

# **Counter Anion Effect on the Photophysical Properties of Emissive Indolizine-Cyanine Dyes in Solution and Solid State**

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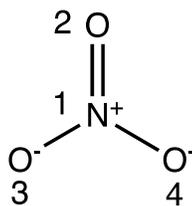
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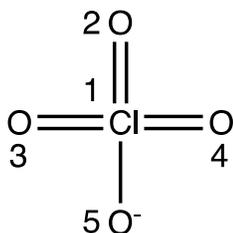
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**Table S1.** Mulliken charges on  $\text{NO}_3^-$  atoms.

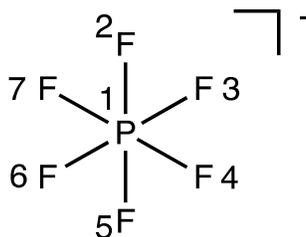
Atom Number	Atom	Charge
1	N	-0.052098
2	O	-0.315967
3	O	-0.315967
4	O	-0.315967

**Table S2.** Mulliken charges on  $\text{ClO}_4^-$  atoms.

Atom Number	Atom	Charge
1	Cl	1.351688
2	O	-0.587922
3	O	-0.587922
4	O	-0.587922
5	O	-0.587922

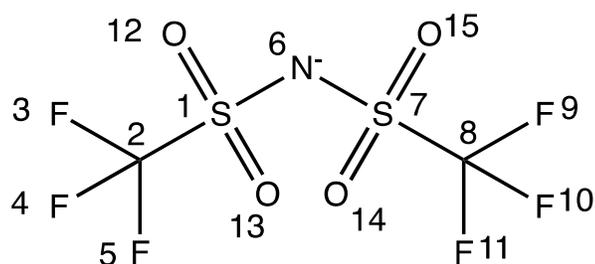
**Table S3.** Mulliken charges on  $\text{PF}_6^-$  atoms.

Atom Number	Atom	Charge
1	P	3.403124
2	F	-0.733854
3	F	-0.733854
4	F	-0.733854
5	F	-0.733854
6	F	-0.733854
7	F	-0.733854



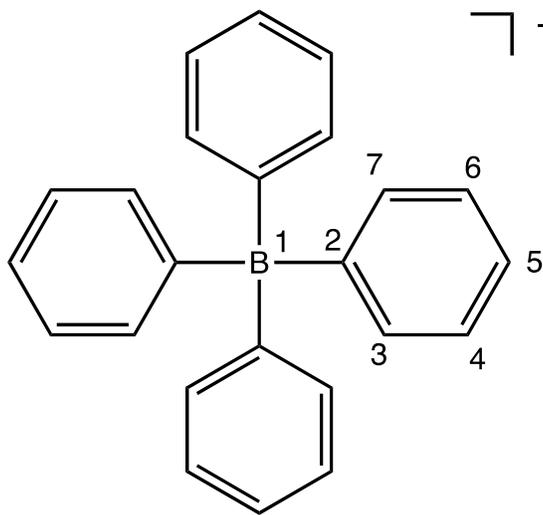
**Table S4.** Mulliken charges on TFSI atoms.

Atom Number	Atom	Charge
1	S	1.176786
2	C	0.742771
3	F	-0.309487
4	F	-0.294206
5	F	-0.266768
6	N	-0.878432
7	S	1.117281
8	C	0.828531
9	F	-0.315792
10	F	-0.282991
11	F	-0.274752
12	O	-0.556669
13	O	-0.568497
14	O	-0.551996
15	O	-0.565780



**Table S5.** Mulliken charges on TPB atoms.

Atom Number	Atom	Charge
1	B	-0.158270
2	C	1.128749
3	C	-0.481455
4	C	-0.418219
5	C	-0.330027
6	C	-0.418219
7	C	-0.481455
8	H	0.178060
9	H	0.145291
10	H	0.143492
11	H	0.145291
12	H	0.178060
13	C	1.128749
14	C	-0.481455
15	C	-0.418219
16	C	-0.330027
17	C	-0.418219
18	C	-0.481455
19	H	0.178060
20	H	0.145291
21	H	0.143492
22	H	0.145291
23	H	0.178060
24	C	1.128749
25	C	-0.481455
26	C	-0.418219
27	C	-0.330027
28	C	-0.418219
29	C	-0.481455
30	H	0.178060
31	H	0.145291
32	H	0.143492
33	H	0.145291
34	H	0.178060
35	C	1.128749
36	C	-0.481455
37	C	-0.418219
38	C	-0.330027
39	C	-0.418219
40	C	-0.481455
41	H	0.178060
42	H	0.145291
43	H	0.143492
44	H	0.145291
45	H	0.178060



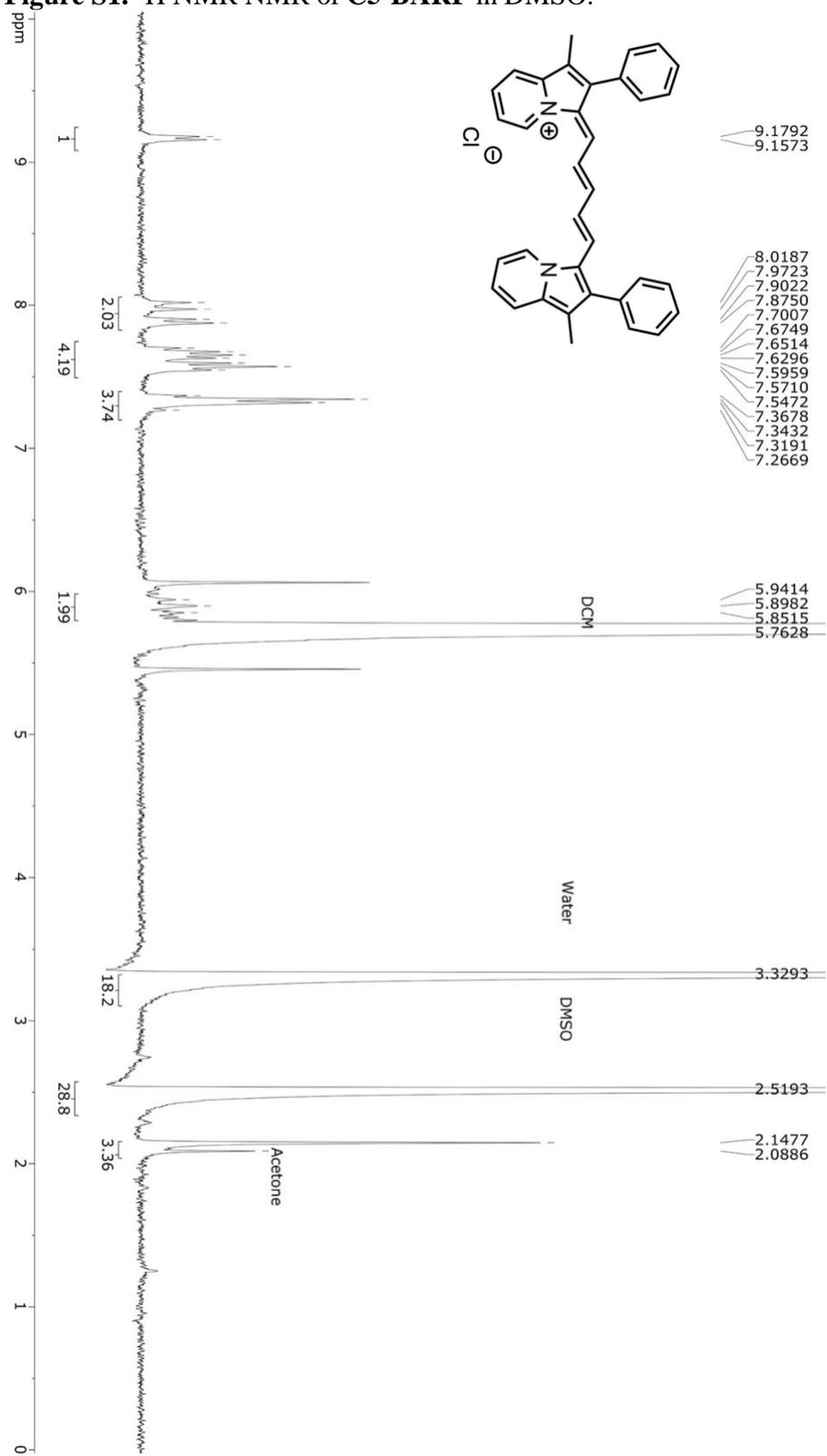
**Table S6.** Mulliken charges on BARF atoms.

