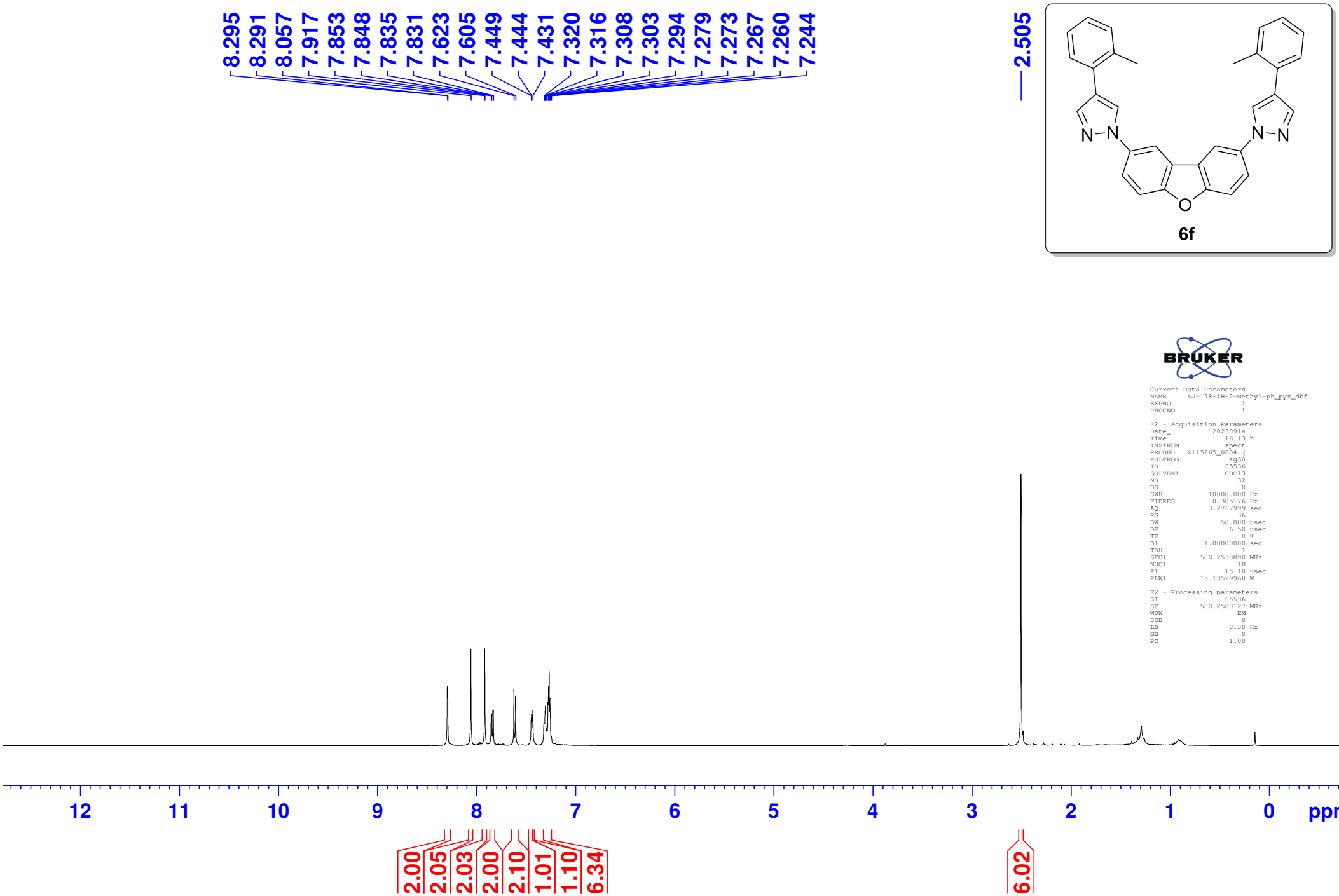
8.321
8.317
8.157
7.879
7.875
7.862
7.858
7.645
7.637
7.635
7.627
7.623
7.620
7.288
7.273
7.260
7.053
7.038
7.021
7.004
3.984
O
O
N–N
N–N
O
6e
BRUKER
Current Data Parameters
NAME MB-SJ-181-1H-2-METHOXY-PH_PYZ_DBF
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230919
Time 18.21 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
F2 - Processing parameters
SI 65536
SF 500.2500144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.04
2.05
2.03
4.00
2.03
4.05
6.07


