

Supplemental Materials

8(*meso*)-Pyridyl-BODIPYs: Effects of 2,6-substitution with Electron-Withdrawing Nitro, Chloro, and Methoxycarbonyl Groups

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Table of Contents

Spectroscopic Properties.....	2
BODIPYs conformations and relative energies	2
Absorption Spectra	3
Emission Spectra	4
NMR spectra	5

Table S1. Spectroscopic properties of BODIPYs in Toluene and relative fluorescence quantum yields using (a) rhodamine 6G ($\Phi_f = 0.86$) in methanol, $\lambda_{exc} = 473$ nm

Solvent	BODIPY	λ_{abs} (nm)	λ_{em} (nm)	Stokes Shift (nm)	Φ_f	ϵ ($M^{-1} cm^{-1}$)
Toluene	2PyCO ₂ Me	508	523	15	0.04	72285
	3PyCO ₂ Me	508	521	13	0.47	77490
	4PyCO ₂ Me	507	520	13	0.45	N/A
	2PyNO ₂	501	518	17	0.03	27390
	3PyNO ₂	500	517	17	0.5	53385
	4PyNO ₂	500	517	17	0.38	57080
	2PyNO ₂ /Cl	520	538	18	0.05	30780
	3PyNO ₂ /Cl	521	536	15	0.47	22940
	4PyNO ₂ /Cl	520	537	17	0.42	20130

Figure S1. Conformations and relative energies for a) 2PyCO₂Me, b) 2PyNO₂, and c) 2PyNO₂Cl. Analogous conformations were also studied for the 3Py and 4Py series.

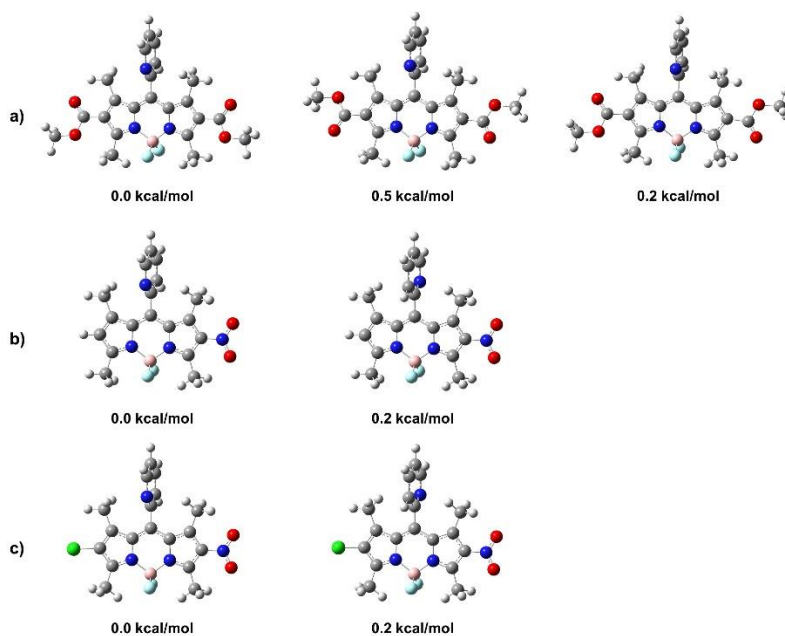


Figure S2. Normalized absorption spectra (1a, b) in CH₃CN (1c,1d) in MeOH and (1e,1f) in toluene.

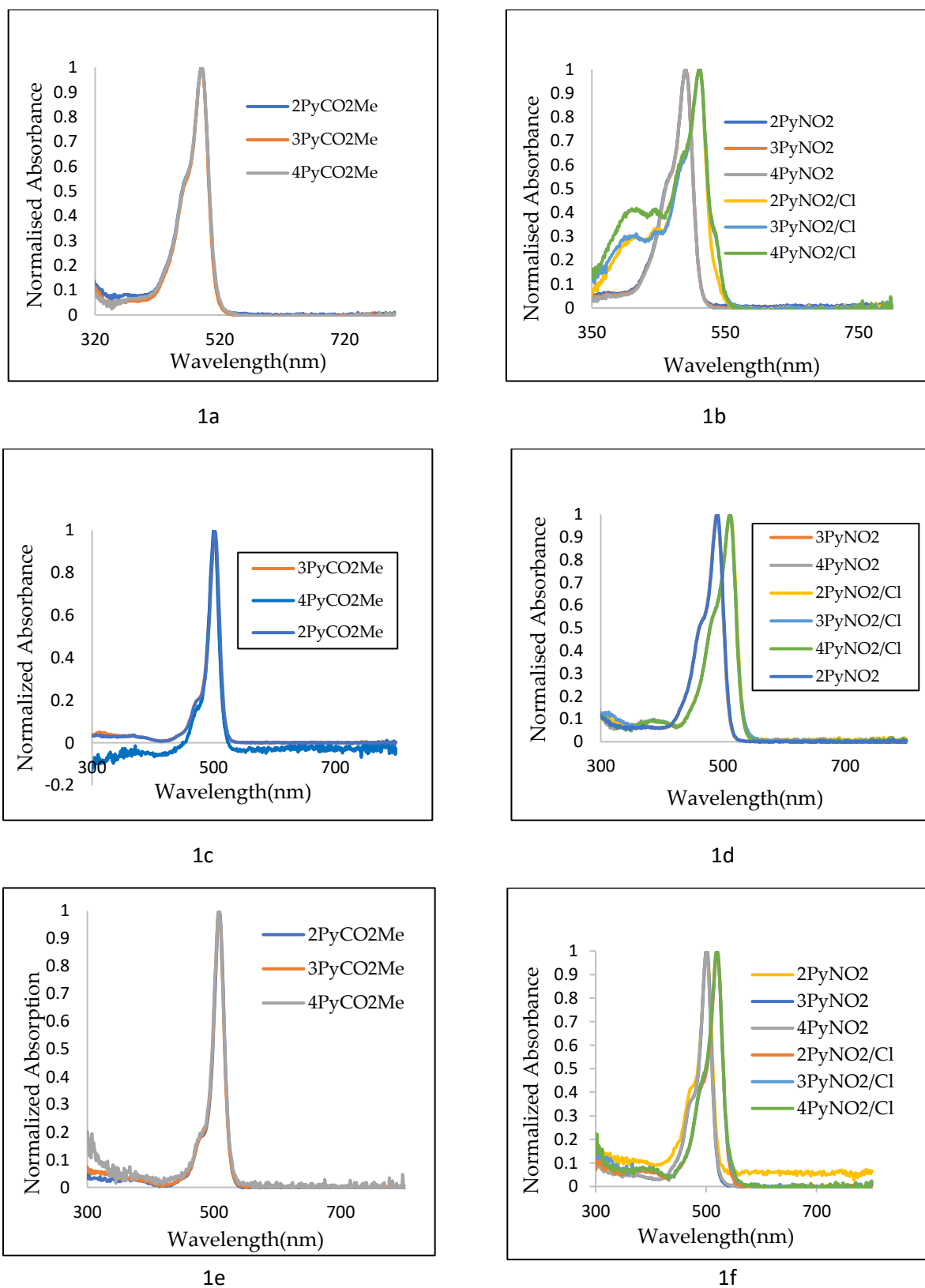
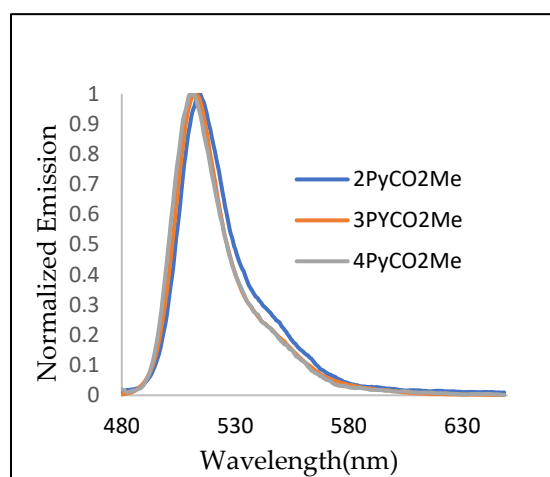
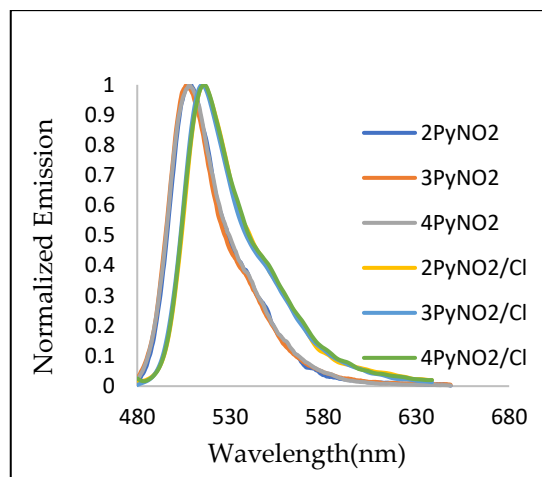


