Supplementary Material

Photophysical and antibacterial properties of symmetrical curcuminoid–BF_2 complexes

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1. HRMS spectra

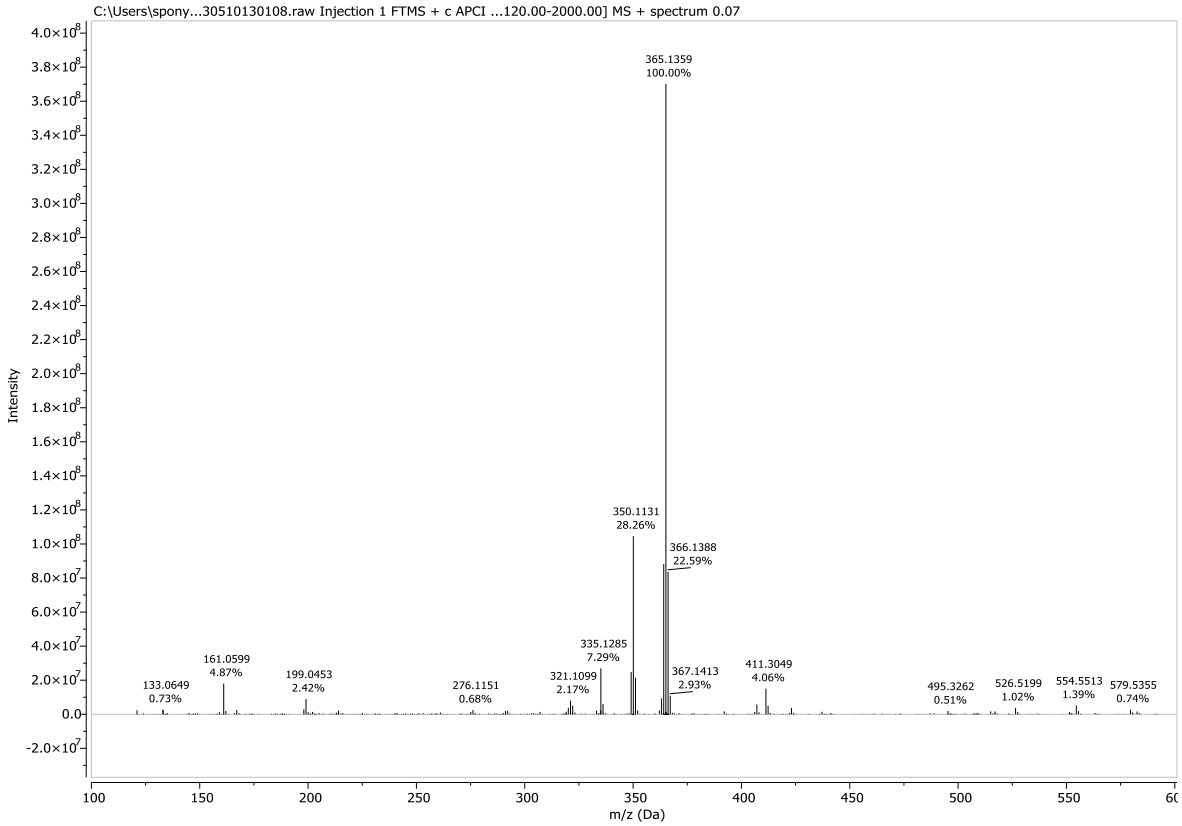


Figure 1.1: APCI (+) HRMS spectrum of **2**

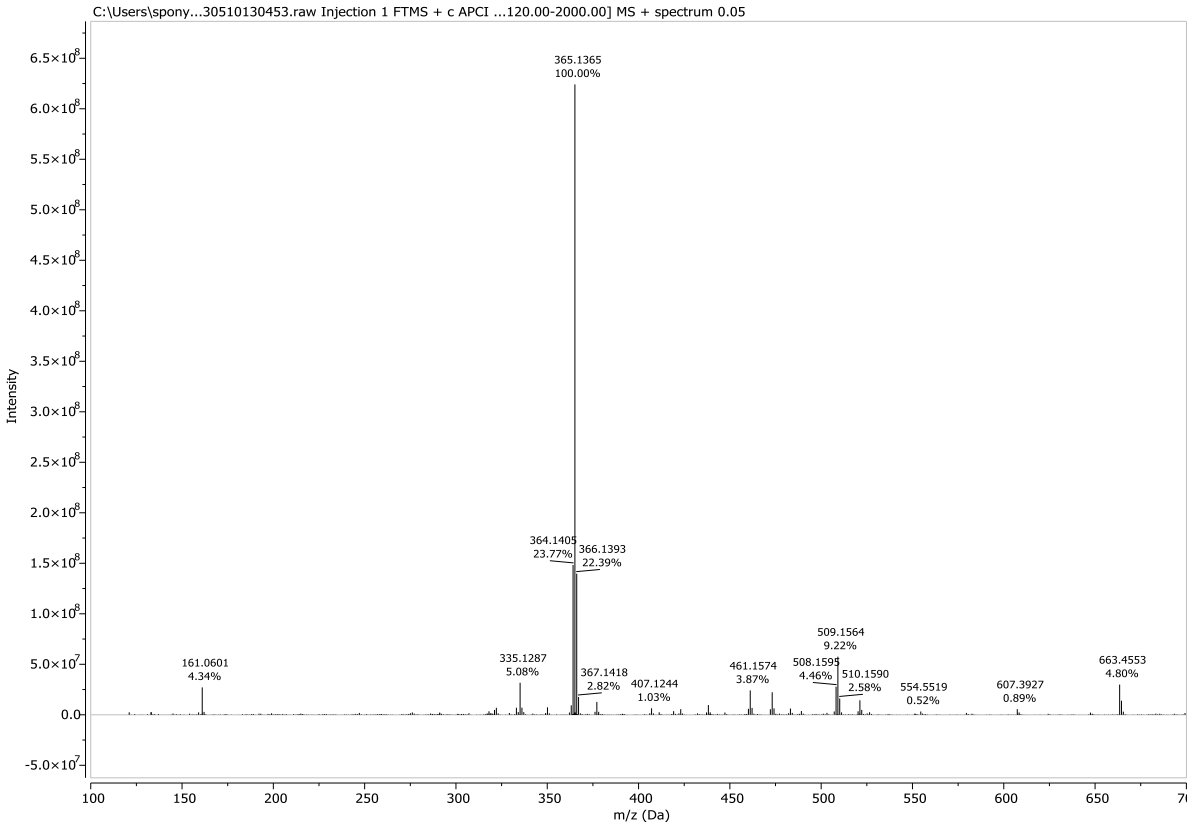


Figure 1.2: APCI (+) HRMS spectrum of **3**

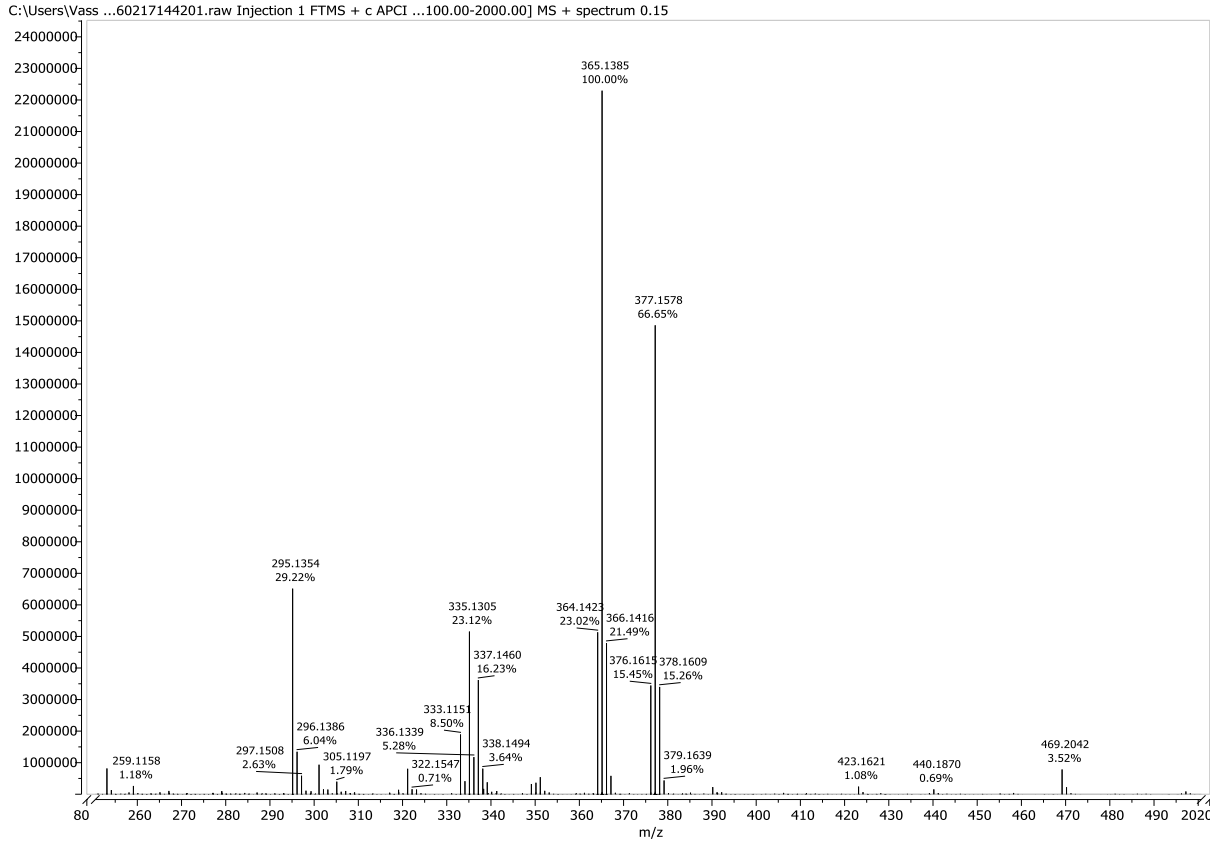


Figure 1.3: APCI (+) HRMS spectrum of 4

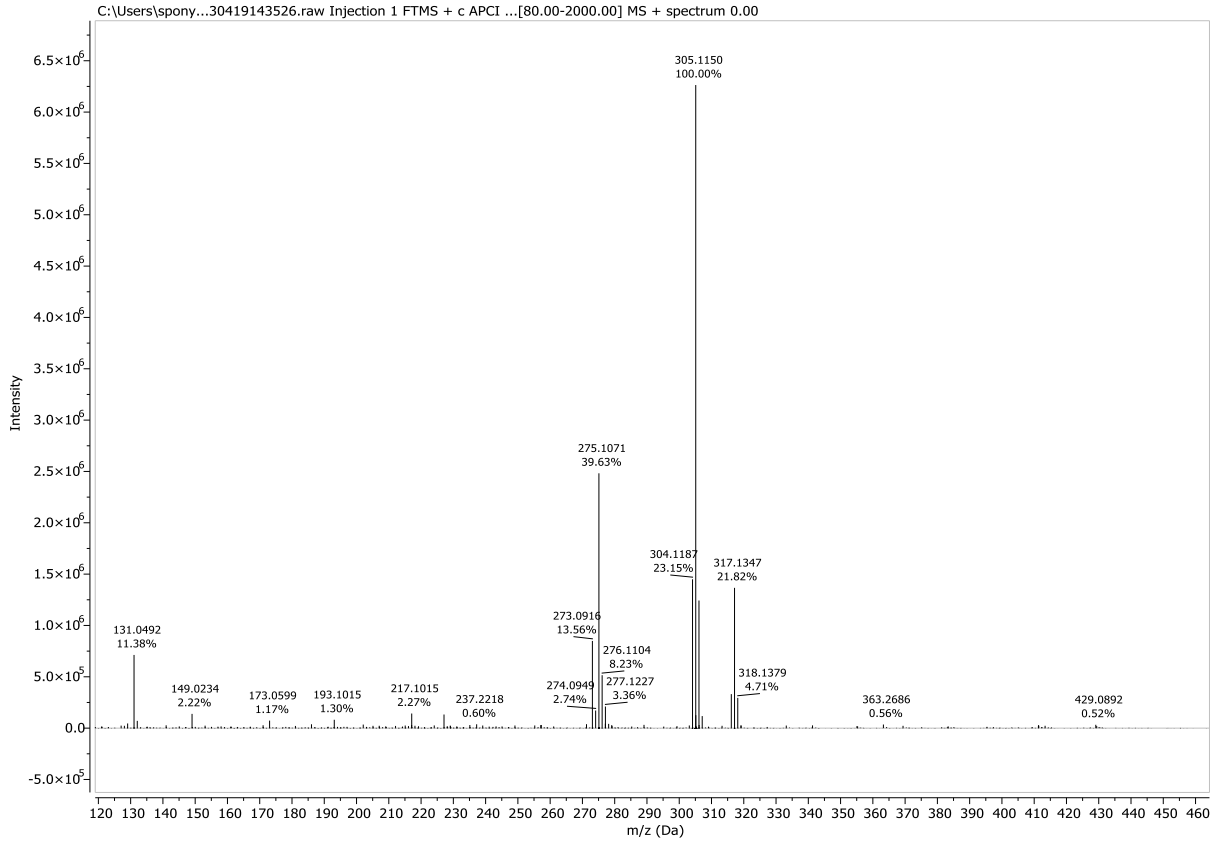


Figure 1.4: APCI (+) HRMS spectrum of **5**

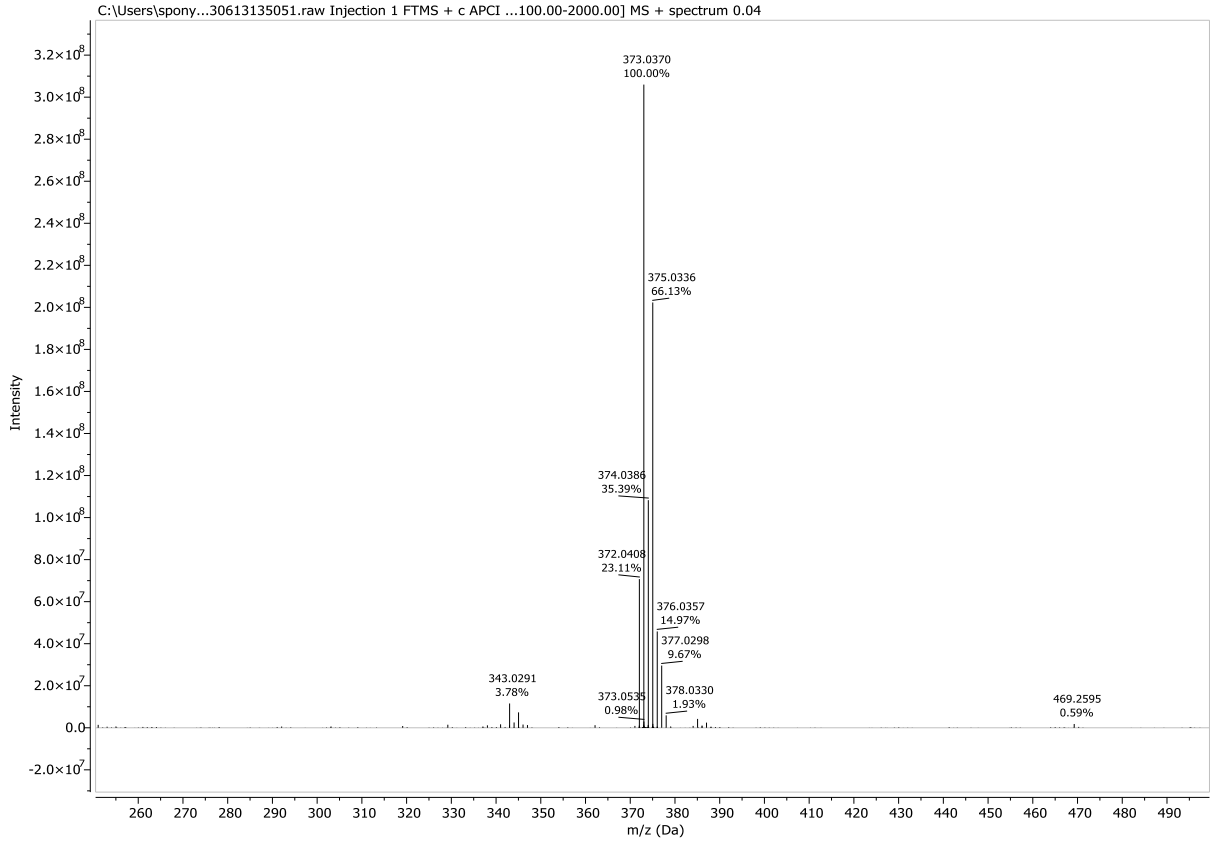


Figure 1.5: APCI (+) HRMS spectrum of **6**

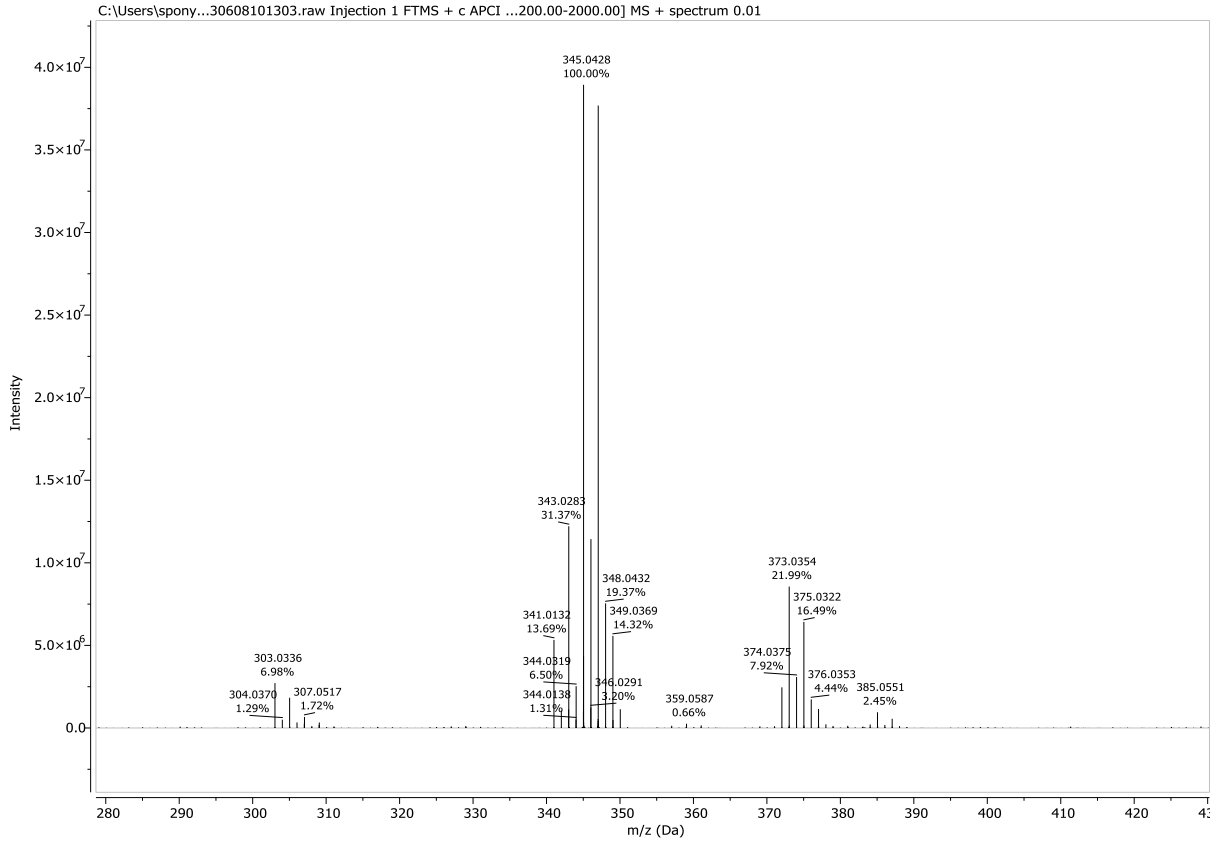


Figure 1.6: APCI (+) HRMS spectrum of **7**

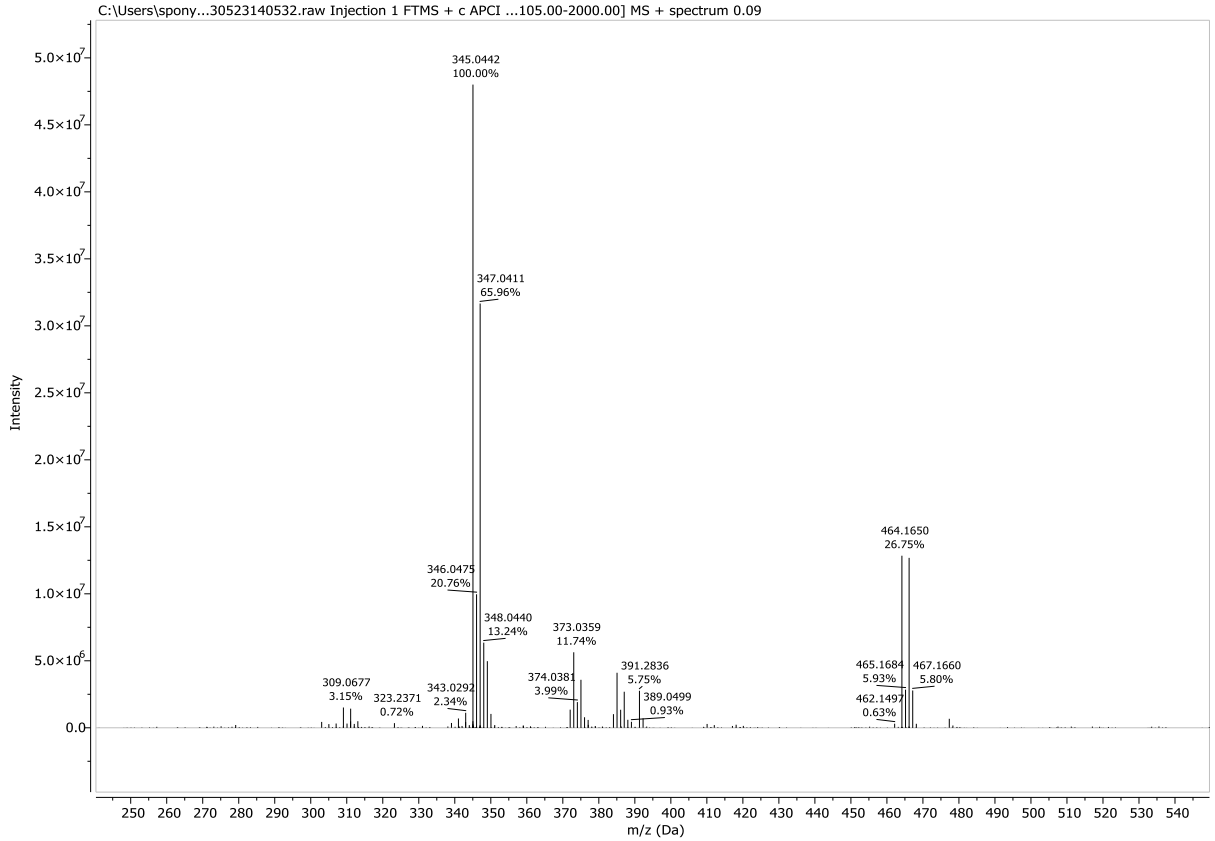


Figure 1.7: APCI (+) HRMS spectrum of **8**

2. ^{1}H, ^{11}B, ^{13}C and ^{19}F NMR spectra

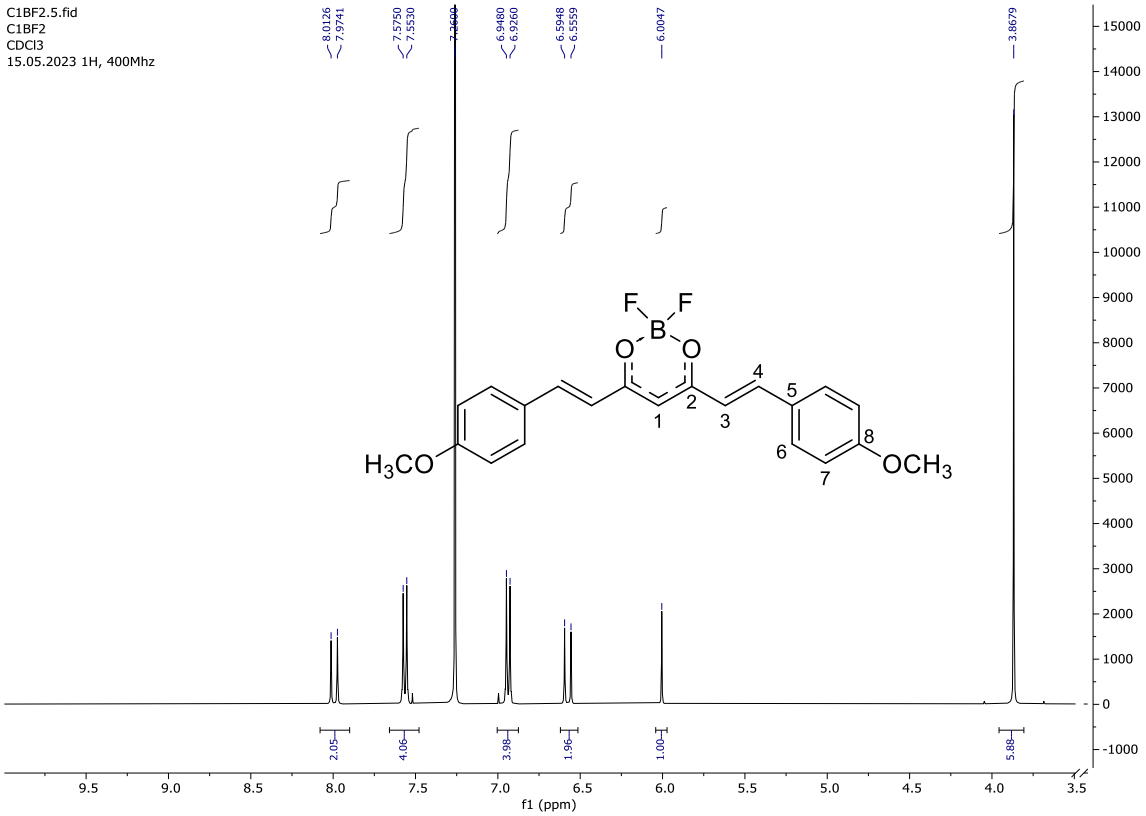


Figure 2.1: ^{1}H NMR spectrum of **2** in $CDCl_3$ at 400 MHz

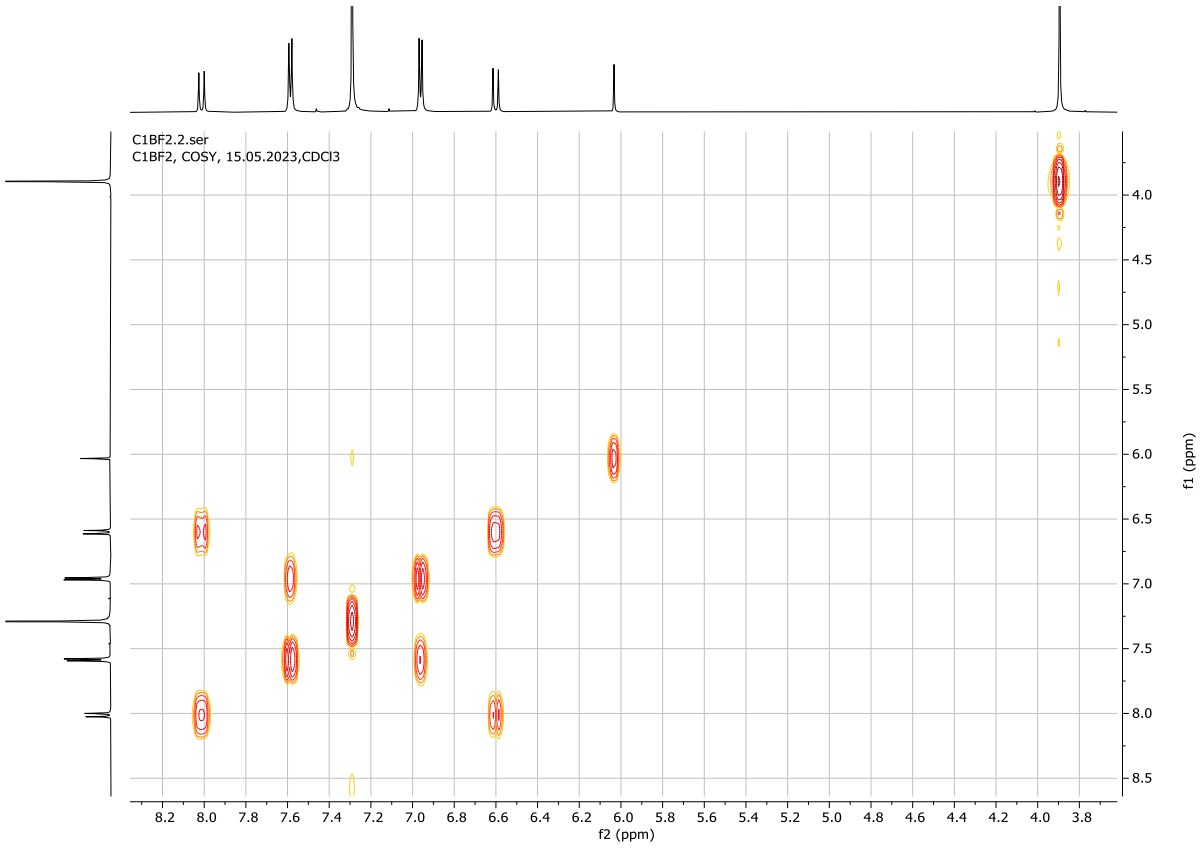


Figure 2.2: ^{1}H-^{1}H COSY NMR spectrum of **2** in $CDCl_3$ at 400 MHz