156.30
155.57
140.43
136.61
128.06
127.88
126.59
125.12
121.25
121.13
120.82
119.83
112.72
112.05
111.60
77.61
77.35
77.10
55.80
O
O
N–N
N–N
O
6e
BRUKER
Current Data Parameters
NAME MB-SJ-181-13C-2-METHOXY-PH-PYZ-DBF
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230919
Time 18.59 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 659
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 812
DW 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
SFO2 500.2520010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.27124000 W
F2 - Processing parameters
SI 32768
SF 125.7879262 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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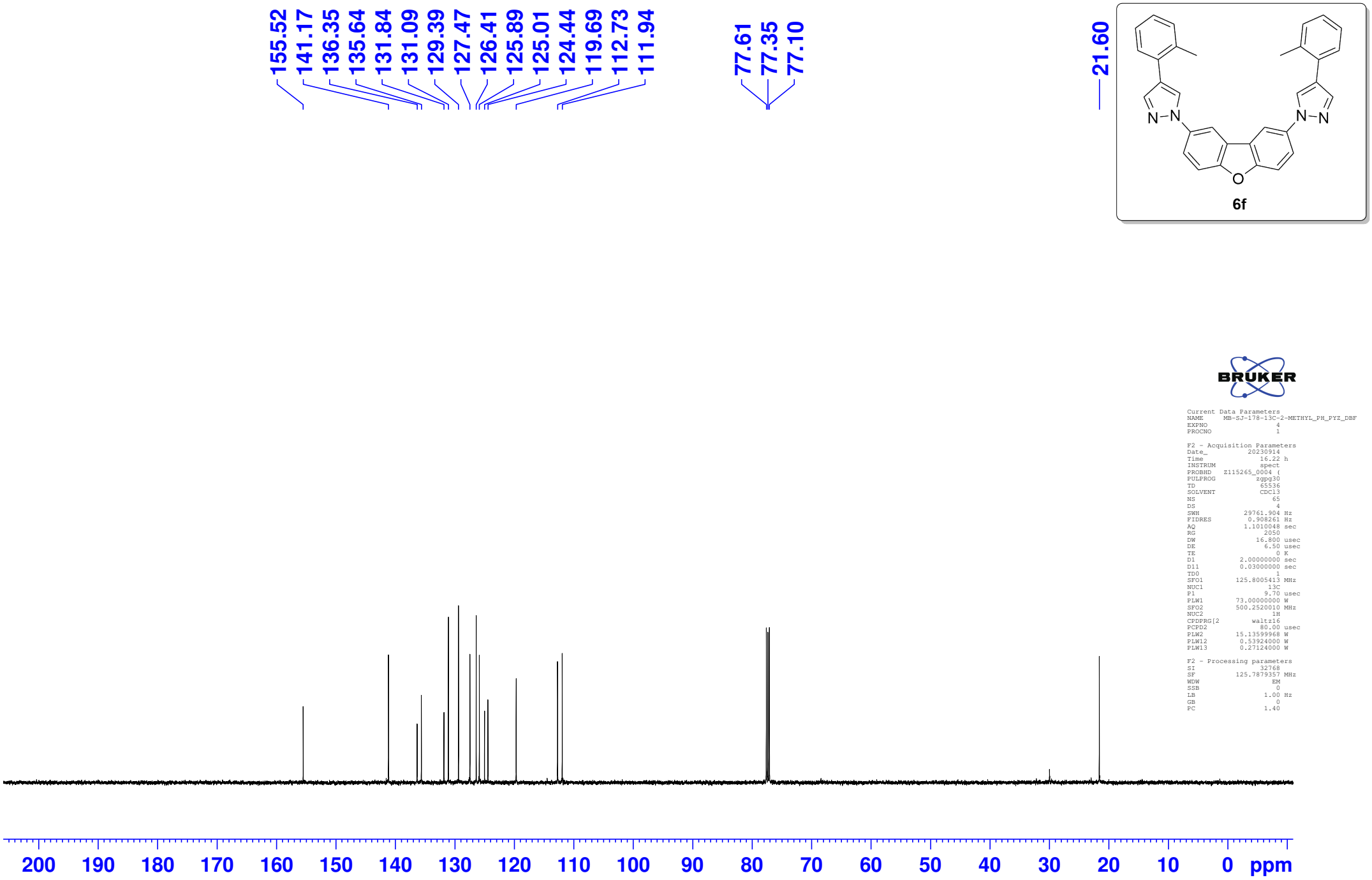
8.057
7.917
7.853
7.848
7.835
7.831
7.623
7.605
7.449
7.444
7.431
7.320
7.316
7.308
7.303
7.294
7.279
7.273
7.267
7.260
7.244
2.505
N–N
N–N
O
6f
BRUKER
Current Data Parameters
NAME SJ-178-1H-2-Methyl-ph_pyz_dbf
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230914
Time 16.13 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 36
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
F2 - Processing parameters
SI 65536
SF 500.2500127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.05
2.03
2.00
2.10
1.01
1.10
6.34
6.02

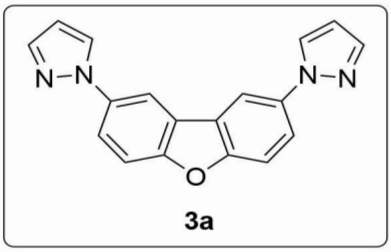

155.52
141.17
136.35
135.64
131.84
131.09
129.39
127.47
126.41
125.89
125.01
124.44
119.69
112.73
111.94
77.61
77.35
77.10
21.60
N–N
N–N
O
6f
BRUKER
Current Data Parameters
NAME MB-SJ-178-13C-2-METHYL_PH_PYZ_DBF
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230914
Time 16.22 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 65
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8005413 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
SFO2 500.2520010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.27124000 W
F2 - Processing parameters
SI 32768
SF 125.7879357 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Target Screening Report