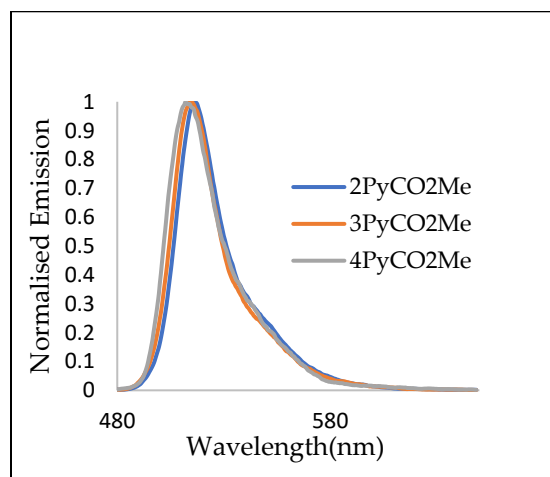
Figure S3. Normalized emission spectra (2a, 2b) in CH₃CN (2c, 2d) in MeOH and (2e,2f) in toluene.



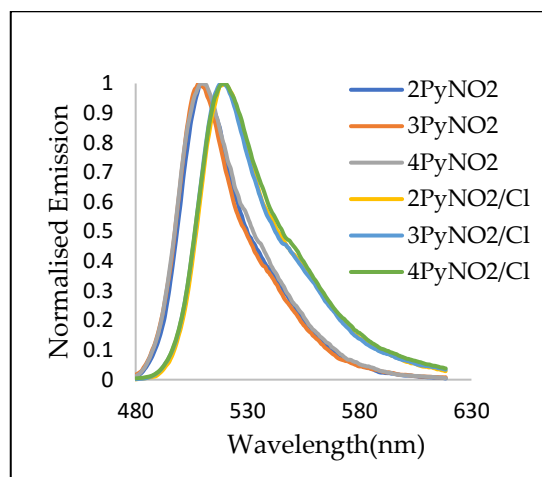
2a



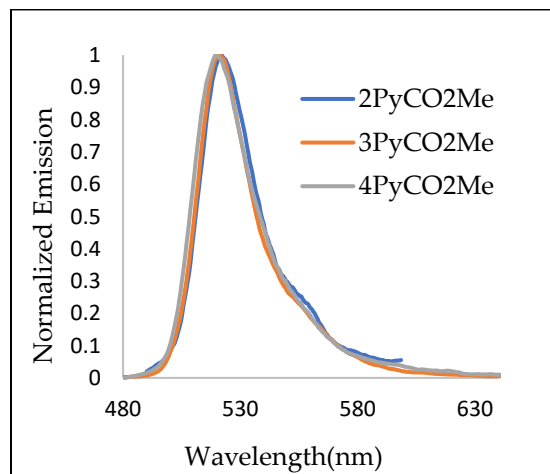
2b



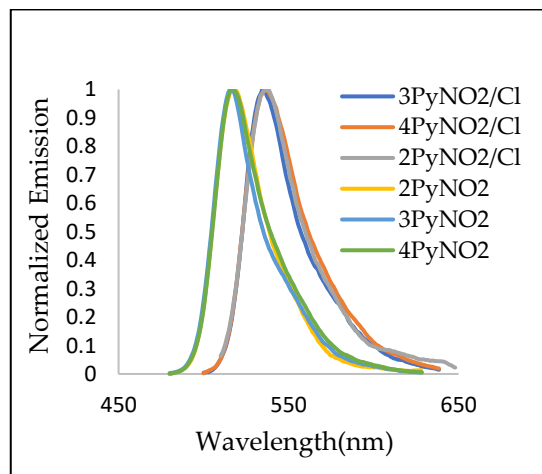
2c



2d



2e