Atom Number	Atom	Charge
1	B	0.246940
2	C	-0.467115
3	C	0.030678
4	C	-1.081474
5	C	-0.353031
6	C	-0.525904
7	C	-0.424496
8	H	0.215602
9	C	1.885359
10	F	-0.322164
11	F	-0.302350
12	F	-0.273043
13	H	0.220926
14	C	1.771129
15	F	-0.296042
16	F	-0.274135
17	F	-0.332978
18	H	0.220021
19	C	-0.337231
20	C	0.010444
21	C	-1.091433
22	C	-0.315577
23	C	-0.594870
24	C	-0.373494
25	H	0.215116
26	C	1.752906
27	F	-0.304481
28	F	-0.268874
29	F	-0.327559
30	H	0.220899
31	C	1.838879
32	F	-0.272759
33	F	-0.301823
34	F	-0.329219
35	H	0.221551
36	C	-0.409728
37	C	-0.022202
38	C	-1.101163
39	C	-0.314471
40	C	-0.573120

Atom Number	Atom	Charge
41	C	-0.341871
42	H	0.215555
43	C	1.737881
44	F	-0.269514
45	F	-0.304927
46	F	-0.328041
47	H	0.221053
48	C	1.828482
49	F	-0.271783
50	F	-0.300031
51	F	-0.329847
52	H	0.220930
53	C	-0.391629
54	C	-0.316589
55	C	-0.740104
56	C	-0.283551
57	C	-1.233593
58	C	0.015076
59	H	0.219623
60	C	1.870671
61	F	-0.332687
62	F	-0.271987
63	F	-0.297009
64	H	0.220620
65	C	1.887648
66	F	-0.265933
67	F	-0.303000
68	F	-0.330092
69	H	0.214931

**Figure S1.**  $^1\text{H}$  NMR of **C5-BARF** in DMSO.



**Figure S2.**  $^1\text{H}$  NMR (DMSO) of C5-NO<sub>3</sub>

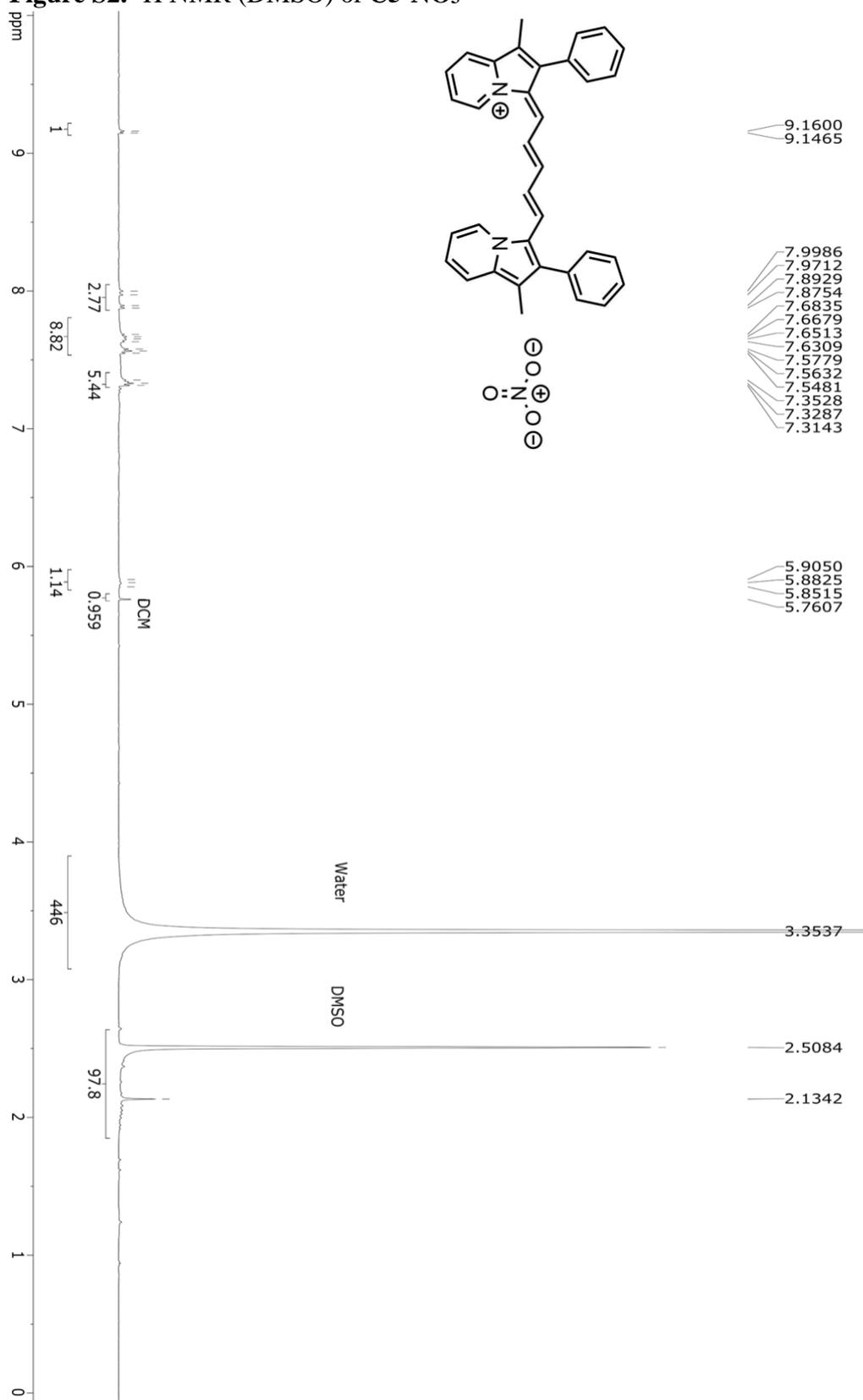
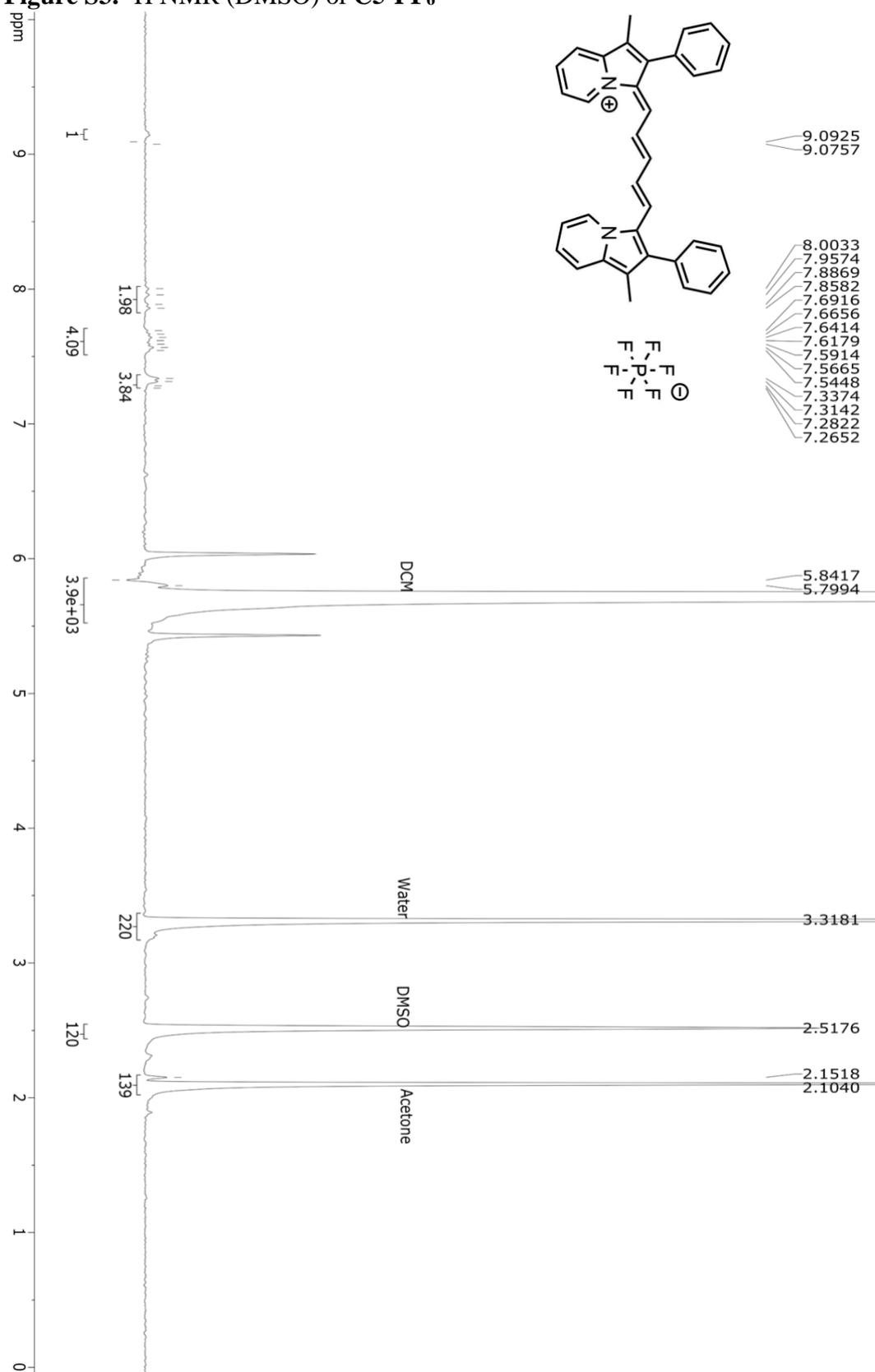