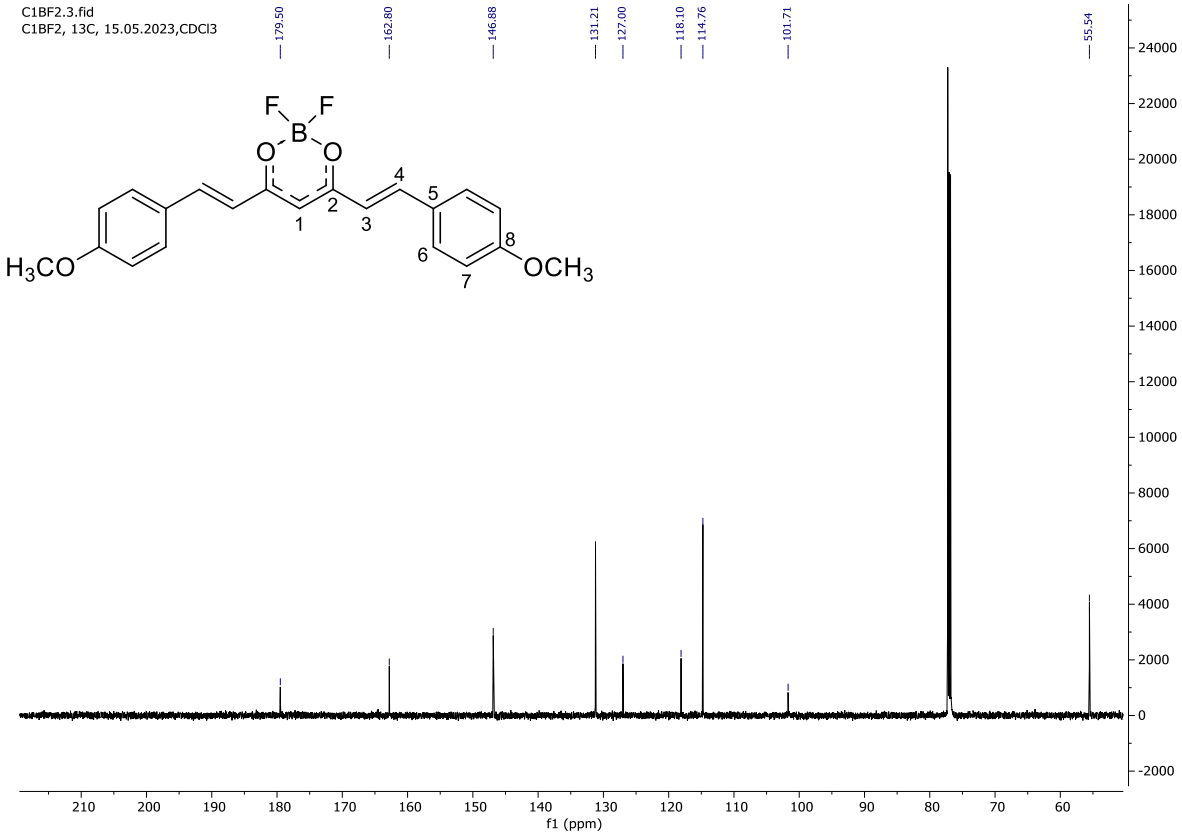


Figure 2.3: ^{13}C NMR spectrum of **2** in $CDCl_3$ at 101 MHz

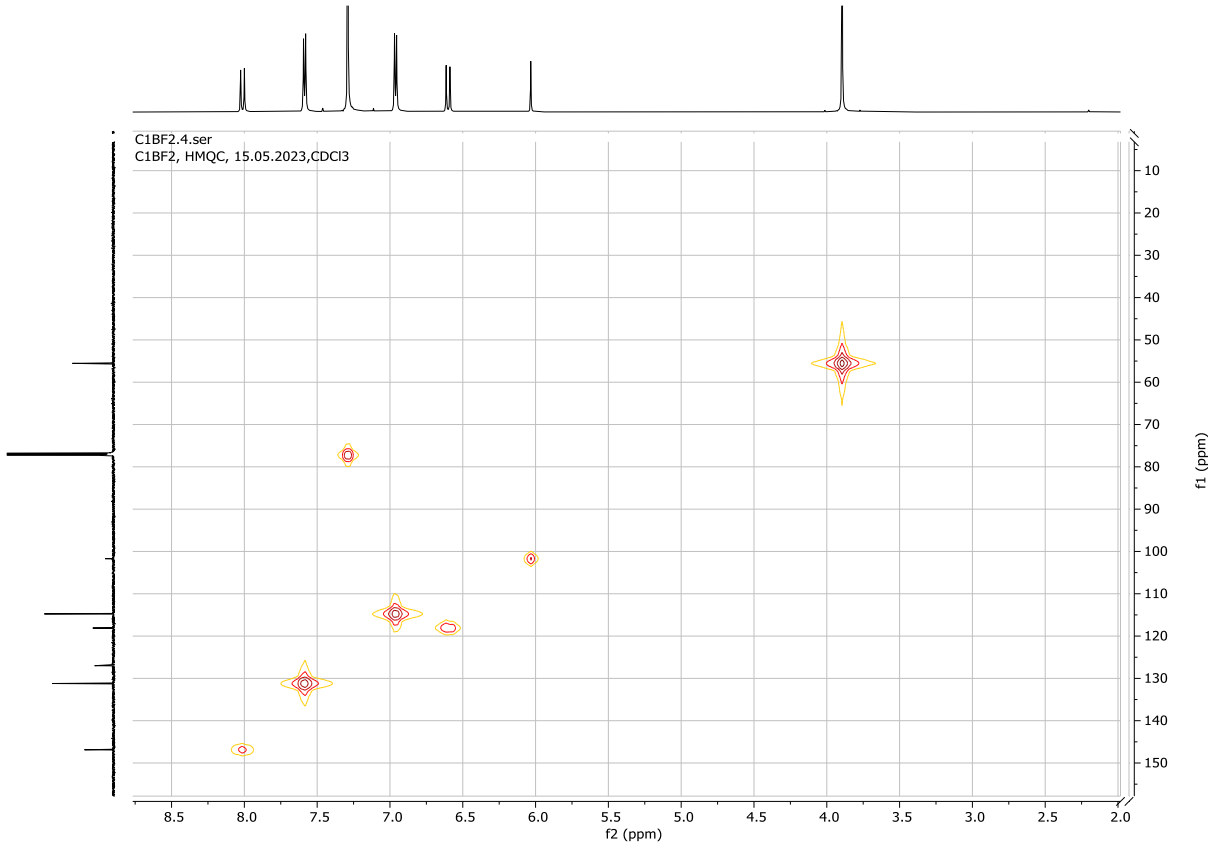


Figure 2.4: ^{1}H-^{13}C HMQC NMR spectrum of **2** in $CDCl_3$

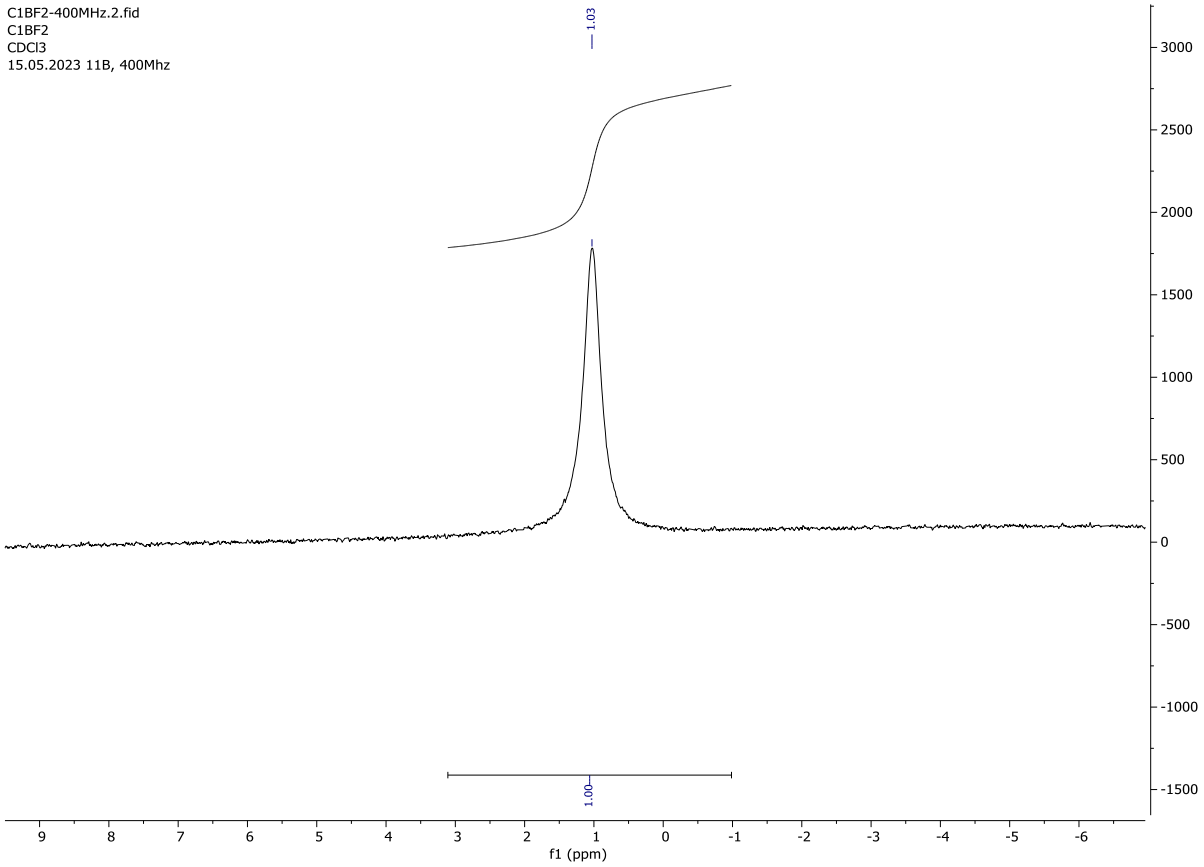


Figure 2.5: ^{11}B NMR spectrum of **2** in $CDCl_3$ at 127 MHz

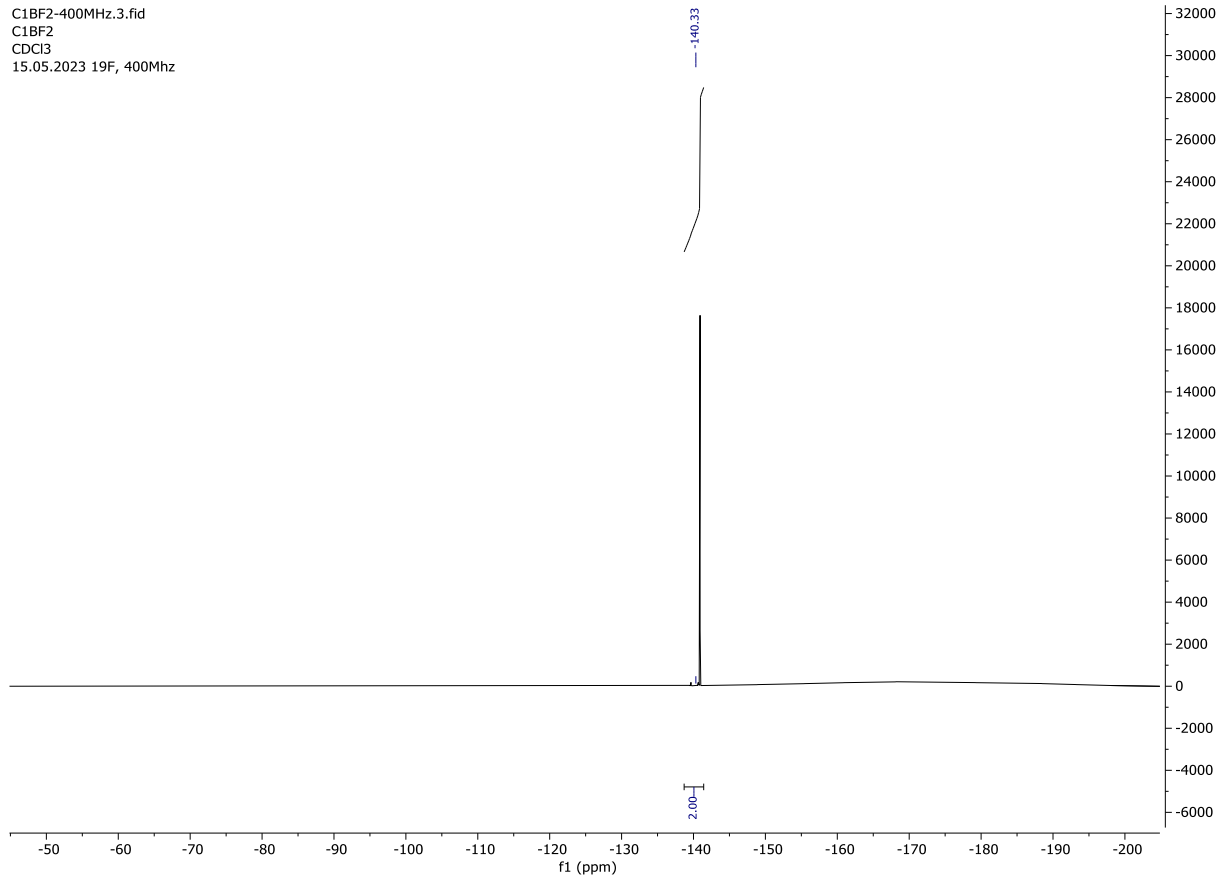


Figure 2.6: ^{19}F NMR spectrum of **2** in $CDCl_3$ at 376 MHz

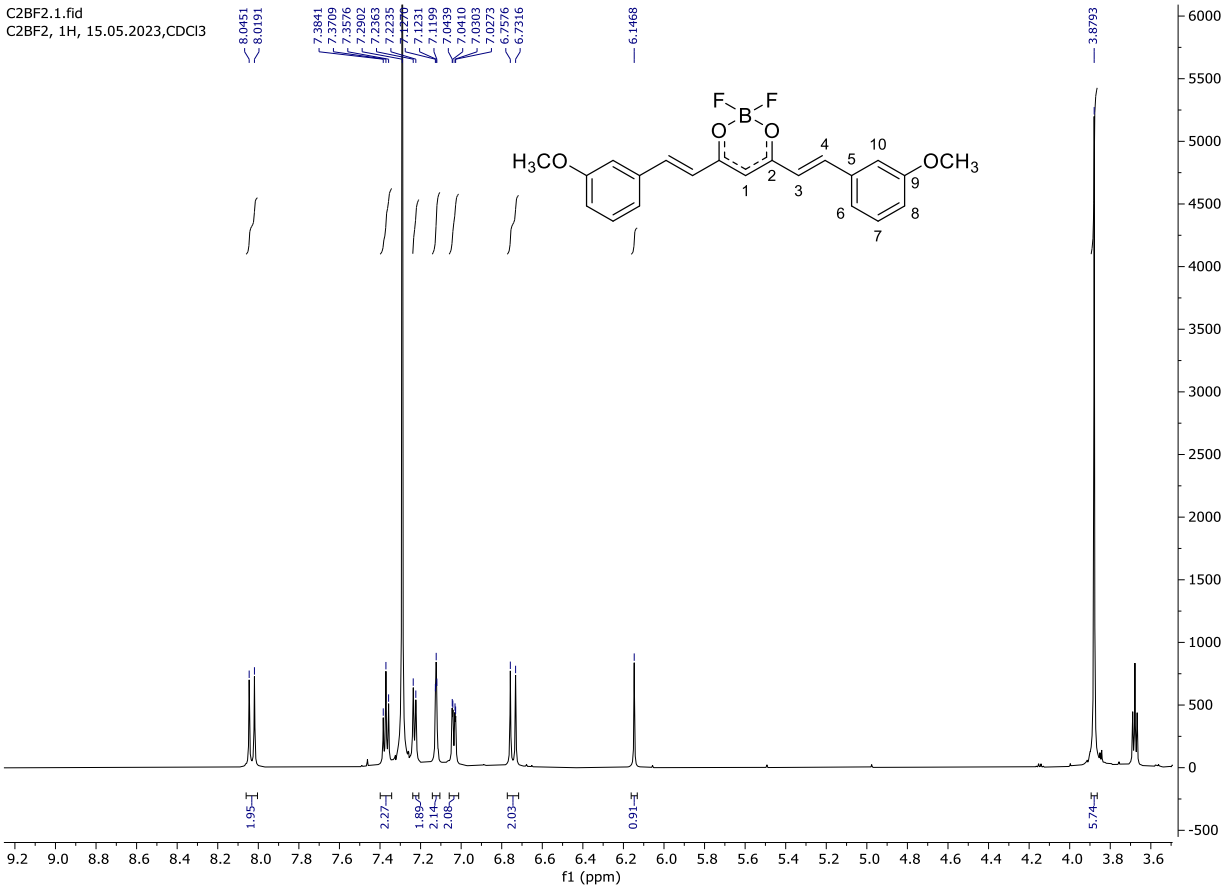


Figure 2.7: ^{1}H NMR spectrum of **3** in $CDCl_3$ at 400 MHz

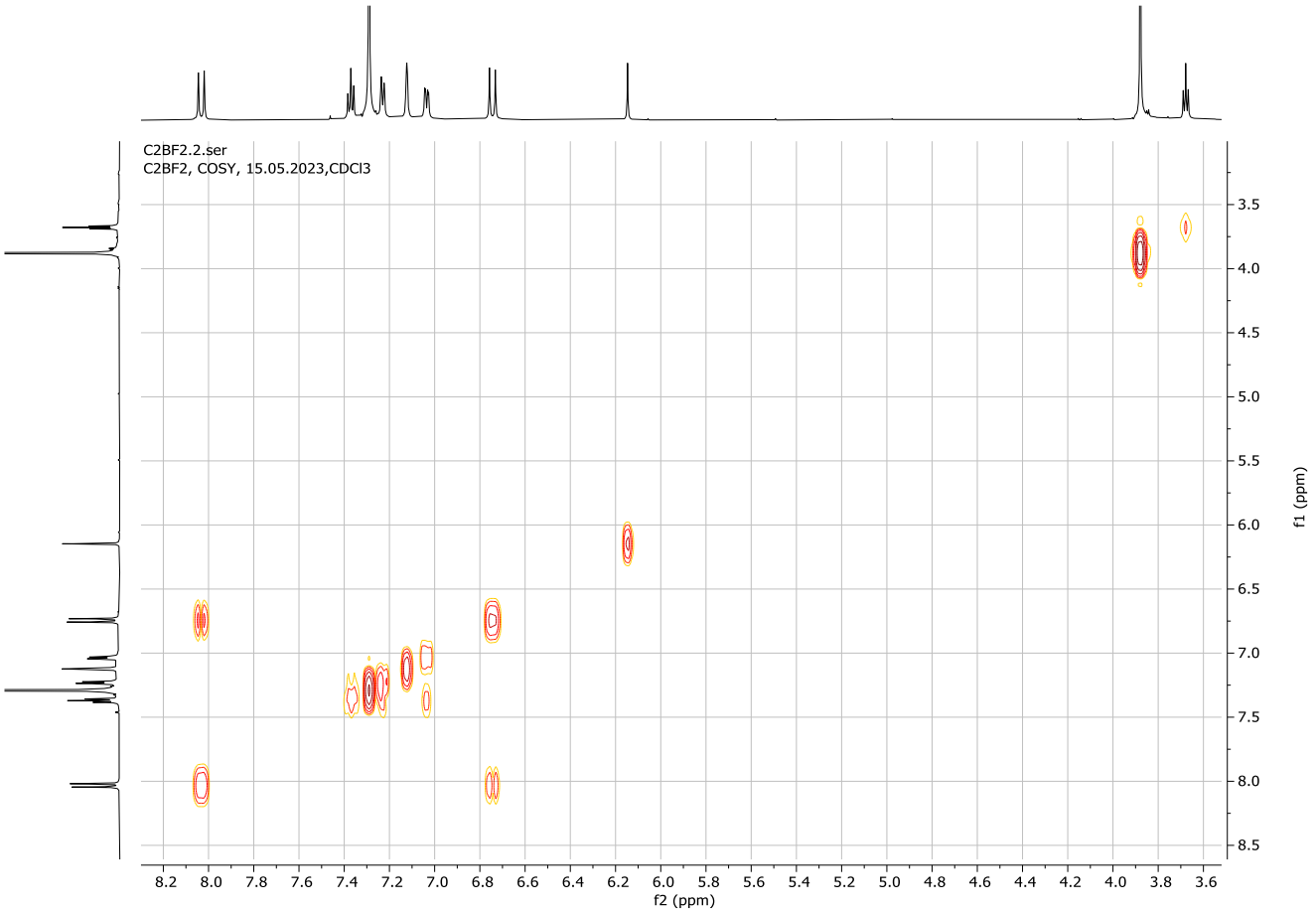


Figure 2.8: ^{1}H-^{1}H COSY NMR spectrum of **3** in $CDCl_3$ at 400 MHz

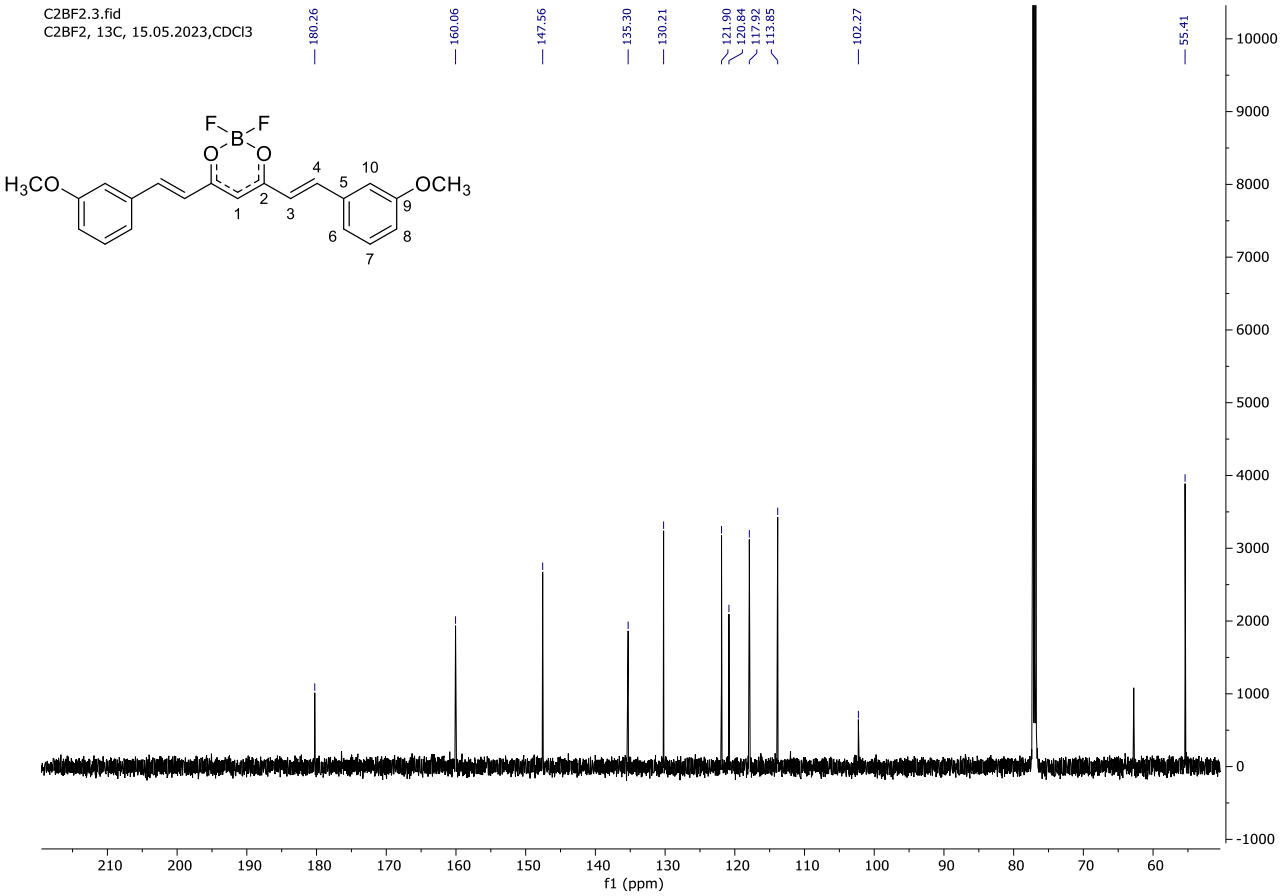


Figure 2.9: ^{13}C NMR spectrum of **3** in $CDCl_3$ at 101 MHz

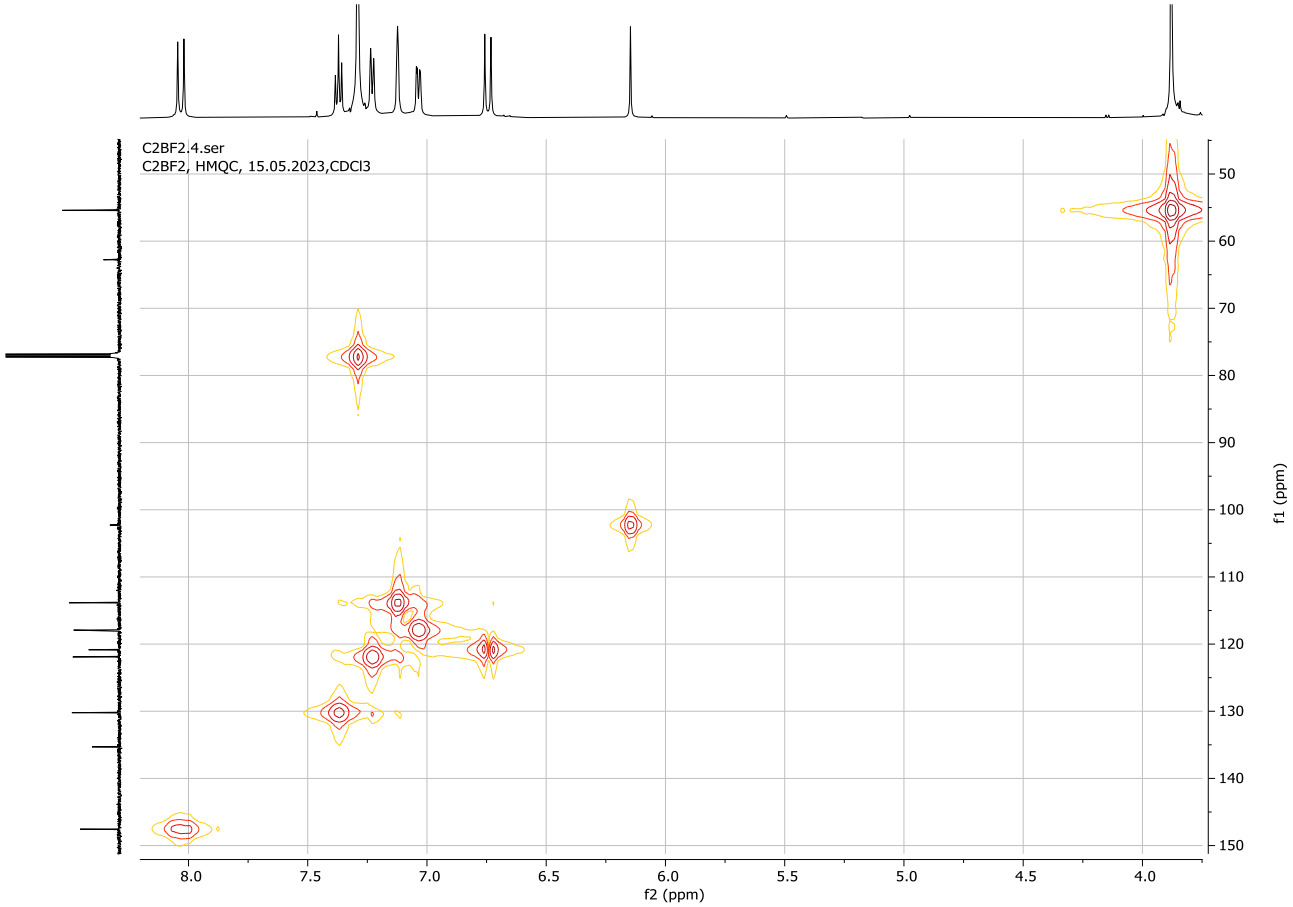


Figure 2.10: ^{1}H-^{13}C HMQC NMR spectrum of **3** in $CDCl_3$

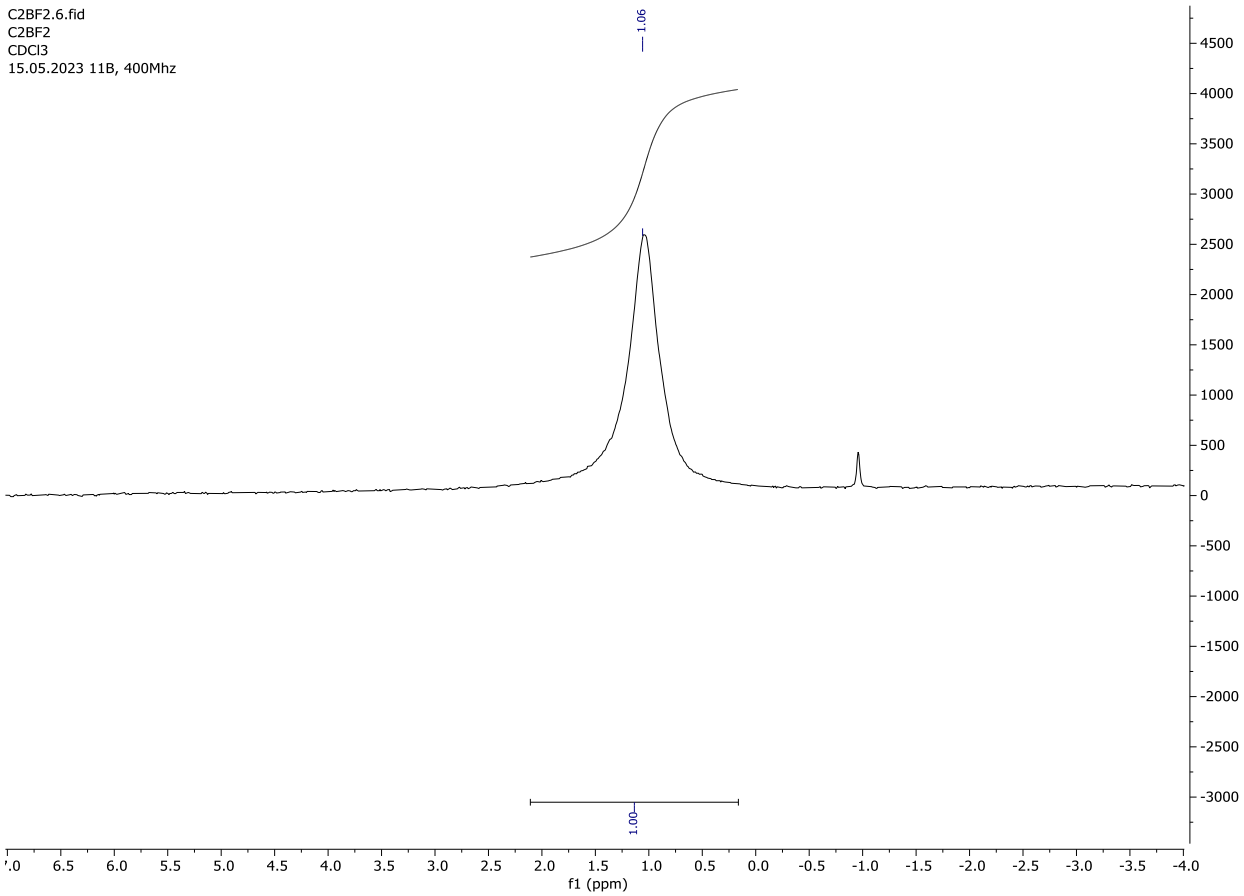


Figure 2.11: ^{11}B NMR spectrum of **3** in $CDCl_3$ at 127 MHz

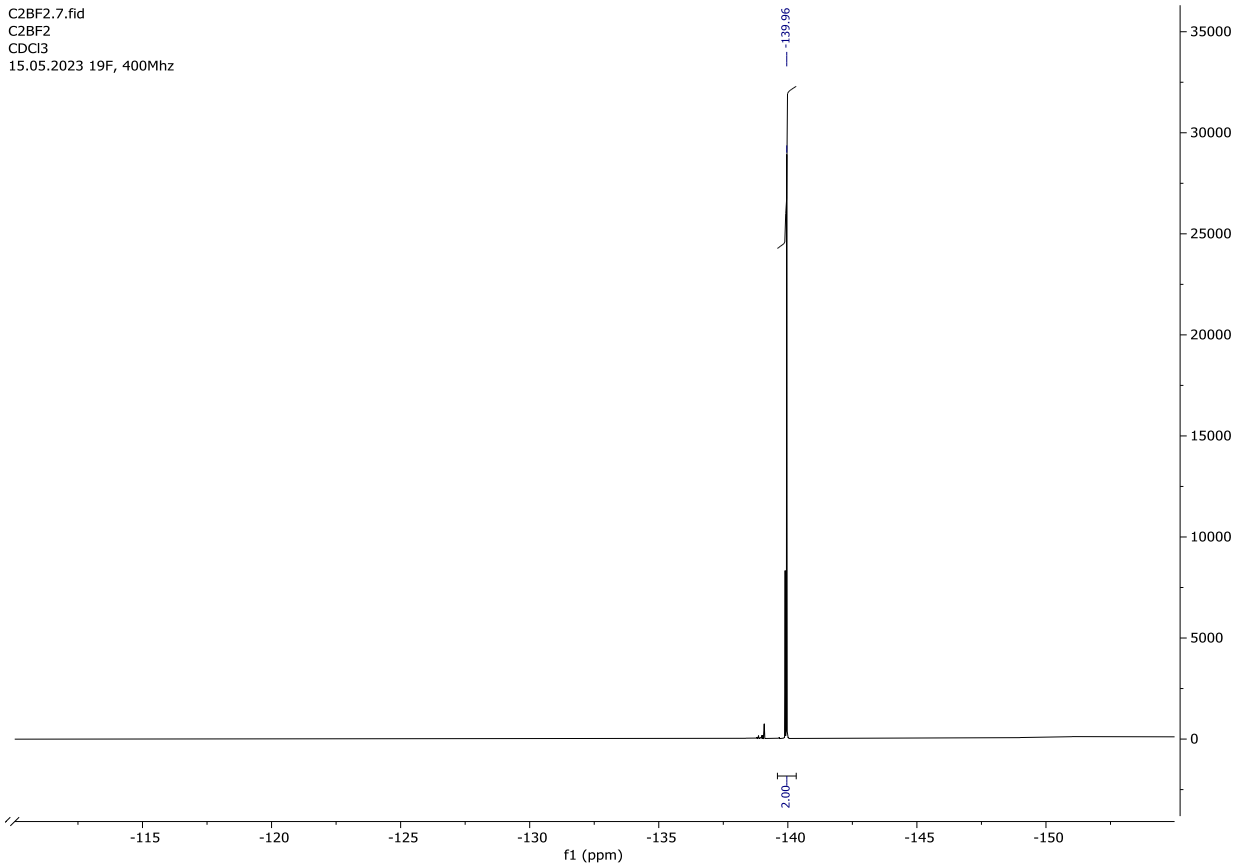