2f

NMR Spectra

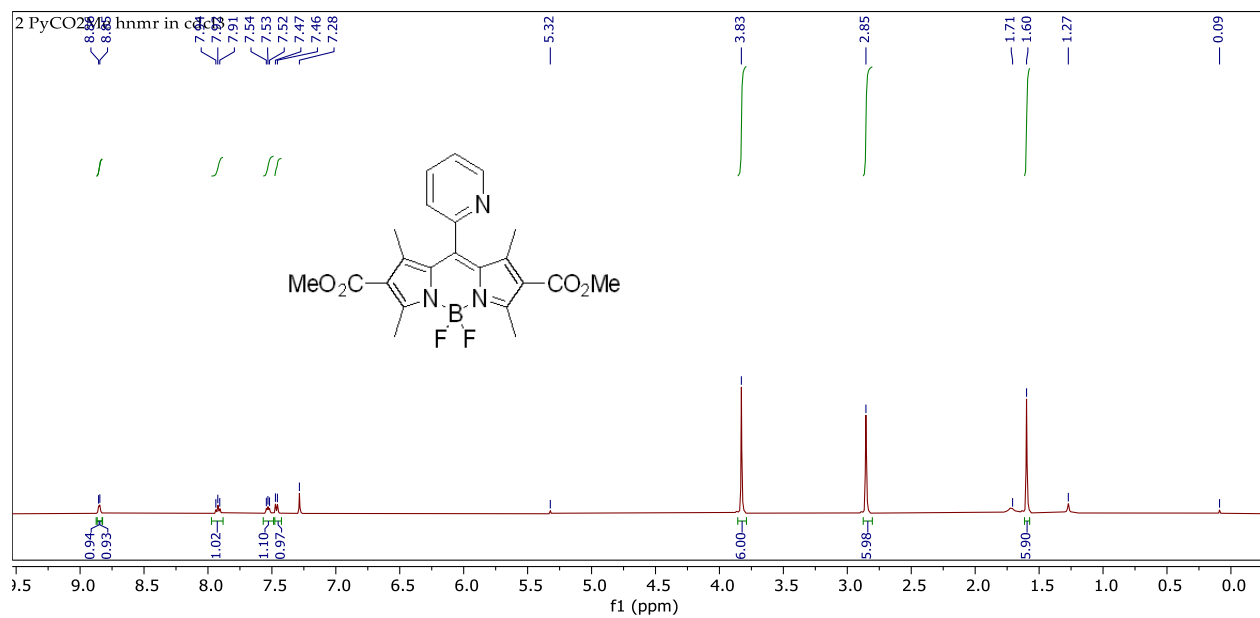


Figure S4. ¹H of BODIPY 2PyCO₂Me in CDCl₃

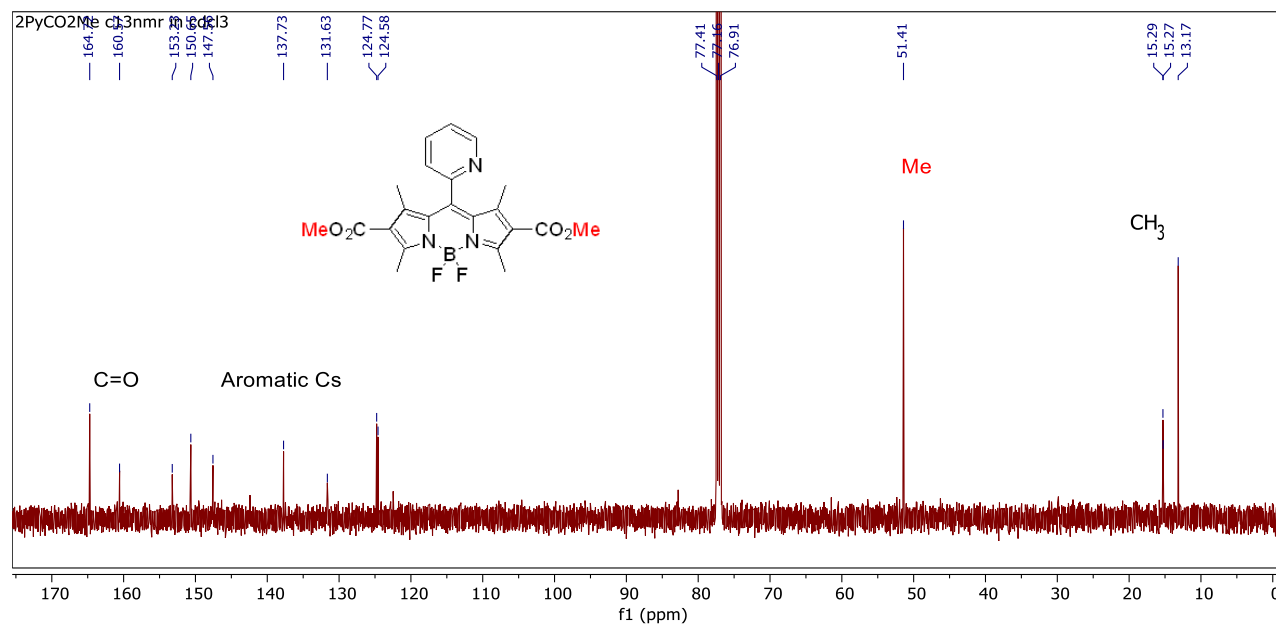


Figure S5. ¹³C of BODIPY 2PyCO₂Me in CDCl₃

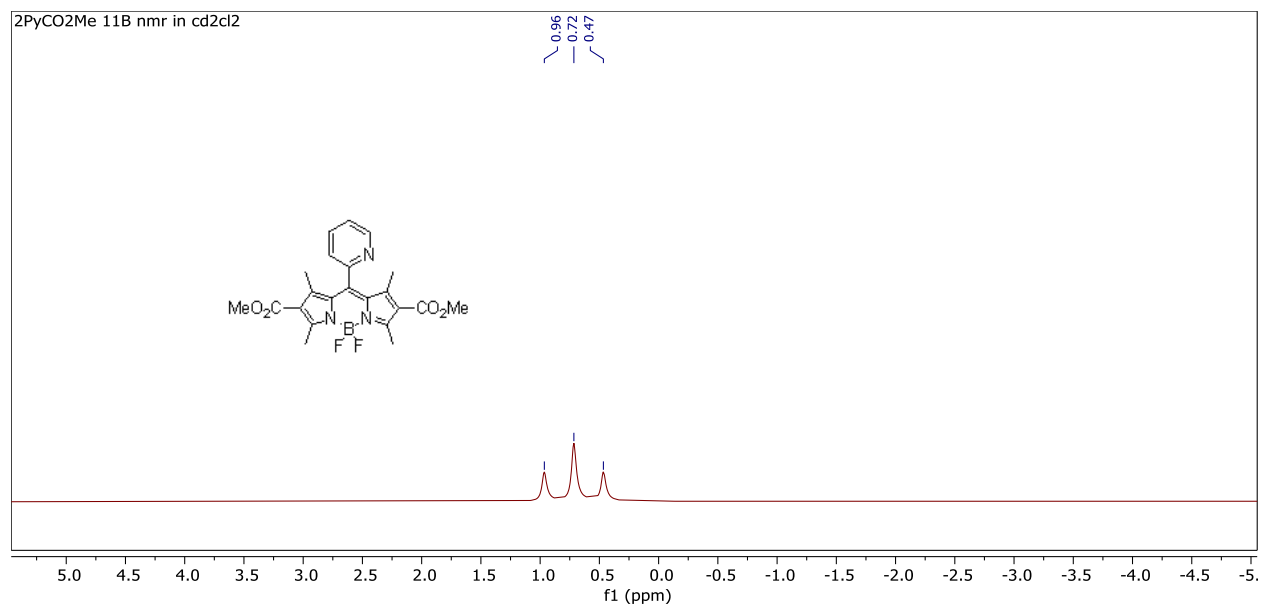


Figure S6. ¹¹B of BODIPY 2PyCO₂Me in CD₂Cl₂

