

## Supplementary Materials

# A Comparison of the Photophysical and Electrochemical Properties of *meso*-(2-, 3- and 4-Pyridyl)-BODIPYs and Their Derivatives

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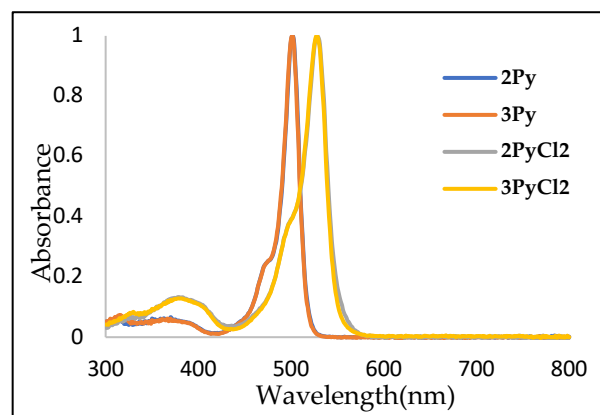
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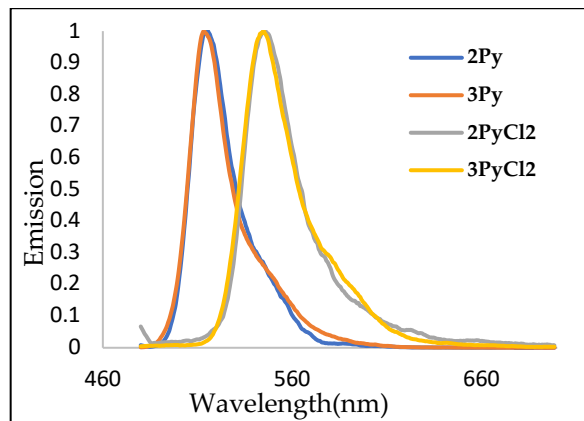
**Table S1.** Relative fluorescence quantum yields determined using rhodamine-6G ( $\Phi=0.86$ ) in methanol,  $\lambda_{\text{exc}}=473\text{nm}$

Solvent	BODIPY	$\lambda_{\text{abs}}$ (nm)	$\lambda_{\text{em}}$ (nm)	Stokes Shift (nm)	$\Phi_f$	$\epsilon$ ( $\text{M}^{-1} \text{cm}^{-1}$ )
CH <sub>3</sub> OH	2Py	504	514	10	0.13	119800
	3Py	503	515	12	0.34	98140
	2PyCl <sub>2</sub>	531	548	17	0.23	69940
	3PyCl <sub>2</sub>	530	546	16	0.57	66880

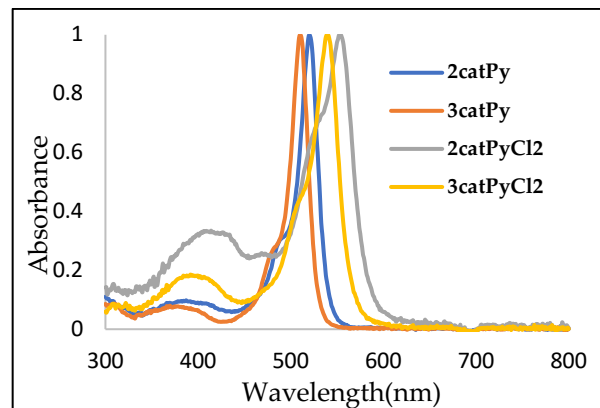
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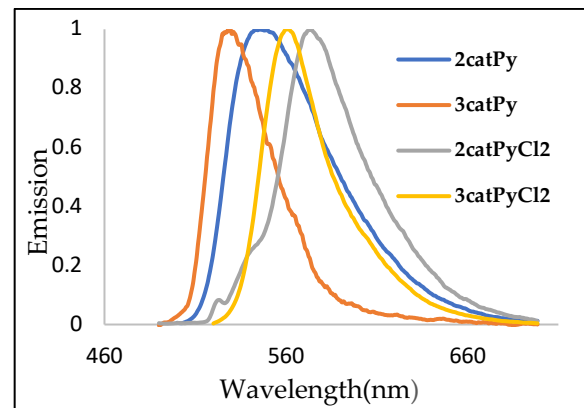
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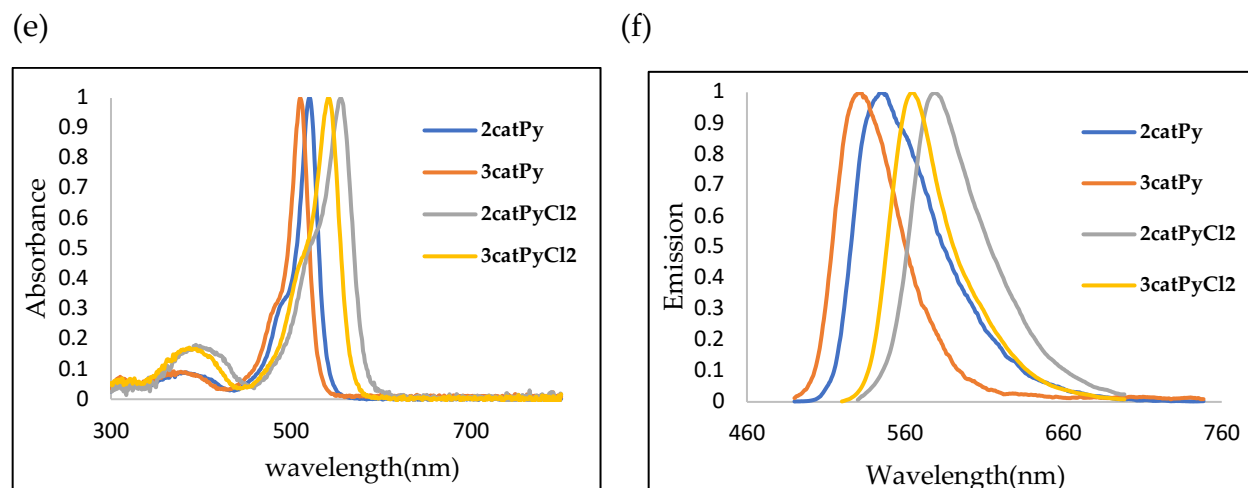


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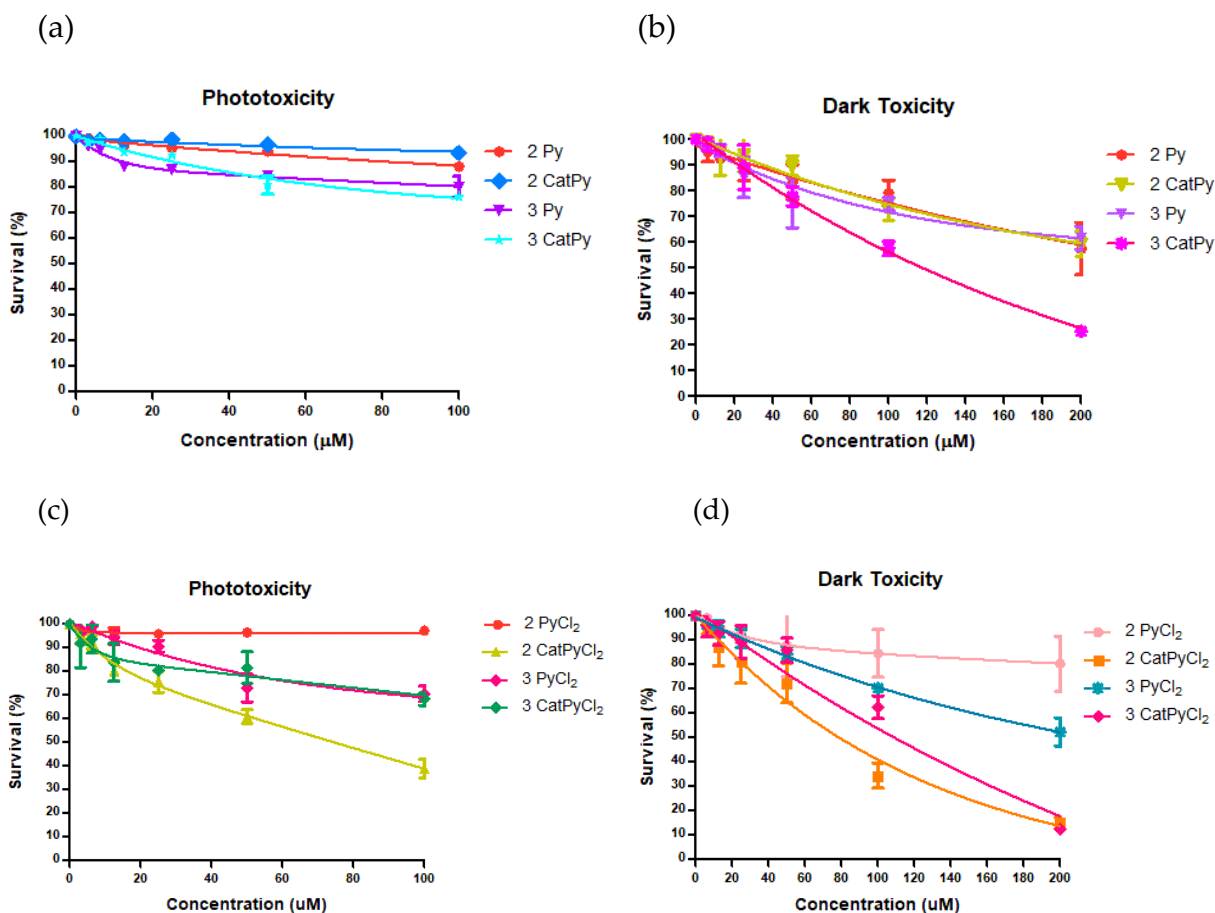


(d)