Figure 2.12: ^{19}F NMR spectrum of **3** in $CDCl_3$ at 376 MHz

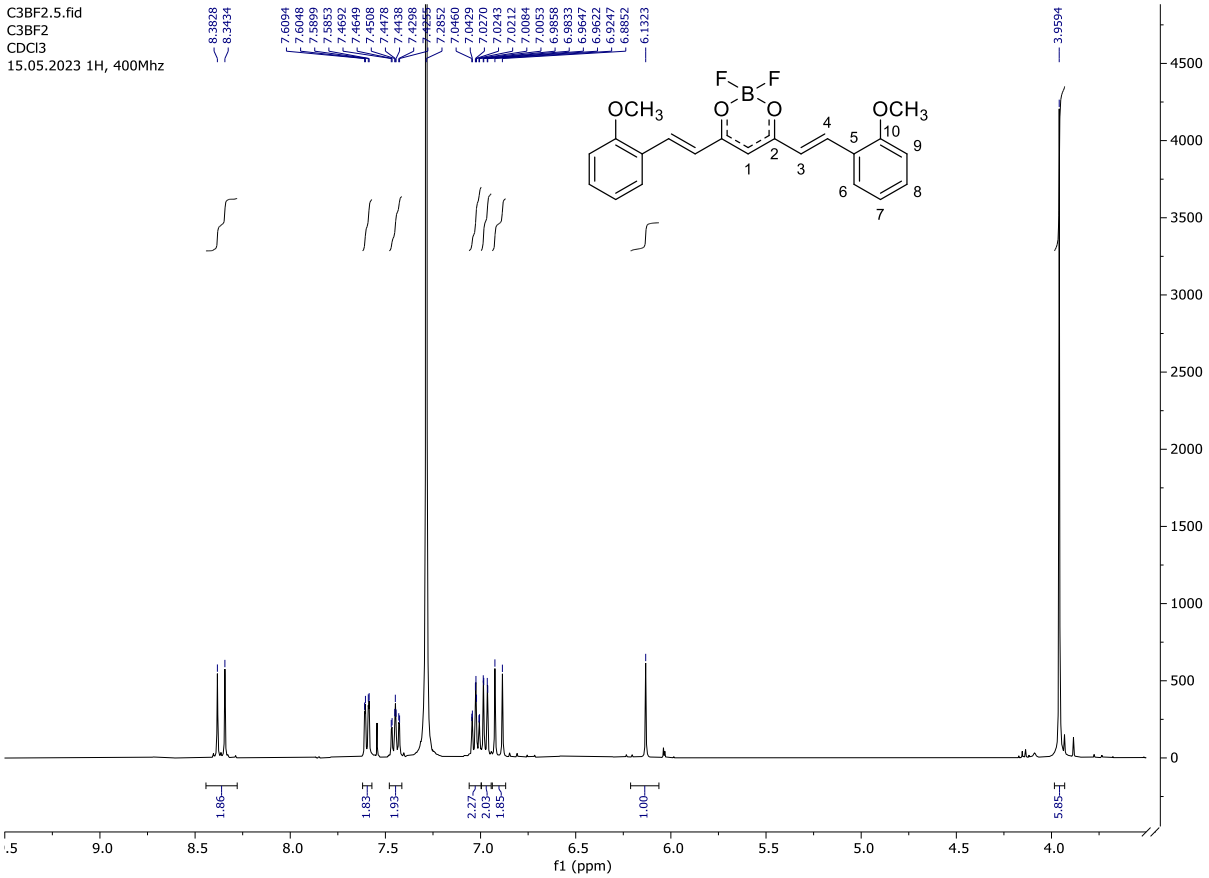


Figure 2.13: ^{1}H NMR spectrum of **4** in $CDCl_3$ at 400 MHz

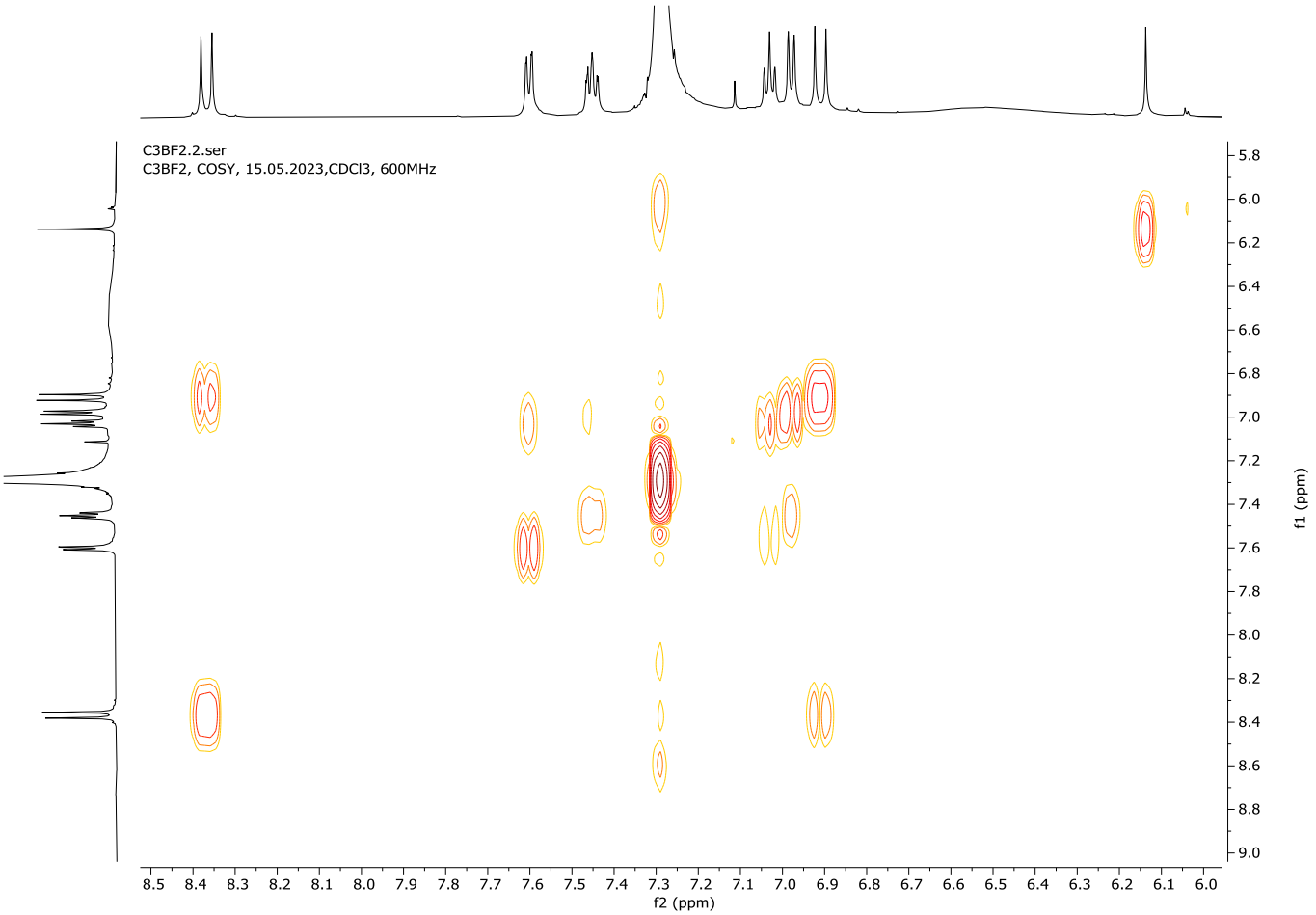


Figure 2.14: ^{1}H-^{1}H COSY NMR spectrum of **4** in $CDCl_3$ at 400 MHz

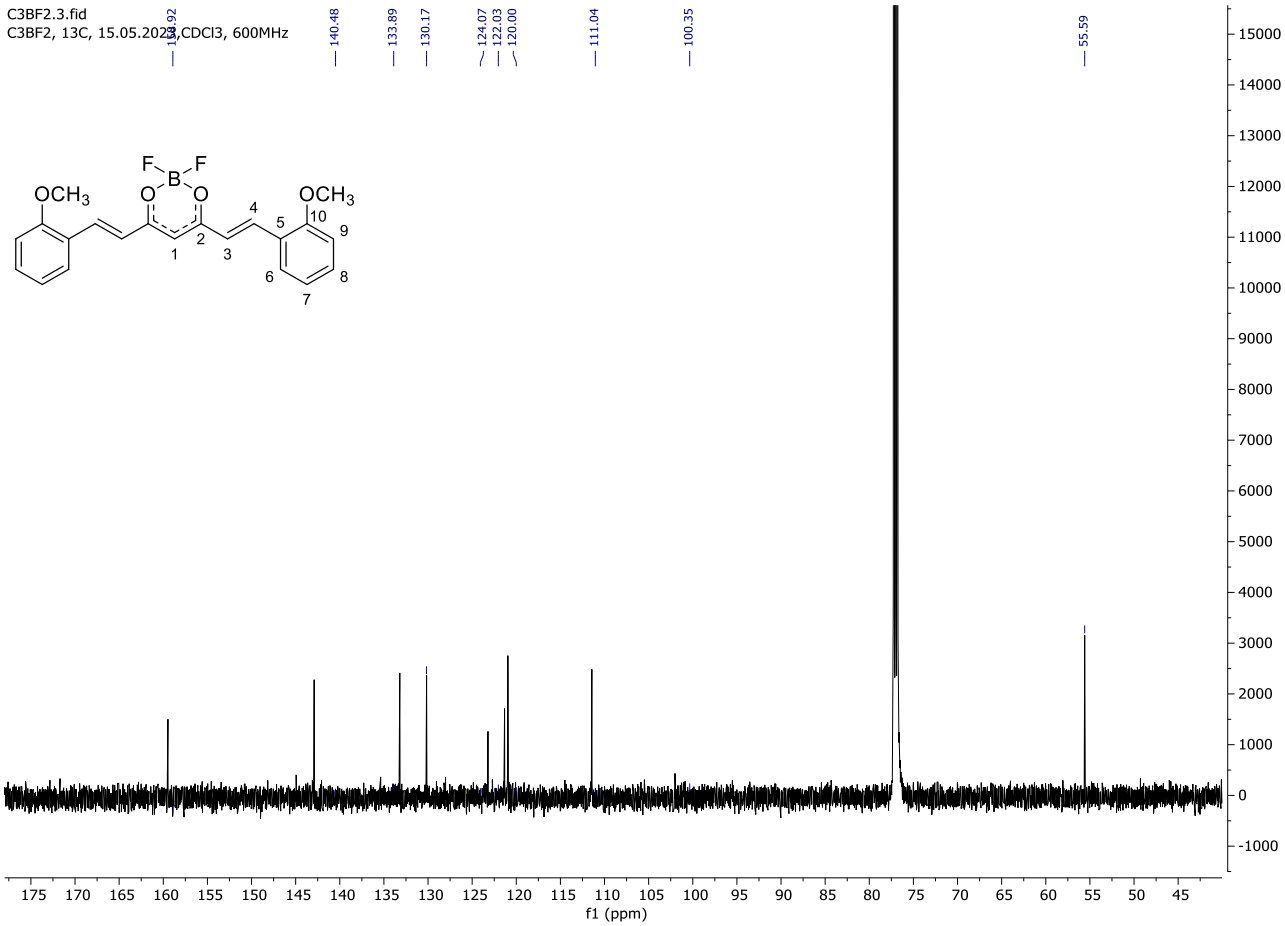


Figure 2.15: ^{13}C NMR spectrum of **4** in $CDCl_3$ at 101 MHz

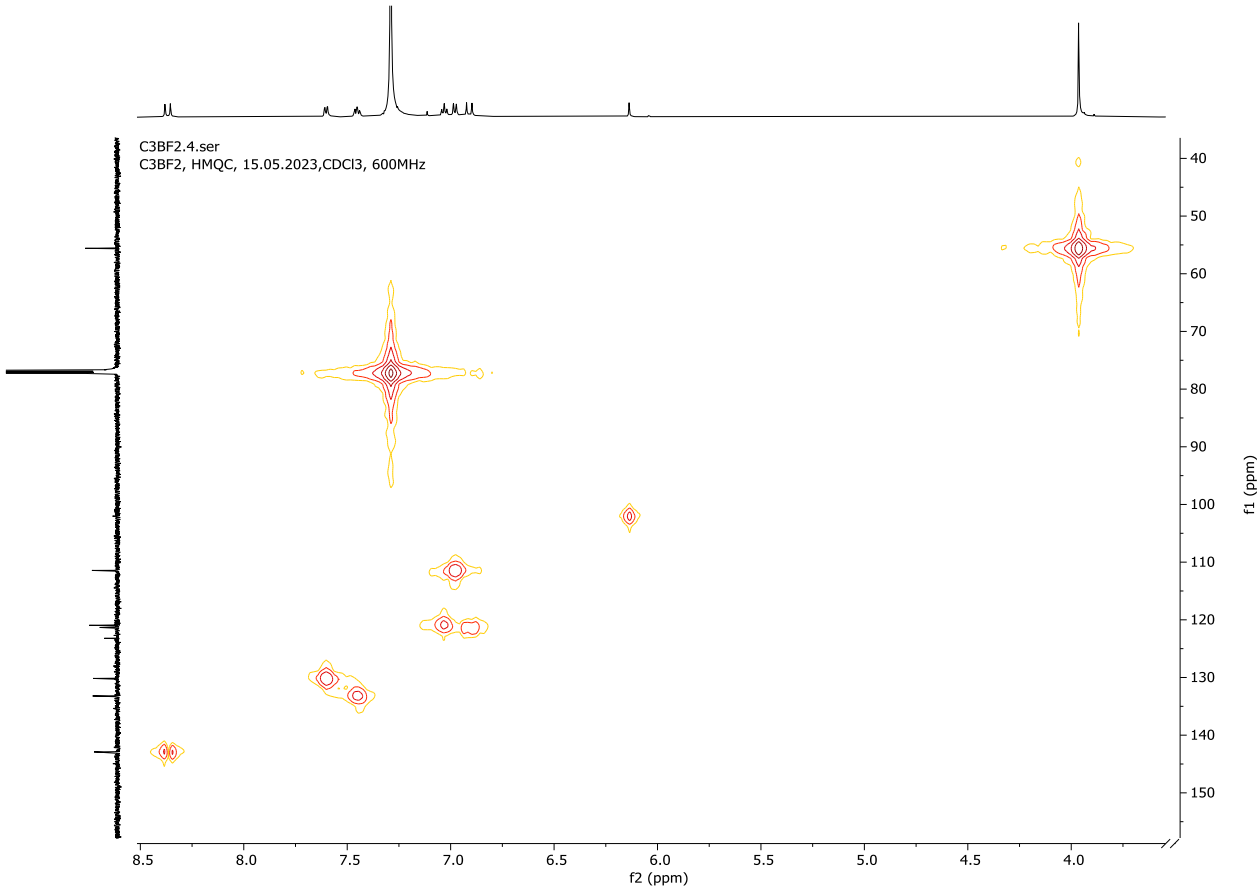


Figure 2.16: ^{1}H-^{13}C HMQC NMR spectrum of **4** in $CDCl_3$

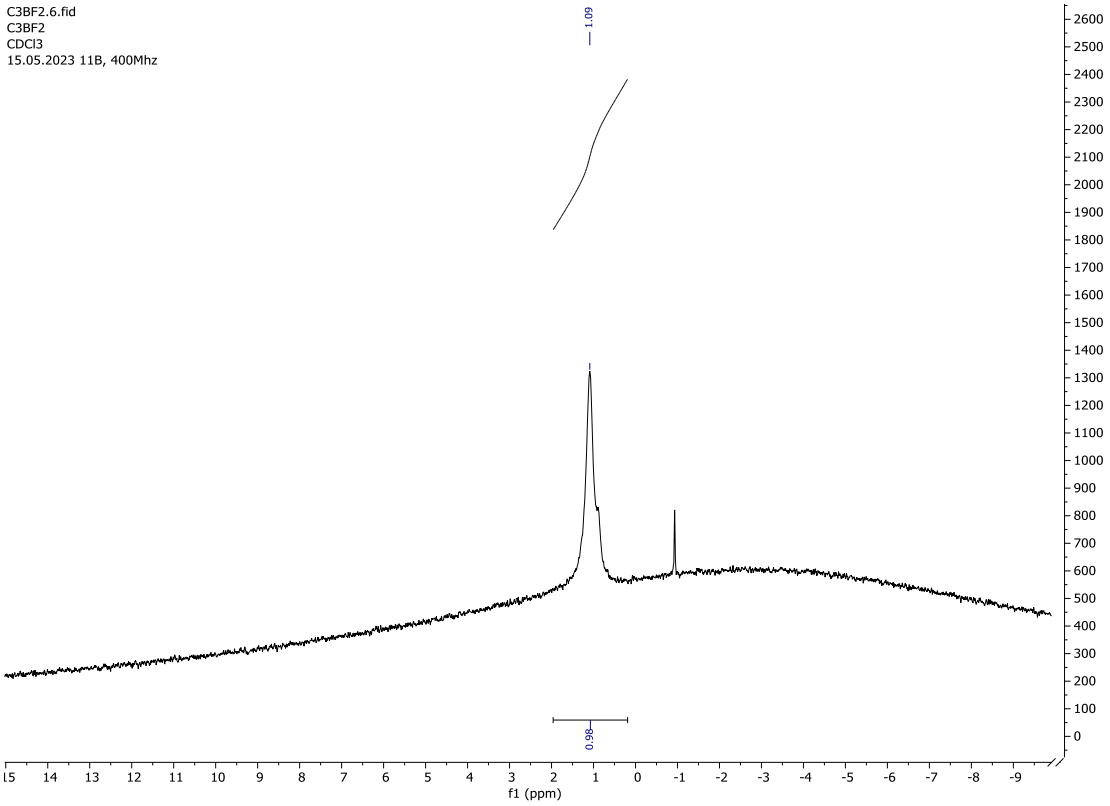


Figure 2.17: ^{11}B NMR spectrum of **4** in $CDCl_3$ at 127 MHz

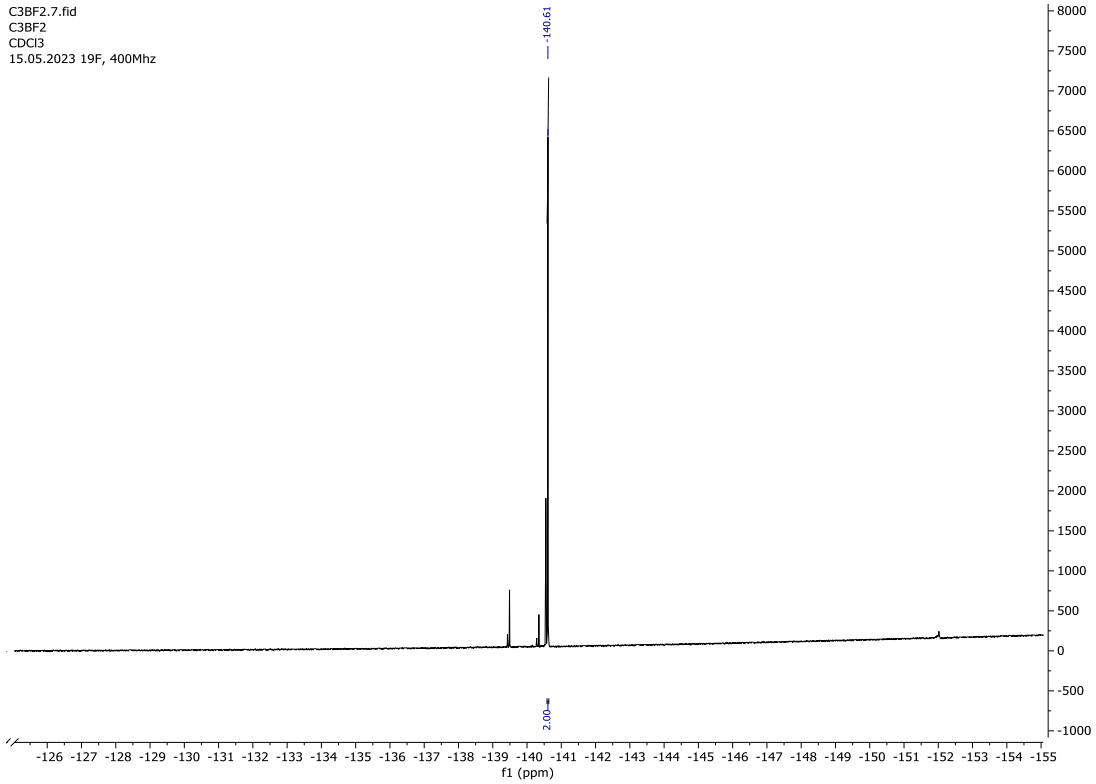


Figure 2.18: ^{19}F NMR spectrum of **4** in $CDCl_3$ at 376 MHz

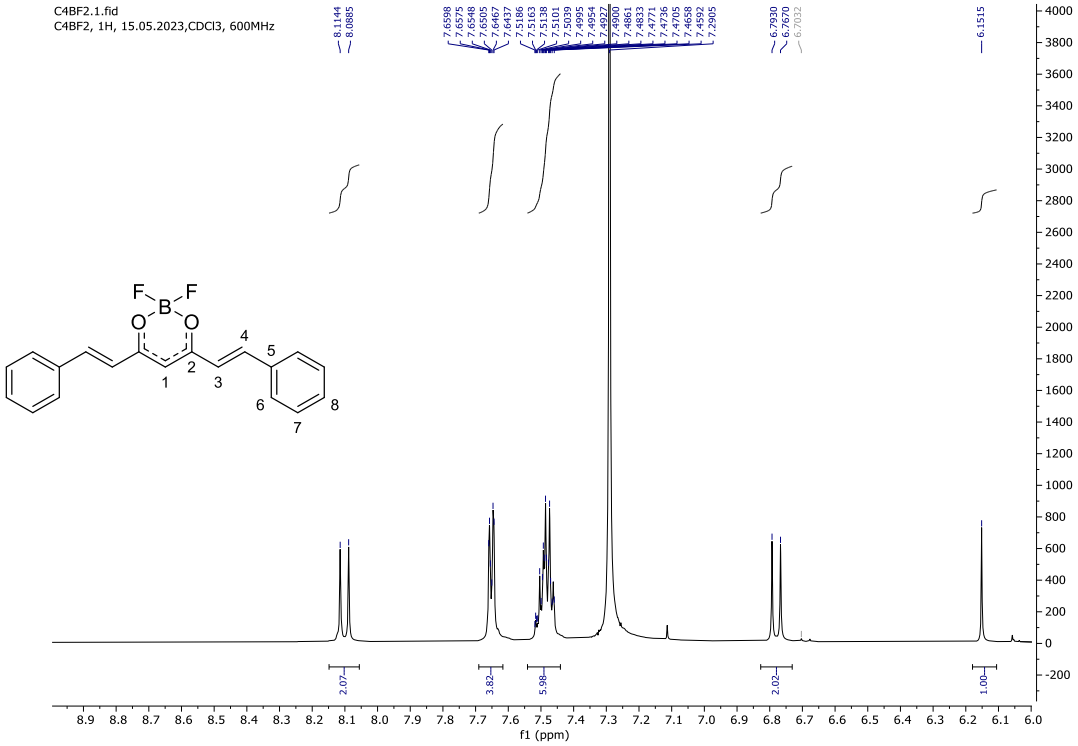


Figure 2.19: ^{1}H NMR spectrum of **5** in $CDCl_3$ at 600 MHz

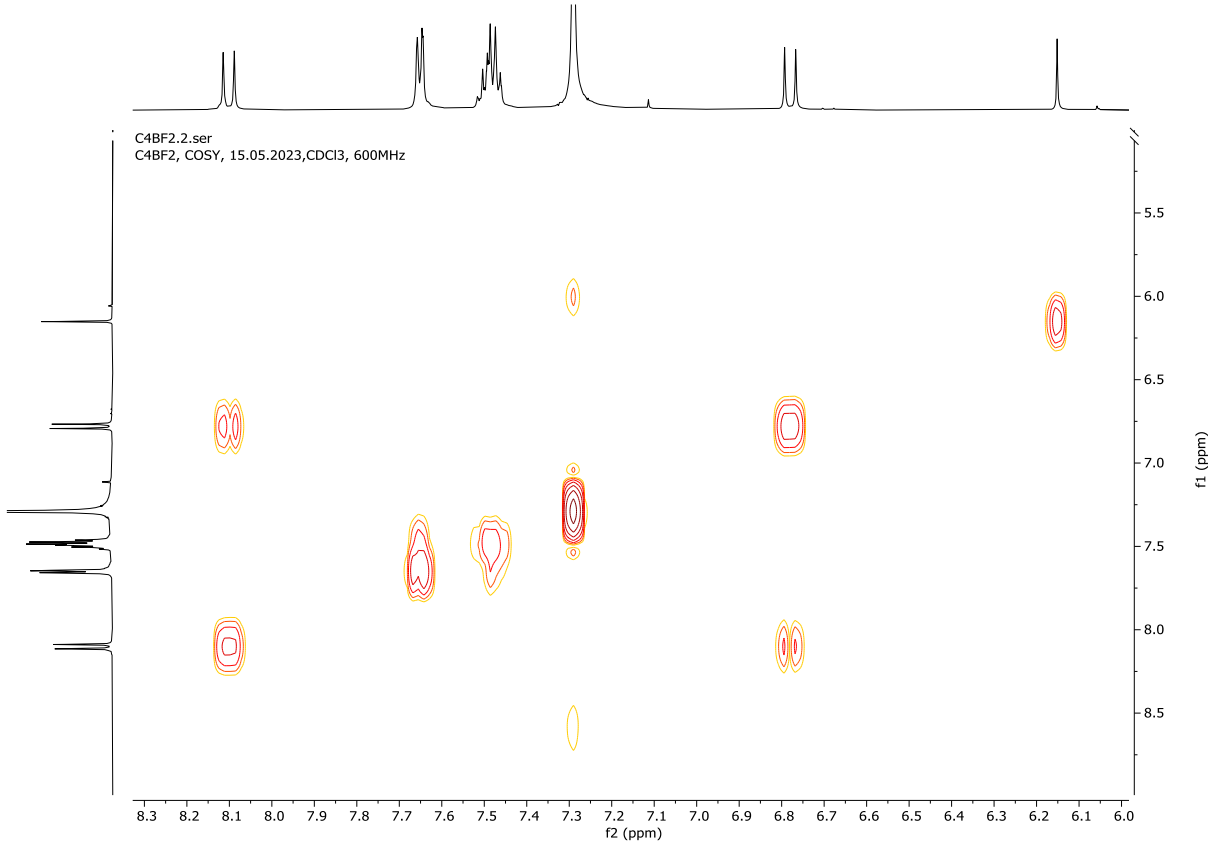


Figure 2.20: ^{1}H-^{1}H COSY NMR spectrum of **5** in $CDCl_3$ at 600 MHz

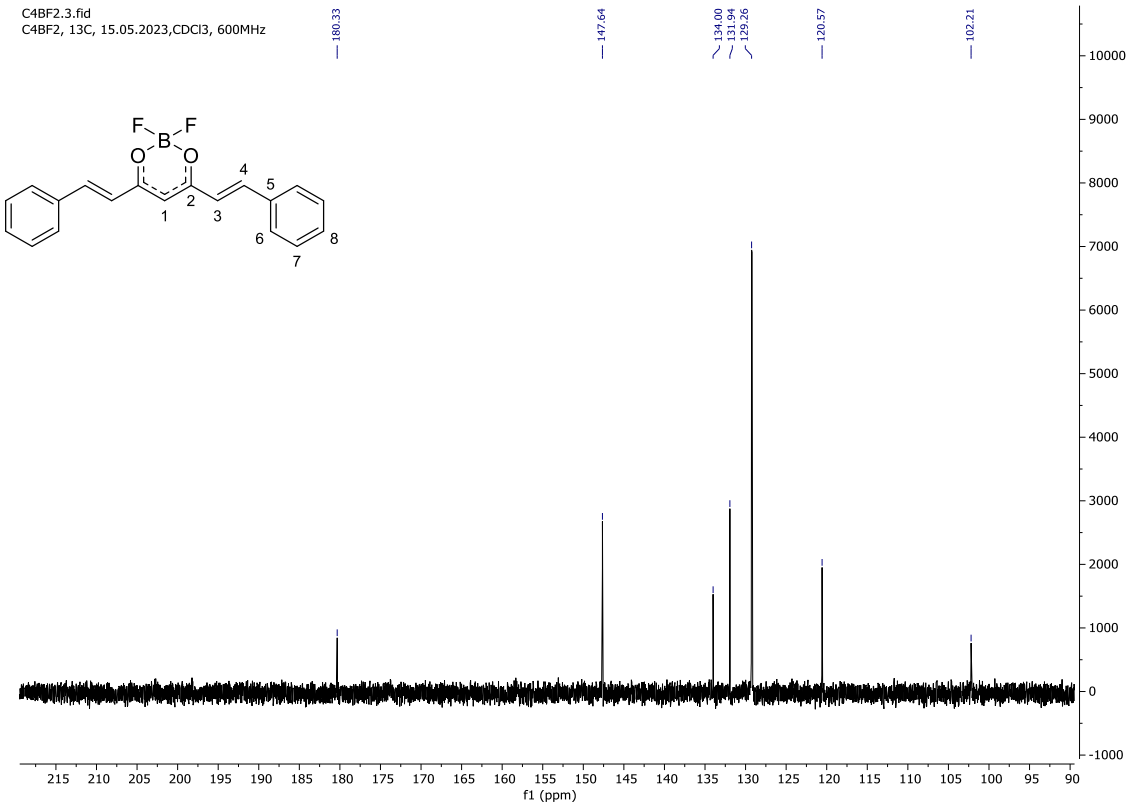


Figure 2.21: ^{13}C NMR spectrum of **5** in $CDCl_3$ at 125 MHz