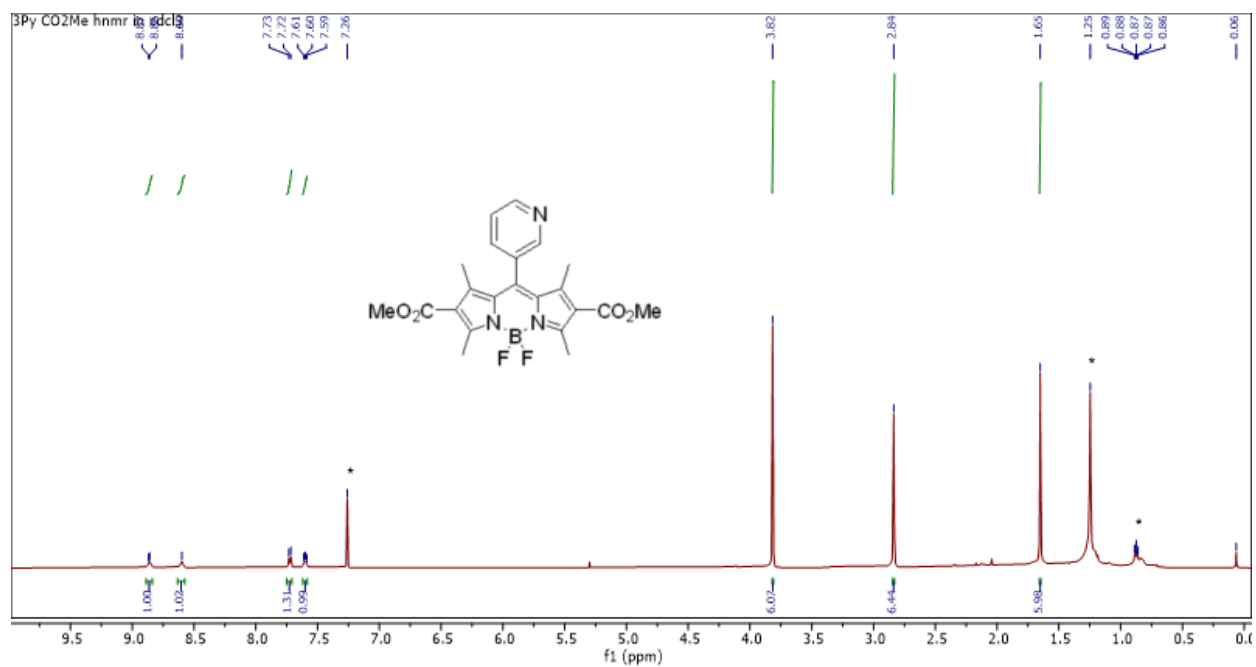


Figure S7. ¹H of BODIPY 3PyCO₂Me in CDCl₃

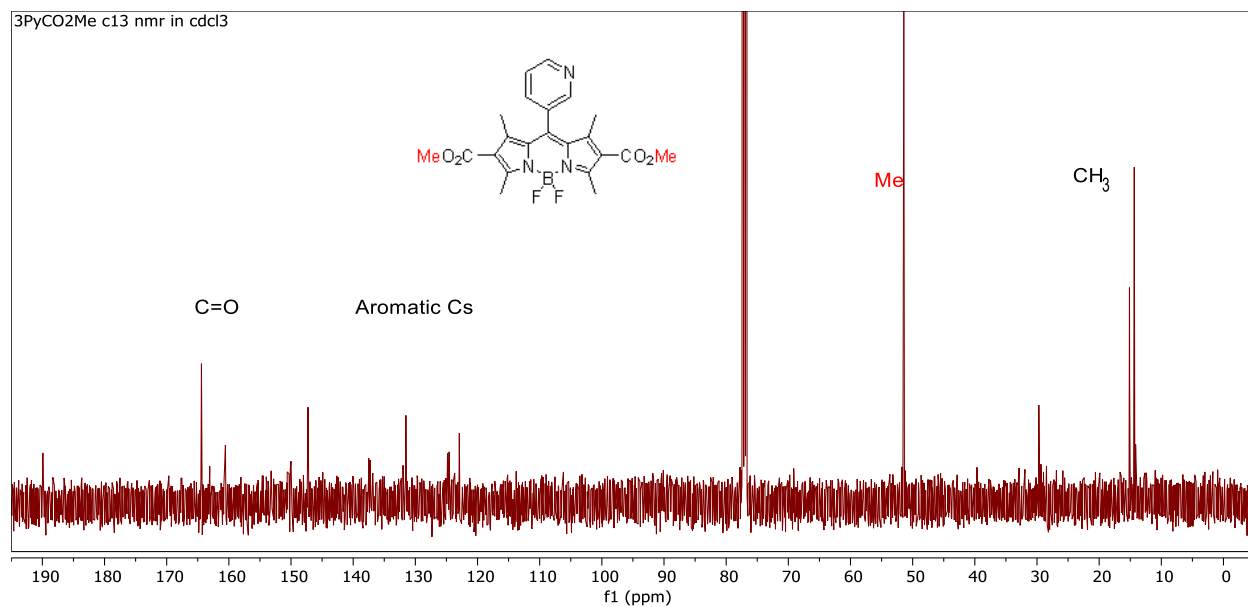


Figure S8. ¹³C of BODIPY 3PyCO₂Me in CDCl₃

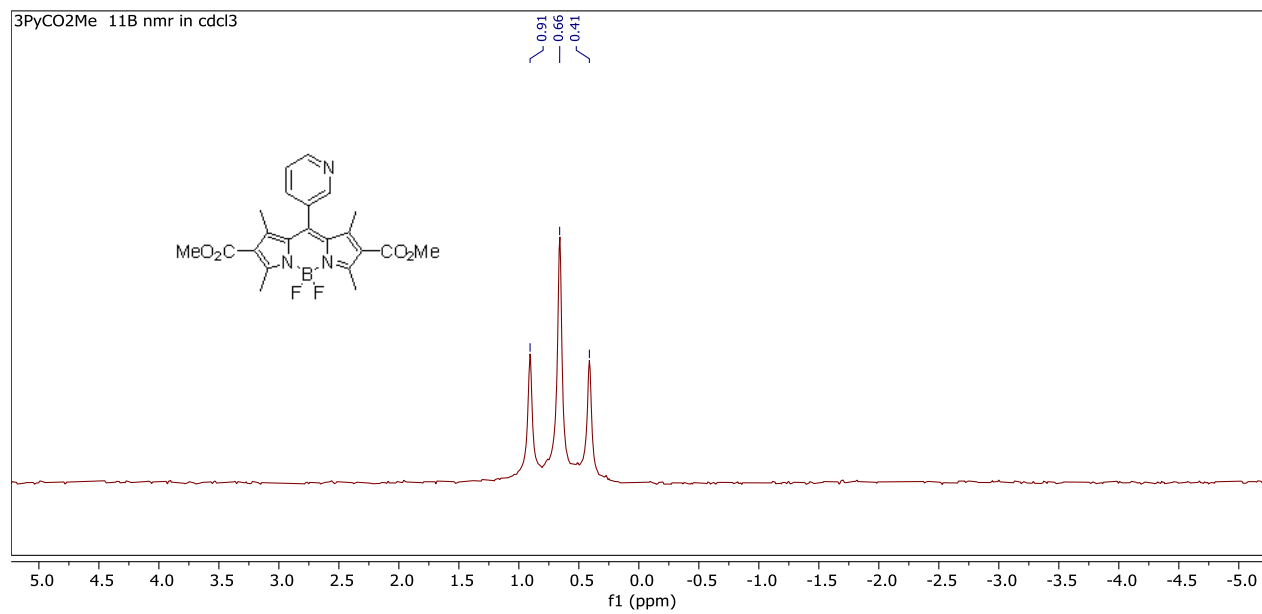


Figure S9. ¹¹B of BODIPY 3PyCO₂Me in CDCl₃

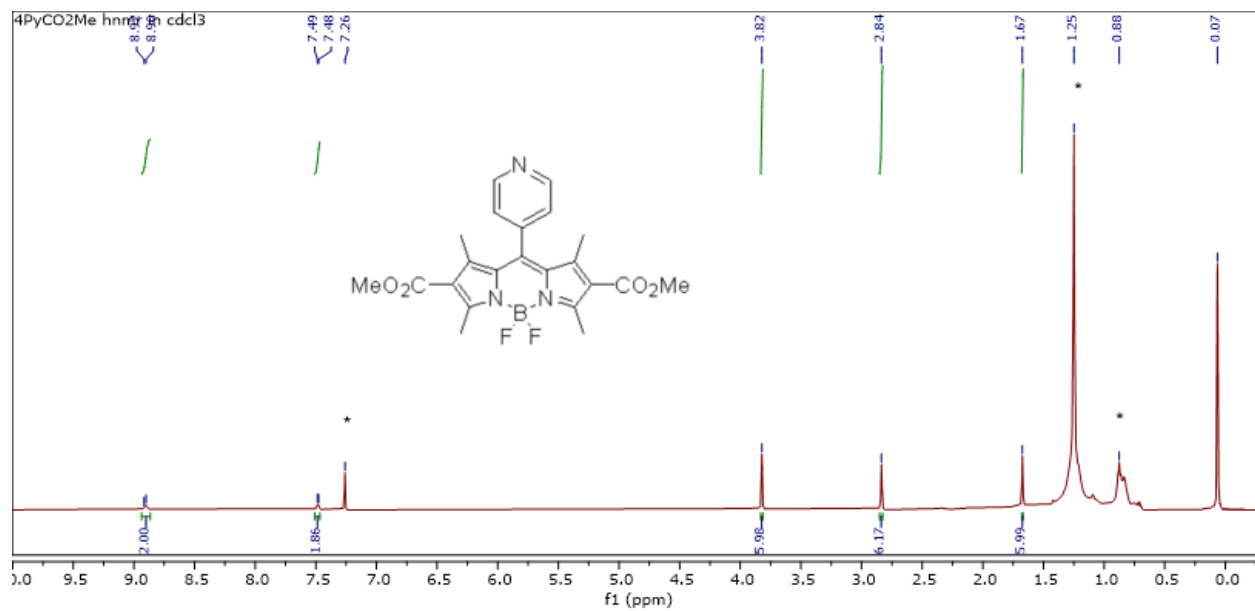