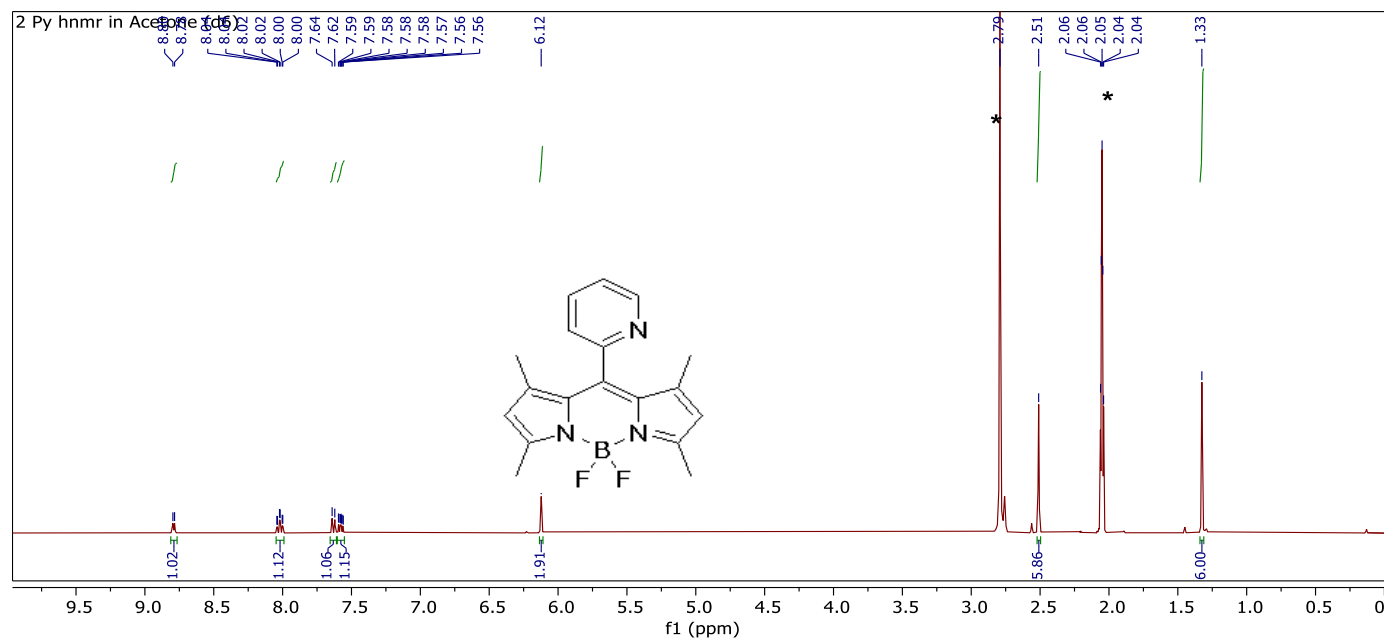


**Figure S1.** Normalized absorption (a, c, e) and emission (b, d, f) spectra of BODIPYs in acetonitrile (a, b, c, d) and water (e, f).

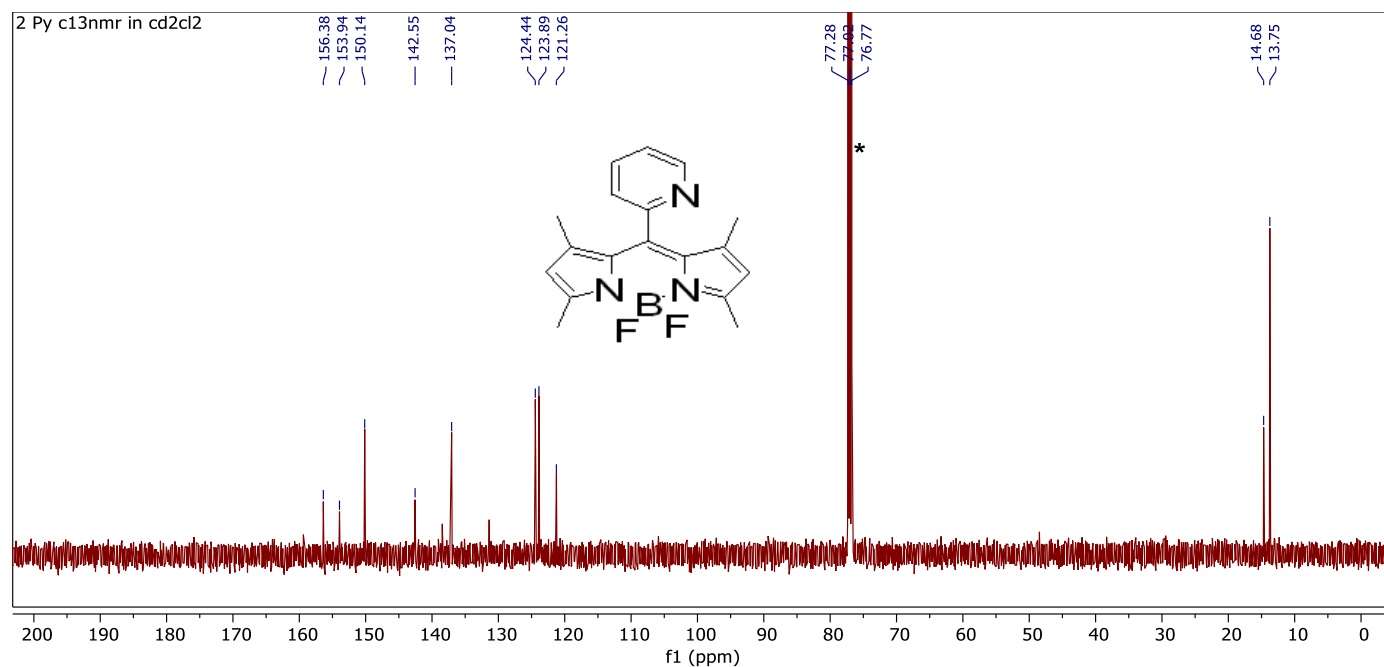


**Figure S2.** Dark (b, d) and photo (a, c) ( $1.5 \text{ J/cm}^2$ ) cytotoxicity of BODIPYs towards HEp2 cells.

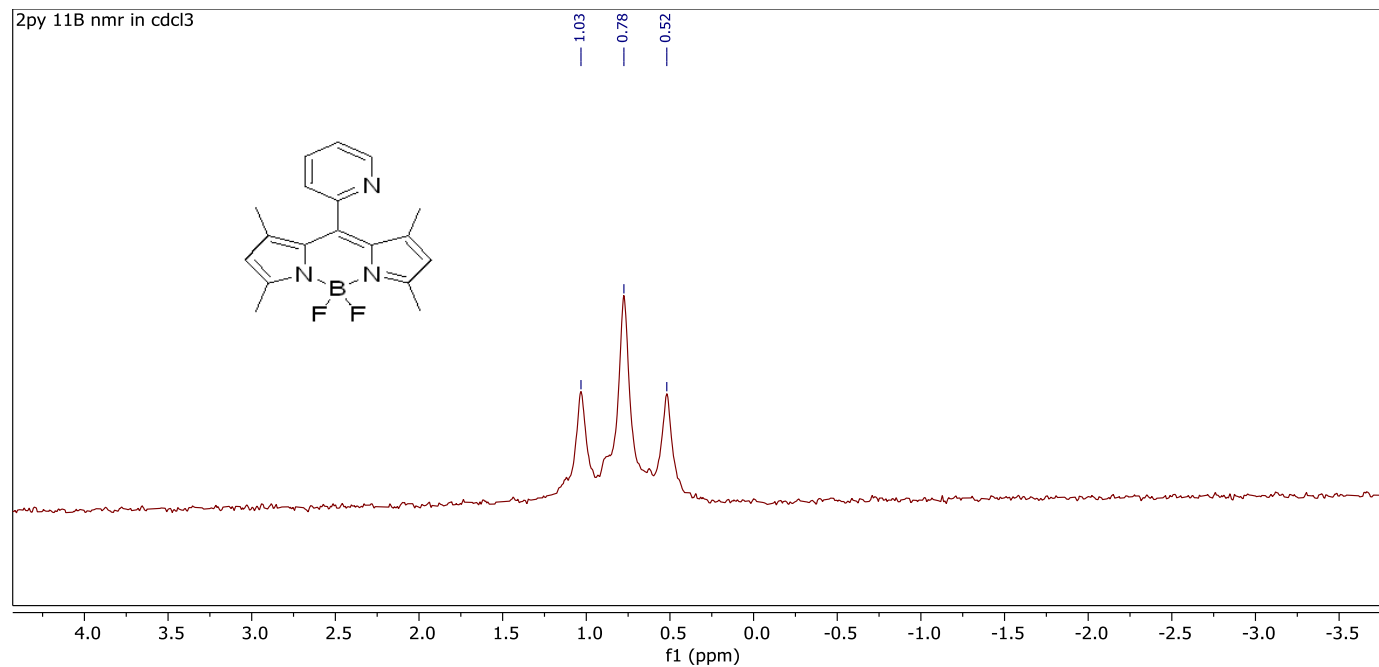
# NMR



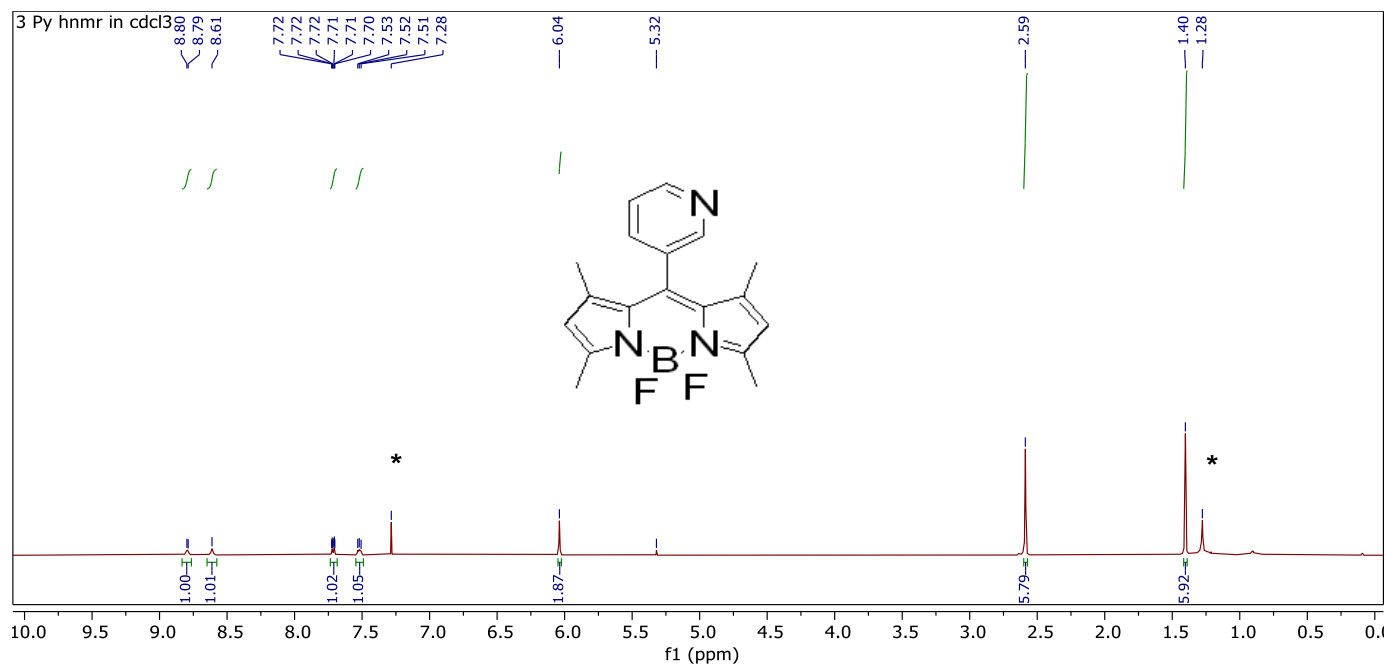
**Figure S3.** <sup>1</sup>H NMR of BODIPY 2Py in acetone-d<sub>6</sub>