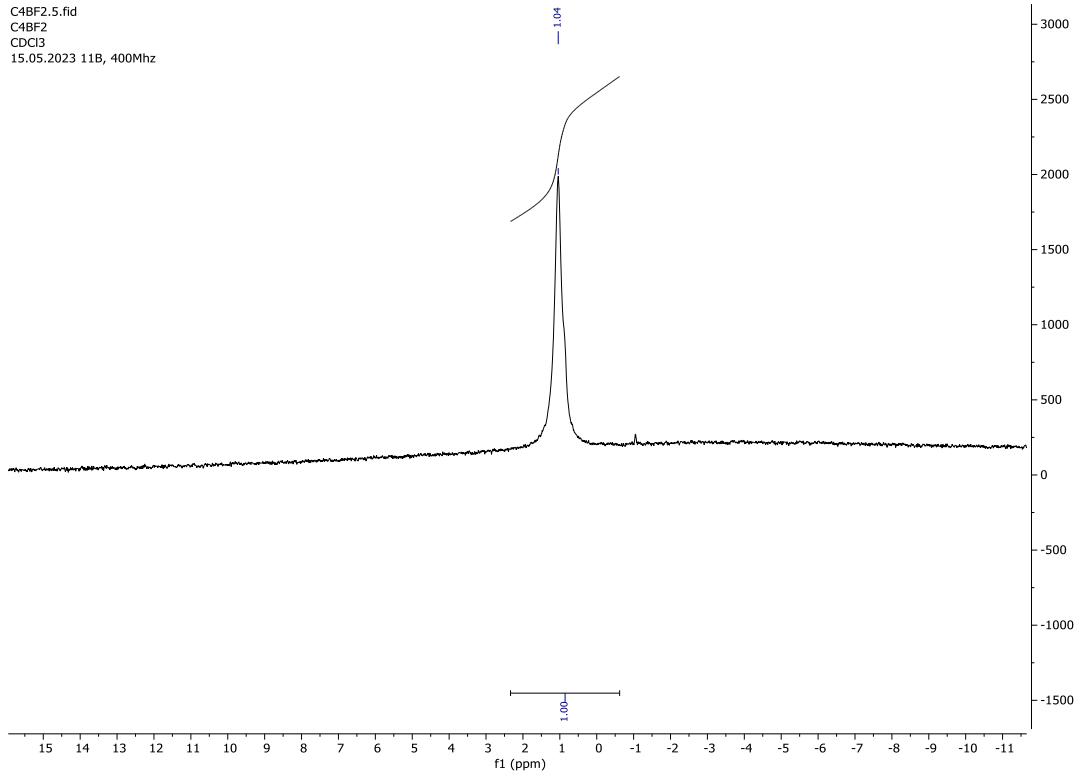


Figure 2.22: ^{11}B NMR spectrum of **5** in $CDCl_3$ at 127 MHz

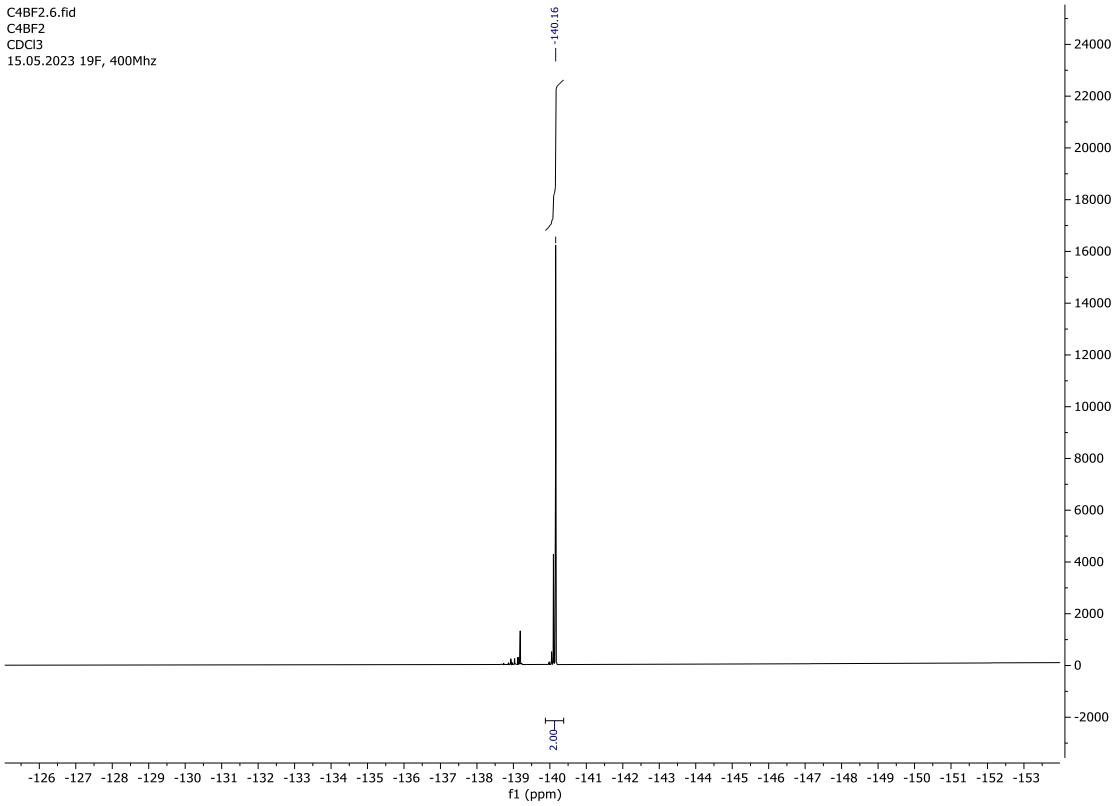


Figure 2.23: ^{19}F NMR spectrum of **5** in $CDCl_3$ at 376 MHz

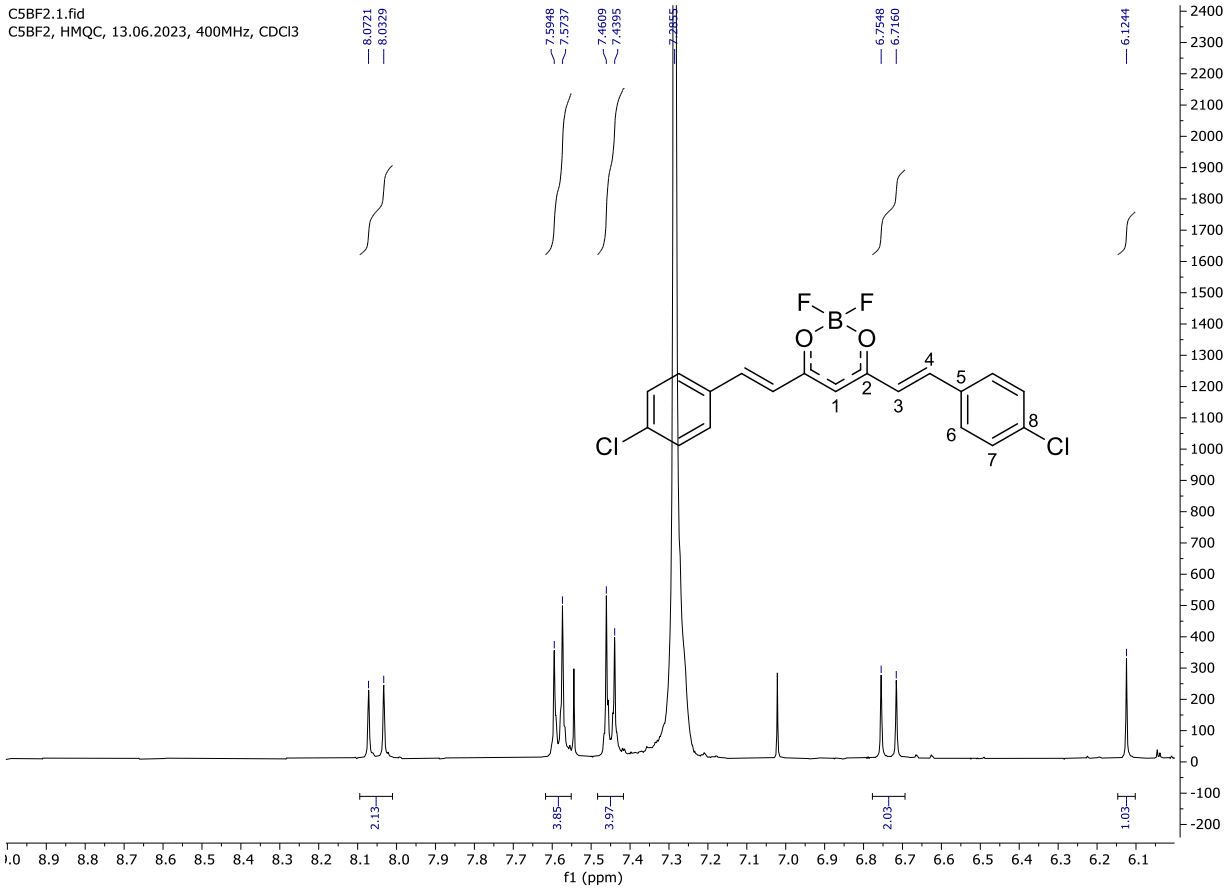


Figure 2.24: ^{1}H NMR spectrum of **6** in $CDCl_3$ at 400 MHz

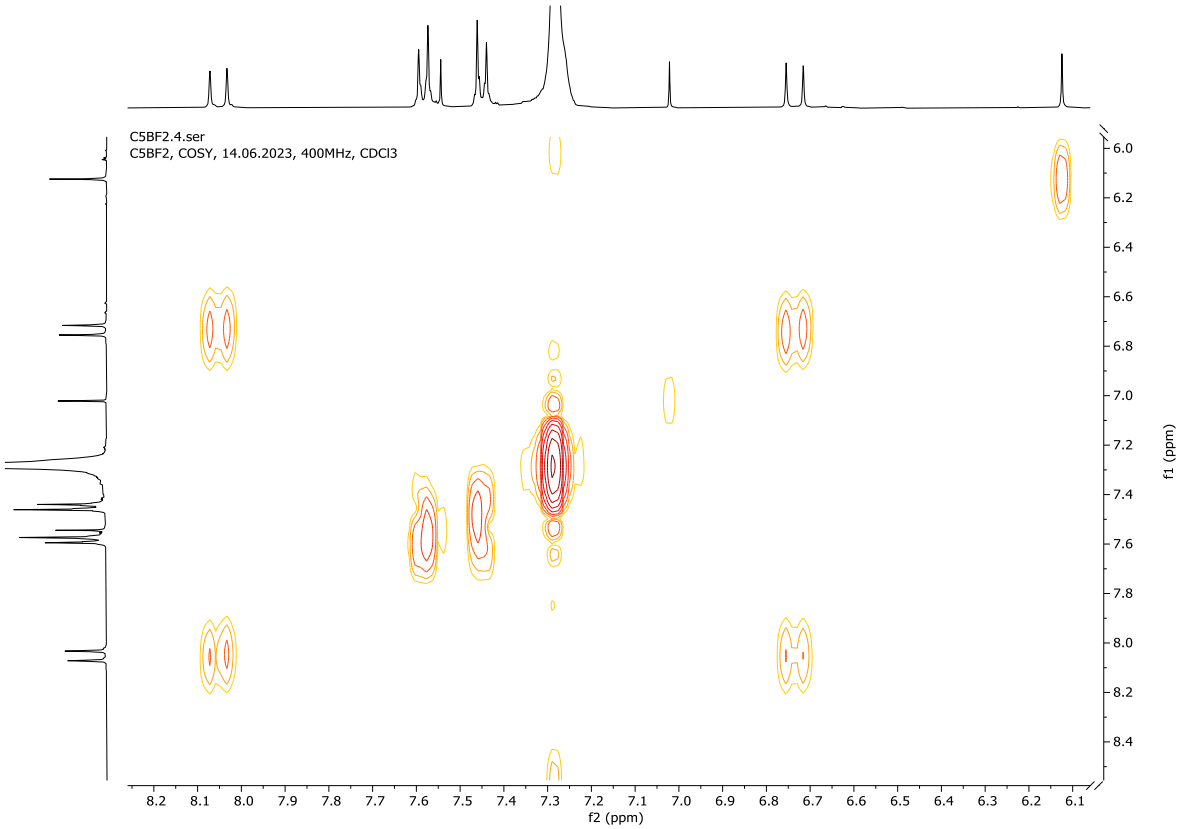


Figure 2.25: ^{1}H-^{1}H COSY NMR spectrum of **6** in $CDCl_3$ at 400 MHz

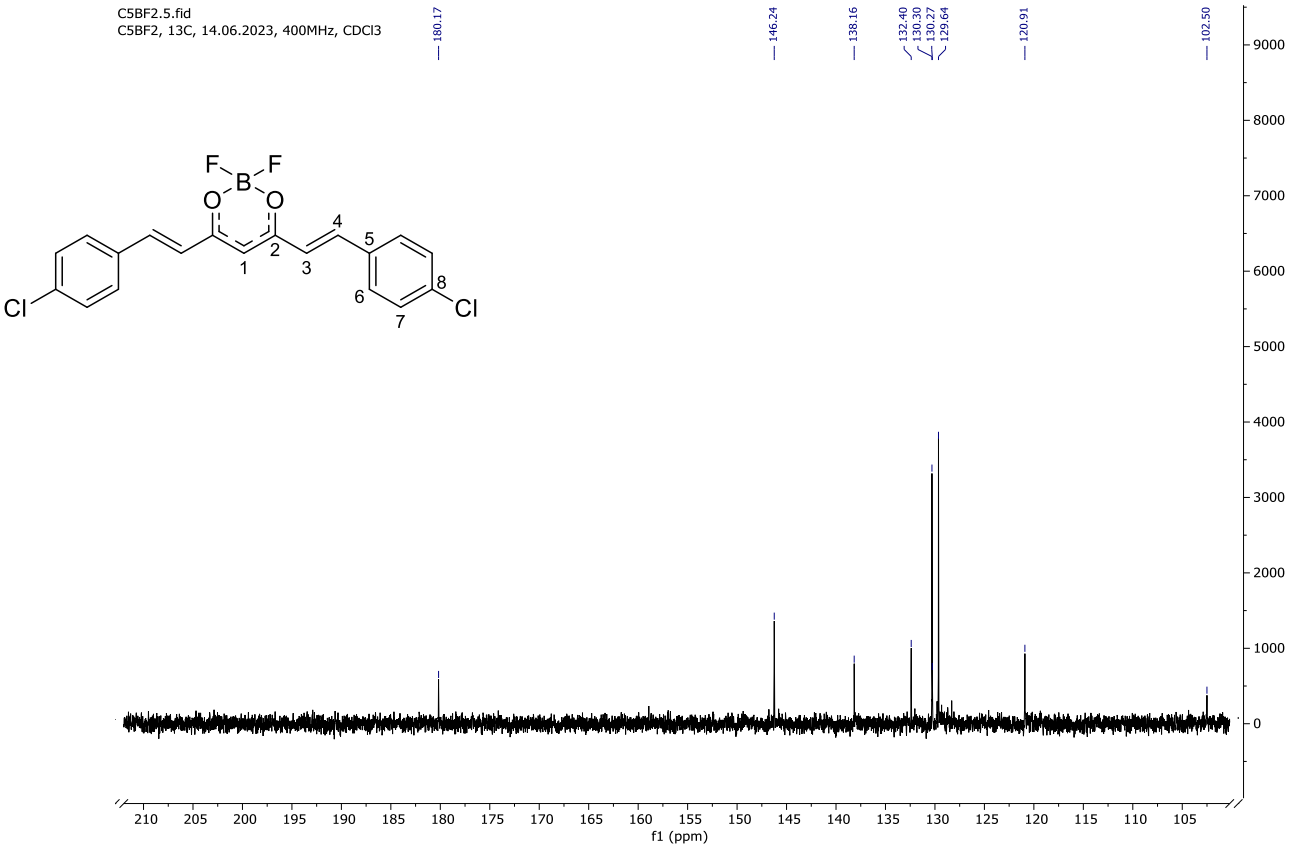


Figure 2.26: ^{13}C NMR spectrum of **6** in $CDCl_3$ at 101 MHz

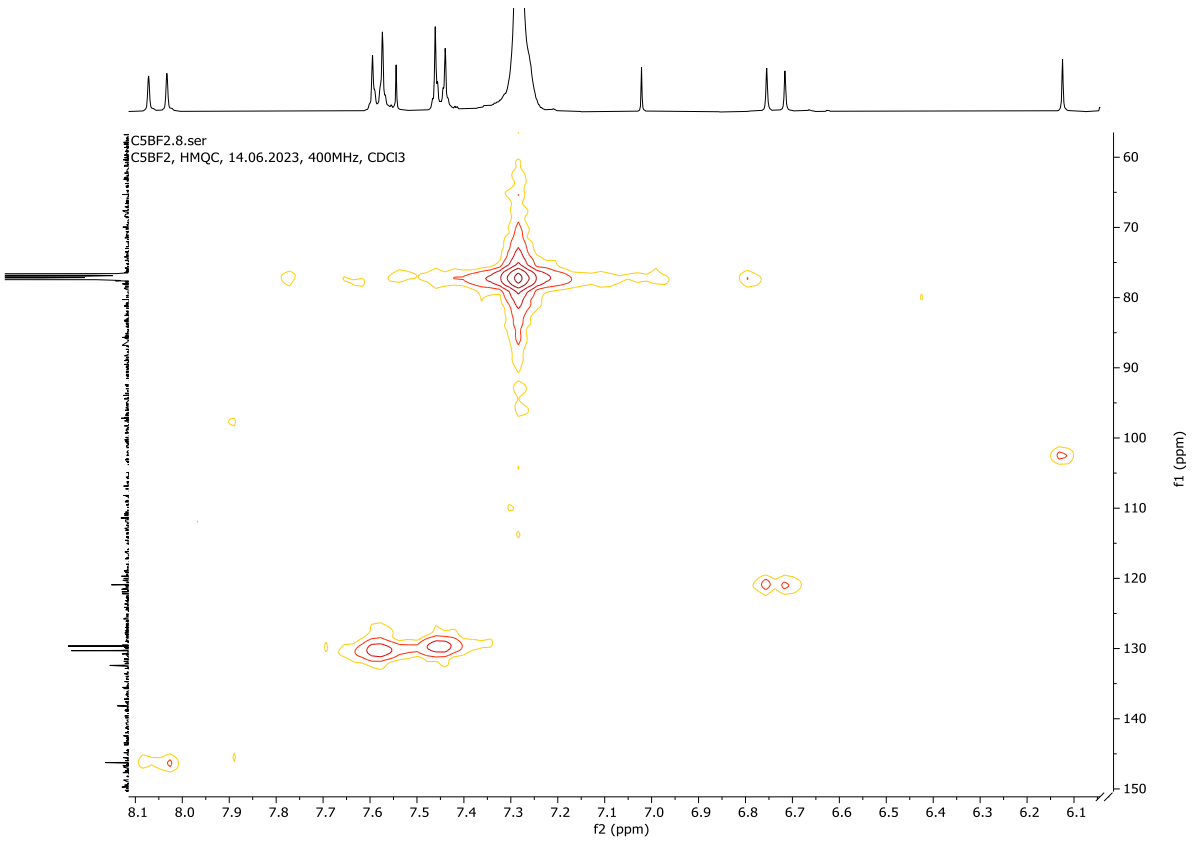


Figure 2.27: ^{1}H-^{13}C HMQC NMR spectrum of **6** in $CDCl_3$

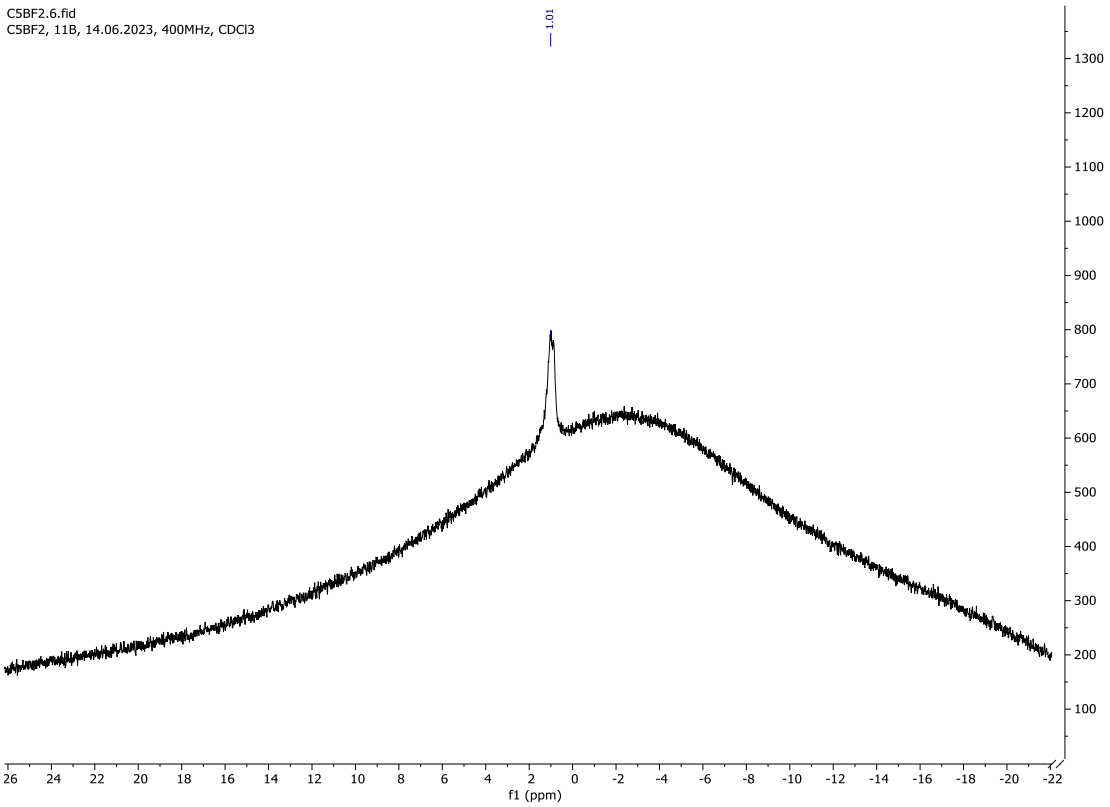


Figure 2.28: ^{11}B NMR spectrum of **6** in $CDCl_3$ at 127 MHz

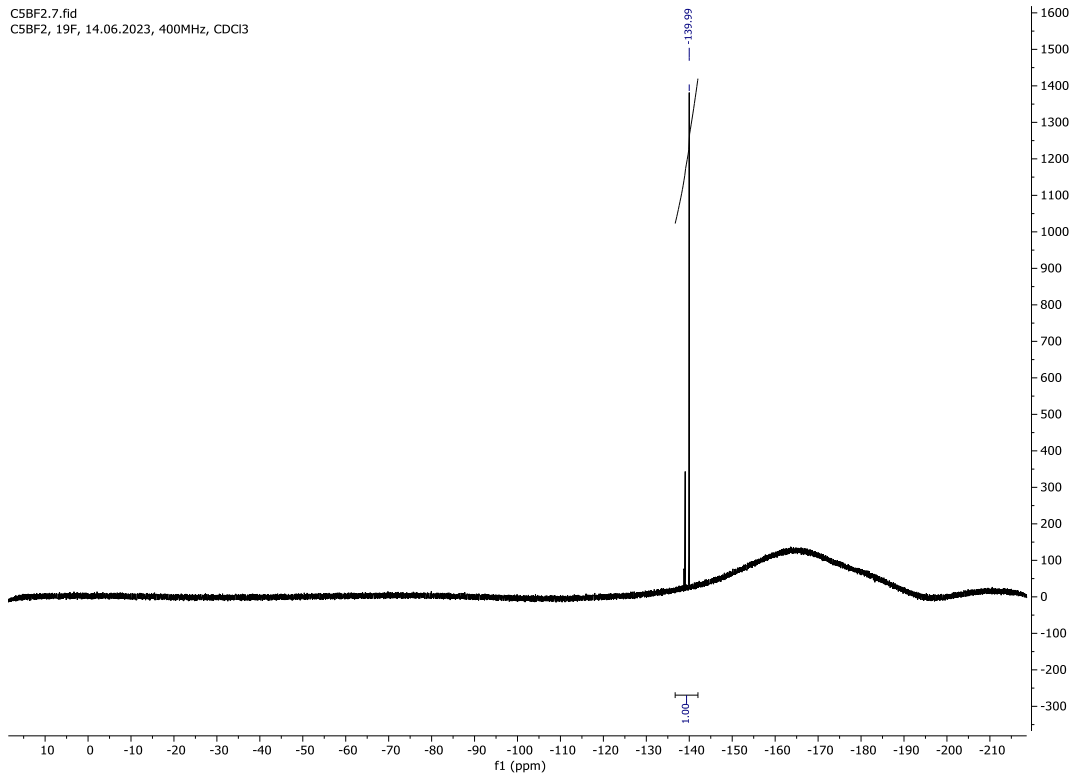


Figure 2.29: ^{19}F NMR spectrum of **6** in $CDCl_3$ at 376 MHz

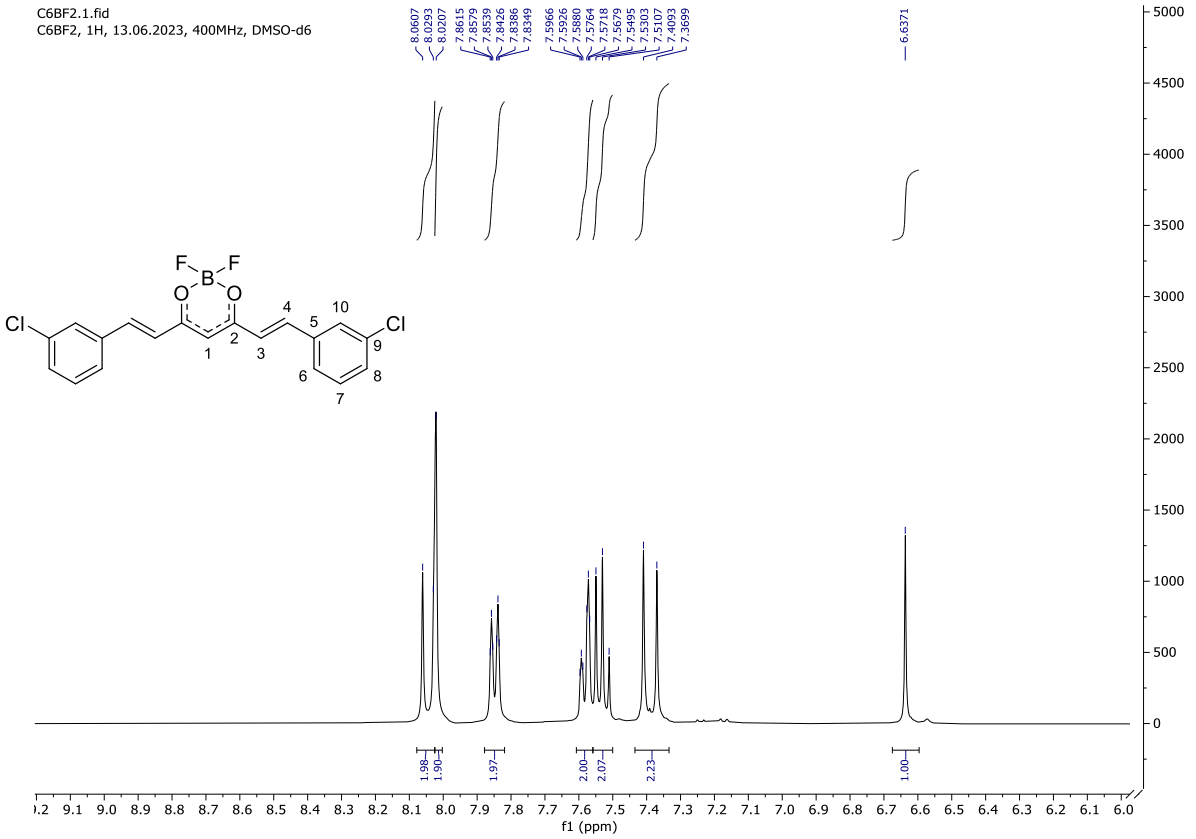


Figure 2.30: ^{1}H NMR spectrum of **7** in DMSO-*d6* at 400 MHz

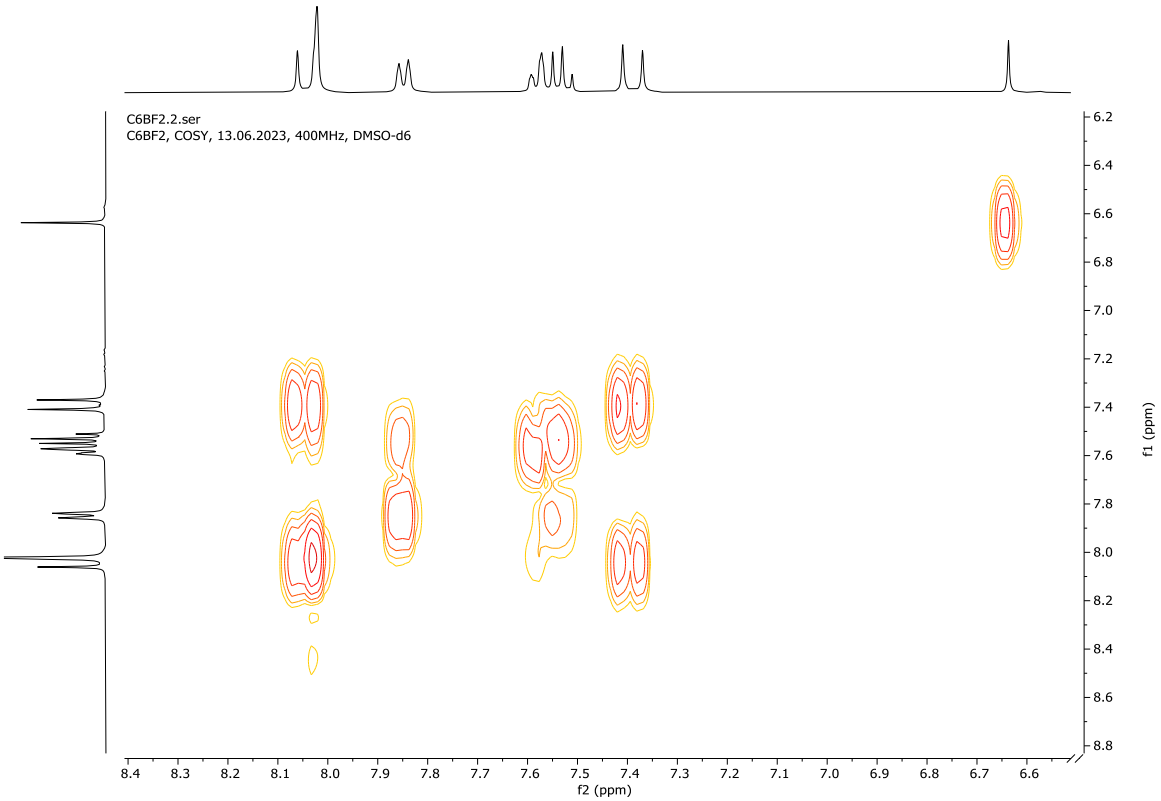