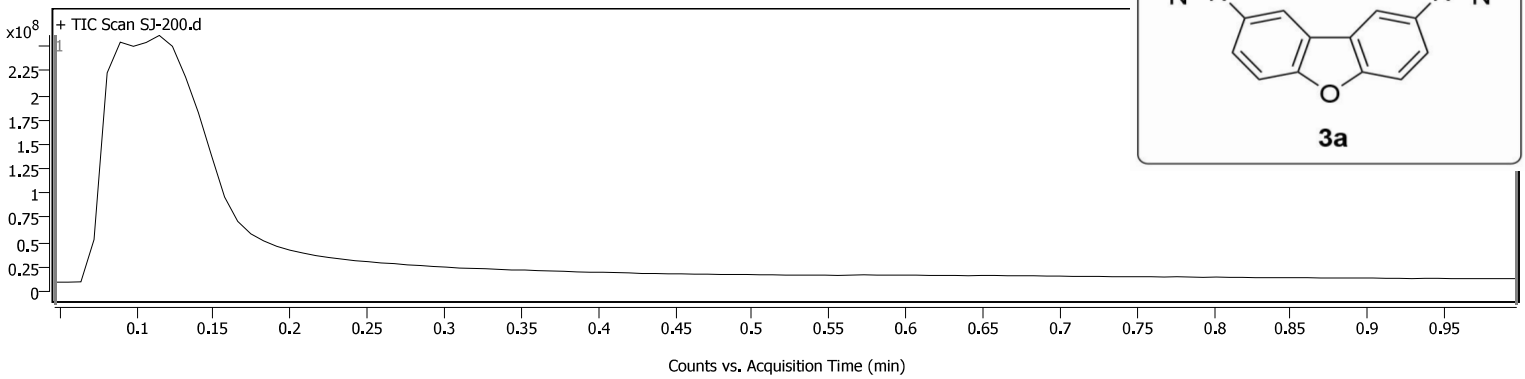
Agilent | Trusted Answers

Sample Information

Name	SJ-200	**Data File Path**	D:\Projects\DEMO TRAINING\Data\17-11-2023\Sonu_Dr. MB\SJ-200.d
Sample ID		**Acq. Time (Local)**	17-11-2023 17:44:06 (UTC+05:30)
Instrument	G6546A	**Method Path (Acq)**	D:\Projects\DEMO TRAINING\Methods\Method_250-650.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	1	**IRM Status**	Success
Position	P1-D10	**Method Path (DA)**	D:\Projects\Installation\Methods\default.m
Plate Pos.		**Target Source Path**	
Operator	SYSTEM (SYSTEM)	**Result Summary**	1 qualified (1 targets)



Sample Chromatograms



Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1		C18 H12 N4 O		0.581	300.1007	300.1011	-1.32	98.82	FBF

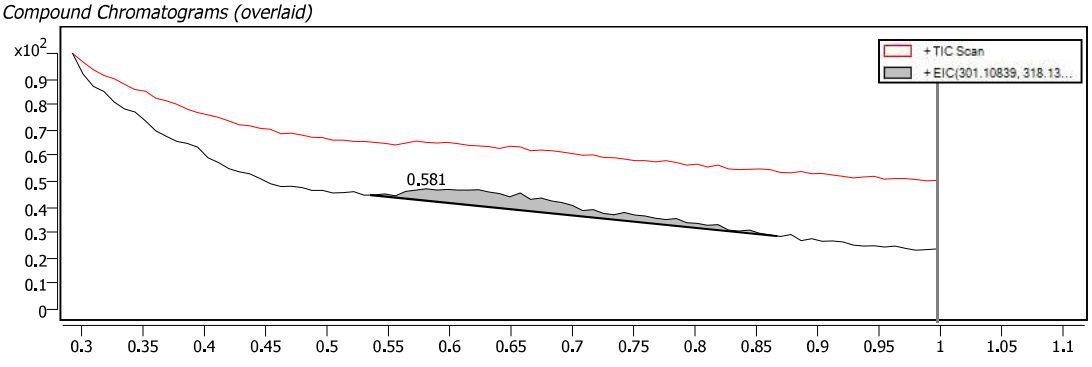
Compound Details

Cpd. 1: C18 H12 N4 O

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C18 H12 N4 O	0.581		300.1007	-1.32		FBF	98.82	FBF