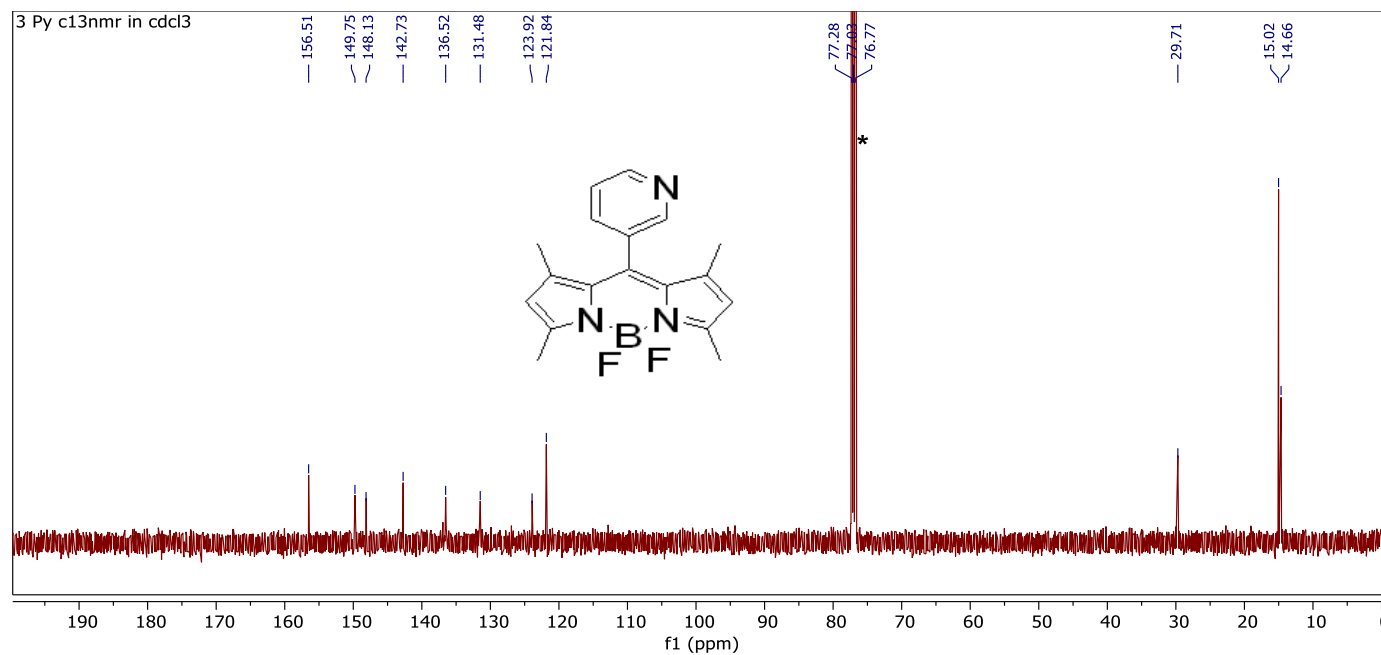
**Figure S4.** <sup>13</sup>C NMR of BODIPY 2Py in CDCl<sub>3</sub>



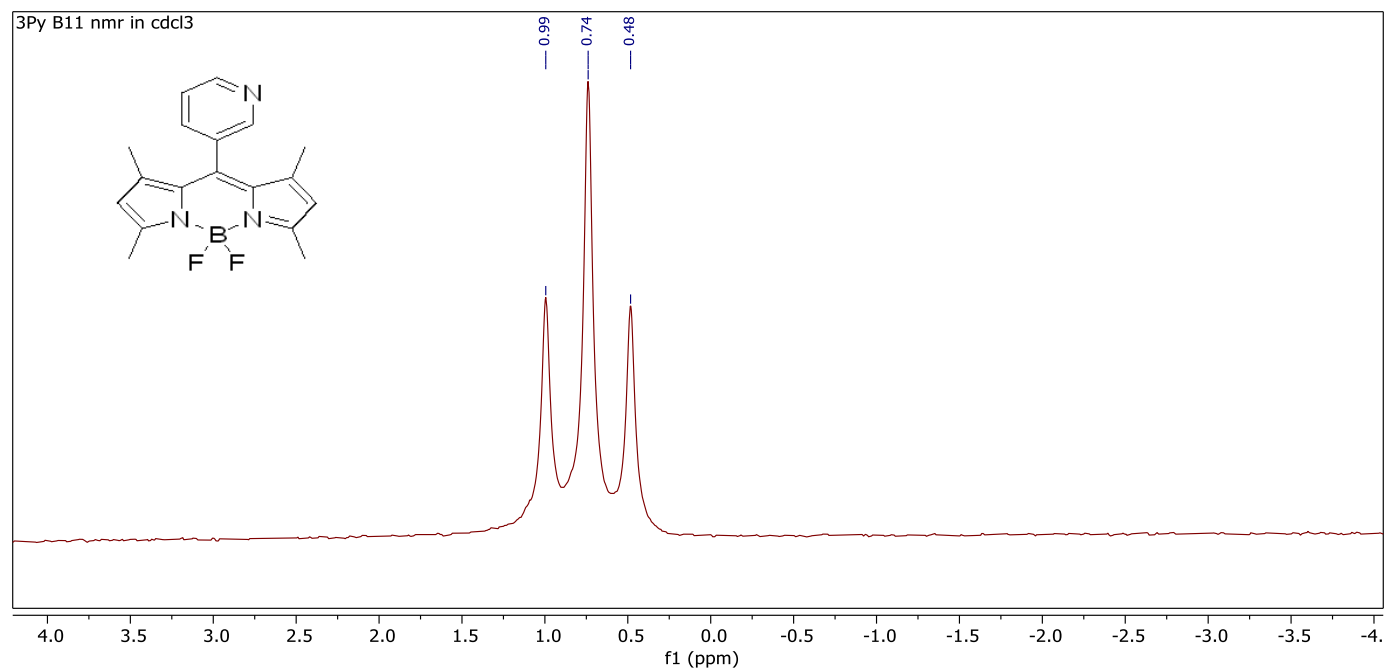
**Figure S5.**  $^{11}\text{B}$  NMR of BODIPY 2Py in  $\text{CDCl}_3$



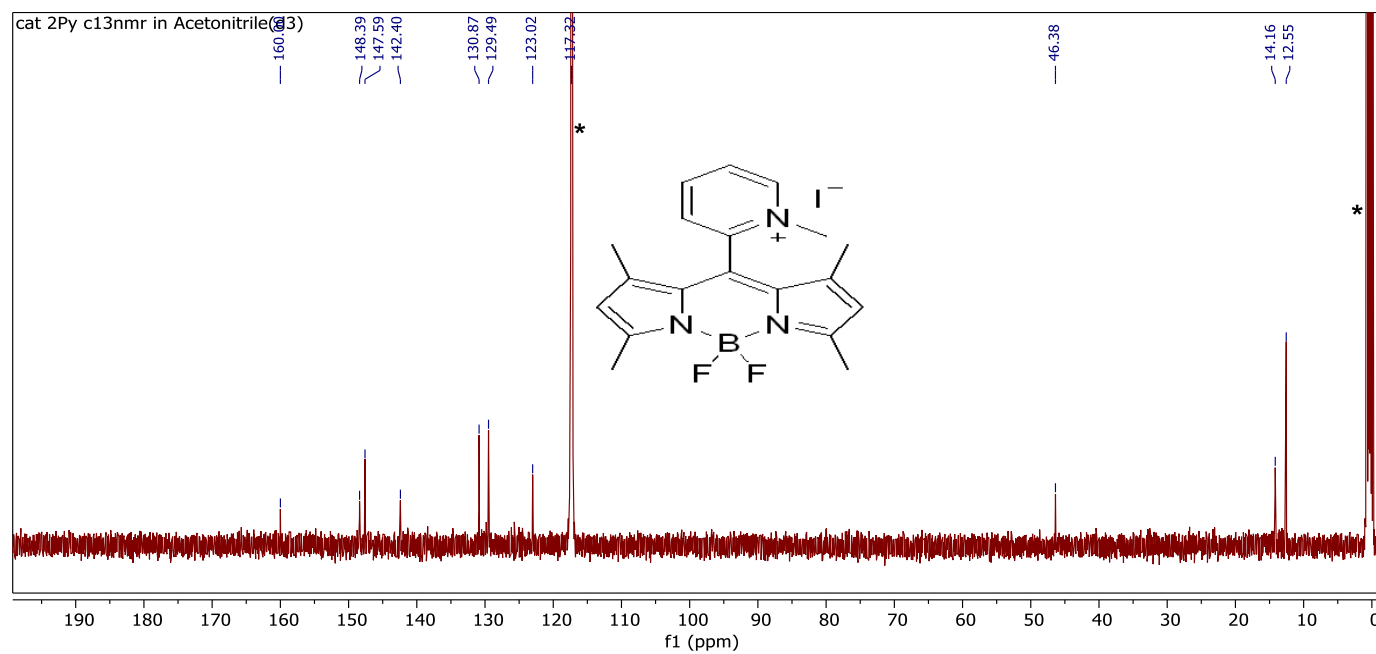
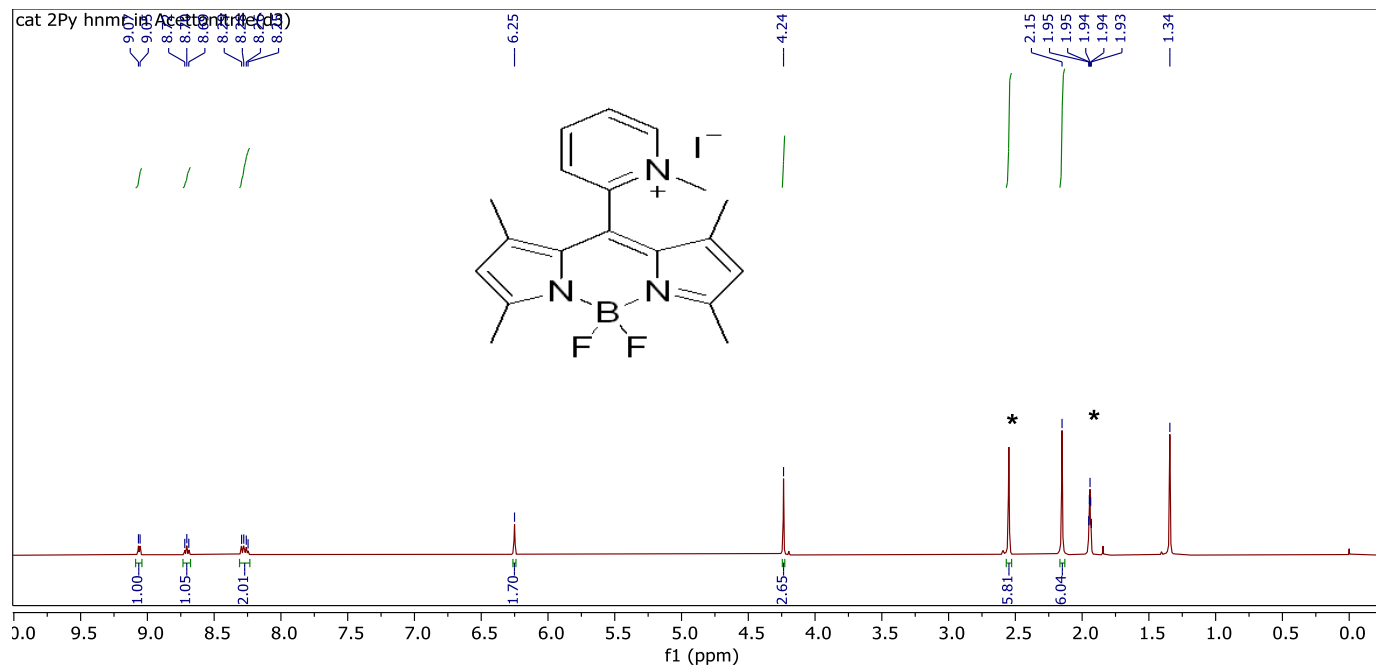
**Figure S6.**  $^1\text{H}$  NMR of BODIPY 3Py in  $\text{CDCl}_3$