Figure 2.31: ^{1}H-^{1}H COSY NMR spectrum of **7** in DMSO-*d6* at 400 MHz

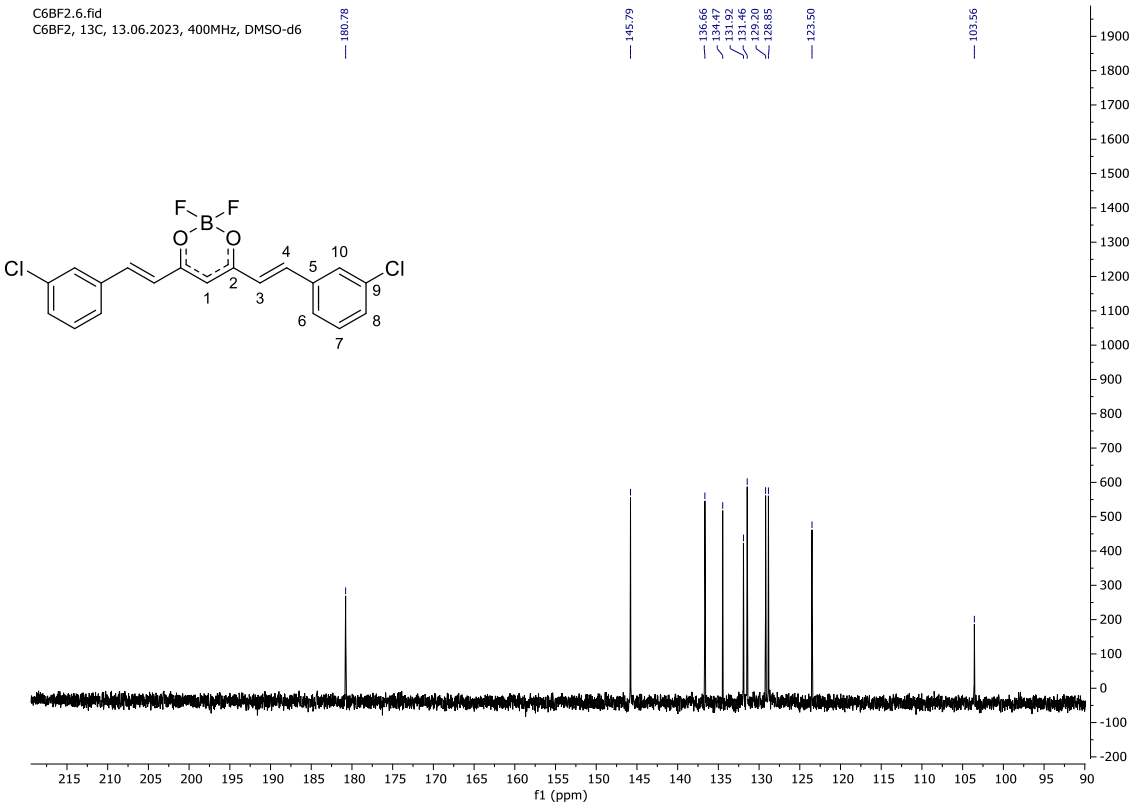


Figure 2.32: ^{13}C NMR spectrum of **7** in DMSO-*d6* at 101 MHz

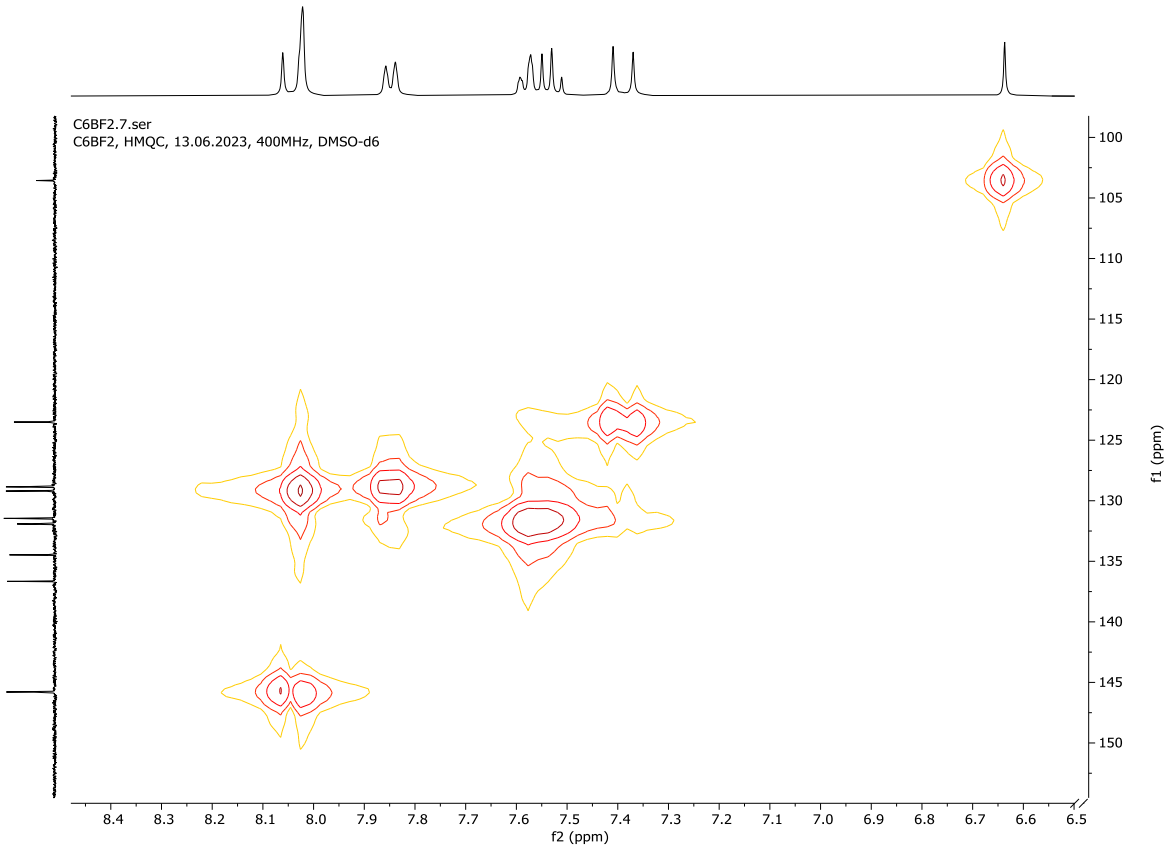


Figure 2.33: ^{1}H-^{13}C HMQC NMR spectrum of **7** in DMSO-*d6*

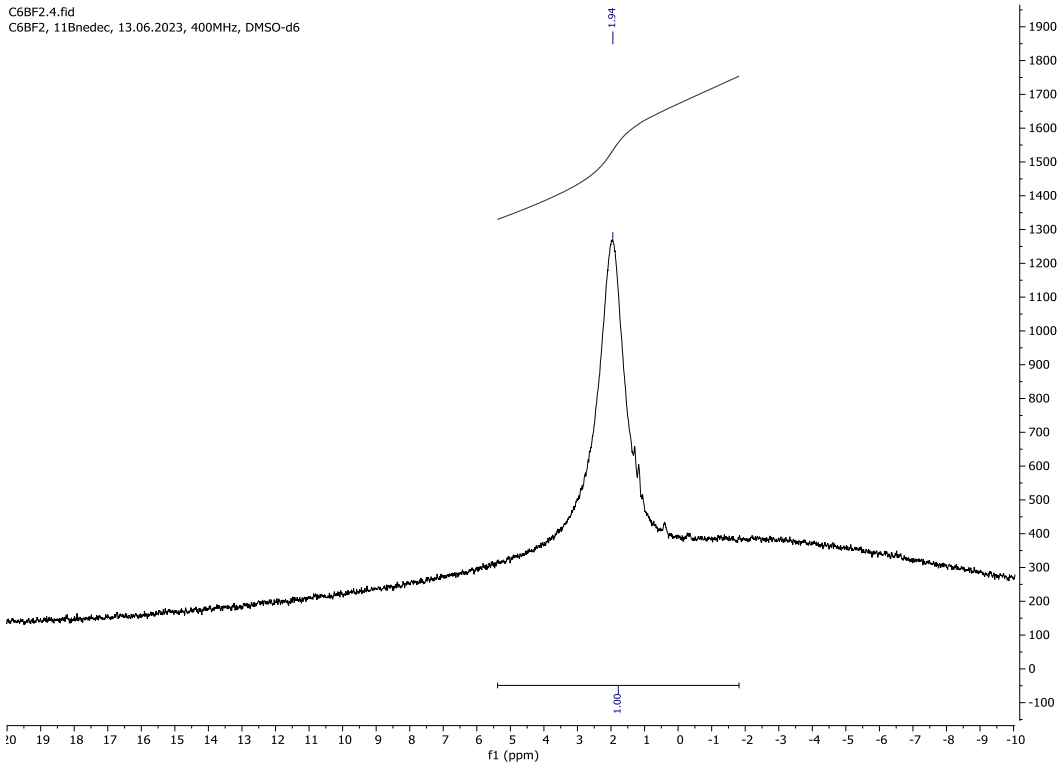


Figure 2.34: ^{11}B NMR spectrum of **7** in DMSO-*d6* at 127 MHz

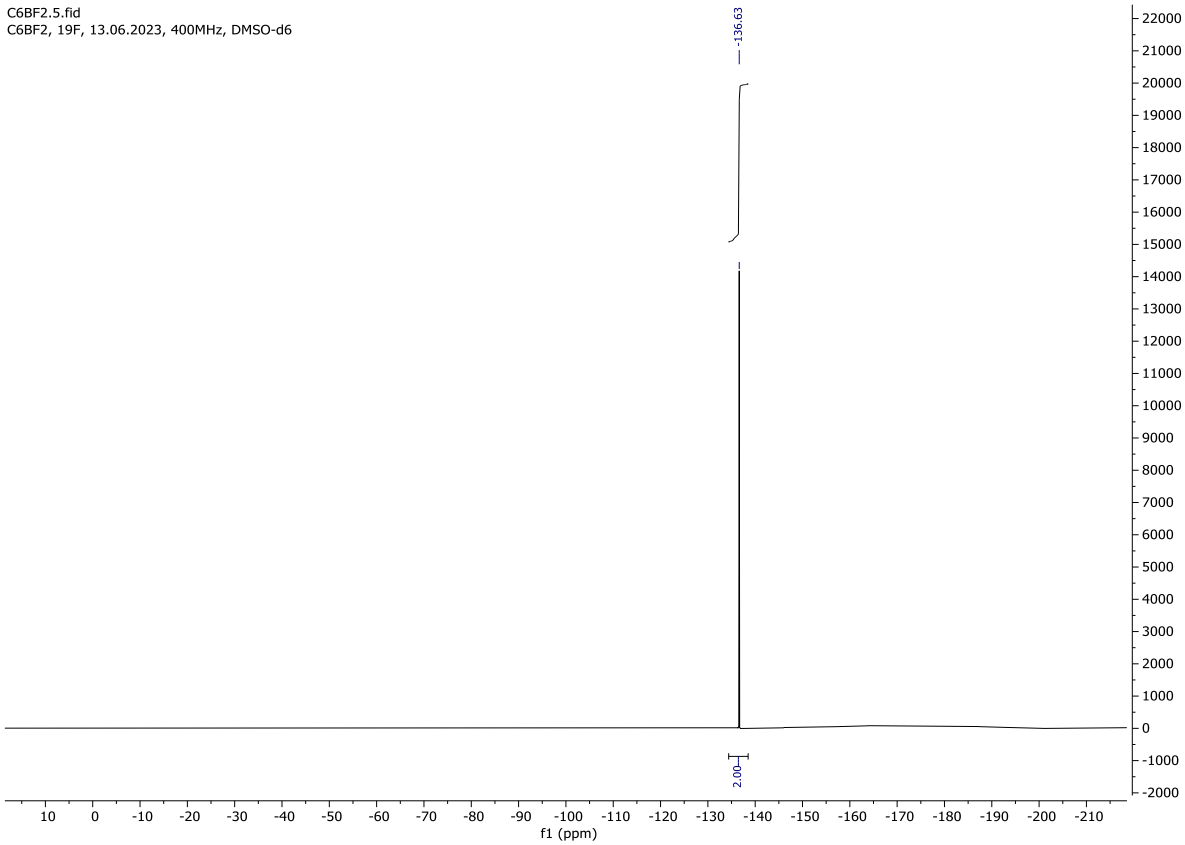


Figure 2.35: ^{19}F NMR spectrum of **7** in DMSO-*d6* at 376 MHz

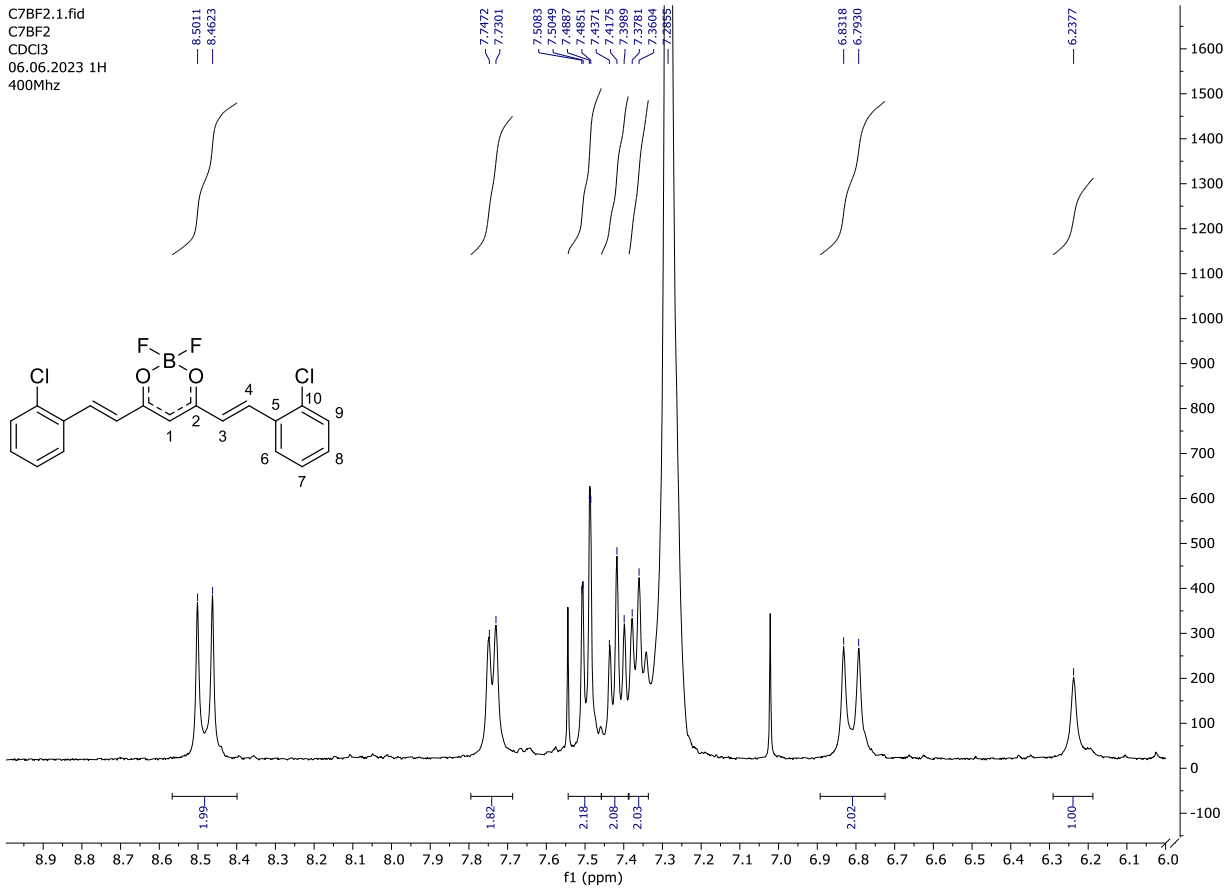


Figure 2.36: ^{1}H NMR spectrum of **8** in $CDCl_3$ at 400 MHz

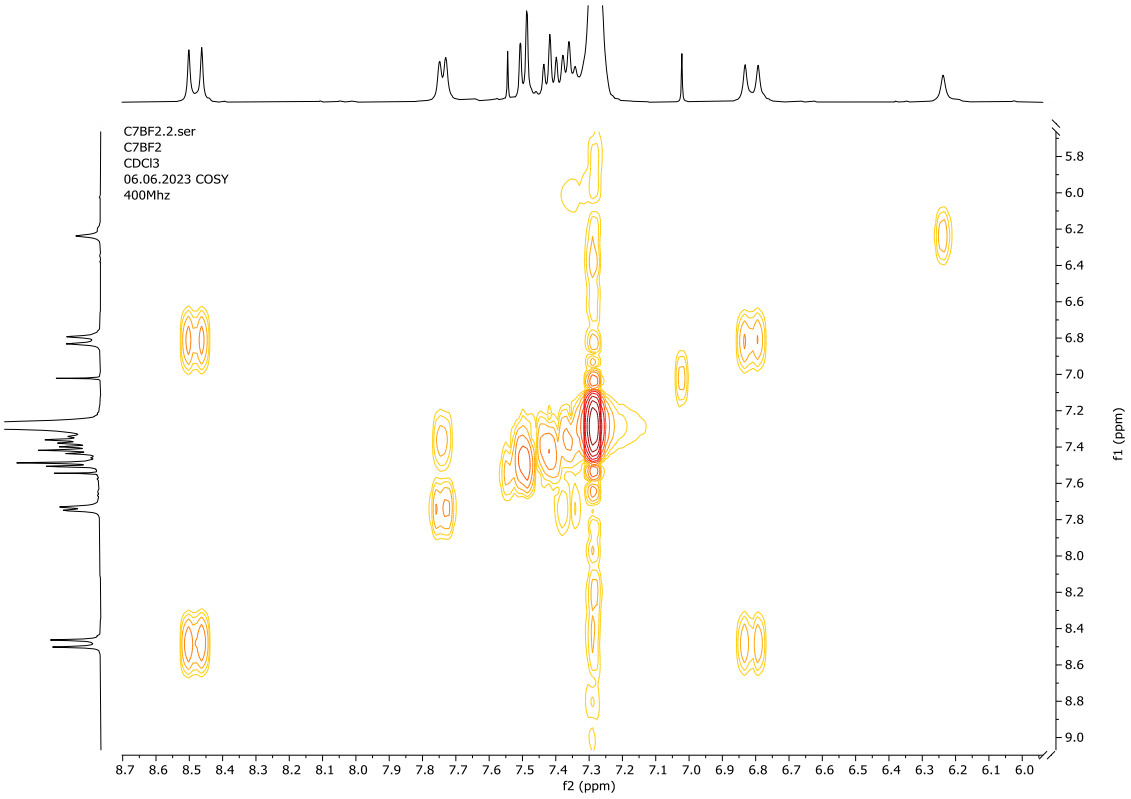


Figure 2.37: ^{1}H-^{1}H COSY NMR spectrum of **8** in $CDCl_3$ at 400 MHz

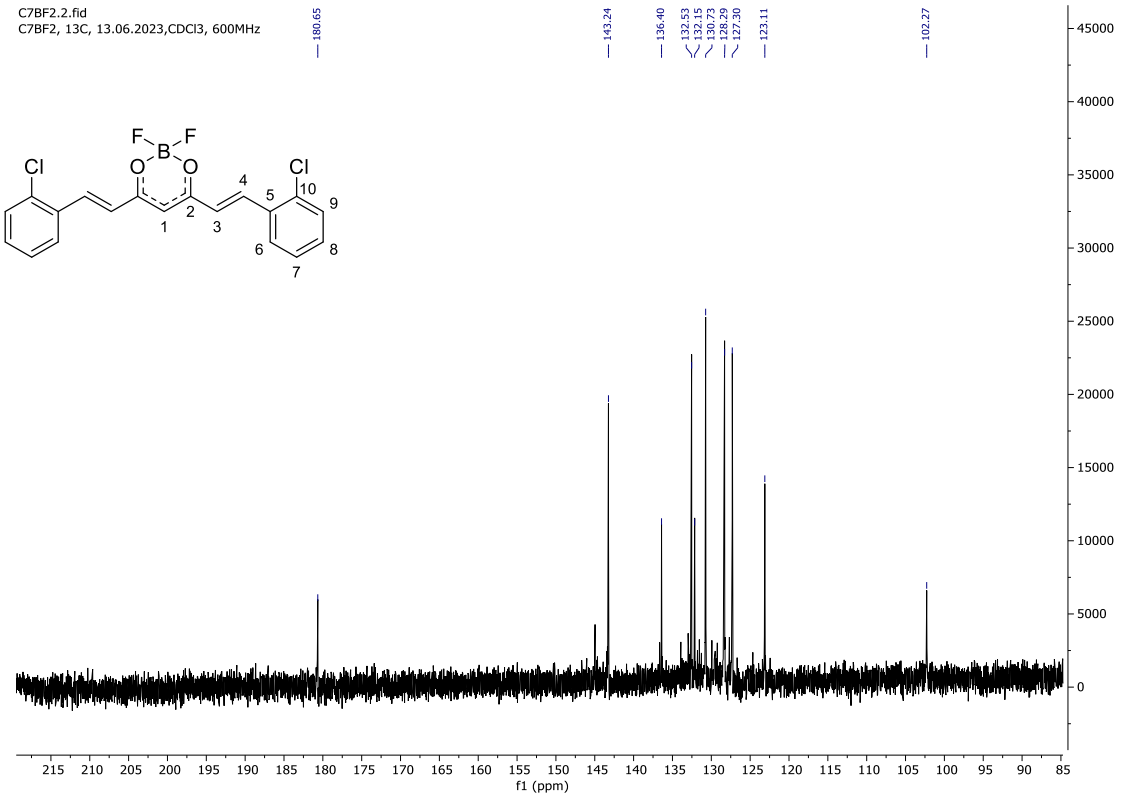


Figure 2.38: ^{13}C NMR spectrum of **8** in $CDCl_3$ at 101 MHz

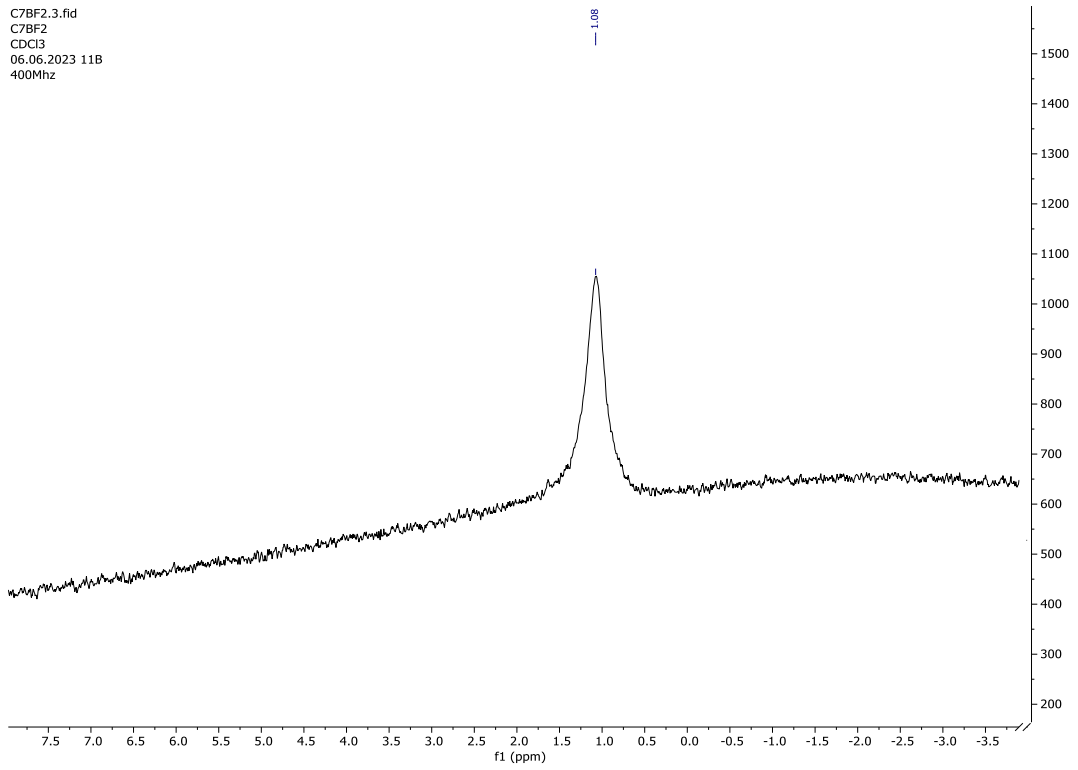


Figure 2.39: ^{11}B NMR spectrum of **8** in $CDCl_3$ at 127 MHz

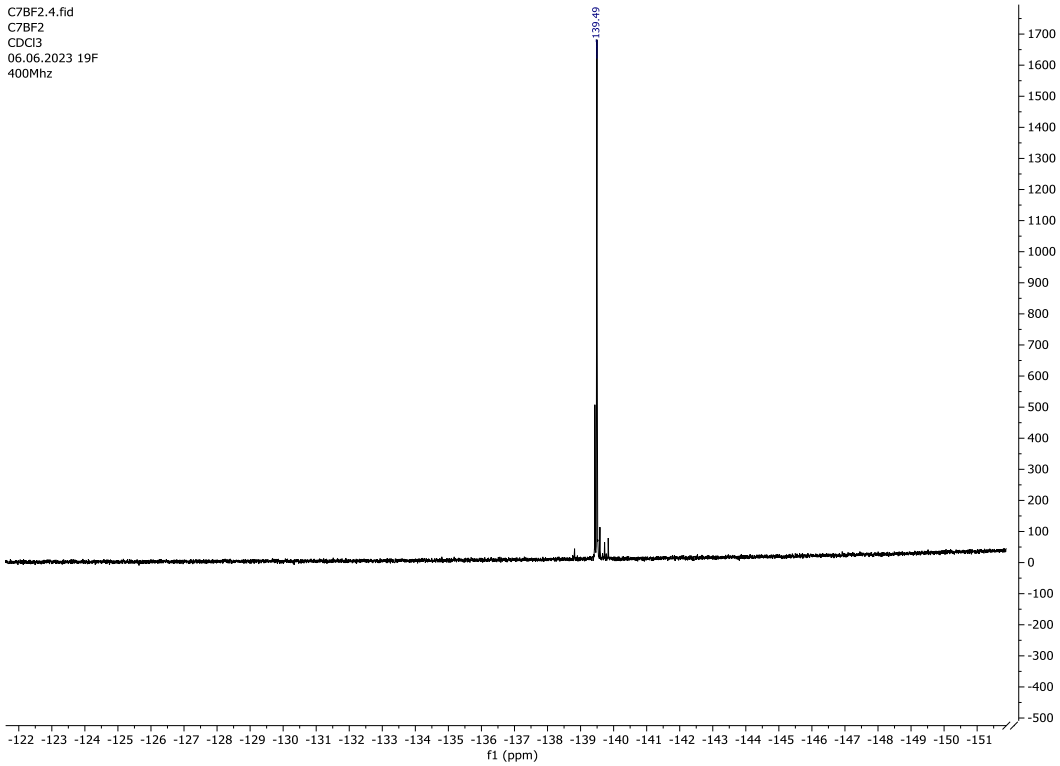