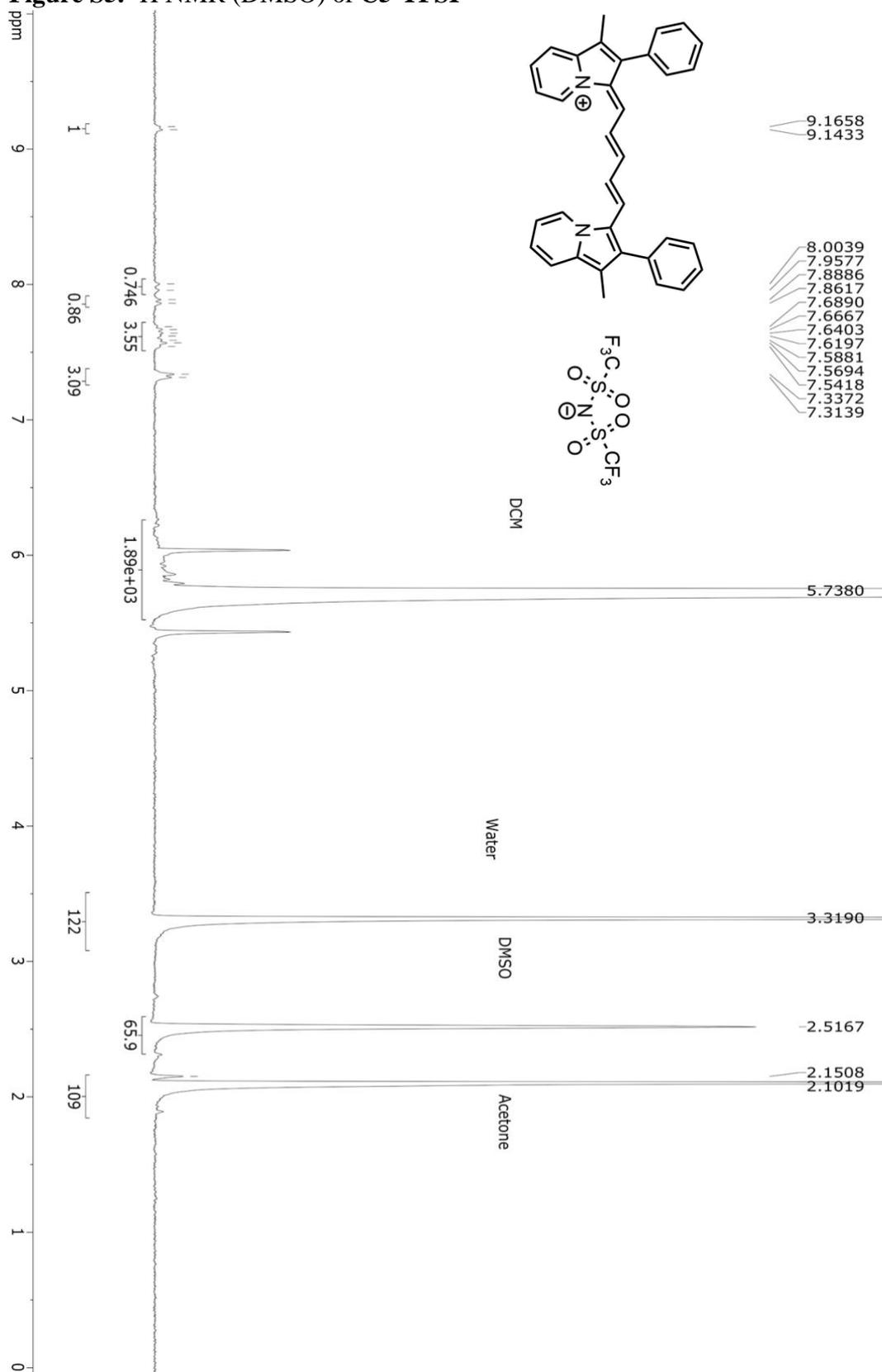
Figure S3. <sup>1</sup>H NMR (DMSO) of C5-PF<sub>6</sub>



**Figure S4.**  $^{19}\text{F}$  NMR (DMSO) of **C5-PF<sub>6</sub>**



**Figure S5.**  $^1\text{H}$  NMR (DMSO) of C5-TFSI



**Figure S6.**  $^{19}\text{F}$  NMR (DMSO) of C5-TFSI

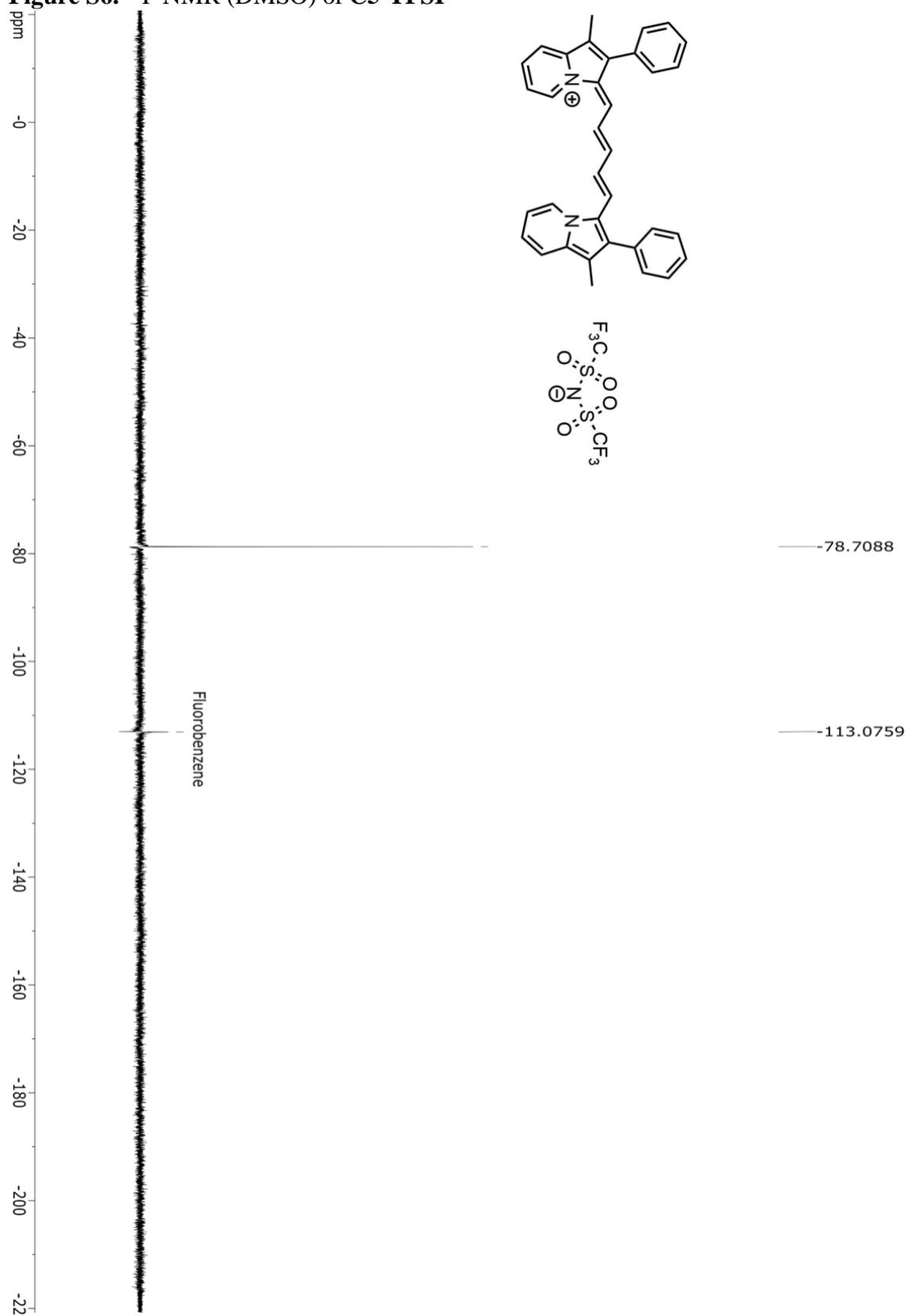
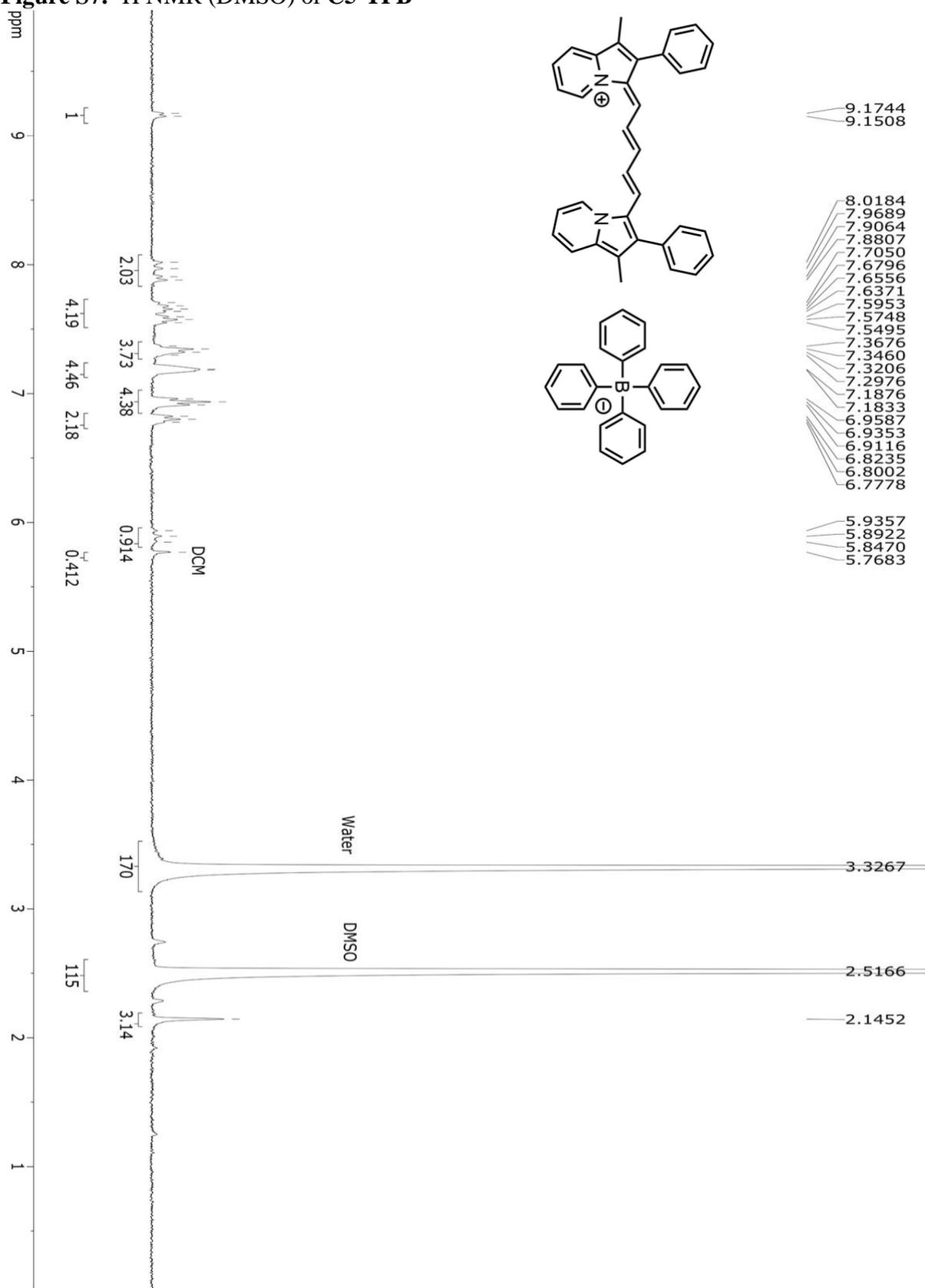