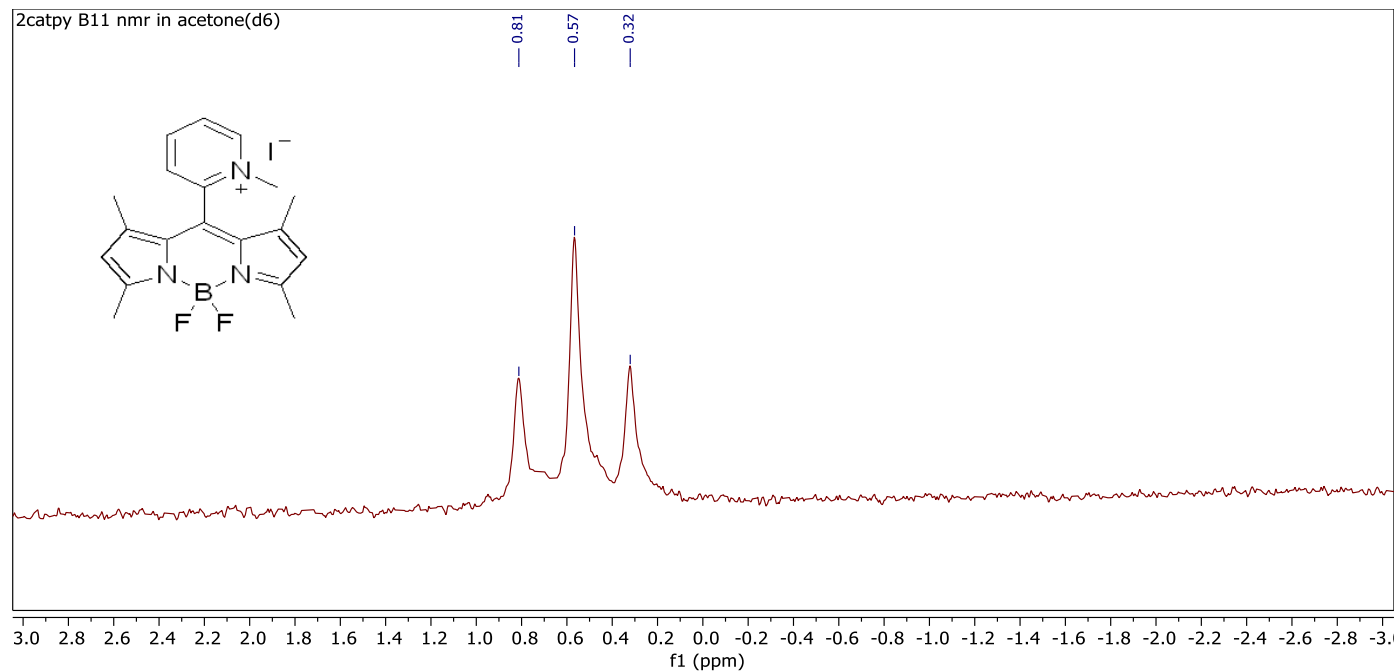


**Figure S7.**  $^{13}\text{C}$  NMR of BODIPY 3Py in  $\text{CDCl}_3$

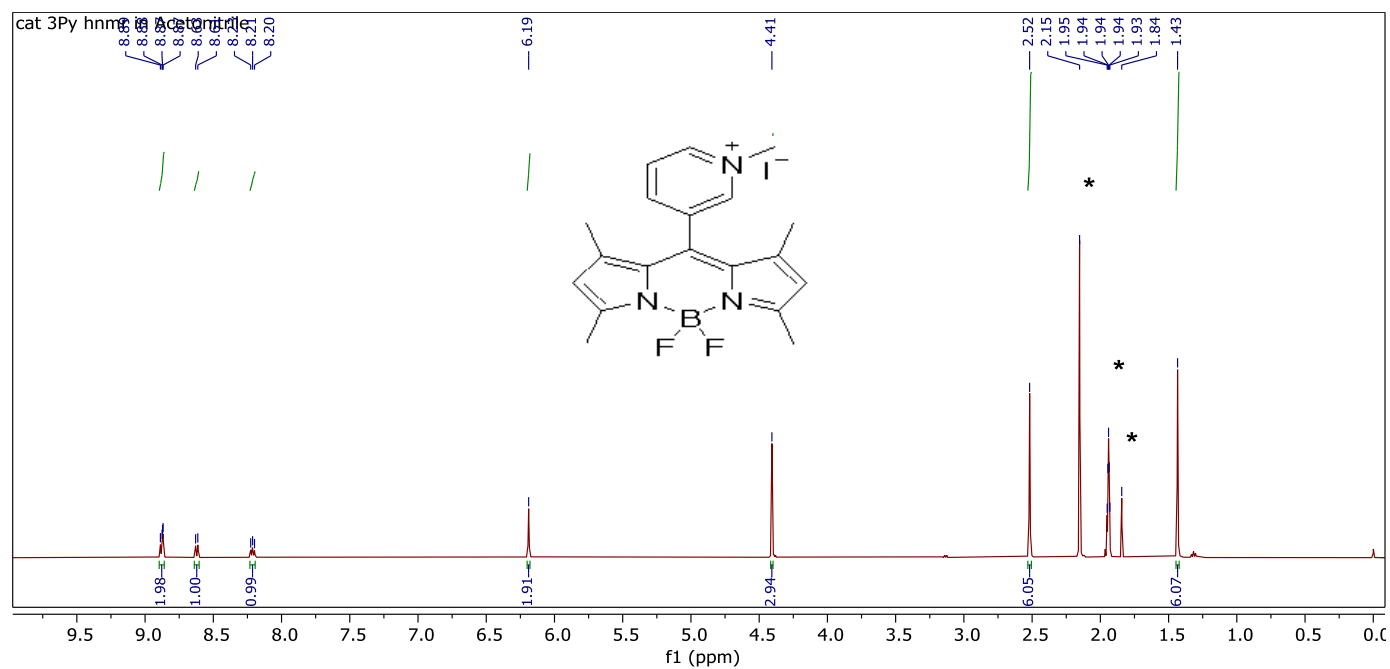


**Figure S8.**  $^{11}\text{B}$  NMR of BODIPY 3Py in  $\text{CDCl}_3$



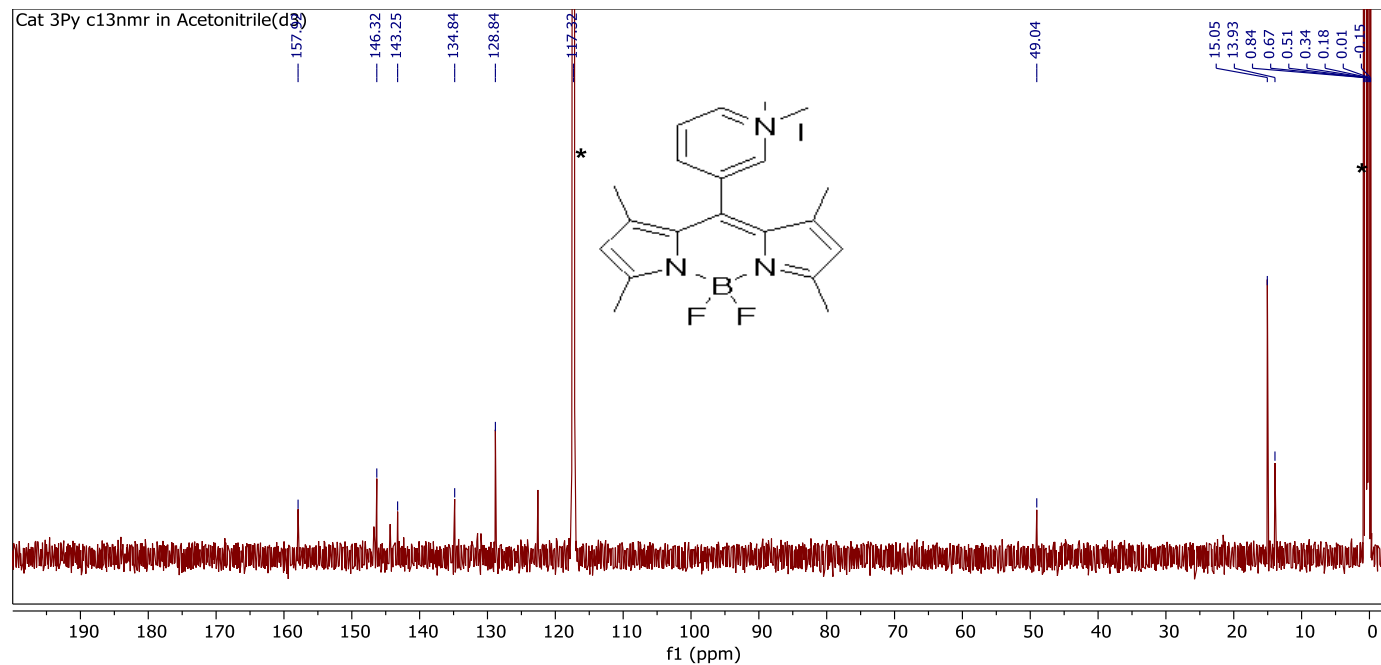


**Figure S11.