Figure 2.40: ^{19}F NMR spectrum of **8** in $CDCl_3$ at 376 MHz

3. UV-Vis and fluorescence measurements

Table S1: Gained absorption and emission maxima

Compound	Solvent	λ_{abs} nm	λ_{em} nm	Stokes shift cm^{-1}
2	Toluene	463, **488**	527	1516
	DCM	469, **489**	541	1966
	DMSO	393, **498**	553	1997
	MeOH	462, **482**	550	2565
3	Toluene	433, **457**	**475**, 499	1842
	DCM	432, **455**	503	2097
	DMSO	441, **463**	508	1913
	MeOH	429, **450**	493	1938
4	Toluene	**453**, 474	520	1866
	DCM	458, **474**	528	2158
	DMSO	486	550	2394
	MeOH	455, **469**	534	2595
5	Toluene	**425**, 449	**465**, 492	1947
	DCM	**425**, 449	**512**, 536	2740
	DMSO	433, **458**	485	1216
	MeOH	**421**, 443	476	1565
6	Toluene	**430**, 456	**471**, 500	698
	DCM	**431**, 456	487, 511	1396
	DMSO	437, **462**	491	1278
	MeOH	**425**, 449	485	1653
7	Toluene	**421**, 447	**465**, 489	866
	DCM	**421**, 446	467	1008
	DMSO	429, **453**	473	933
	MeOH	**416**, 440	467	1314
8	Toluene	**429**, 450	**481**, 497	1432
	DCM	**427**, 448	478, 501	1401
	DMSO	**434**, 455	492	1653
	MeOH	**433**, 463	479	721