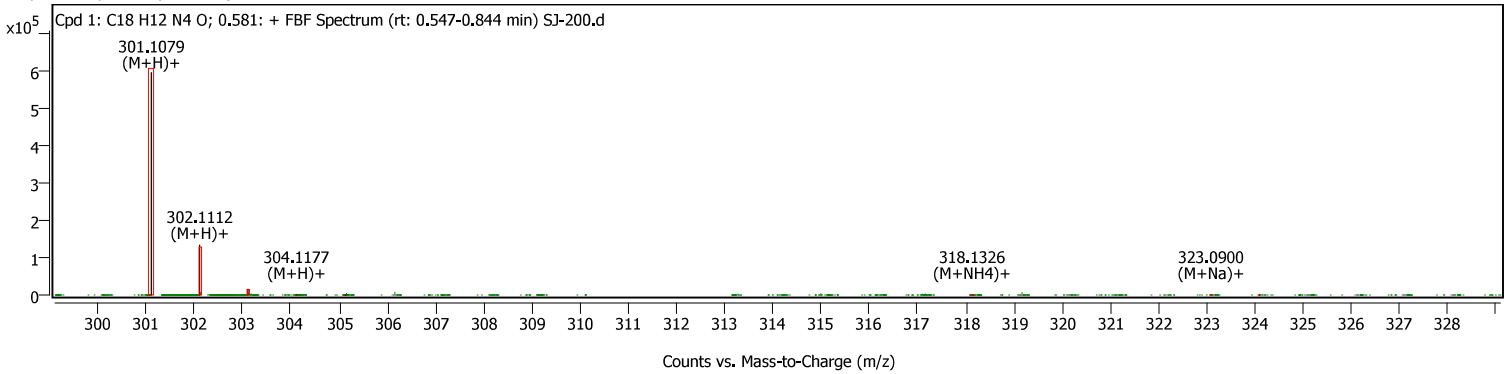
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+NH4)+ (M+Na)+	301.1079 318.1326 323.0900	98.82				

Compound Chromatograms (overlaid)

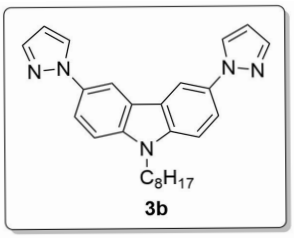


Structure

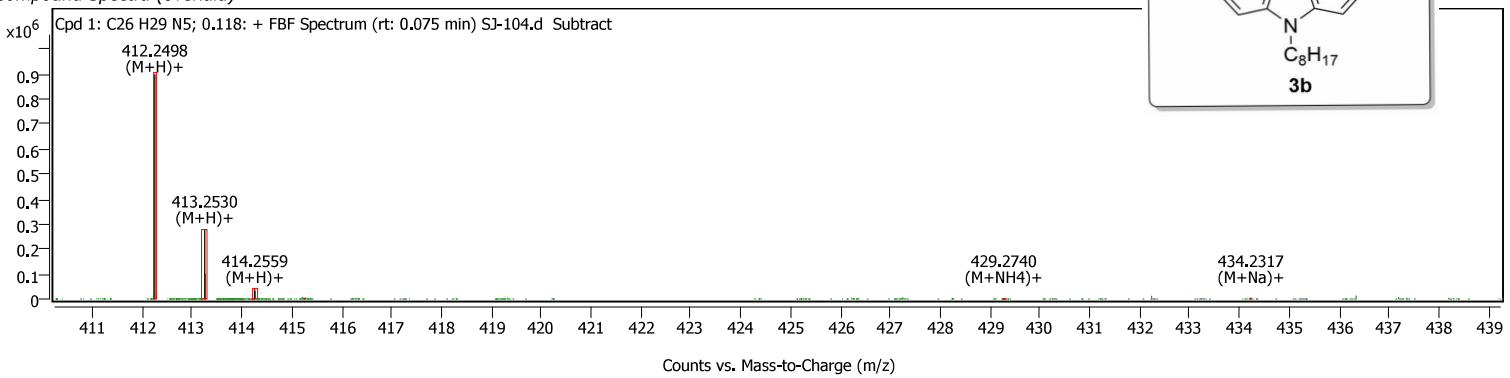
Compound Spectra (overlaid)



Target Screening Report



Compound Spectra (overlaid)

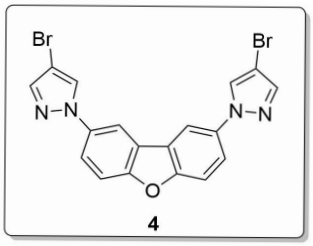


Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C26 H29 N5	(M+H)+ (M+NH4)+ (M+Na)+	0.118		411.2426		FBF	99.67		99.67

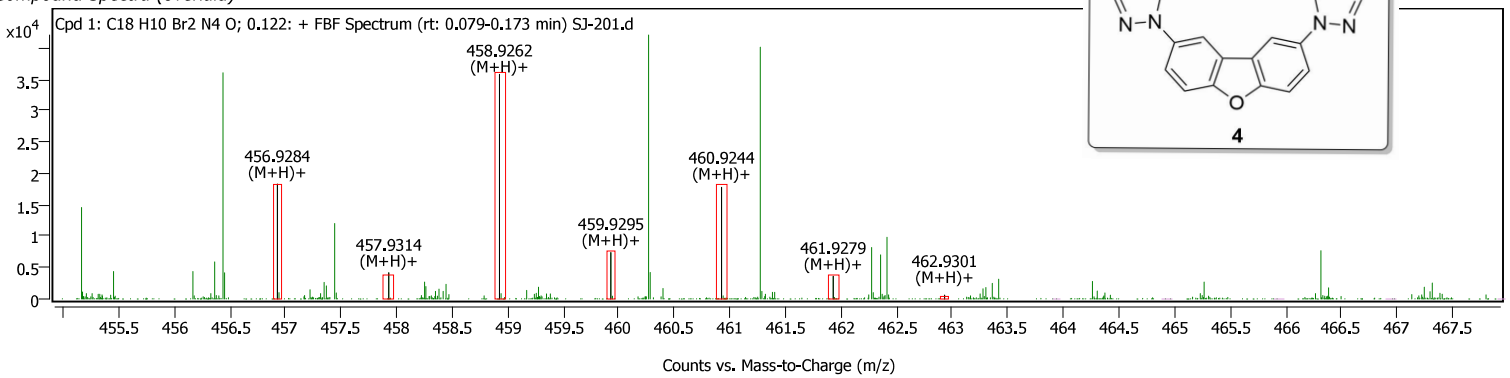
MassHunter Qual 10.0
(End of Report)