**  $^{11}\text{B}$  NMR of BODIPY 2catPy in acetone- $\text{d}_6$

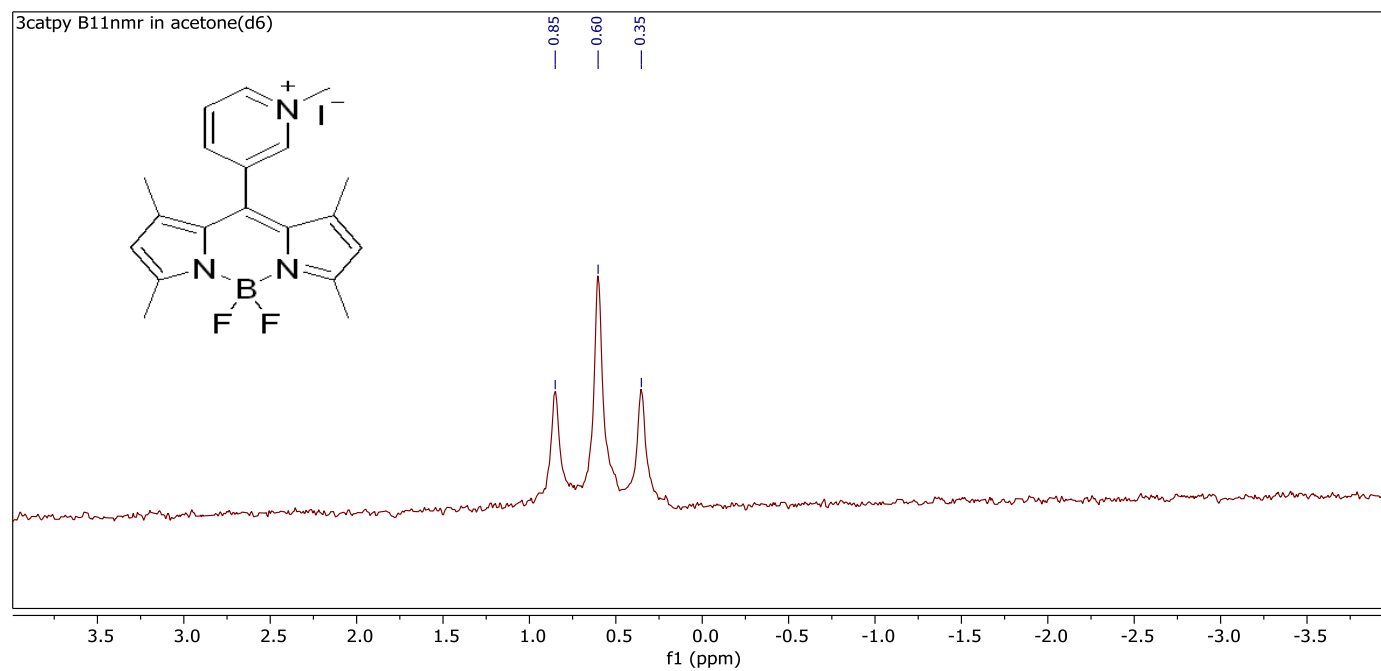


**Figure S12.**  $^1\text{H}$  NMR of BODIPY 3catPy in acetone- $\text{d}_6$

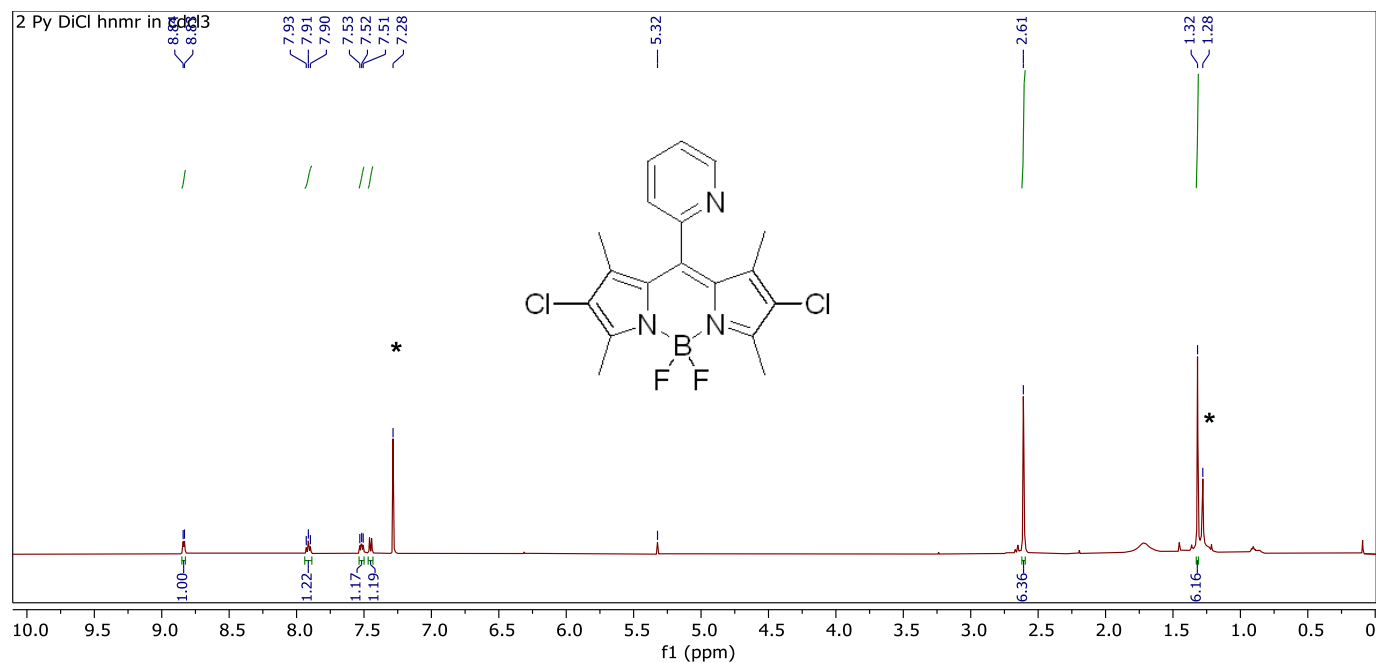




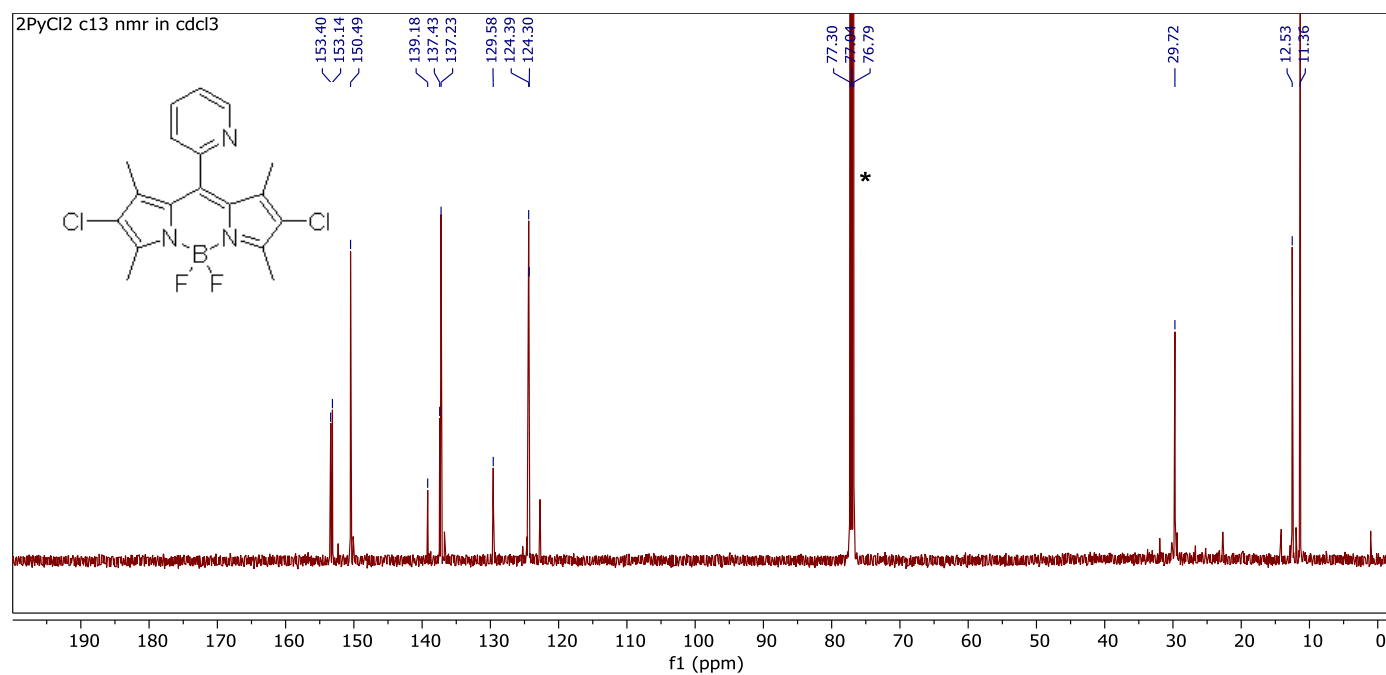
**Figure S13.**  $^{13}\text{C}$  NMR of BODIPY 3catPy in acetonitrile- $\text{d}_3$