Table S2: The obtained molar absorptivity for each compound

Compound	Solvent	C_{UV-Vis} µM	A	ε L·mol^{-1}·cm^{-1}	C_{fluo} µM
2	Toluene	13	0.6702	51496	0.07
	DCM	13	0.8227	63214	0.07
	DMSO	13	0.6893	52964	0.07
	MeOH	13	0.7152	54954	0.07
3	Toluene	23	0.7464	31862	0.47
	DCM	23	0.8096	34560	0.47
	DMSO	23	0.8096	34560	0.47
	MeOH	23	0.7240	30906	0.47
4	Toluene	25	0.8513	33544	0.25
	DCM	25	0.9621	37910	0.25
	DMSO	25	0.9992	39372	0.25
	MeOH	25	0.7970	31405	0.25
5	Toluene	12	0.5480	46499	0.59
	DCM	12	0.7346	62332	0.59
	DMSO	12	0.7152	60686	0.59
	MeOH	12	0.5552	47110	0.59
6	Toluene	12	0.5675	48698	0.58
	DCM	12	0.8298	71207	0.58
	DMSO	12	0.7081	60763	0.58
	MeOH	12	0.5682	48758	0.58
7	Toluene	16	0.6642	41834	1.07
	DCM	16	0.8158	51382	1.07
	DMSO	16	0.7273	45808	1.07
	MeOH	16	0.7996	50362	1.07
8	Toluene	15	0.2558	16896	5.56
	DCM	15	0.3232	21348	5.56
	DMSO	15	0.3114	20569	5.56
	MeOH	15	0.2003	13230	5.56

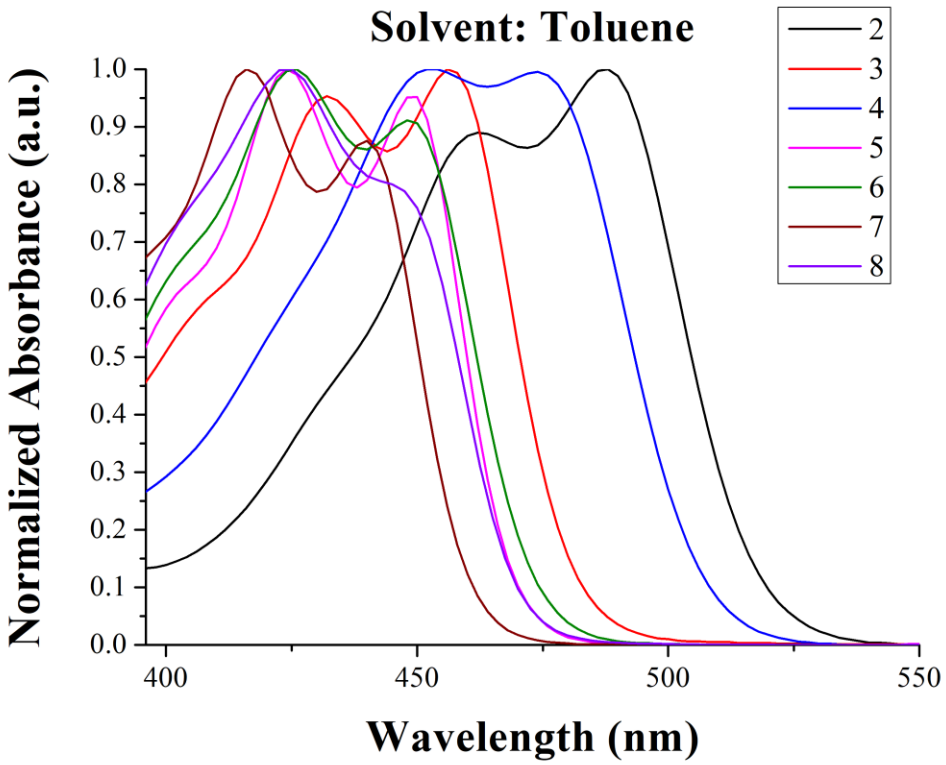


Figure 3.1: Obtained Normalized UV-Vis spectra in Toluene (20 °C, 10^{-5} M)

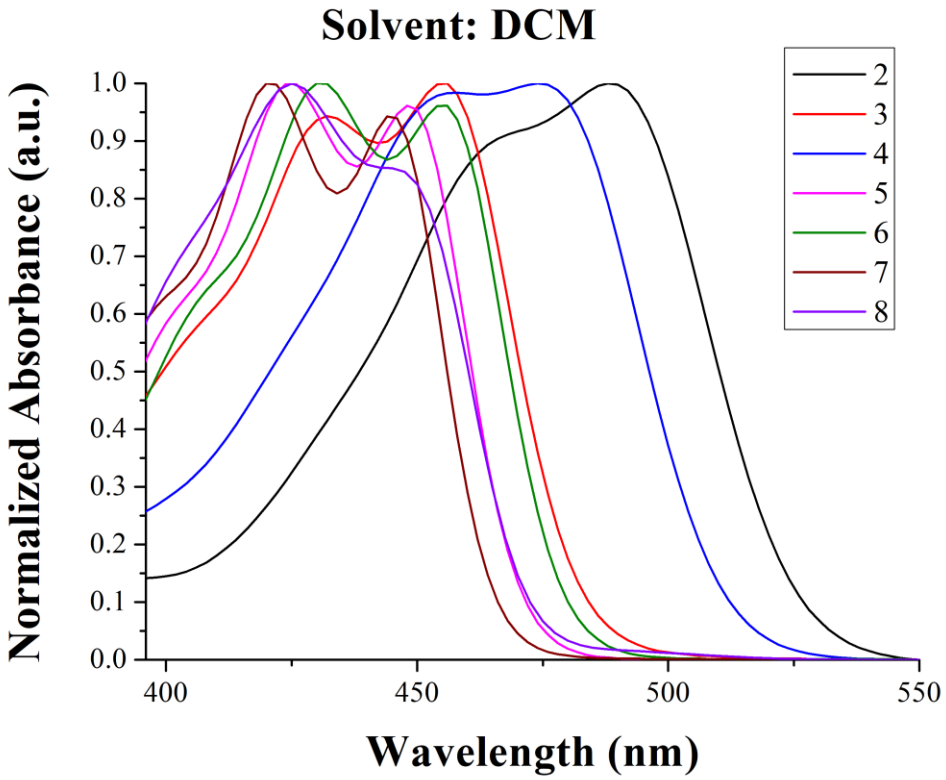


Figure 3.2: Obtained Normalized UV-Vis spectra in DCM (20 °C, 10^{-5} M)

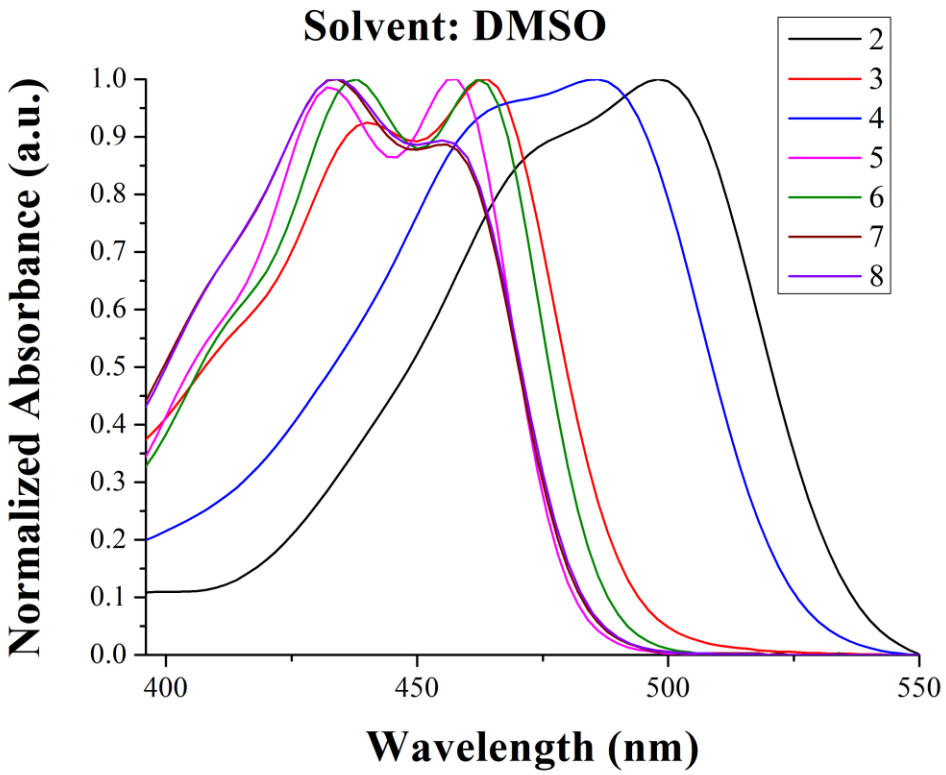


Figure 3.3: Obtained Normalized UV-Vis spectra in DMSO (20 °C, 10^{-5} M)

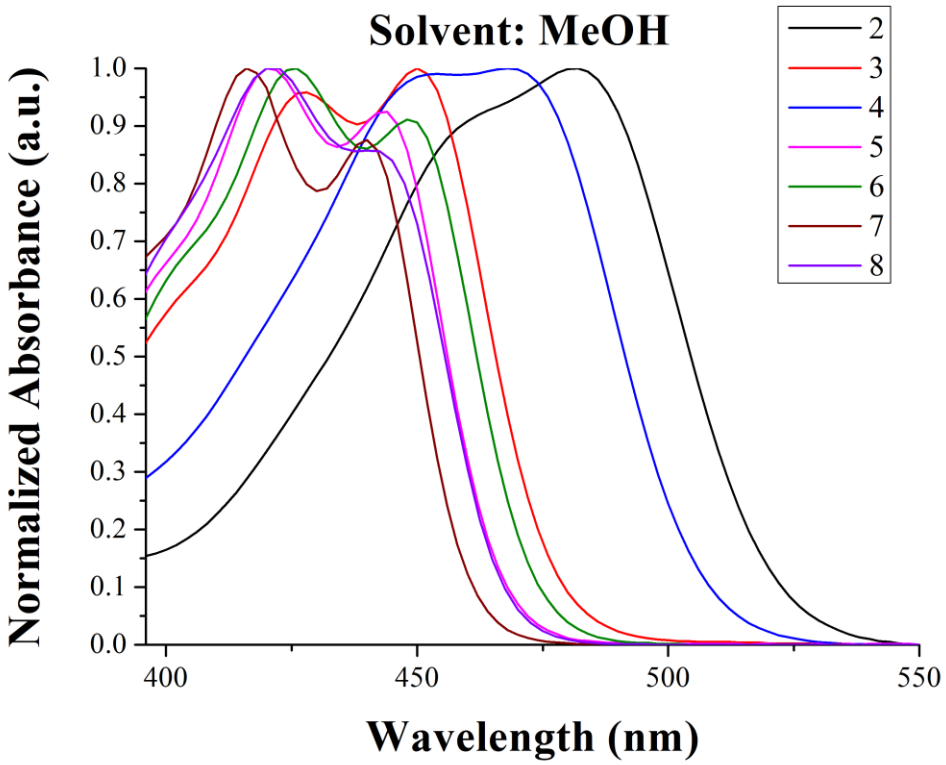


Figure 3.4: Obtained Normalized UV-Vis spectra in MeOH (20 °C, 10^{-5} M)

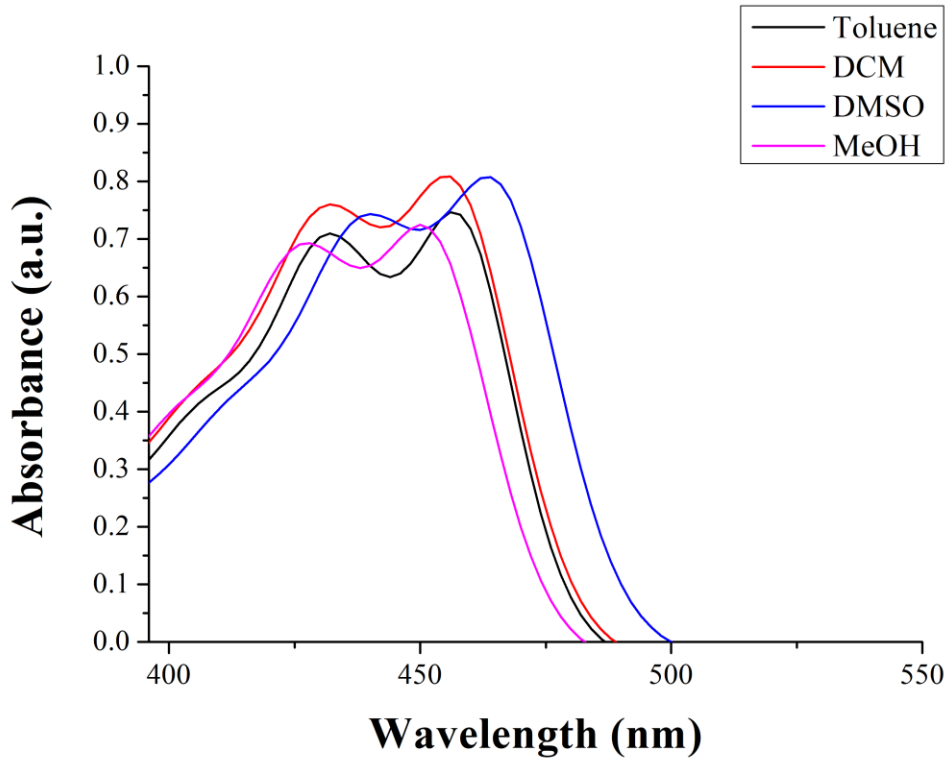


Figure 3.5: Obtained UV-Vis spectra of compound **3** in several solvents (20 °C, 13 µM)

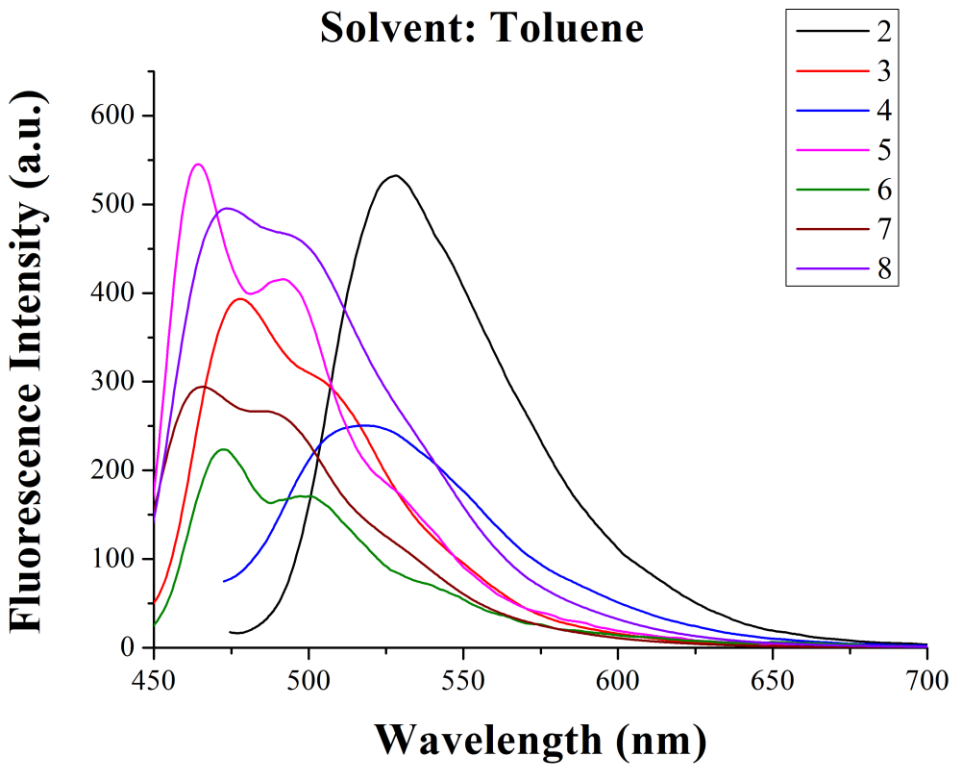


Figure 3.6: Obtained Fluorescence spectra in Toluene (20 °C, **2** at 0.07 µM, **3** at 0.47 µM, **4** at 0.25 µM, **5** at 0.59 µM, **6** 0.58 at µM, **7** at 1.07 µM, **8** at 5.50 µM)

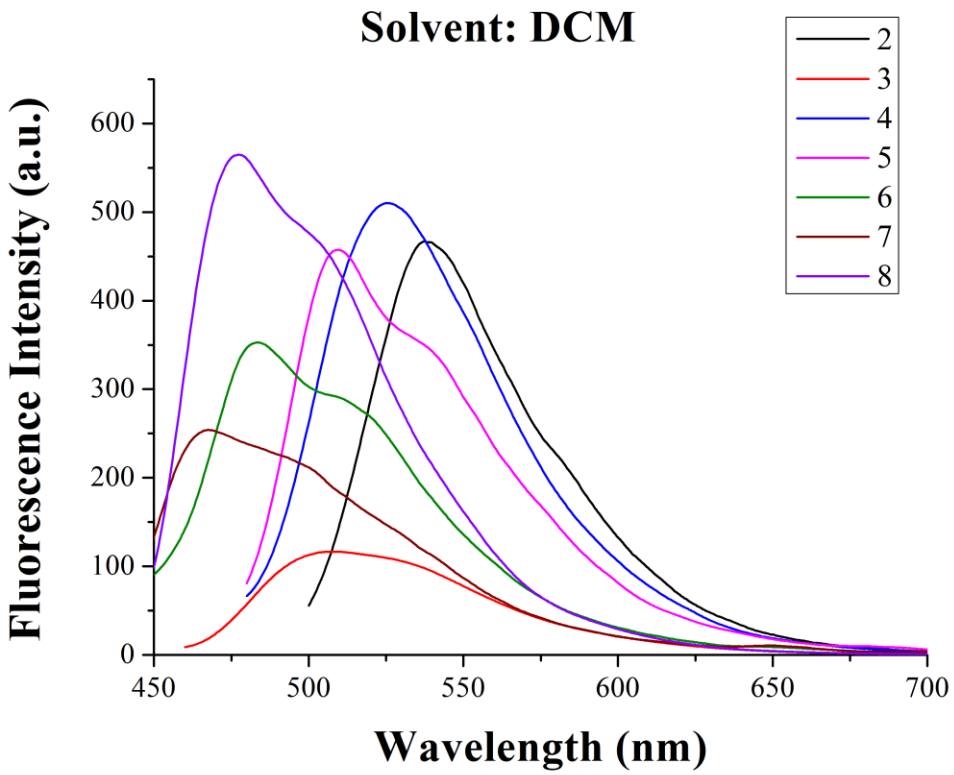


Figure 3.7: Obtained Fluorescence spectra in DCM (20 °C, **2** at 0.07 µM, **3** at 0.47 µM, **4** at 0.25 µM, **5** at 0.59 µM, **6** 0.58 at µM, **7** at 1.07 µM, **8** at 5.50 µM)

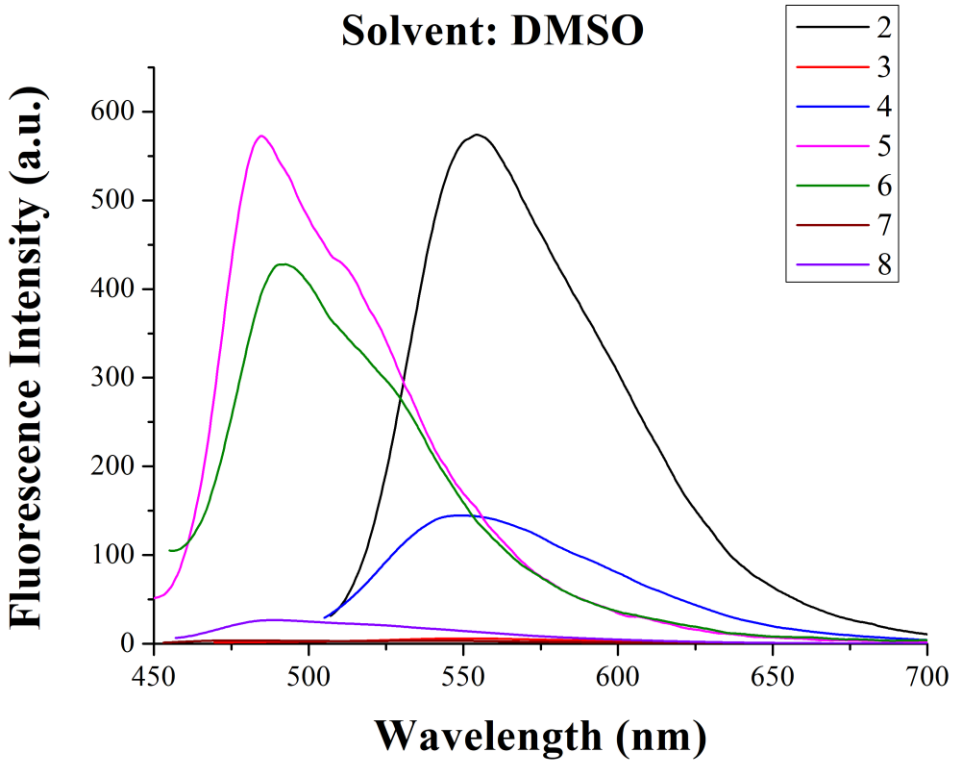


Figure 3.8: Obtained Fluorescence spectra in DMSO (20 °C, **2** at 0.07 µM, **3** at 0.47 µM, **4** at 0.25 µM, **5** at 0.59 µM, **6** 0.58 at µM, **7** at 1.07 µM, **8** at 5.50 µM)

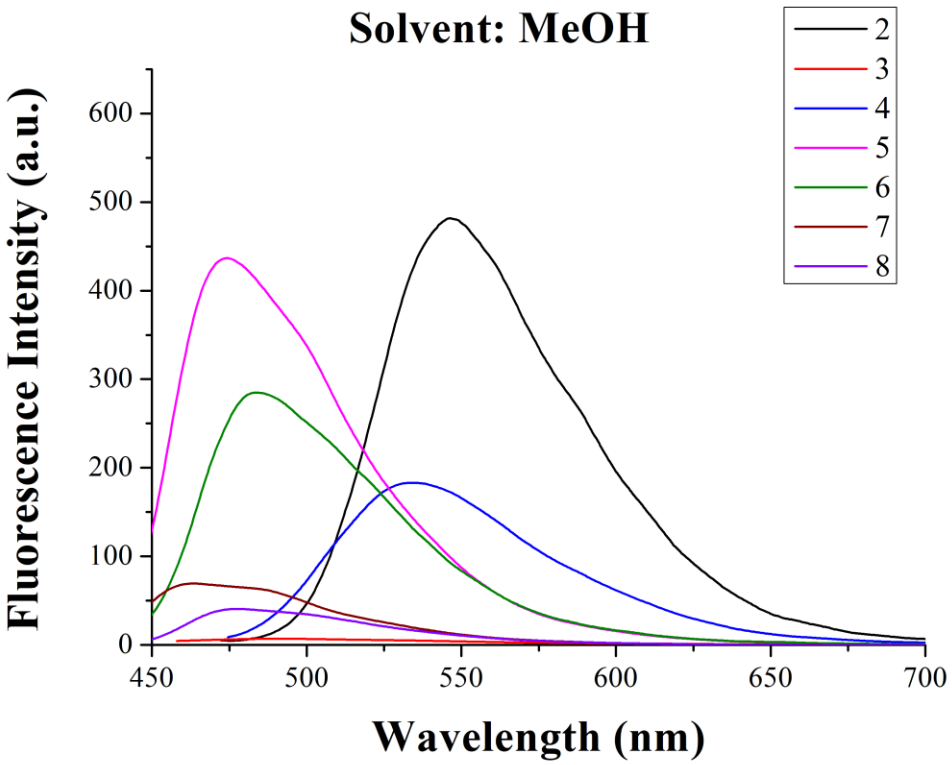


Figure 3.9: Obtained Fluorescence spectra in MeOH (20 °C, **2** at 0.07 µM, **3** at 0.47 µM, **4** at 0.25 µM, **5** at 0.59 µM, **6** 0.58 at µM, **7** at 1.07 µM, **8** at 5.50 µM)