Figure S7. <sup>1</sup>H NMR (DMSO) of C5-TPB



**Figure S8.**  $^1\text{H}$  NMR (DMSO) of C5-BARF

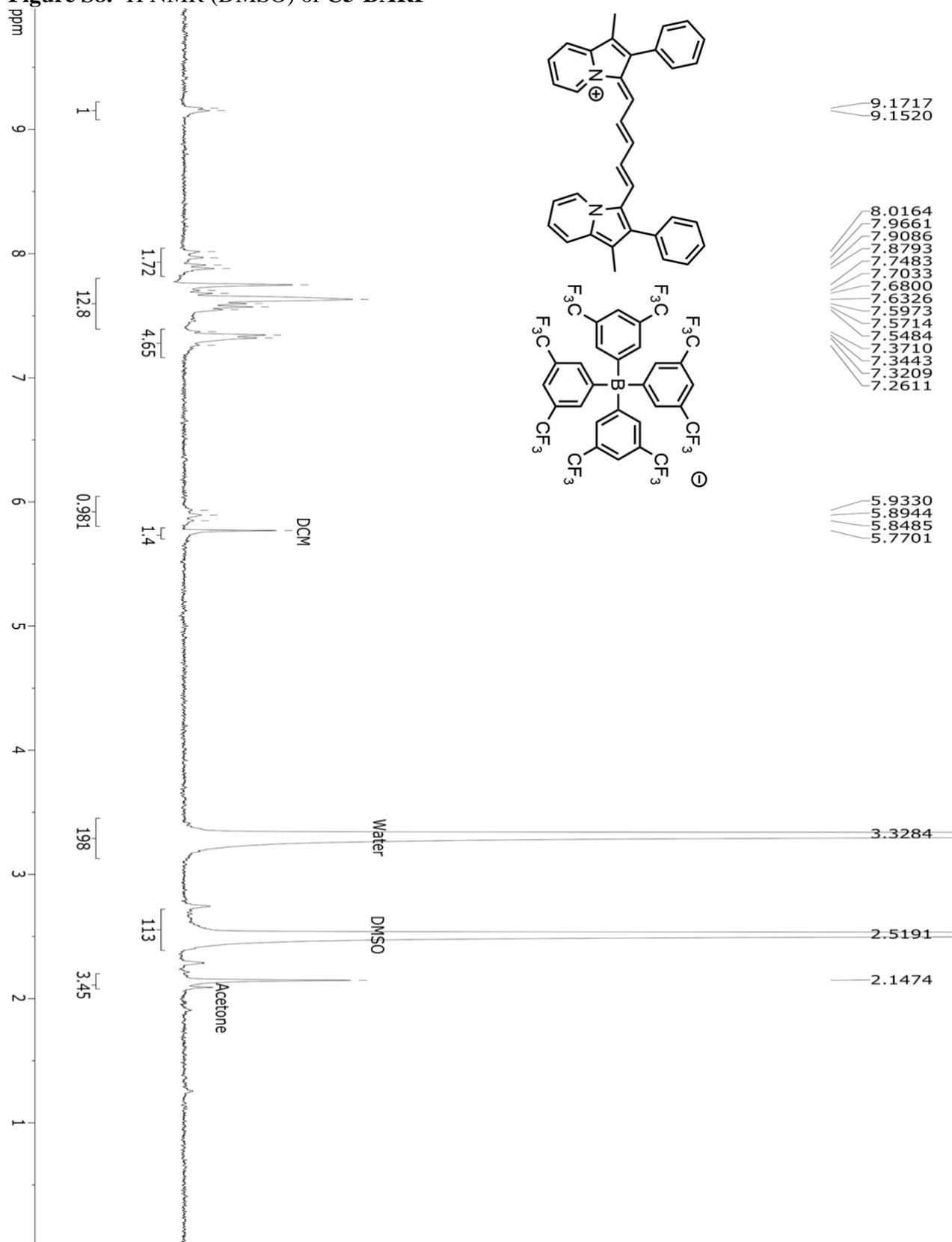
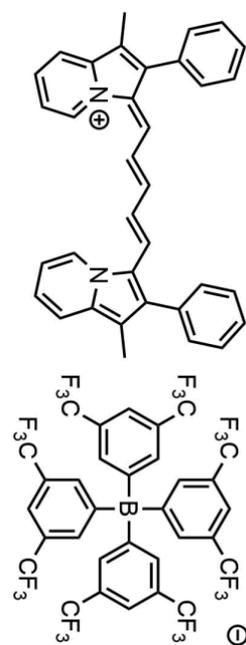
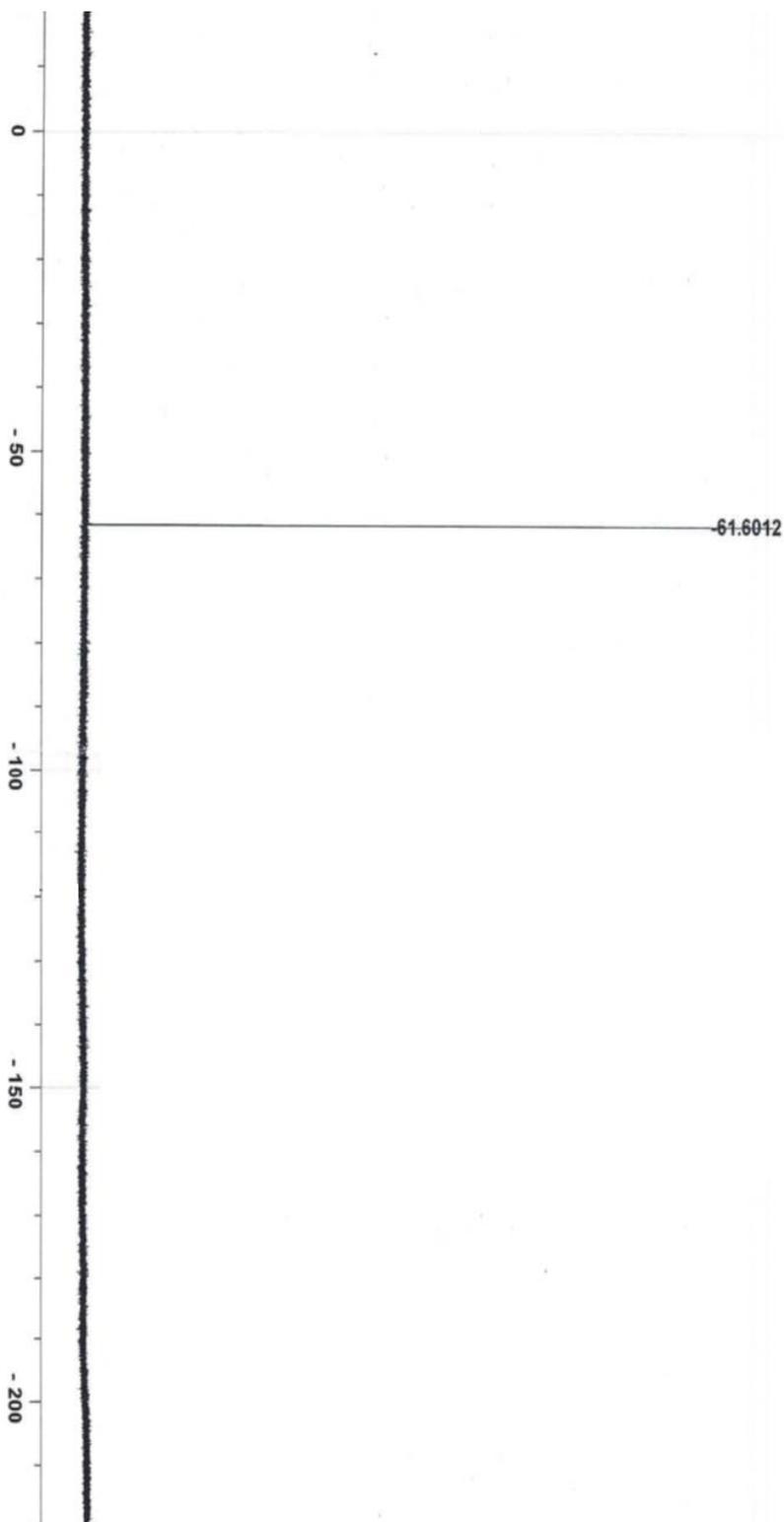
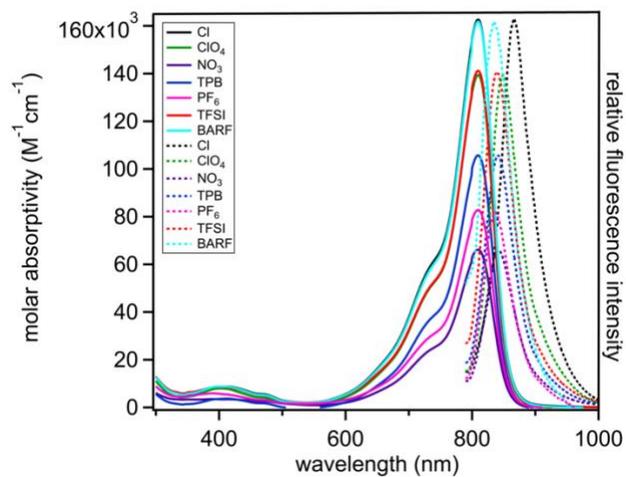
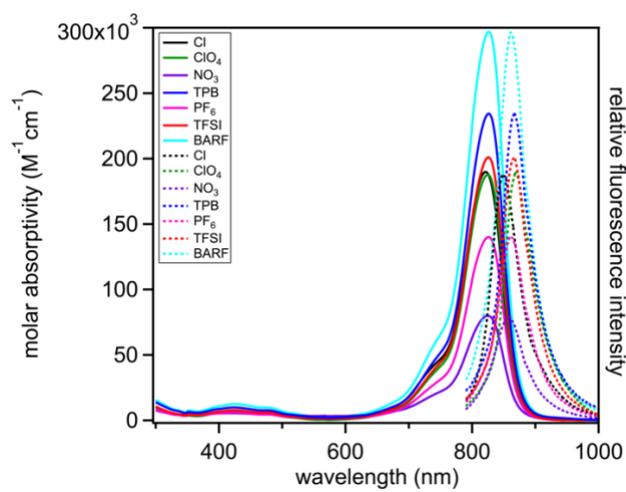