Target Screening Report



Trusted Answers

Compound Spectra (overlaid)



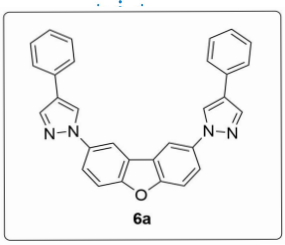
Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C18 H10 Br2 N4 O	(M+H)+	0.122		455.9210		FBF	96.90		96.90

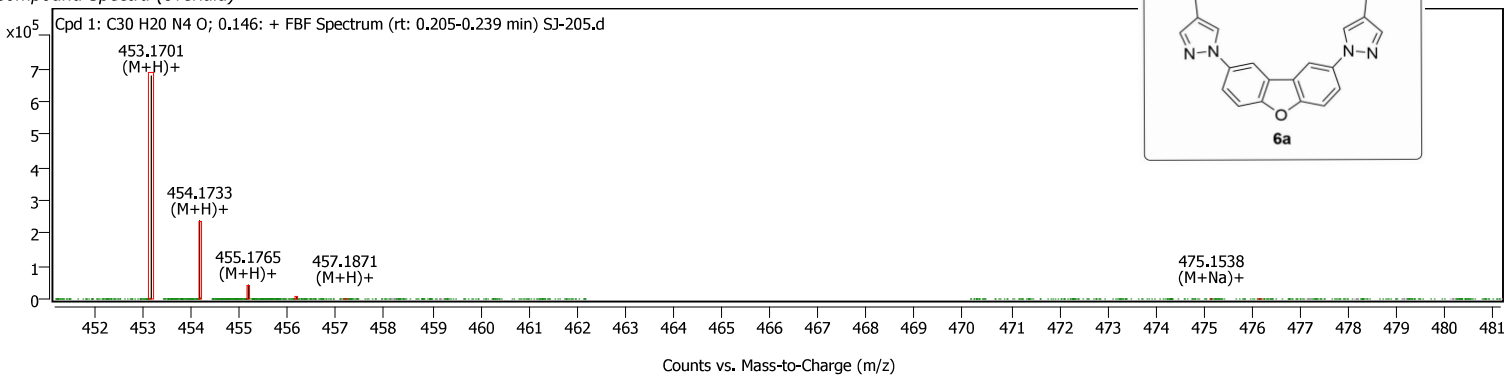
MassHunter Qual 10.0
(End of Report)

Target Screening Report

Trusted Answers



Compound Spectra (overlaid)

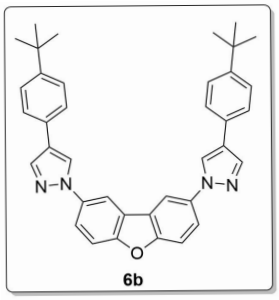


Compound ID Table

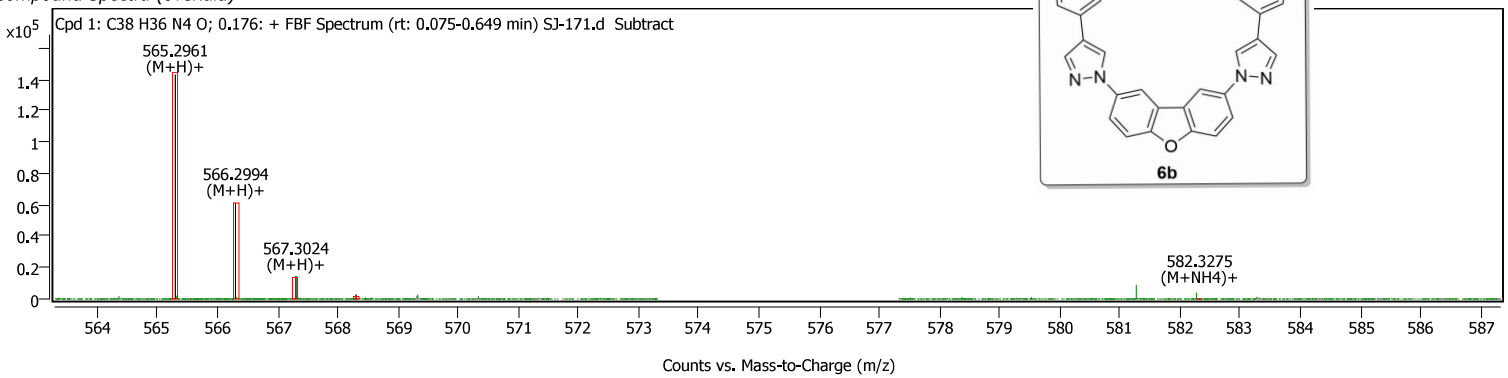
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C30 H20 N4 O	(M+H)+ (M+Na)+	0.146		452.1629		FBF	98.24		98.24