**Figure S14.**  $^{11}\text{B}$  NMR of BODIPY 3catPy in acetone- $\text{d}_6$



**Figure S15.** <sup>1</sup>H NMR of BODIPY 2PyCl<sub>2</sub> in CDCl<sub>3</sub>



**Figure S16.** <sup>13</sup>C NMR of BODIPY 2PyCl<sub>2</sub> in CDCl<sub>3</sub>

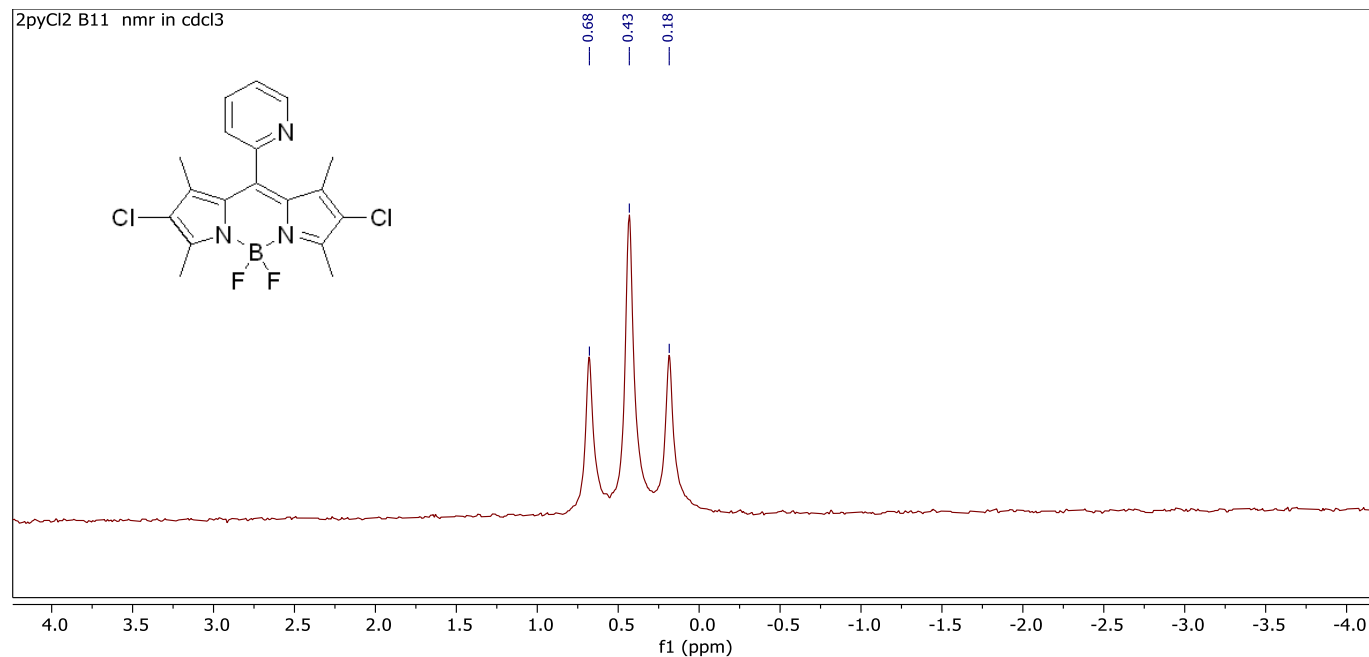


Figure S17. <sup>11</sup>B NMR of BODIPY 2PyCl<sub>2</sub> in CDCl<sub>3</sub>

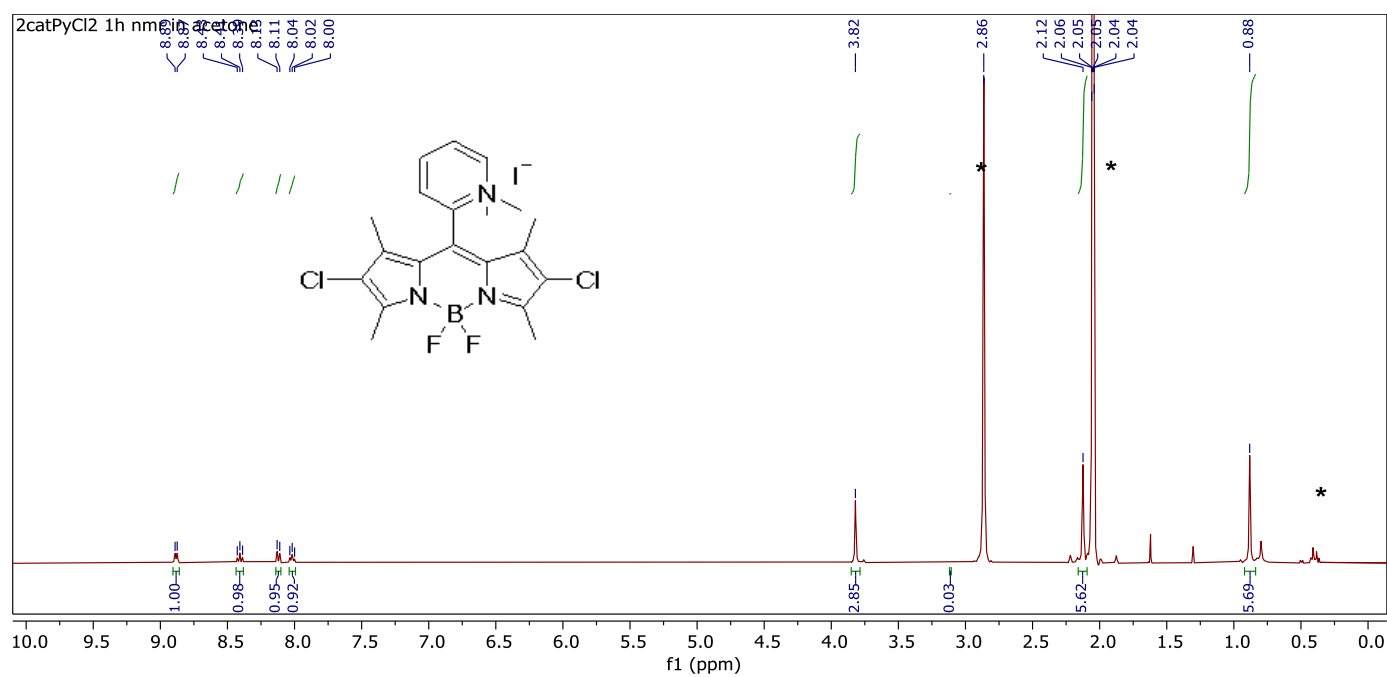
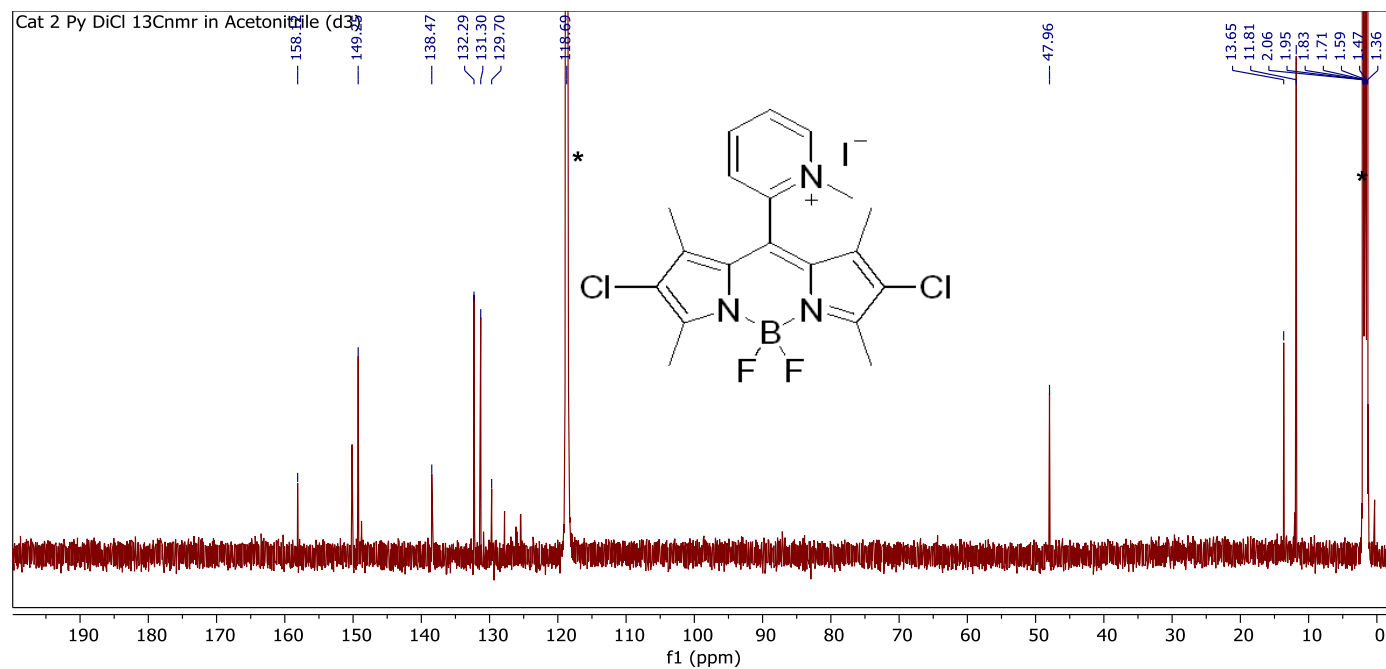
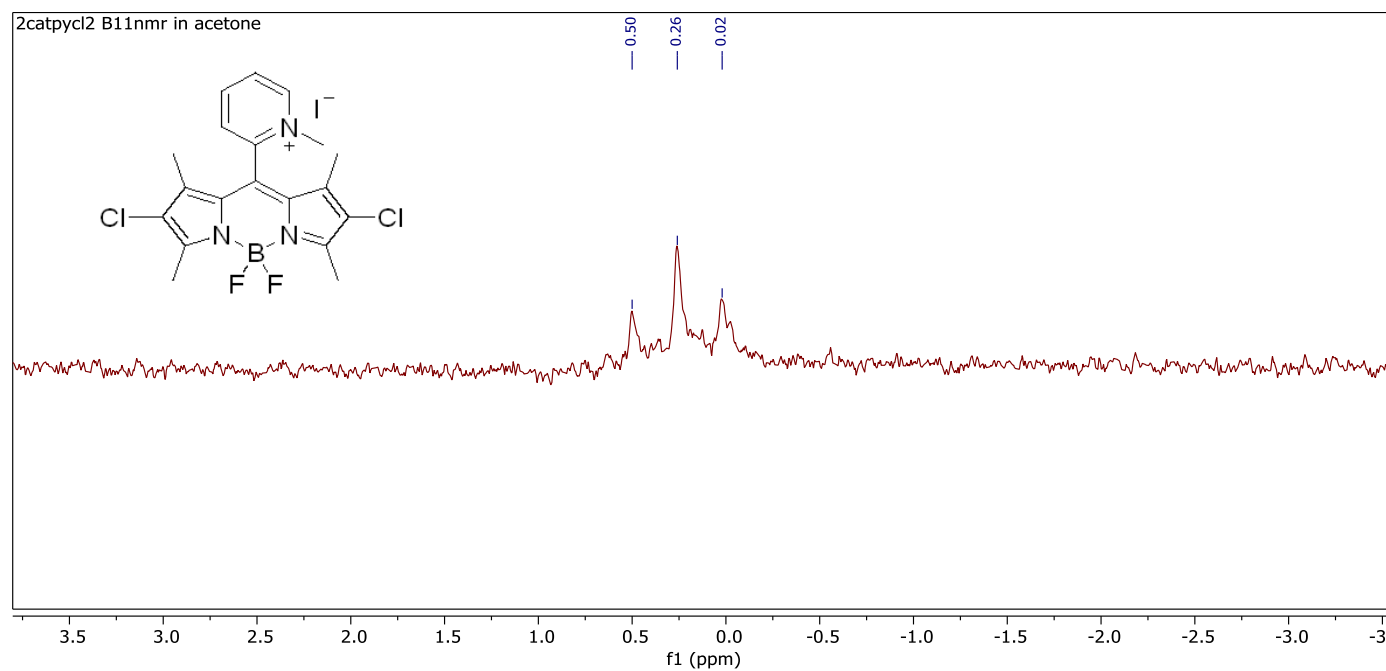