Figure S10. ¹H of BODIPY 4PyCO₂Me in CDCl₃

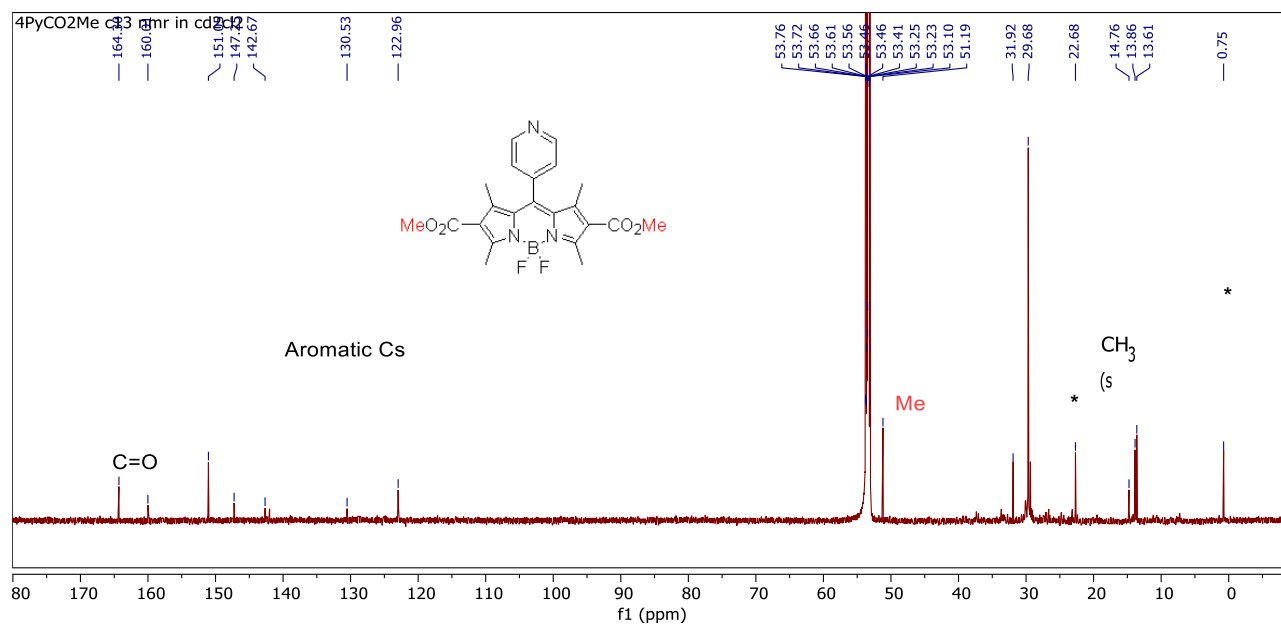


Figure S11. ¹³C of BODIPY 4PyCO₂Me in CD₂Cl₂

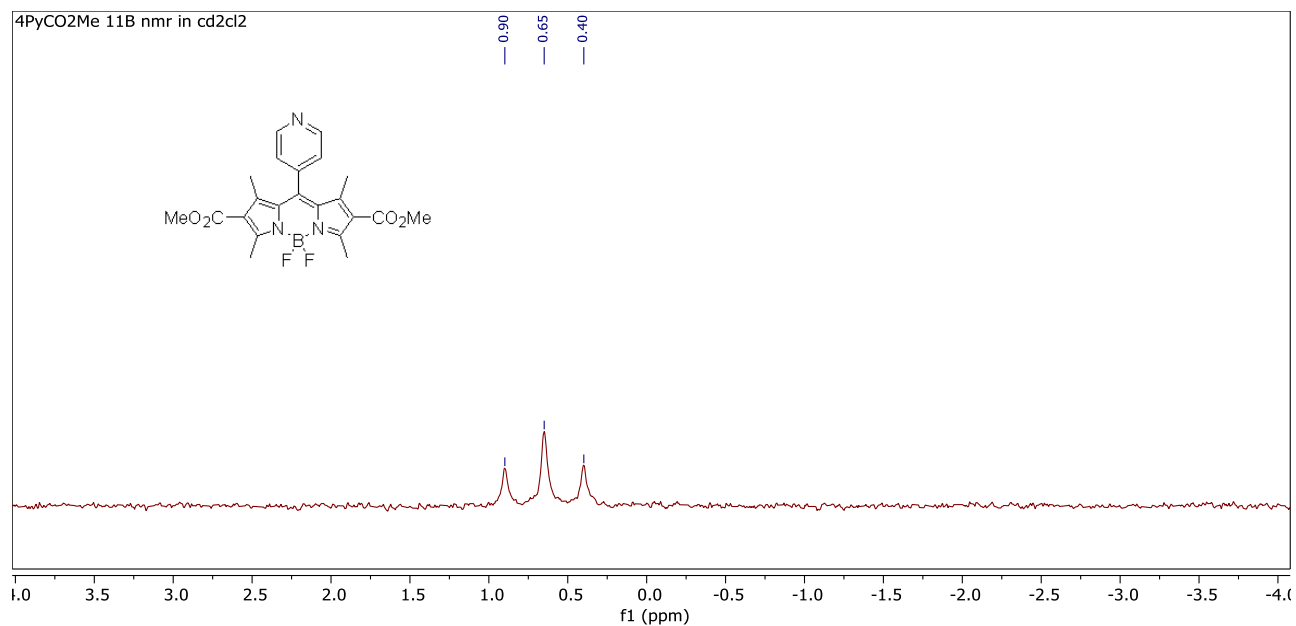


Figure S12. ¹¹B of BODIPY 4PyCO₂Me in CD₂Cl₂

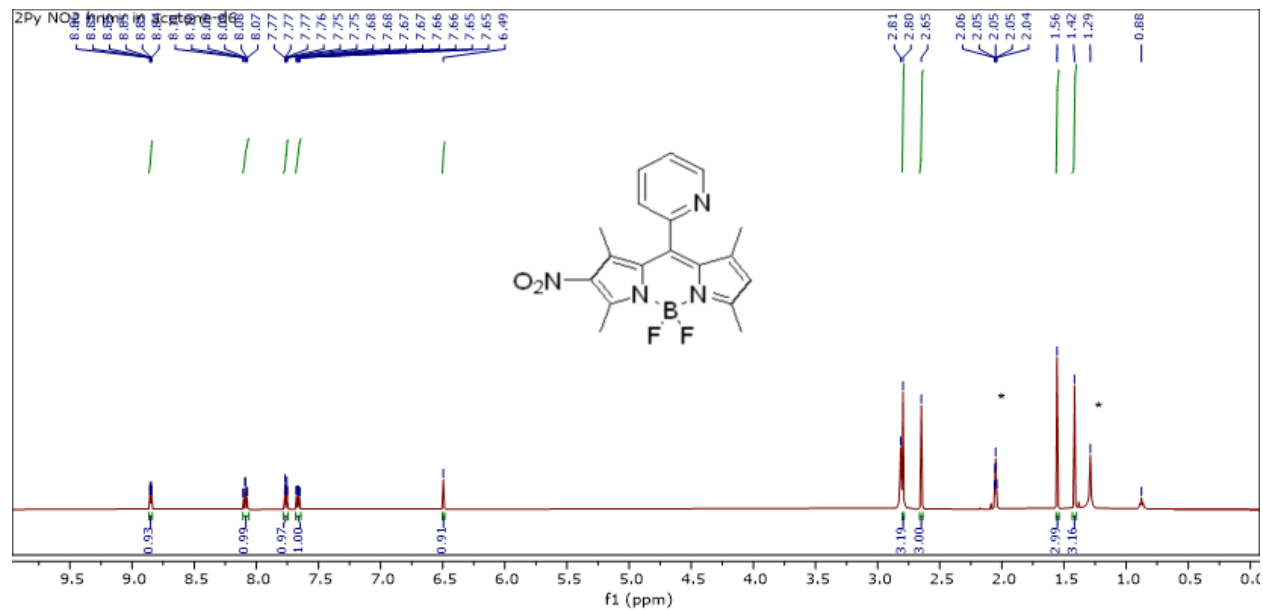


Figure S13. ¹H of BODIPY 2PyNO₂ in acetone-d₆