MassHunter Qual 10.0
(End of Report)

Target Screening Report



Compound Spectra (overlaid)



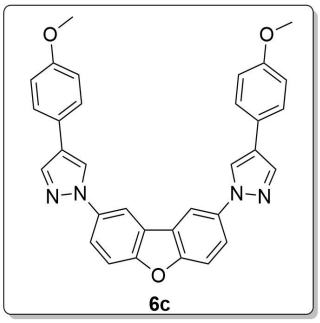
Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C38 H36 N4 O	(M+H)+ (M+NH4)+	0.176		564.2889		FBF	99.72		99.72

MassHunter Qual 10.0
(End of Report)

Sample Information

Name	SJ-155	**Data File Path**	D:\Projects\ANALYSIS\Data\2026\February\SJ-155.d
Sample ID		**Acq. Time (Local)**	26-02-2026 17:36:26 (UTC+05:30)
Instrument	G6546A	**Method Path (Acq)**	D:\Projects\ANALYSIS\Methods\Mass_scan.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	1	**IRM Status**	Success
Position	P1-D1	**Method Path (DA)**	D:\Projects\ANALYSIS\Methods\default.m
Plate Pos.		**Target Source Path**	
Operator	SYSTEM (SYSTEM)	**Result Summary**	1 qualified (1 targets)



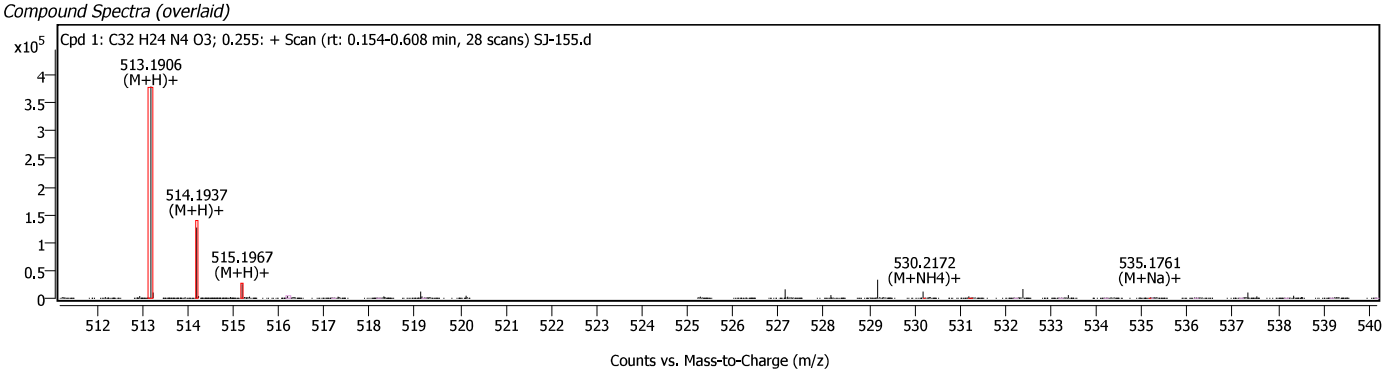
6c

Compound Details

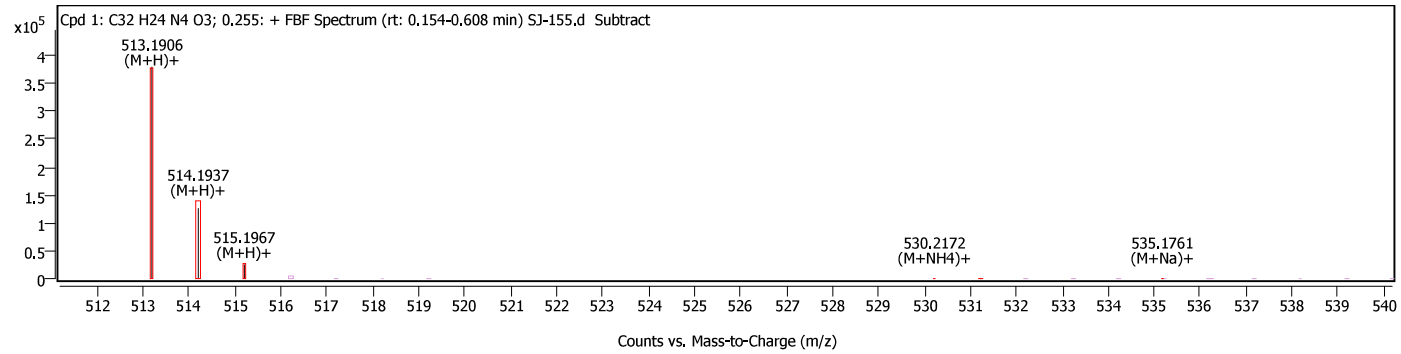
Cpd. 1: C32 H24 N4 O3

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+NH4)+ (M+Na)+	513.1906 530.2172 535.1761					

Compound Spectra (overlaid)