Figure S18. <sup>1</sup>H NMR of BODIPY 2catPyCl<sub>2</sub> in acetone-d<sub>6</sub>



**Figure S19.** <sup>13</sup>C NMR of BODIPY 2catPyCl<sub>2</sub> in acetonitrile-d<sub>3</sub>



**Figure S20.** <sup>11</sup>B NMR of BODIPY 2catPyCl<sub>2</sub> in acetone-d<sub>6</sub>

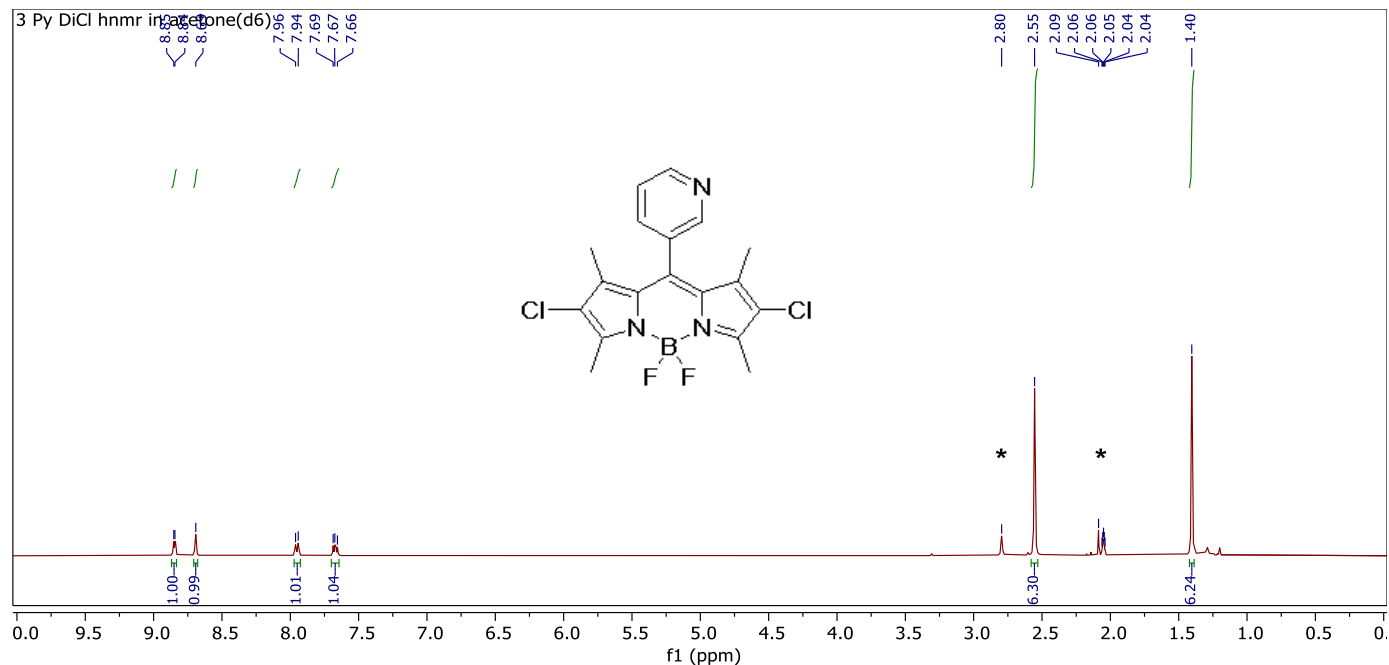


Figure S21. <sup>1</sup>H NMR of BODIPY 3PyCl<sub>2</sub> in acetone-d<sub>6</sub>

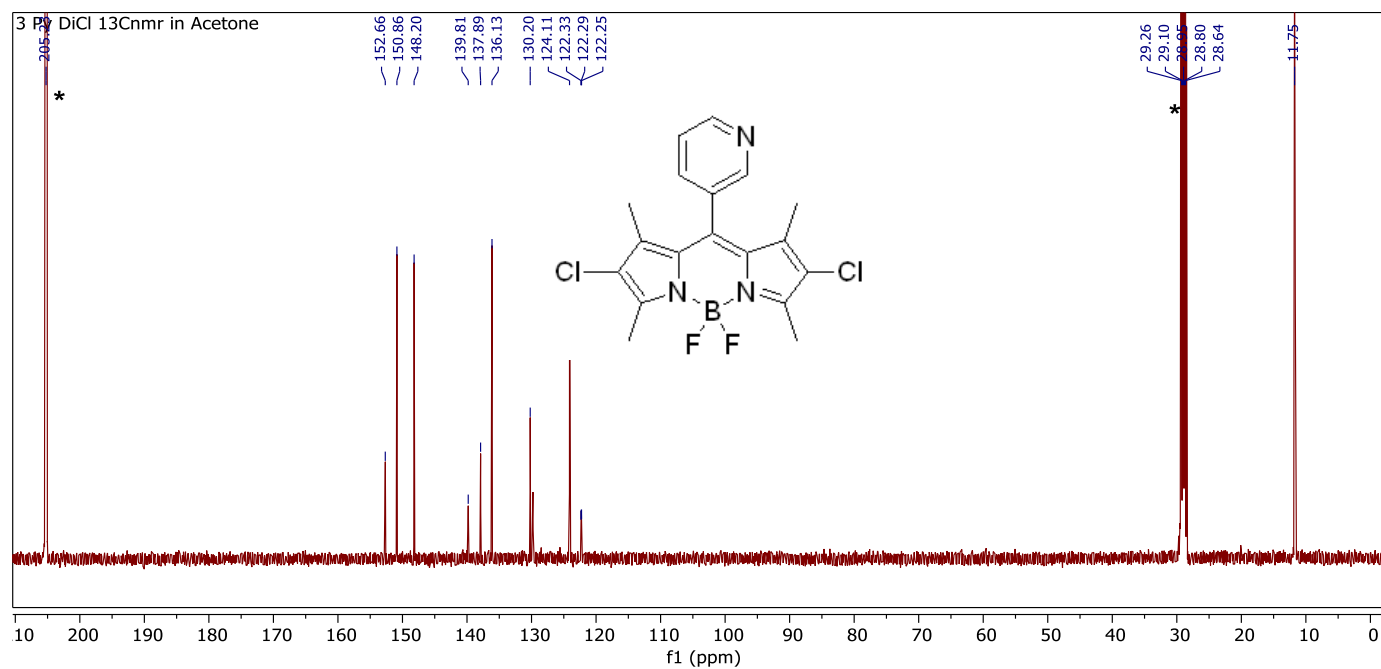
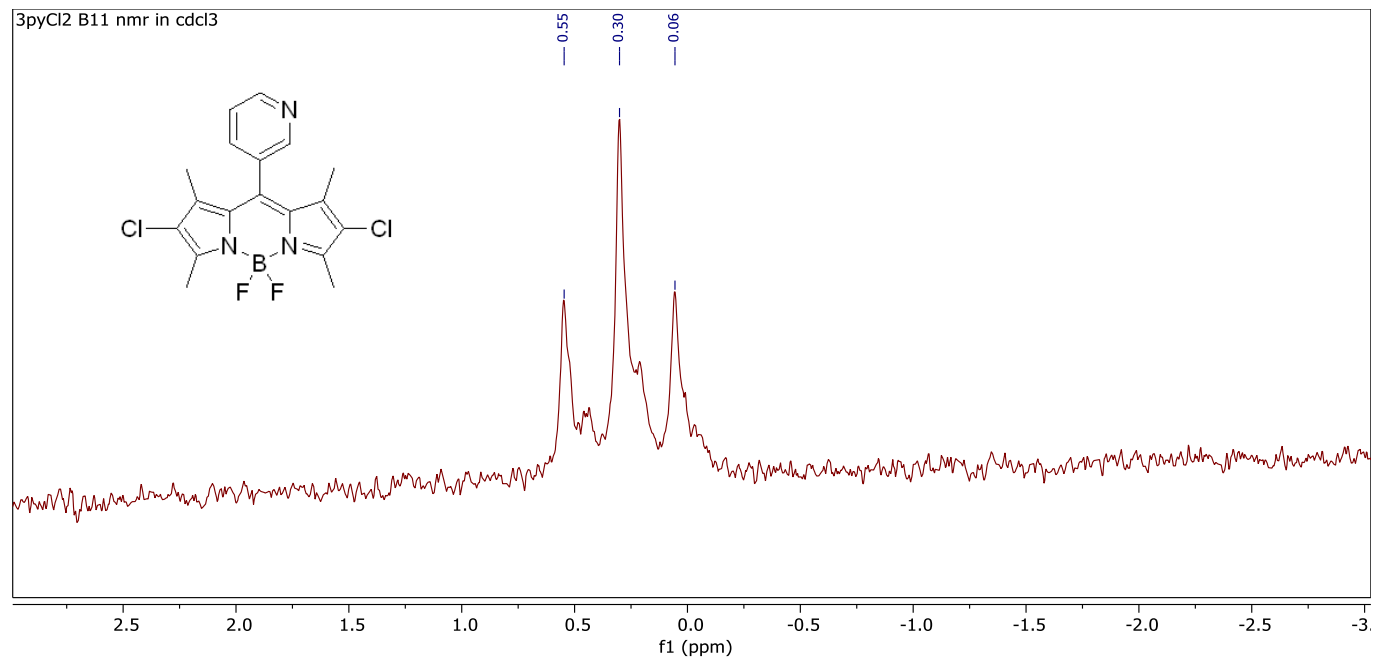
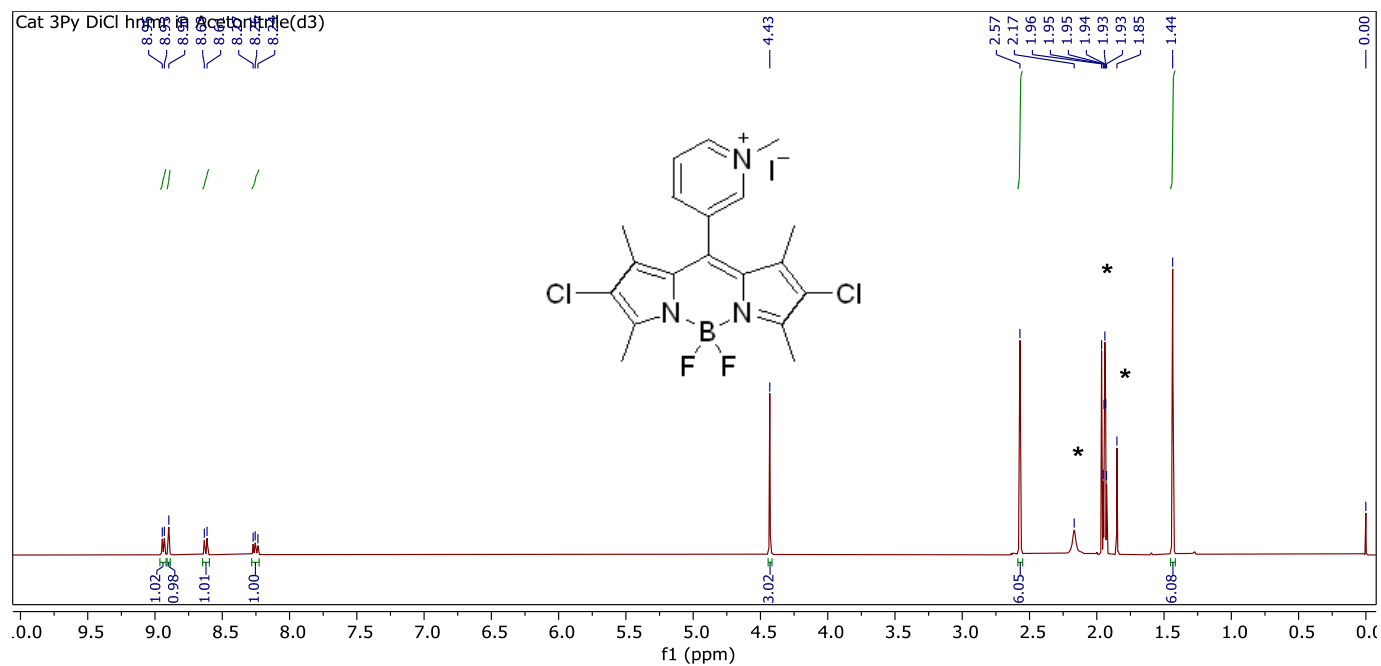