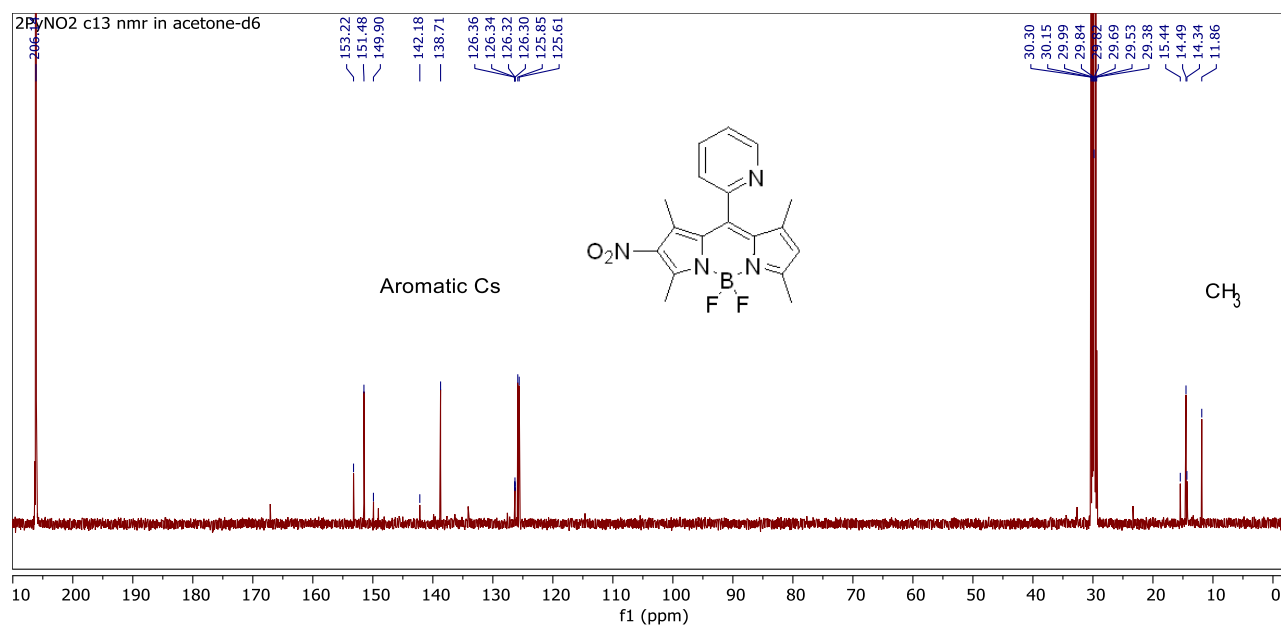


Figure S14. ¹³C of BODIPY 2PyNO₂ in acetone-d₆

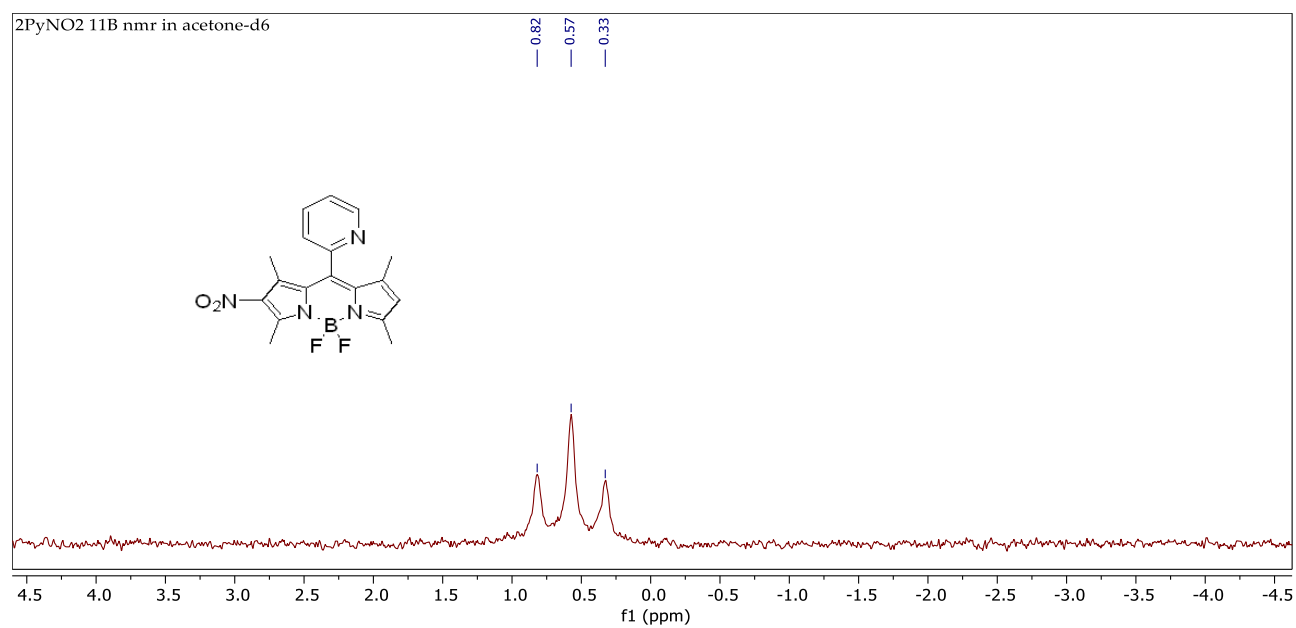


Figure S15. ¹¹B of BODIPY 2PyNO₂ in acetone-d₆

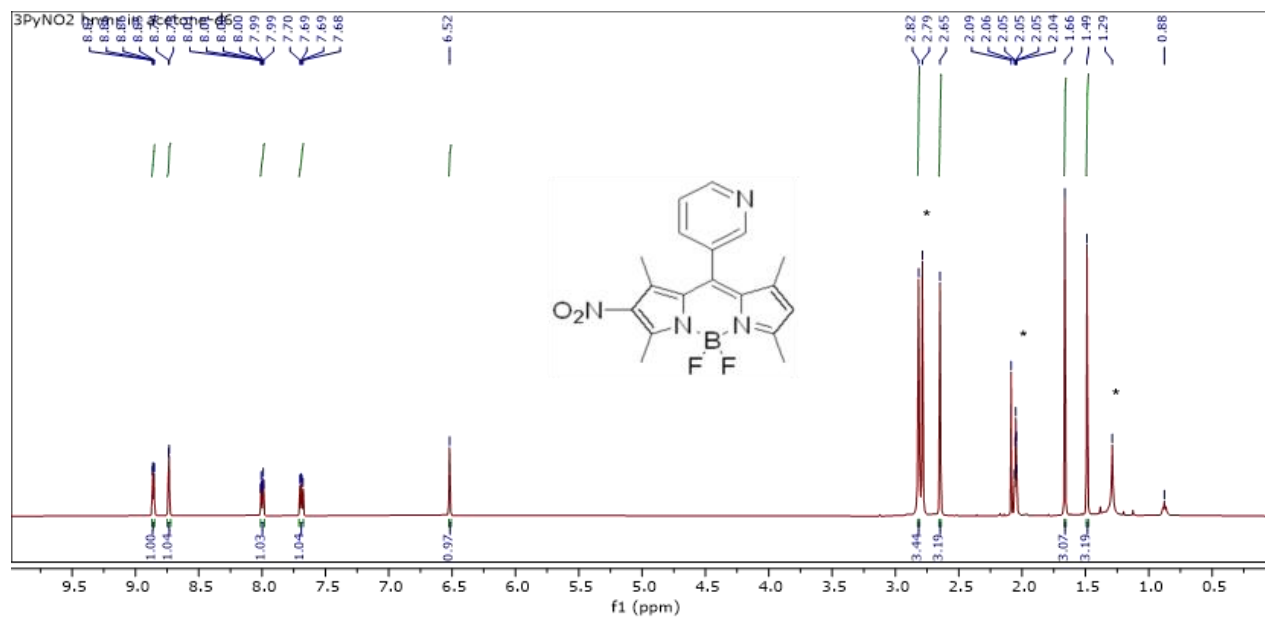


Figure S16. ¹H of BODIPY 3PyNO₂ in acetone-d₆

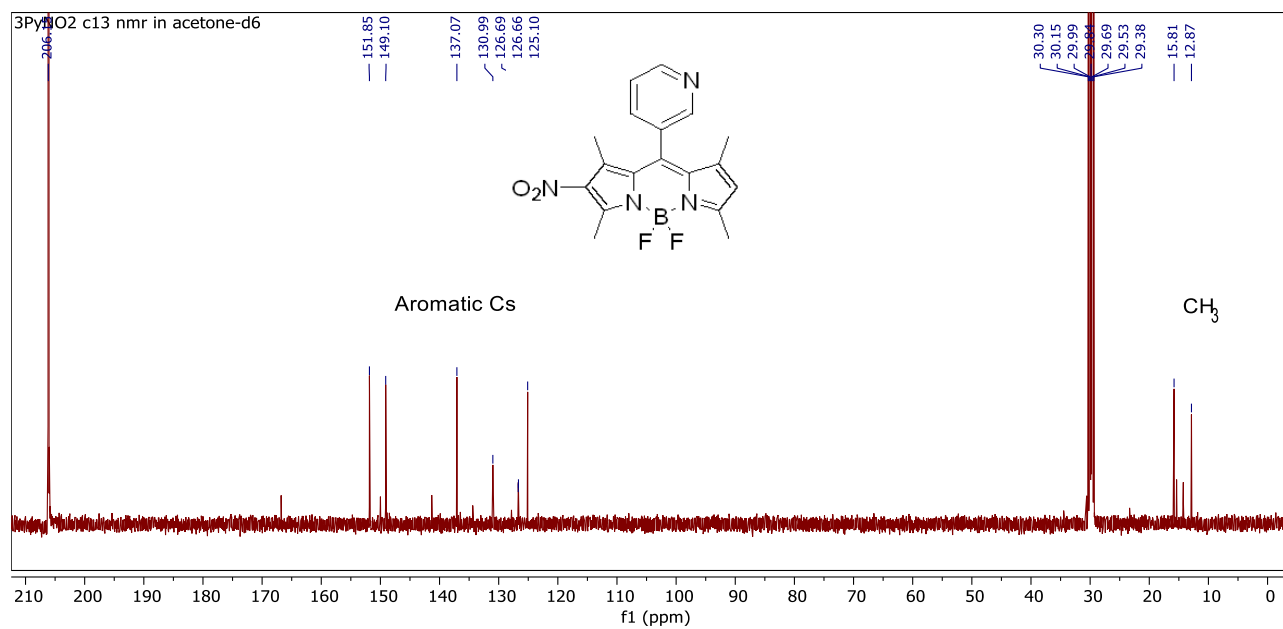