Figure S9.  $^{19}\text{F}$  NMR (DMSO) of C5-BARF

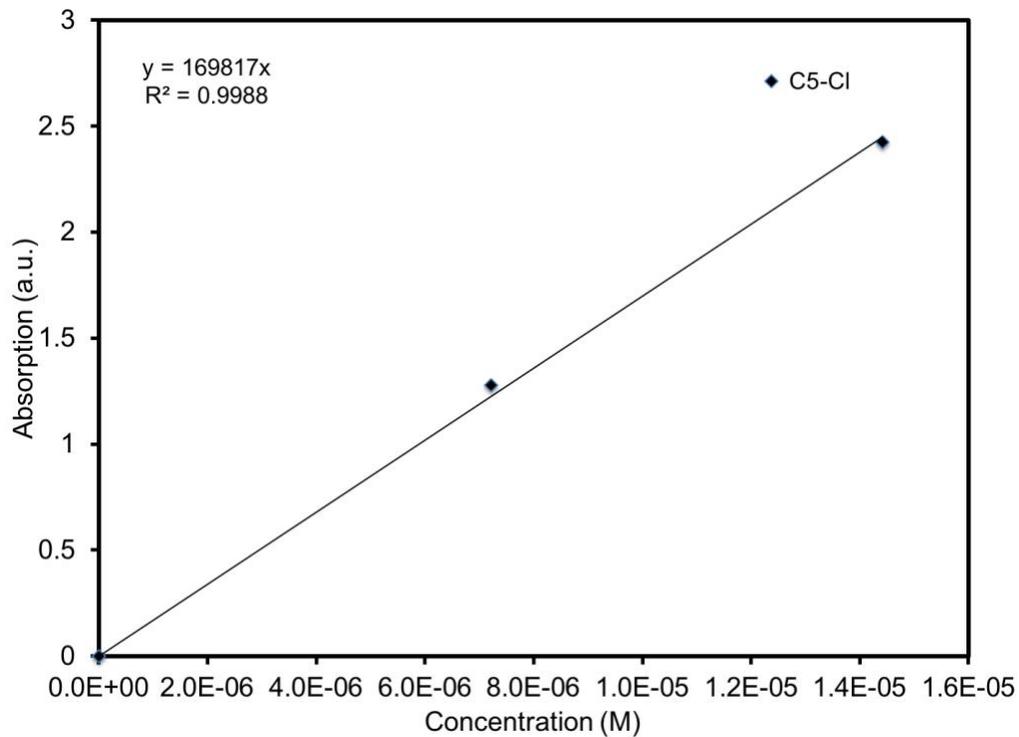




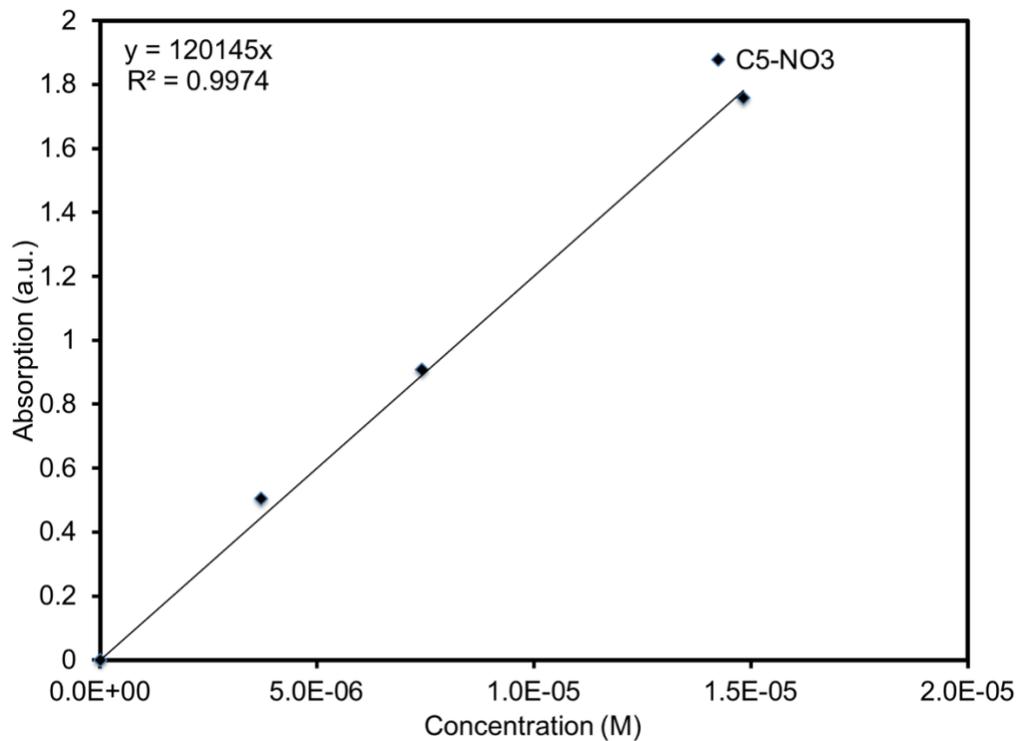
**Figure S10.** Full spectrum (300-1000 nm) of molar absorptivity and emission plot in MeCN.



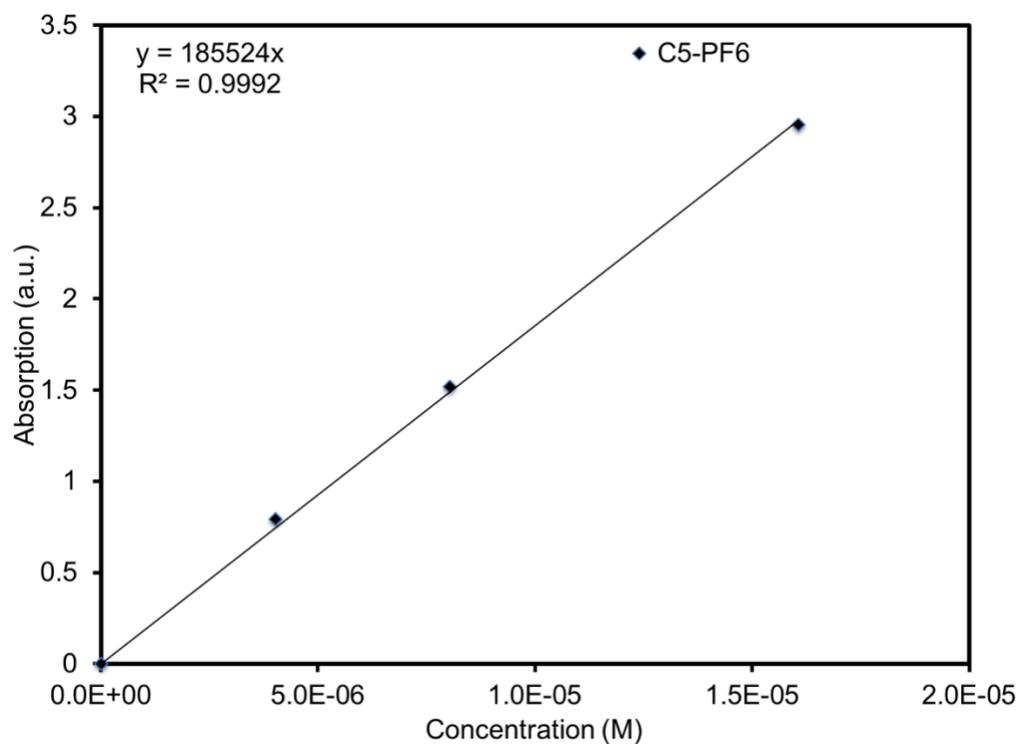
**Figure S11.** Full spectrum (300-1000 nm) of molar absorptivity and emission plot in DCM.