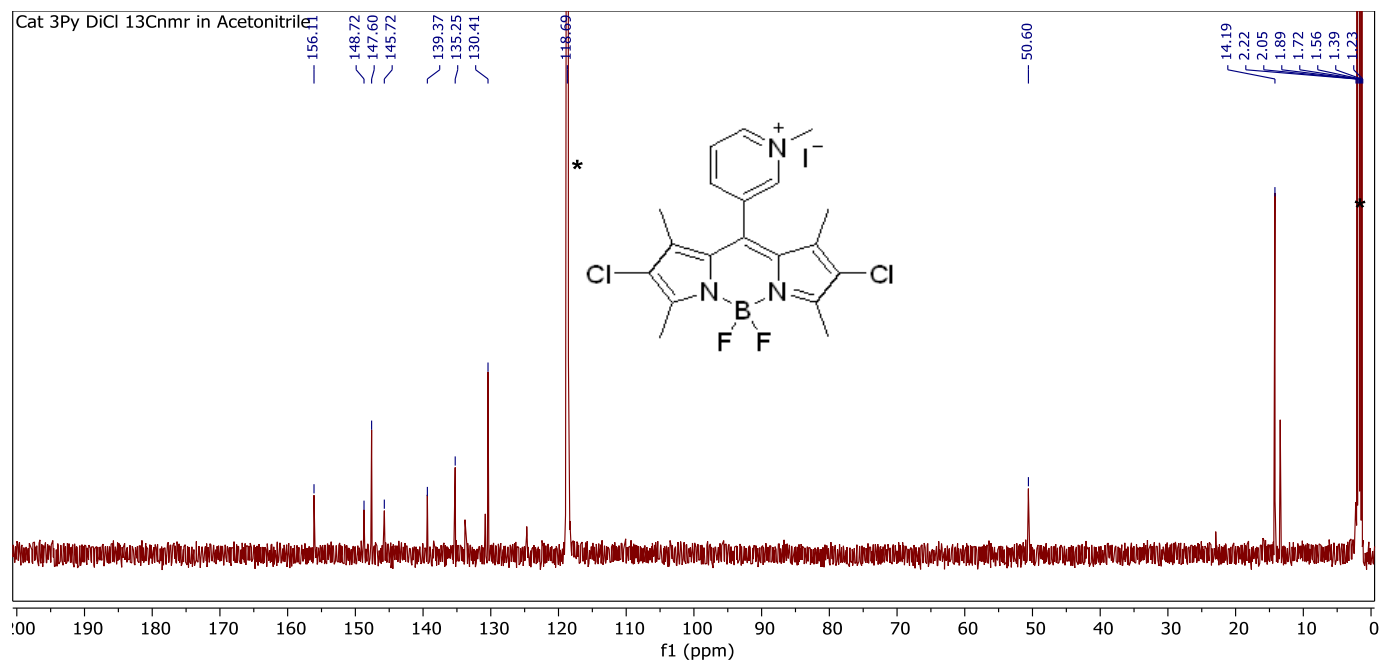
Figure S22. <sup>13</sup>C NMR of BODIPY 3PyCl<sub>2</sub> in acetone-d<sub>6</sub>



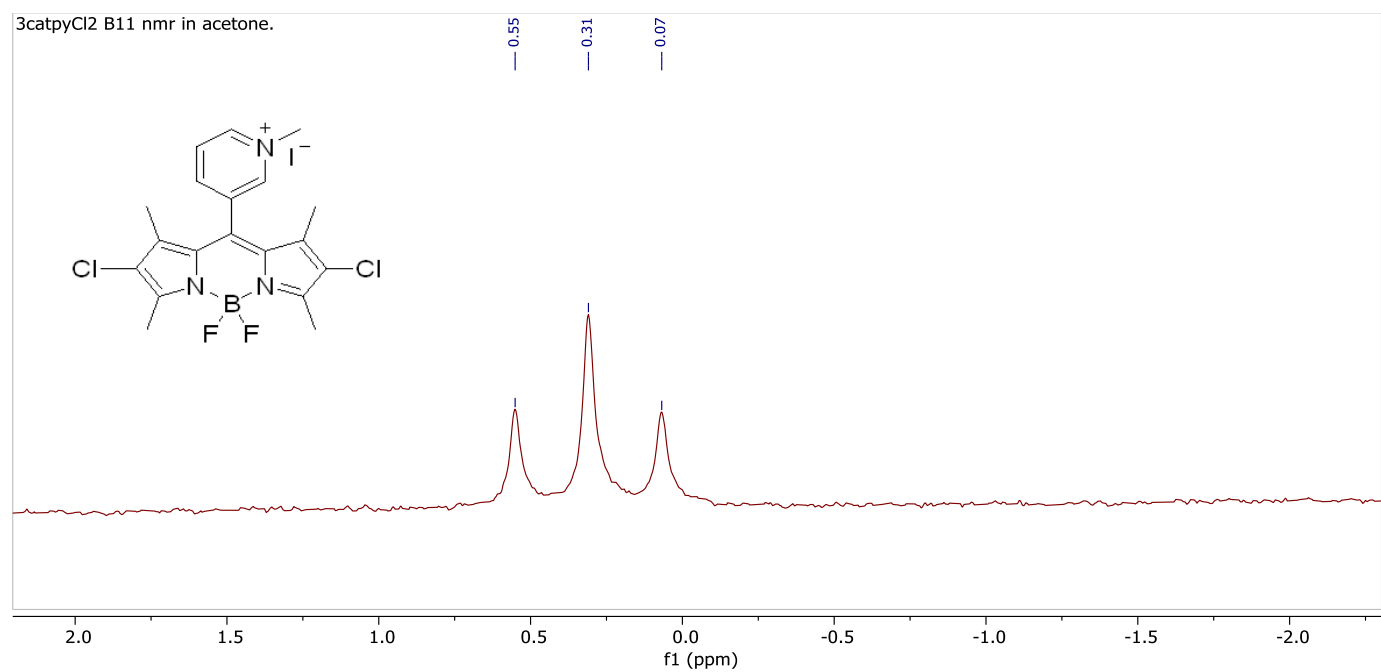
**Figure S23.**  $^{11}\text{B}$  NMR of BODIPY 3PyCl<sub>2</sub> in CDCl<sub>3</sub>



**Figure S24.**  $^1\text{H}$  NMR of BODIPY 3catPyCl<sub>2</sub> in acetonitrile-d<sub>3</sub>



**Figure S25.** <sup>13</sup>C NMR of BODIPY 3catPyCl<sub>2</sub> in acetonitrile-d<sub>3</sub>



**Figure S26.** <sup>11</sup>B NMR of BODIPY 3catPyCl<sub>2</sub> in acetone-d<sub>6</sub>