Compound Spectra



Spectrum Peaks

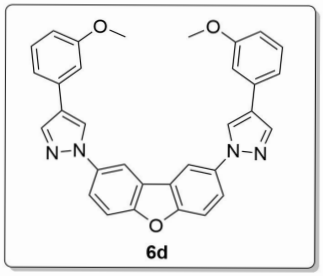
m/z	m/z (Calc)	Diff (ppm)	Abund	Height %	Height % (Calc)	Ion Species	Z
513.1906	513.1921	-2.98	380094	100.00	100.00	(M+H)+	1
514.1937	514.1952	-3.01	126519	33.29	36.47	(M+H)+	1
515.1967	515.1982	-2.97	25217	6.63	7.08	(M+H)+	1
530.2172	530.2187	-2.75	602	100.00	100.00	(M+NH4)+	1
531.2167	531.2217	-9.42	130	21.67	36.87	(M+NH4)+	1
535.1761	535.1741	3.78	209	100.00	100.00	(M+Na)+	1

Spectrum Peaks

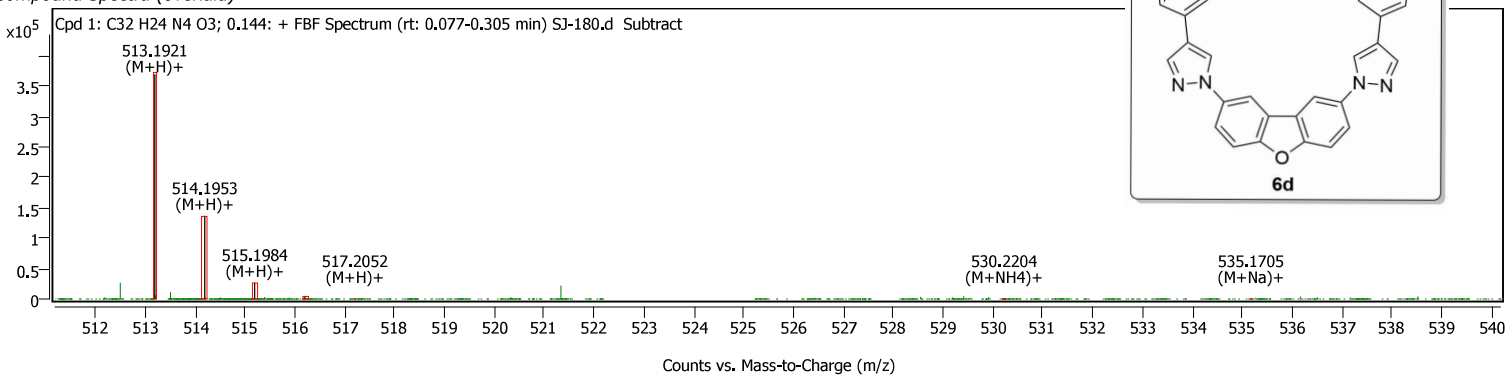
m/z	m/z (Calc)	Diff (ppm)	Abund	Height %	Height % (Calc)	Ion Species	Z
513.1906	513.1921	-2.98	380094	100.00	100.00	(M+H)+	1
514.1937	514.1952	-3.01	126519	33.29	36.47	(M+H)+	1
515.1967	515.1982	-2.97	25217	6.63	7.08	(M+H)+	1
530.2172	530.2187	-2.75	602	100.00	100.00	(M+NH4)+	1
531.2167	531.2217	-9.42	130	21.67	36.87	(M+NH4)+	1
535.1761	535.1741	3.78	209	100.00	100.00	(M+Na)+	1

MassHunter Qual 10.0
(End of Report)

Target Screening Report



Compound Spectra (overlaid)



Compound ID Table

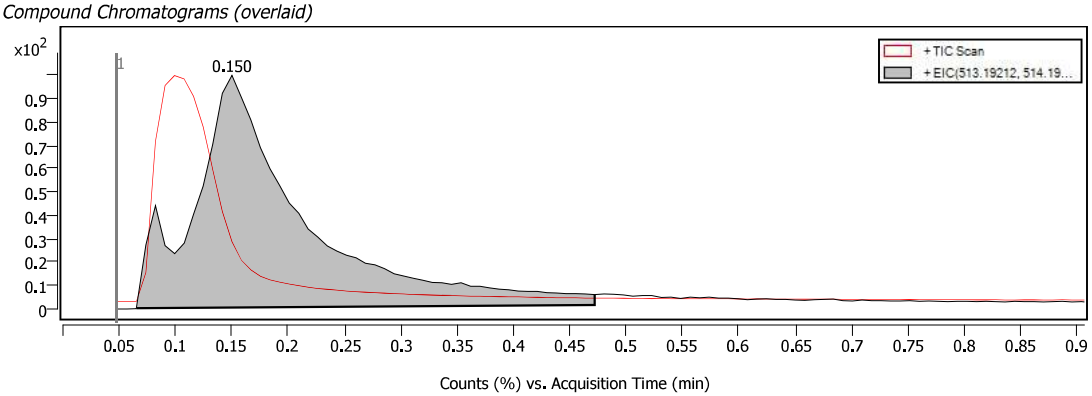
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C32 H24 N4 O3	(M+H)+ (M+NH4)+ (M+Na)+	0.144		512.1848		FBF	99.95		99.95