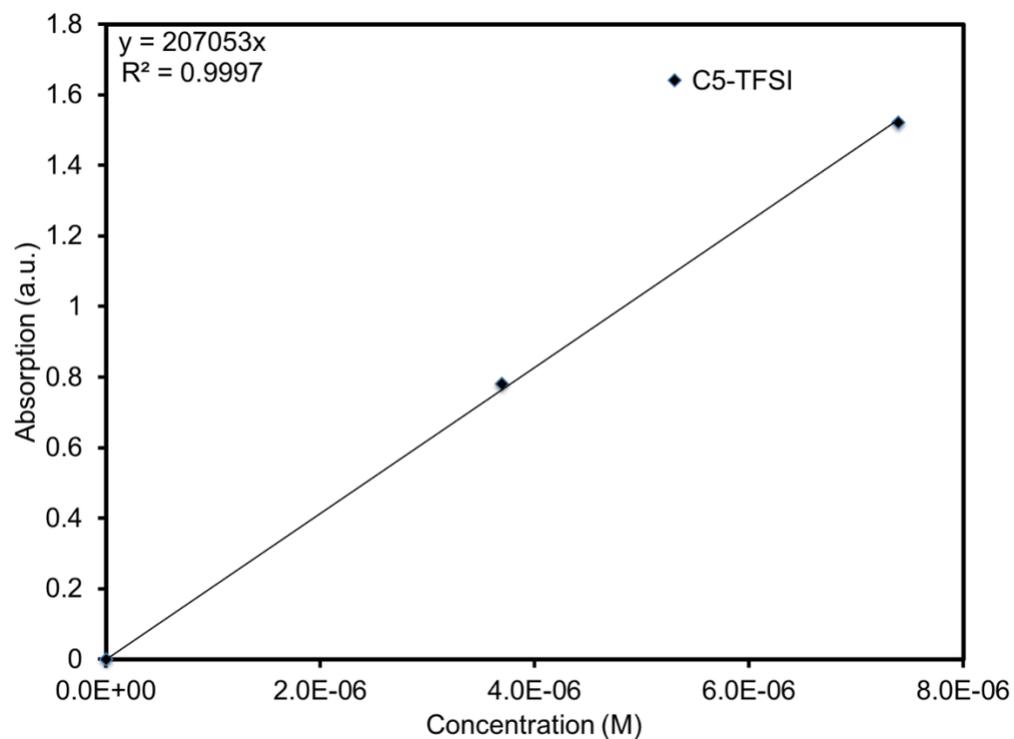
**Figure S12.** Concentration versus absorbance plot for **C5-Cl** in DCM.



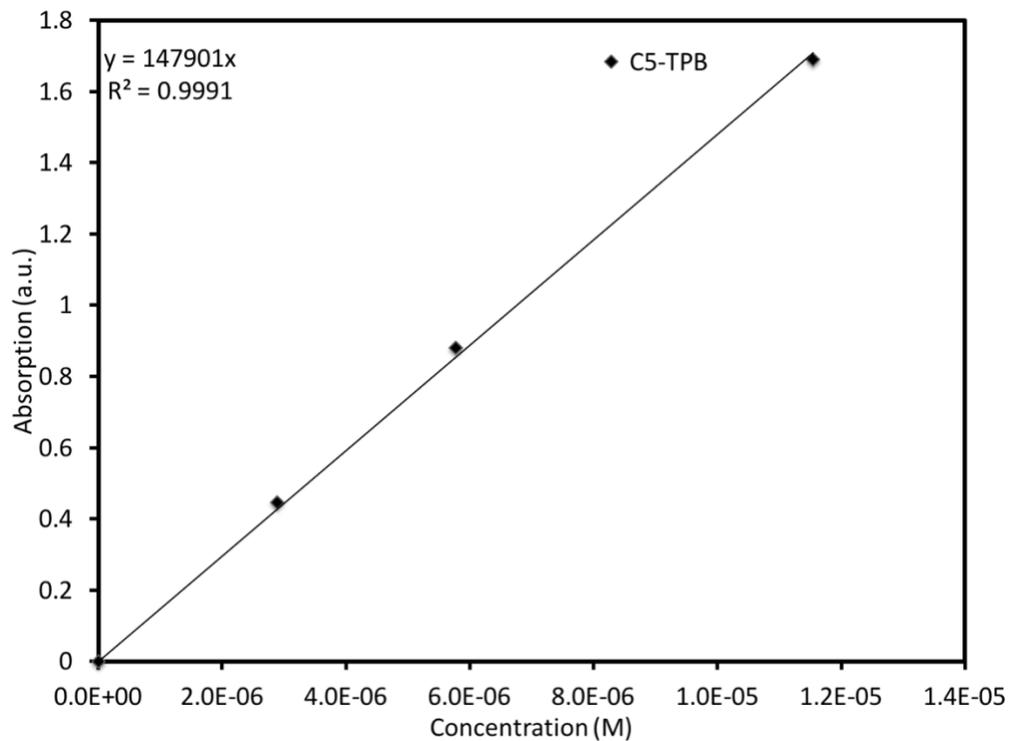
**Figure S13.** Concentration versus absorbance plot for **C5-NO<sub>3</sub>** in DCM.



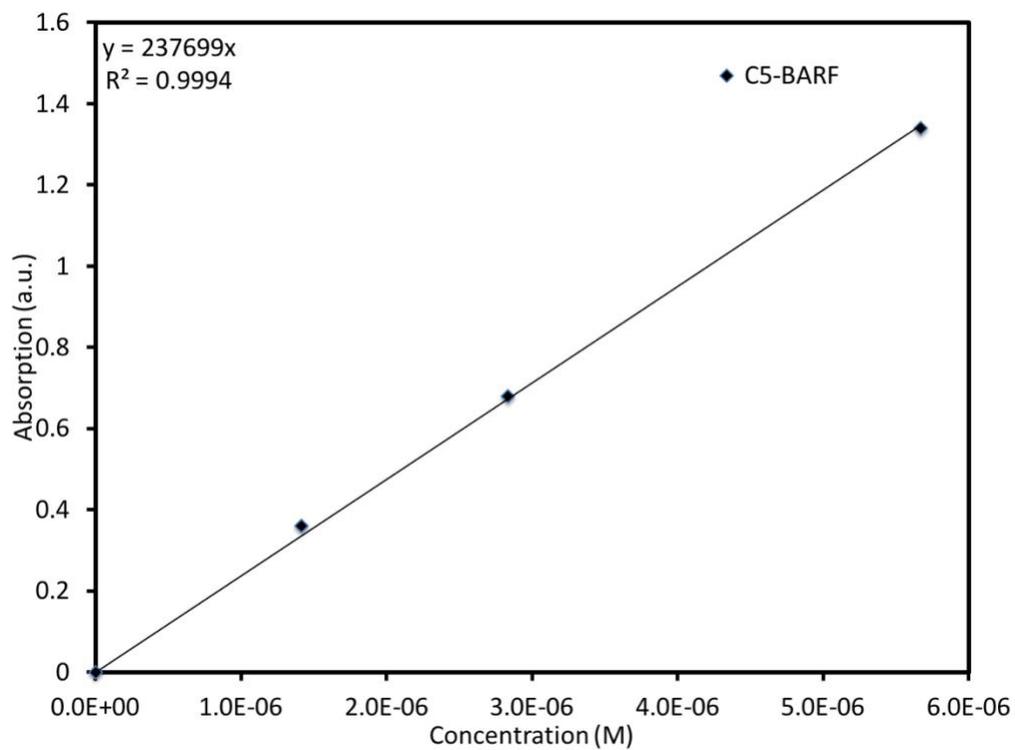
**Figure S14.** Concentration versus absorbance plot for **C5-PF<sub>6</sub>** in DCM.



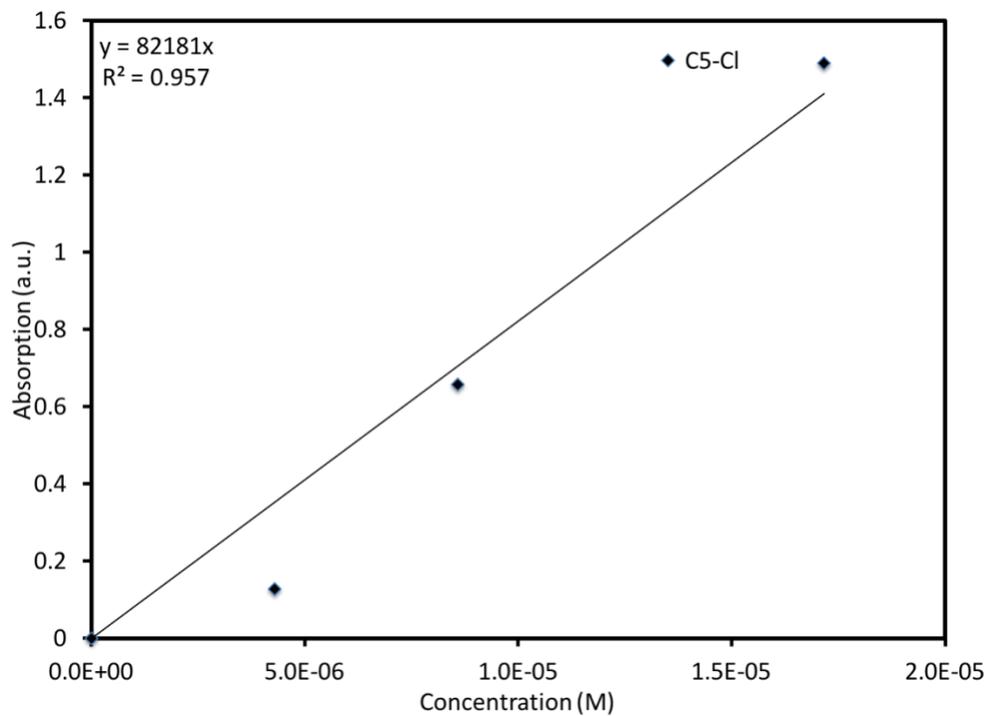
**Figure S15.** Concentration versus absorbance plot for **C5-TFSI** in DCM.