Figure S17. ¹³C of BODIPY 3PyNO₂ in acetone-d₆

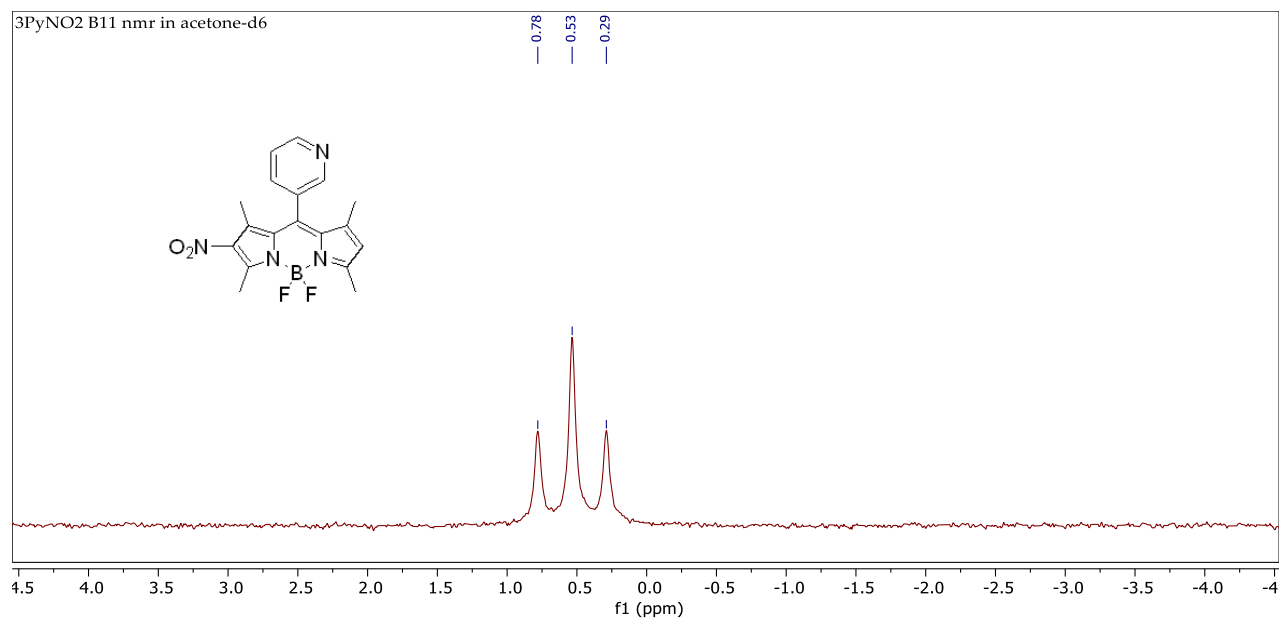


Figure S18. ¹¹B of BODIPY 3PyNO₂ in acetone-d₆

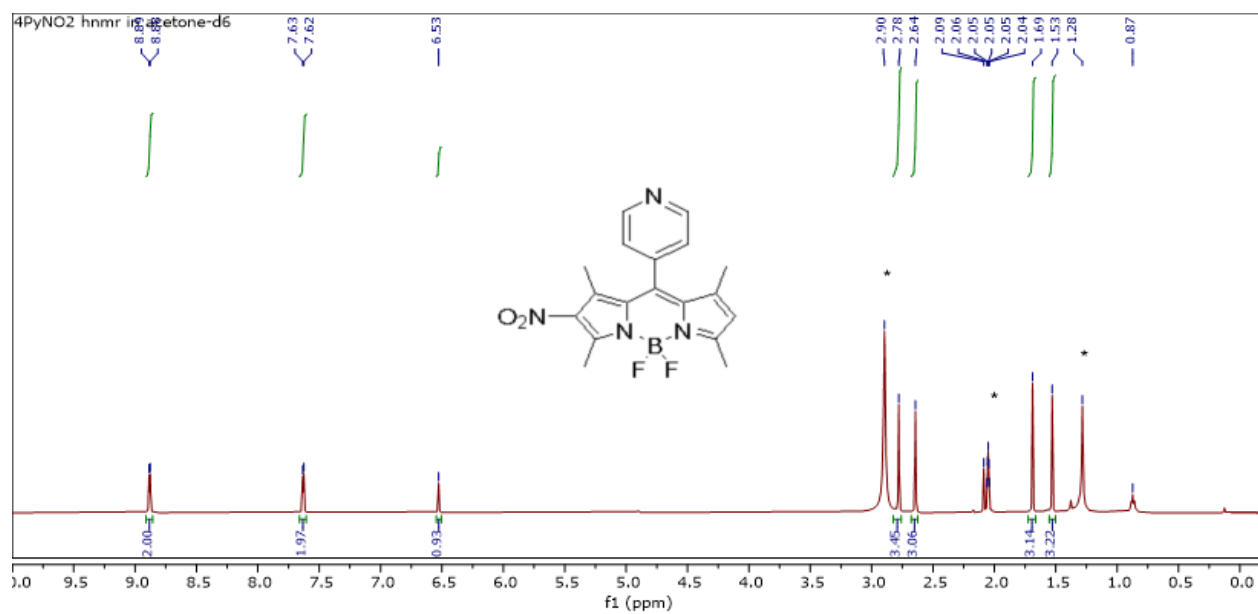


Figure S19. ¹H of BODIPY 4PyNO₂ in Acetone-d₆

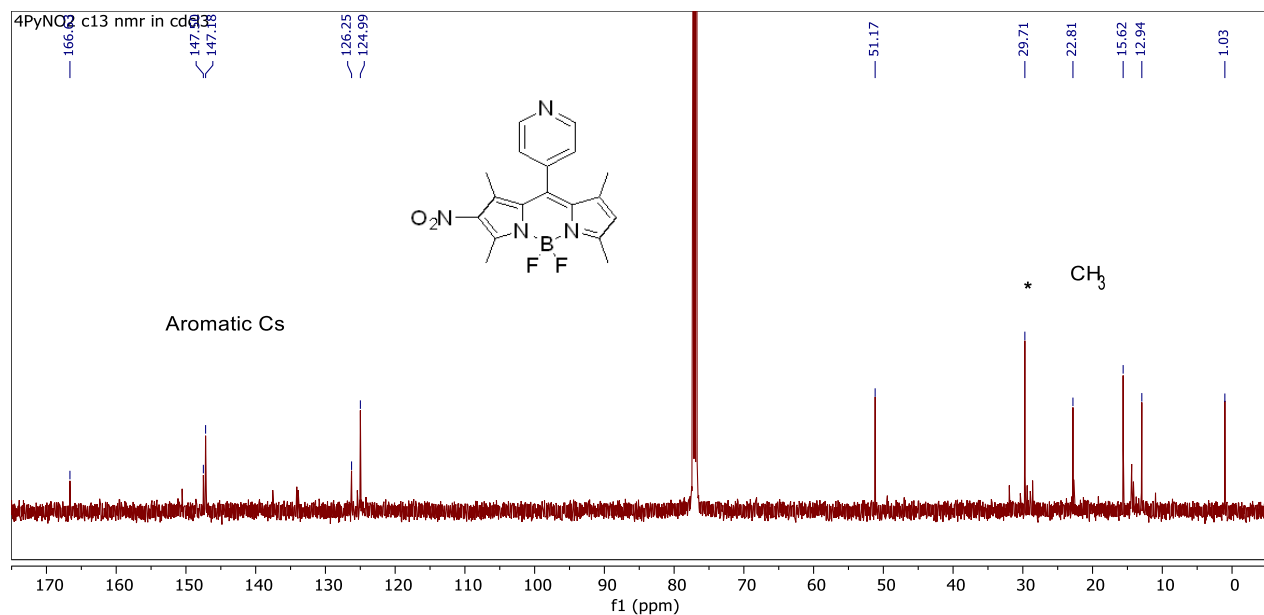