MassHunter Qual 10.0
(End of Report)

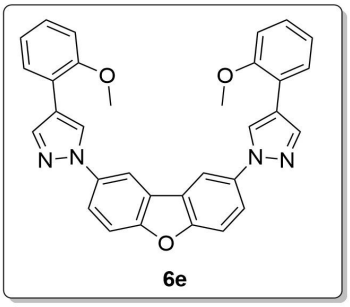
Target Screening Report

Agilent | Trusted Answers

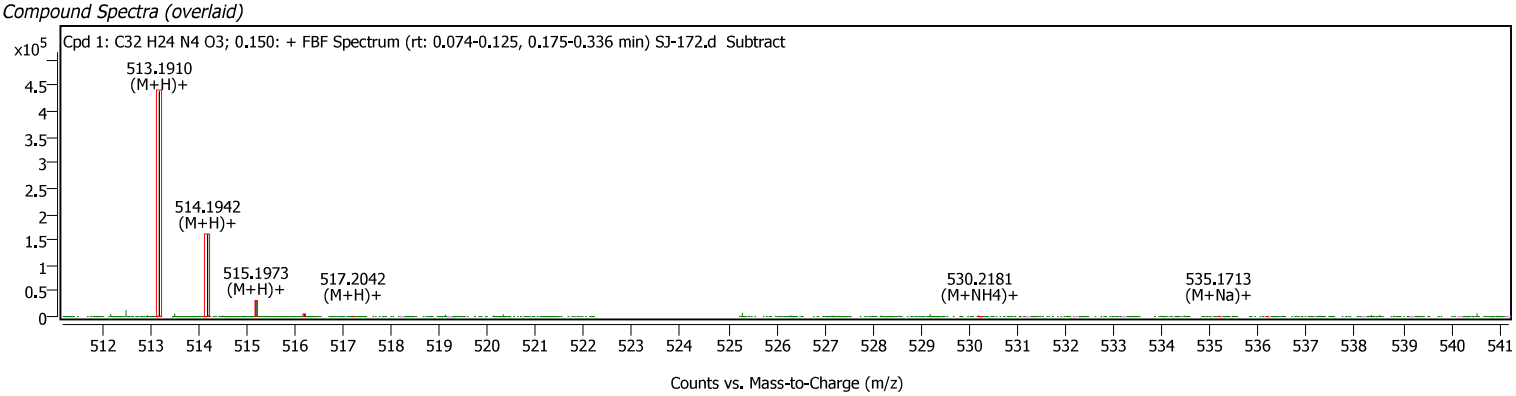
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)

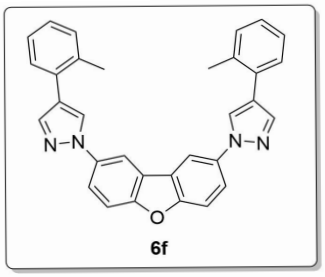


Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C32 H24 N4 O3	(M+H)+ (M+NH4)+ (M+Na)+	0.150		512.1838		FBF	97.67		97.67

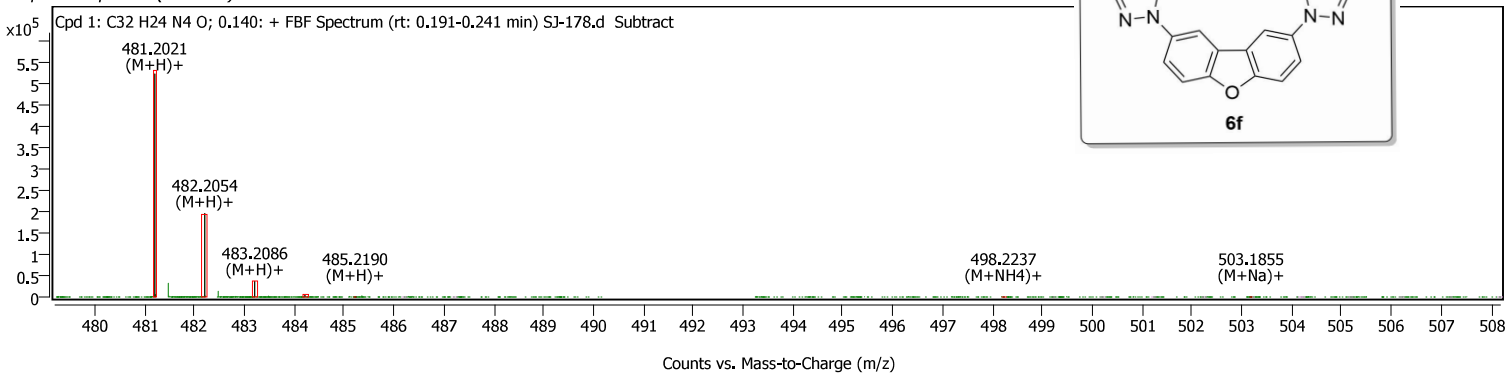
MassHunter Qual 10.0
(End of Report)

Target Screening Report



Trusted Answers

Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C32 H24 N4 O	(M+H)+ (M+NH4)+ (M+Na)+	0.140		480.1949		FBF	99.77		99.77

MassHunter Qual 10.0
(End of Report)