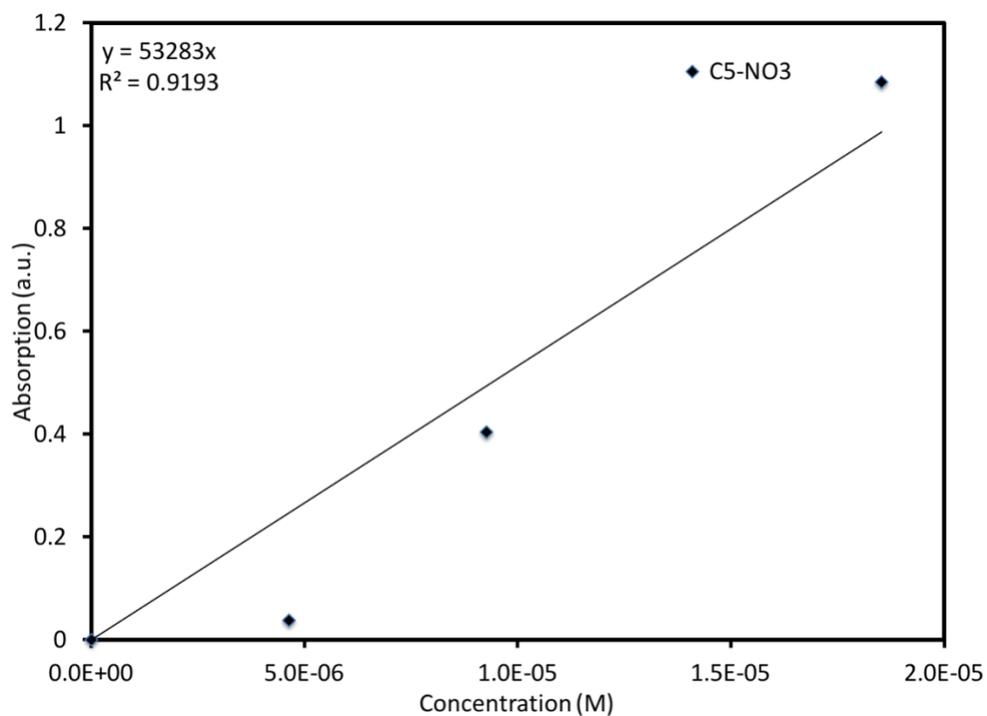
**Figure S16.** Concentration versus absorbance plot for **C5-TPB** in DCM.



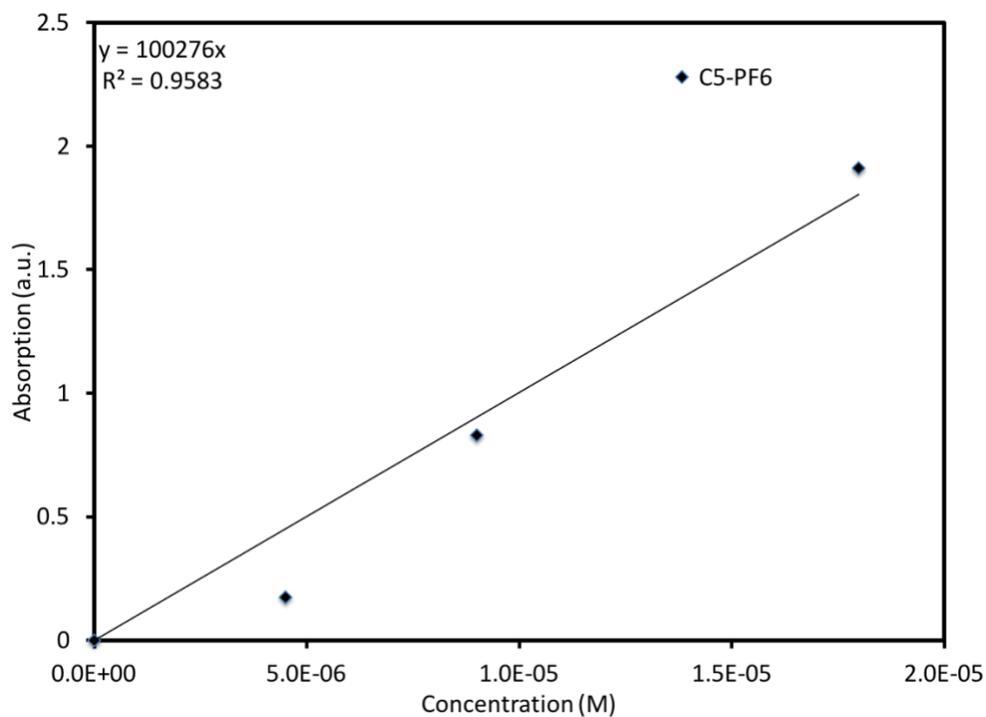
**Figure S17.** Concentration versus absorbance plot for **C5-BARF** in DCM.



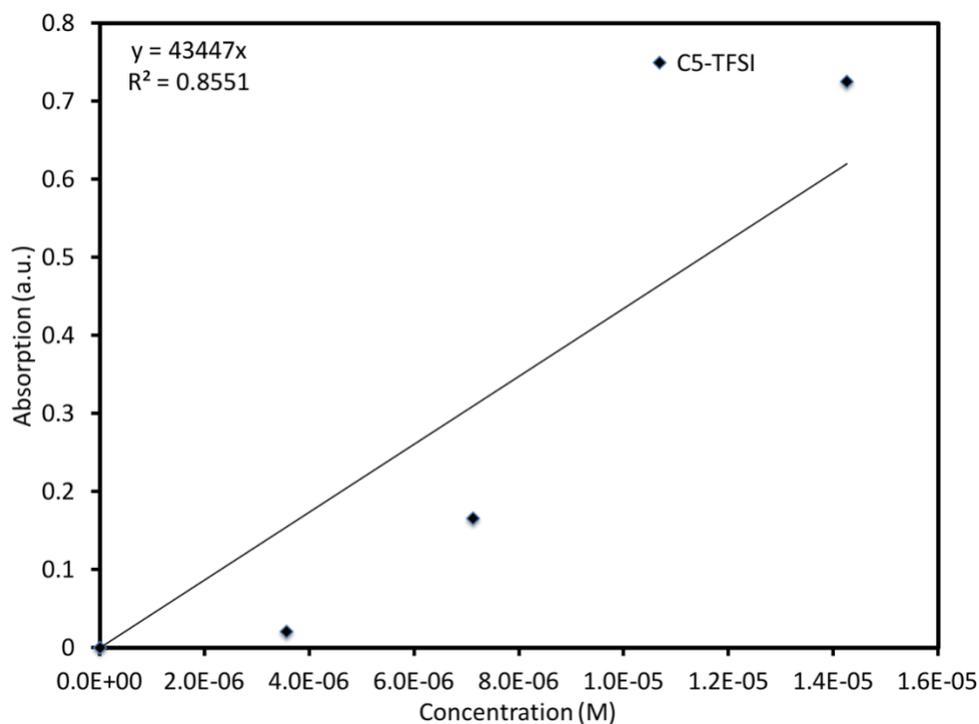
**Figure S18.** Concentration versus absorbance plot for **C5-Cl** in MeCN. A positive deviation from the Beer-Lambert Law is observed.



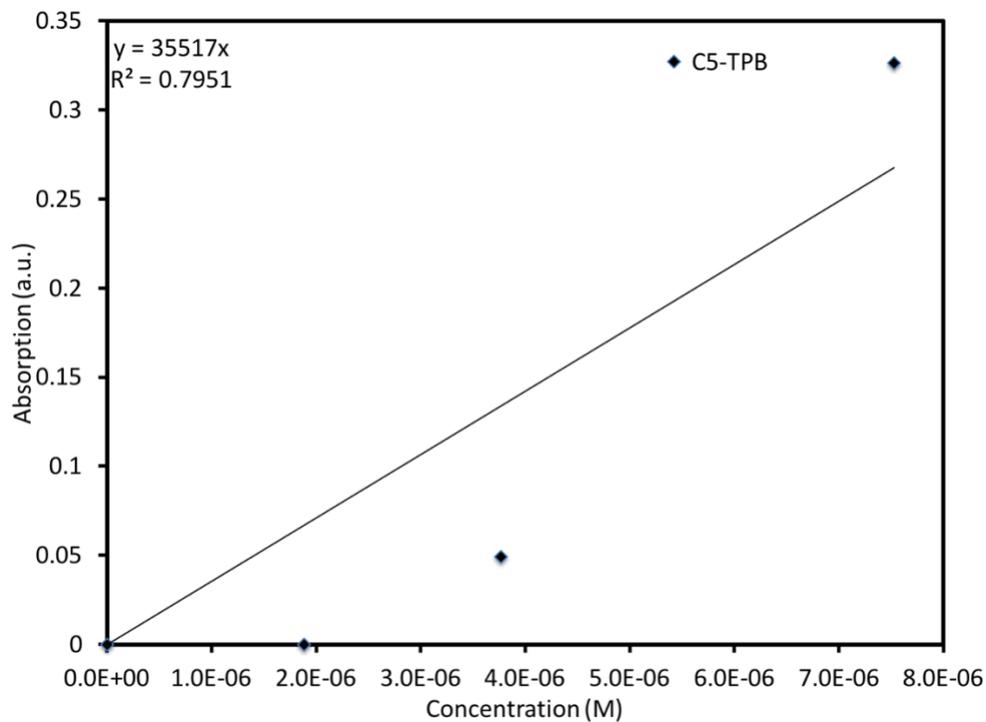
**Figure S19.** Concentration versus absorbance plot for **C5-NO<sub>3</sub>** in MeCN. A positive deviation from the Beer-Lambert Law is observed.