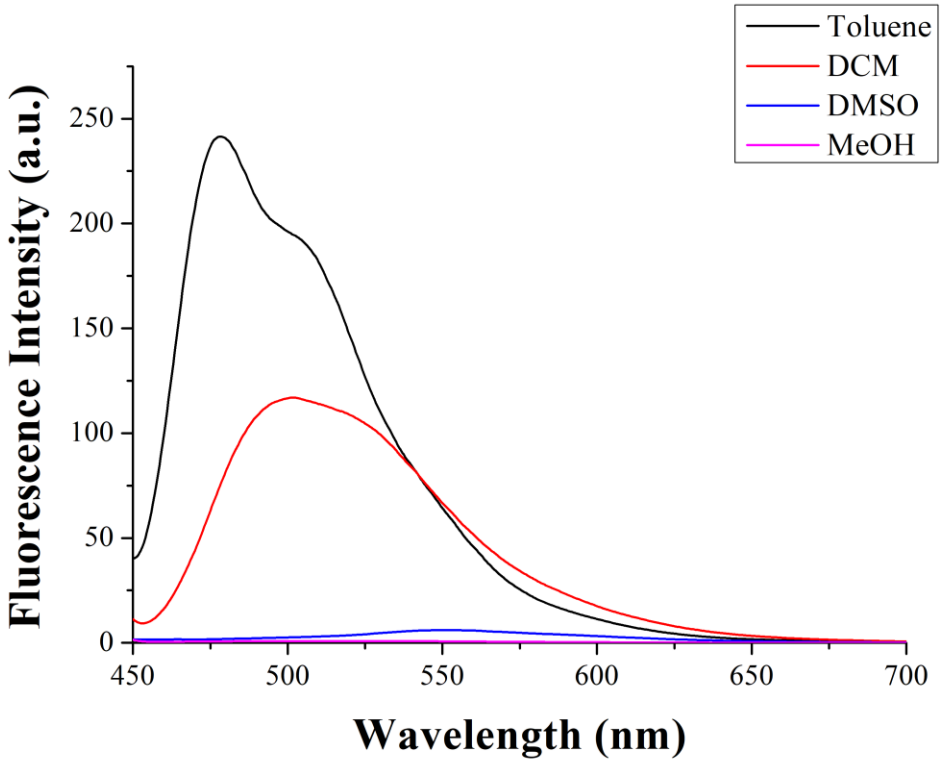


Figure 3.10: Obtained fluorescence spectra of compound **3** (20 °C, 0.47 µM)

4. DFT results

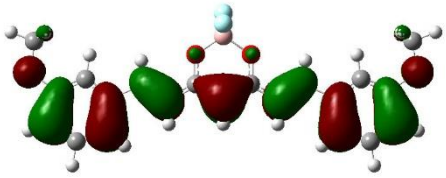
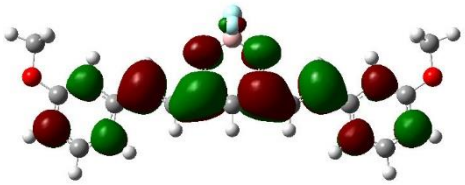
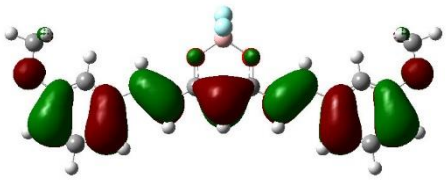
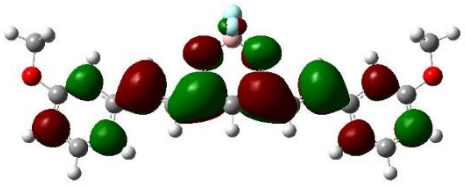
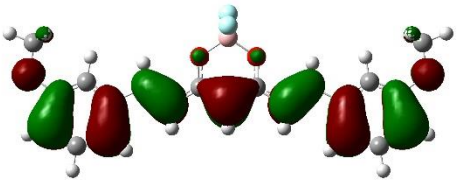
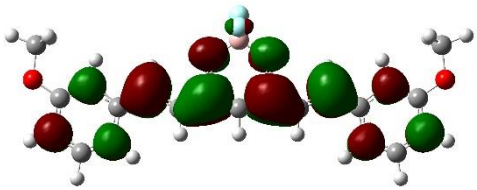
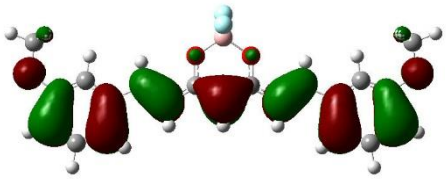
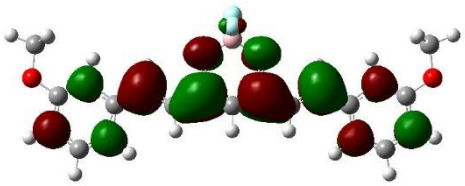
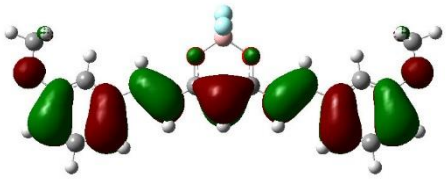
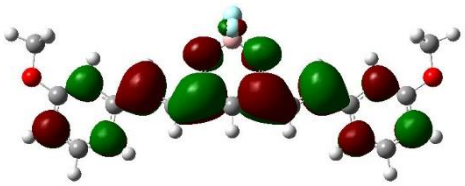
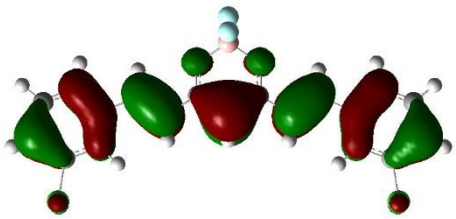
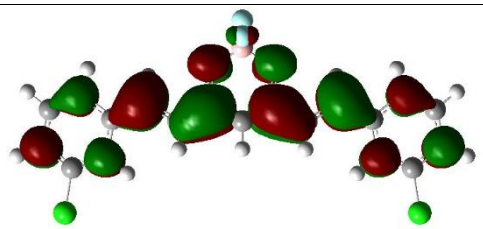
Table S3: The DFT-calculated dipole moment values

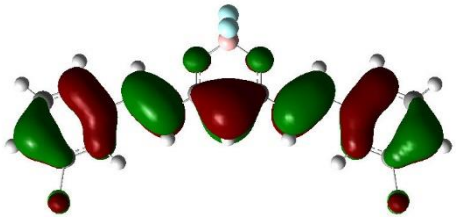
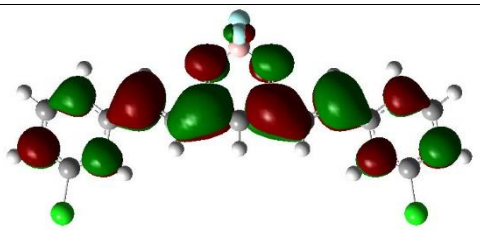
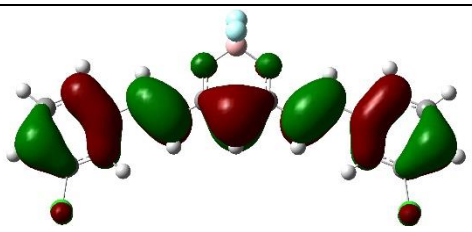
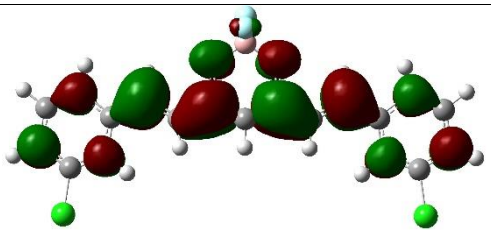
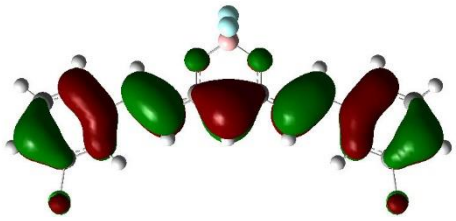
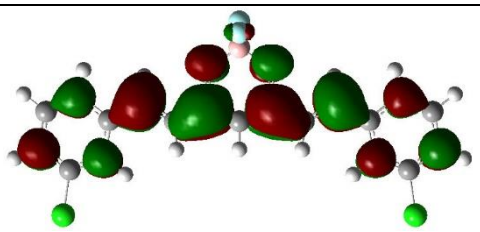
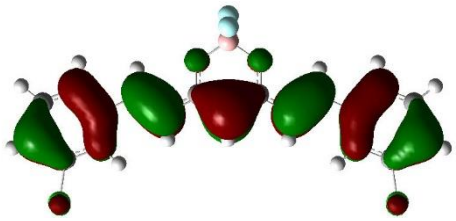
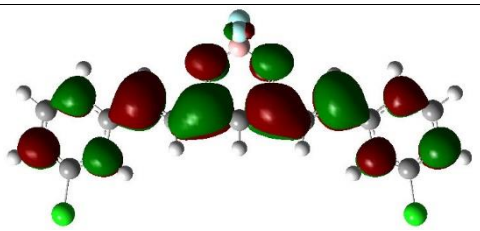
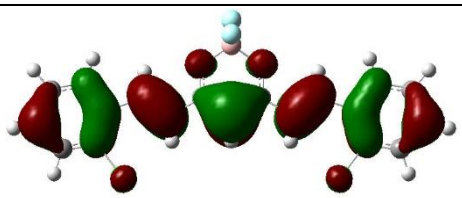
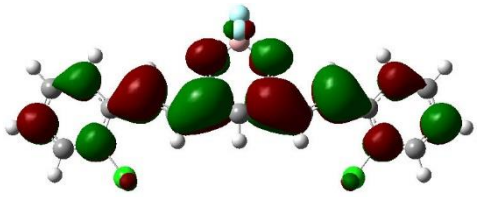
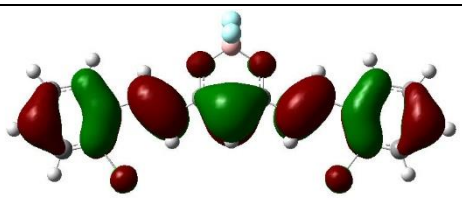
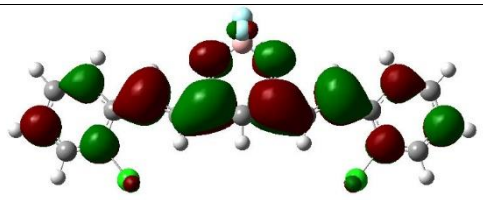
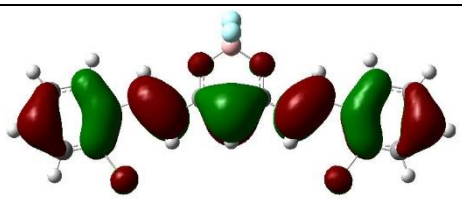
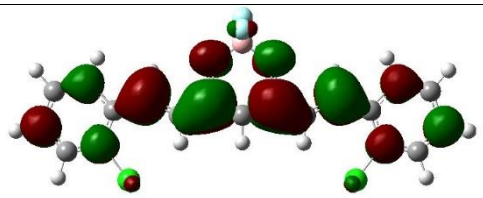
Compound	Solvent	Polarity (Debye)	
		Ground state	Excited state
2	–	6.08 D	6.73 D
	Toluene	7.25 D	8.14 D
	DCM	8.30 D	9.46 D
	DMSO	8.73 D	10.01 D
	MeOH	8.68 D	9.95 D
3	–	4.83 D	5.42 D
	Toluene	5.87 D	6.40 D
	DCM	5.85 D	7.55 D
	DMSO	7.25 D	8.04 D
	MeOH	7.21 D	7.99 D
4	–	10.96 D	11.51 D
	Toluene	12.89 D	13.67 D
	DCM	14.58 D	15.63 D
	DMSO	15.26 D	16.44 D
	MeOH	15.19 D	16.35 D
5	–	7.63 D	8.03 D
	Toluene	9.03 D	9.62 D
	DCM	10.30 D	11.09 D
	DMSO	10.82 D	11.71 D
	MeOH	10.77 D	11.64 D
6	–	6.38 D	6.75 D
	Toluene	7.55 D	8.12 D
	DCM	8.64 D	9.42 D
	DMSO	9.11 D	9.97 D
	MeOH	9.06 D	9.91 D
7	–	4.03 D	4.44 D
	Toluene	4.82 D	5.44 D
	DCM	5.91 D	6.42 D
	DMSO	5.95 D	6.86 D
	MeOH	5.91 D	6.81 D
8	–	4.89 D	5.34 D
	Toluene	5.81 D	6.46 D
	DCM	6.67 D	7.55 D
	DMSO	7.04 D	8.03 D
	MeOH	7.00 D	7.97 D

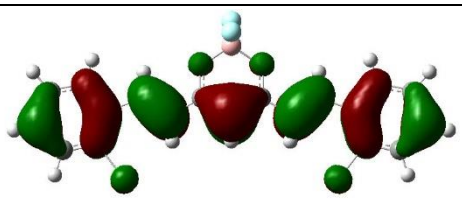
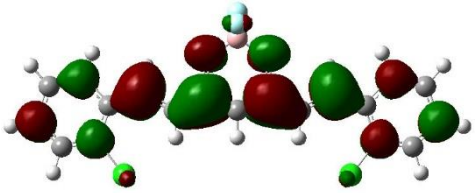
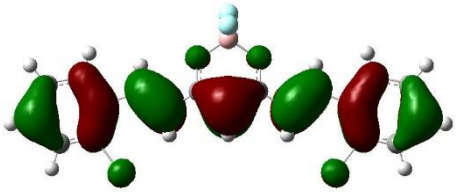
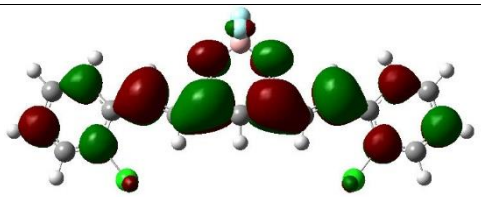
Table S4: *In silico* obtained absorbance and emission values

Compound	Solvent	λ_{abs} (nm)	f	λ_{em} (nm)	f
2	Gas phase	443	1.9009	464	1.9779
	Toluene	485	2.1114	515	2.2134
	DCM	497	2.1405	564	2.3590
	DMSO	503	2.1551	585	2.4069
	MeOH	498	2.1334	583	2.4018
3	Gas phase	443	1.0910	506	0.4550
	Toluene	476	1.3325	510	1.4059
	DCM	485	1.2772	549	1.6250
	DMSO	489	1.2701	566	1.6998
	MeOH	486	1.2243	564	1.6919
4	Gas phase	430	1.4480	456	1.5480
	Toluene	468	1.6374	502	1.7630
	DCM	482	1.5821	547	1.9035
	DMSO	488	1.5648	566	1.9501
	MeOH	483	1.5312	564	1.9452
5	Gas phase	414	1.6480	443	1.6916
	Toluene	447	1.8558	485	1.9316
	DCM	454	1.8767	525	2.0762
	DMSO	457	1.8876	542	2.1219
	MeOH	453	1.8660	540	2.1171
6	Gas phase	427	1.8098	456	1.8759
	Toluene	459	2.0118	499	2.1070
	DCM	465	2.0310	538	2.2417
	DMSO	468	2.0414	555	2.2828
	MeOH	464	2.0209	553	2.2786
7	Gas phase	414	1.6209	455	1.6740
	Toluene	444	1.8232	484	1.9061
	DCM	449	1.8414	521	2.0457
	DMSO	452	1.8515	537	2.0896
	MeOH	448	1.8304	535	2.0850
8	Gas phase	412	1.5579	445	1.6191
	Toluene	442	1.7765	484	1.8701
	DCM	448	1.7875	520	2.0266
	DMSO	451	1.7942	535	2.0775
	MeOH	447	1.7692	553	2.0721

Table S5. Frontier molecular orbitals FMO predicted for curcuminoid BF_2-complexes **3**, **7** and **8**

No	Solvent	HOMO	LUMO
3	**Gas phase** ΔE = 3.0817 eV	 **-6.3022 eV**	 **-3.2205 eV**
	Toluene ΔE = 2.9856 eV	 **-6.2706 eV**	 **-3.2850 eV**
	DCM ΔE = 3.0817 eV	 **-6.2597 eV**	 **-3.3465 eV**
	DMSO ΔE = 2.8878 eV	 **-6.2571 eV**	 **-3.3693 eV**
	MeOH ΔE = 2.8906 eV	 **-6.2575 eV**	 **-3.3669 eV**
7	**Gas phase** ΔE = 3.2564 eV	 **-6.7533 eV**	 **-3.4969 eV**

	Toluene ΔE = 3.1873 eV	 **-6.6573 eV**	 **-3.4700 eV**
	DCM ΔE = 3.1249 eV	 **-6.6001 eV**	 **-3.4752 eV**
	DMSO ΔE = 3.1007 eV	 **-6.5808 eV**	 **-3.4801 eV**
	MeOH ΔE = 3.1035 eV	 **-6.5827 eV**	 **-3.4792 eV**
8	**Gas phase** ΔE = 3.2808 eV	 **-6.6322 eV**	 **-3.3514 eV**
	Toluene ΔE = 3.2120 eV	 **-6.5960 eV**	 **-3.3840 eV**
	DCM ΔE = 3.1468 eV	 **-6.5803 eV**	 **-3.4335 eV**

	DMSO ΔE = 3.1220 eV	 **-6.5765 eV**	 **-3.4545 eV**
	MeOH ΔE = 3.1247 eV	 **-6.5770 eV**	 **-3.4523 eV**

4.1. Cartesian Coordinates

Compound 3 in gas phase

1	6	0	1.210346	-0.102168	0.095770
2	6	0	-0.000000	-0.798014	0.220280
3	6	0	-1.210344	-0.102170	0.095731
4	8	0	1.227880	1.193149	-0.052687
5	8	0	-1.227875	1.193148	-0.052724
6	5	0	-0.000003	2.037970	0.178761
7	9	0	-0.000022	2.453727	1.499489
8	9	0	0.000011	3.070336	-0.724992
9	1	0	-0.000001	-1.873099	0.342936
10	6	0	-2.482972	-0.801519	0.090583
11	6	0	-3.663500	-0.145221	-0.008334
12	1	0	-2.432339	-1.882377	0.175858
13	6	0	-5.004777	-0.721741	-0.026703
14	1	0	-3.610595	0.939134	-0.080077
15	6	0	-6.097719	0.169386	-0.101334
16	6	0	-5.251753	-2.105350	0.027174
17	6	0	-7.408894	-0.314325	-0.118845
18	1	0	-5.897249	1.233615	-0.143052

19	6	0	-6.563687	-2.578332	0.008357
20	1	0	-4.429139	-2.809950	0.080897
21	6	0	-7.641267	-1.697586	-0.063601
22	8	0	-8.521281	0.471493	-0.188117
23	1	0	-6.752033	-3.647020	0.049440
24	1	0	-8.665436	-2.055386	-0.079005
25	6	0	-8.358807	1.885697	-0.246003
26	1	0	-9.367412	2.296809	-0.294822
27	1	0	-7.853267	2.265870	0.650056
28	1	0	-7.799077	2.186446	-1.140048
29	6	0	2.482975	-0.801514	0.090662
30	6	0	3.663501	-0.145222	-0.008322
31	1	0	2.432346	-1.882365	0.176031
32	6	0	5.004779	-0.721739	-0.026655
33	1	0	3.610591	0.939127	-0.080157
34	6	0	6.097717	0.169385	-0.101371
35	6	0	5.251760	-2.105343	0.027336
36	6	0	7.408894	-0.314323	-0.118855
37	1	0	5.897244	1.233610	-0.143177
38	6	0	6.563696	-2.578323	0.008546
39	1	0	4.429148	-2.809941	0.081126
40	6	0	7.641272	-1.697579	-0.063497
41	8	0	8.521278	0.471493	-0.188204
42	1	0	6.752045	-3.647006	0.049717
43	1	0	8.665442	-2.055377	-0.078880
44	6	0	8.358798	1.885691	-0.246207
45	1	0	9.367402	2.296802	-0.295071
46	1	0	7.799059	2.186363	-1.140272
47	1	0	7.853267	2.265938	0.649825

Compound 7 in gas phase

1	6	0	-1.209462	-0.822140	0.041114
2	6	0	0.000000	-0.125625	0.169443
3	6	0	1.209461	-0.822138	0.041096
4	8	0	-1.228376	-2.114955	-0.112888
5	8	0	1.228375	-2.114954	-0.112903
6	5	0	0.000003	-2.964861	0.112794
7	9	0	0.000009	-3.385367	1.429944
8	9	0	-0.000003	-3.987124	-0.799304
9	1	0	-0.000000	0.948843	0.296945
10	6	0	2.483465	-0.121505	0.038145
11	6	0	3.662827	-0.776917	-0.064929
12	1	0	2.430684	0.958910	0.128785
13	6	0	5.004097	-0.198099	-0.080685
14	1	0	3.615029	-1.860786	-0.144023
15	6	0	6.108961	-1.066012	-0.174548
16	6	0	5.239774	1.190102	-0.005687
17	6	0	7.410149	-0.565572	-0.191700
18	1	0	5.939108	-2.136969	-0.233299
19	6	0	6.542777	1.671097	-0.024270
20	1	0	4.417503	1.892371	0.065059
21	6	0	7.640436	0.808970	-0.116534
22	1	0	8.252663	-1.246243	-0.263943
23	17	0	6.819438	3.404341	0.069292
24	1	0	8.647775	1.209905	-0.129375
25	6	0	-2.483467	-0.121509	0.038180
26	6	0	-3.662822	-0.776910	-0.065037
27	1	0	-2.430694	0.958894	0.128966

28	6	0	-5.004093	-0.198095	-0.080782
29	1	0	-3.615017	-1.860769	-0.144268
30	6	0	-6.108950	-1.065999	-0.174803
31	6	0	-5.239777	1.190097	-0.005623
32	6	0	-7.410138	-0.565561	-0.191954
33	1	0	-5.939091	-2.136948	-0.233681
34	6	0	-6.542781	1.671090	-0.024206
35	1	0	-4.417512	1.892359	0.065248
36	6	0	-7.640433	0.808971	-0.116628
37	1	0	-8.252648	-1.246225	-0.264320
38	17	0	-6.819451	3.404321	0.069557
39	1	0	-8.647773	1.209905	-0.129466

Compound 8 in gas phase

1	6	0	1.209721	0.504672	0.049725
2	6	0	-0.000002	-0.190734	0.178175
3	6	0	-1.209722	0.504663	0.049724
4	8	0	1.228027	1.797890	-0.105744
5	8	0	-1.228029	1.797890	-0.105755
6	5	0	-0.000020	2.647911	0.113130
7	9	0	-0.000010	3.081376	1.426771
8	9	0	-0.000006	3.664811	-0.806724
9	1	0	0.000001	-1.265047	0.305741
10	6	0	-2.481796	-0.204638	0.048795
11	6	0	-3.652725	0.469076	-0.053395
12	1	0	-2.425935	-1.279519	0.139025
13	6	0	-5.042193	0.017327	-0.075669
14	1	0	-3.553445	1.549705	-0.129500
15	6	0	-5.543450	-1.305548	-0.024376
16	6	0	-6.012467	1.046513	-0.160903

17	6	0	-6.912474	-1.571571	-0.054469
18	17	0	-4.491220	-2.711847	0.076176
19	6	0	-7.378006	0.793060	-0.190742
20	1	0	-5.659183	2.072610	-0.202979
21	6	0	-7.832539	-0.526394	-0.136792
22	1	0	-7.249585	-2.601355	-0.013240
23	1	0	-8.081115	1.617121	-0.255698
24	1	0	-8.895000	-0.748128	-0.159040
25	6	0	2.481793	-0.204639	0.048791
26	6	0	3.652722	0.469071	-0.053417
27	1	0	2.425925	-1.279517	0.139047
28	6	0	5.042194	0.017326	-0.075664
29	1	0	3.553440	1.549698	-0.129542
30	6	0	5.543455	-1.305551	-0.024436
31	6	0	6.012463	1.046523	-0.160785
32	6	0	6.912484	-1.571561	-0.054452
33	17	0	4.491231	-2.711870	0.075880
34	6	0	7.378007	0.793082	-0.190551
35	1	0	5.659174	2.072620	-0.202819
36	6	0	7.832545	-0.526371	-0.136645
37	1	0	7.249601	-2.601345	-0.013268
38	1	0	8.081115	1.617150	-0.255427
39	1	0	8.895010	-0.748094	-0.158830