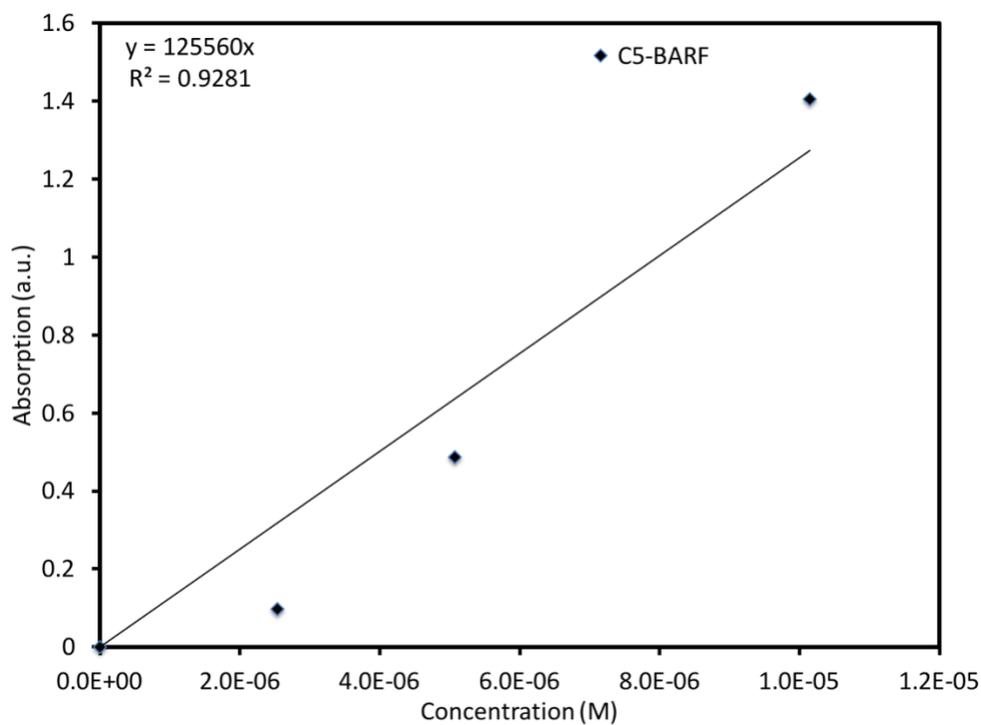
**Figure S20.** Concentration versus absorbance plot for **C5-PF<sub>6</sub>** in MeCN. A positive deviation from the Beer-Lambert Law is observed.



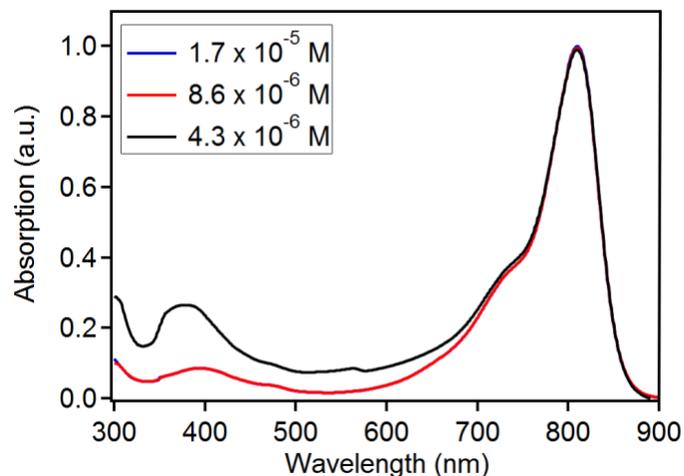
**Figure S21.** Concentration versus absorbance plot for **C5-TFSI** in MeCN. A positive deviation from the Beer-Lambert Law is observed.



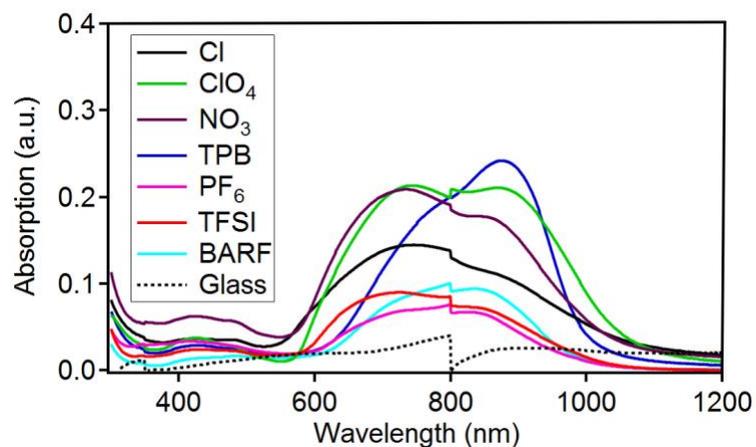
**Figure S22.** Concentration versus absorbance plot for **C5-TPB** in MeCN. A positive deviation from the Beer-Lambert Law is observed.



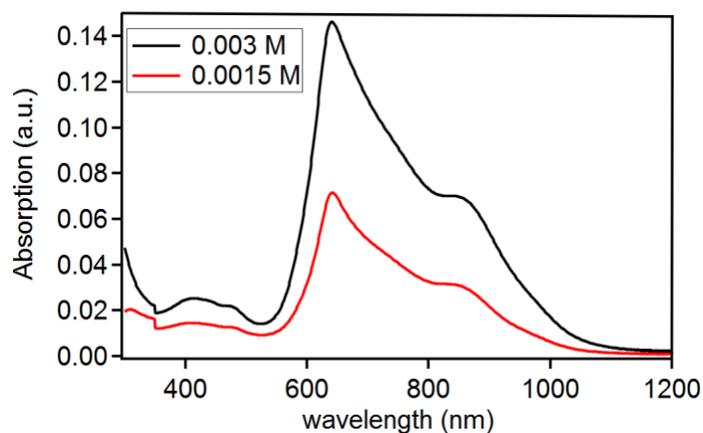
**Figure S23.** Concentration versus absorbance plot for **C5-BARF** in MeCN. A positive deviation from the Beer-Lambert Law is observed.



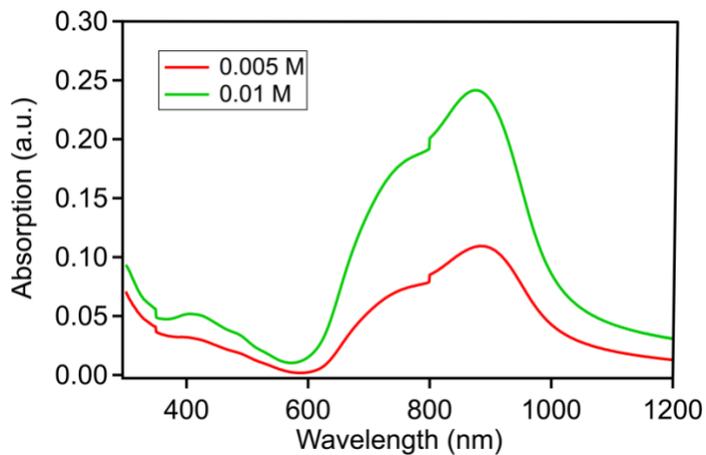
**Figure S24.** Absorption spectrum of varying concentrations of C5-Cl in MeCN showing a change in features as concentration changes.



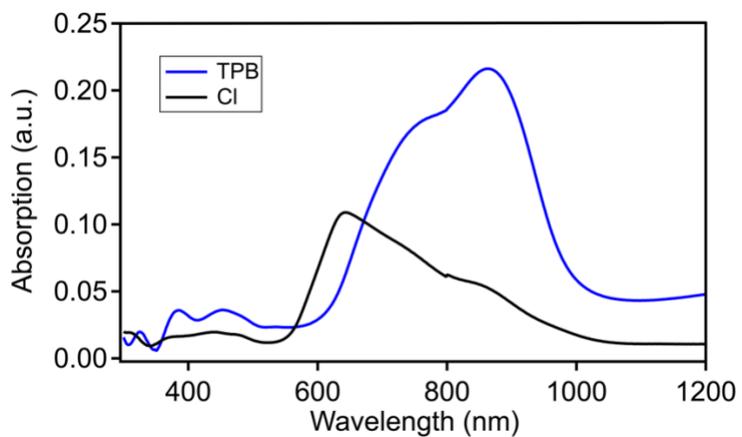
**Figure S25.** Raw film absorption spectrum not normalized. The blank glass absorption spectrum with no dye is shown for comparison.



**Figure S26.** Film absorption with C5-Cl on glass prepared with varying concentrations of the dye.



**Figure S27.** Film absorption with **C5-TPB** on glass prepared with varying concentrations of the dye.



**Figure S28.** Film absorption with **C5-TPB** and **C5-Cl** on fluorine doped tin oxide (FTO).