Figure S20. ¹³C of BODIPY 4PyNO₂ in CDCl₃

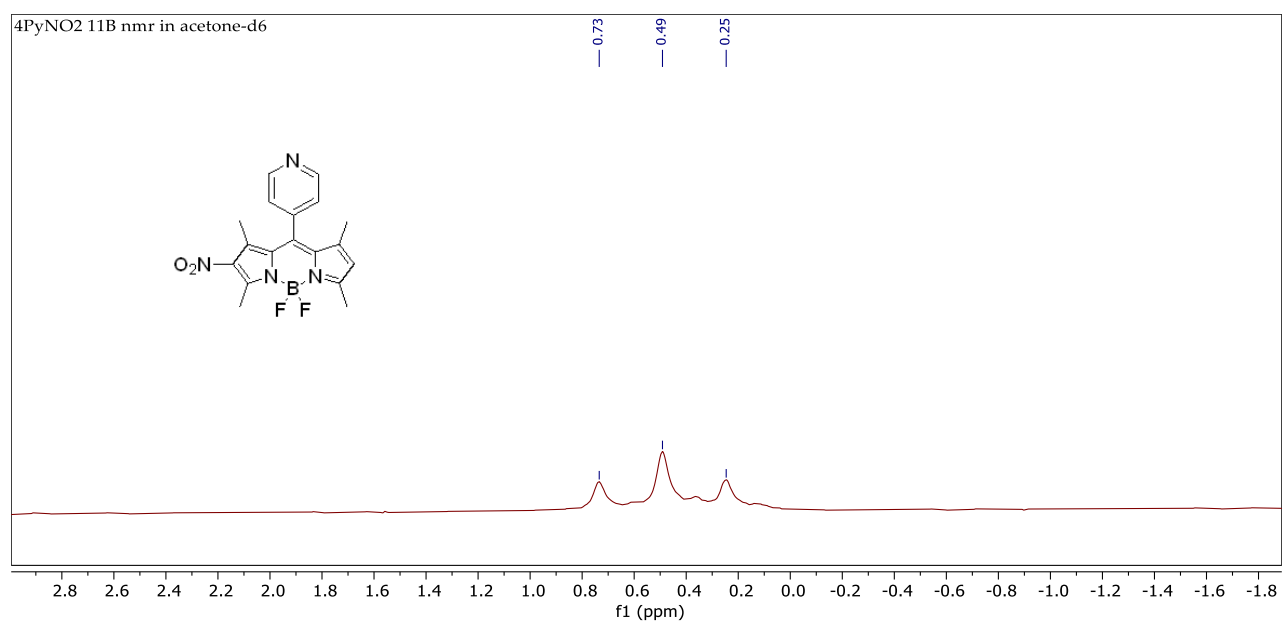


Figure S21. ¹¹B of BODIPY 4PyNO₂ in acetone-d₆

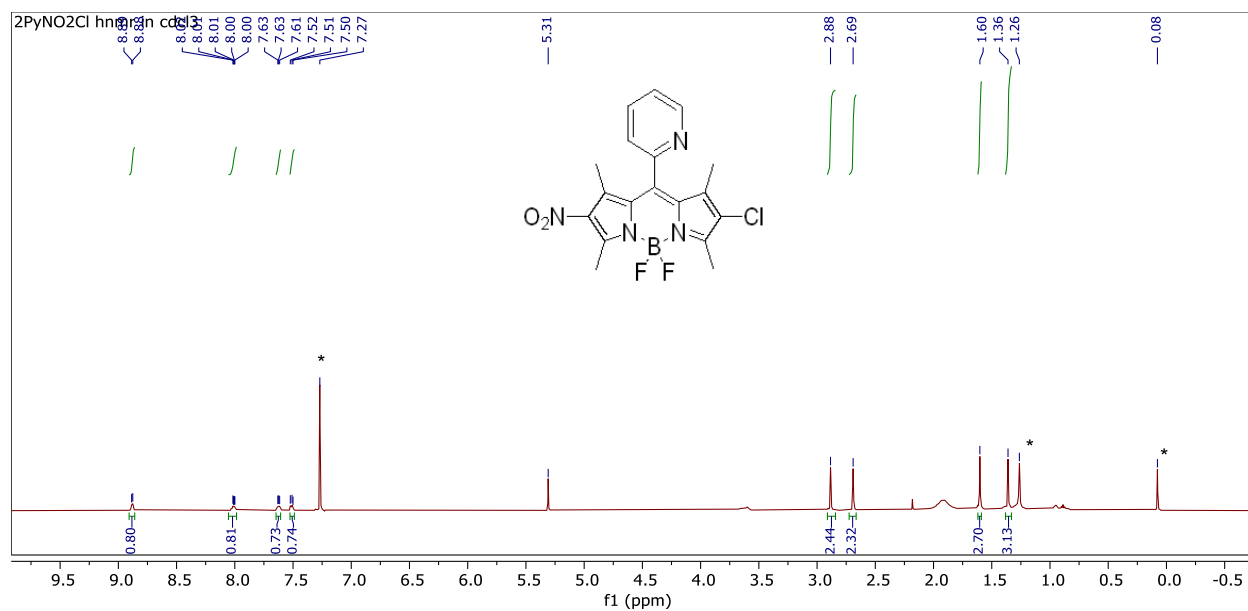


Figure S22. ¹H of BODIPY 2PyNO₂Cl in CDCl₃

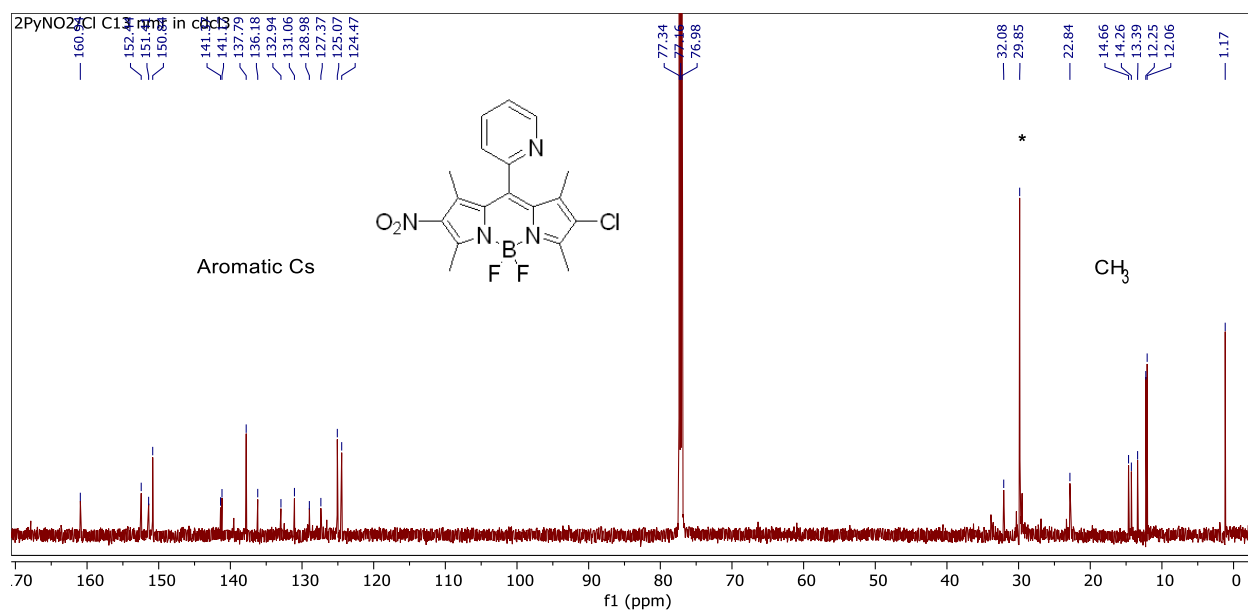
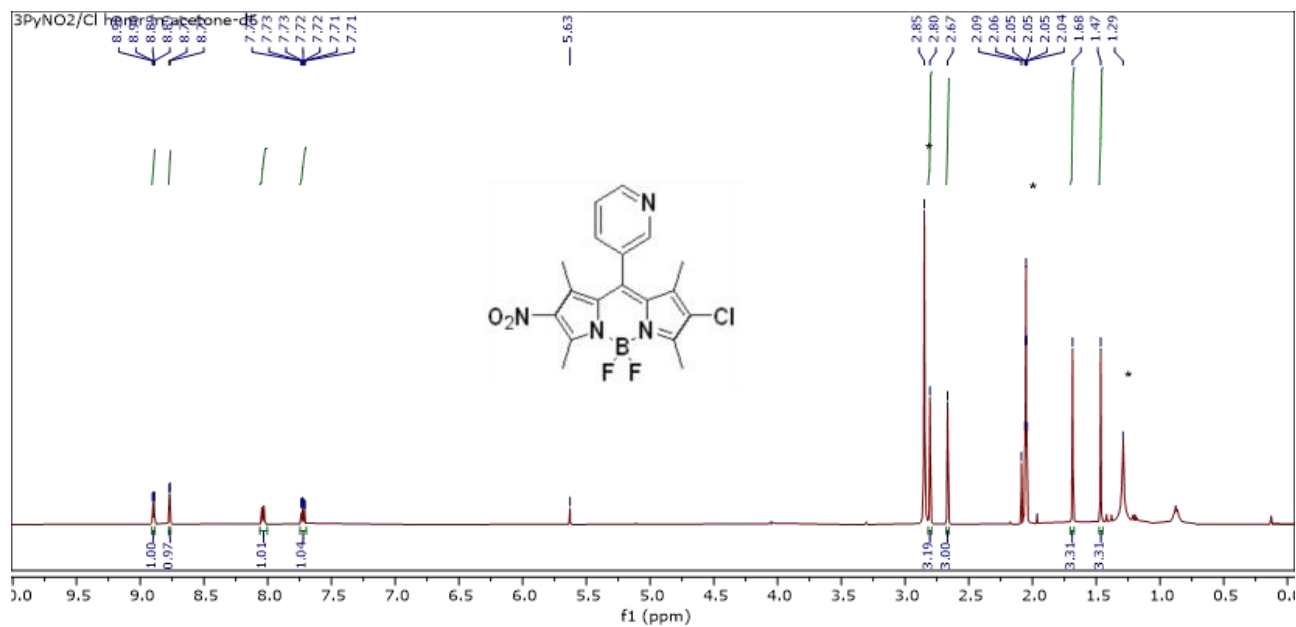
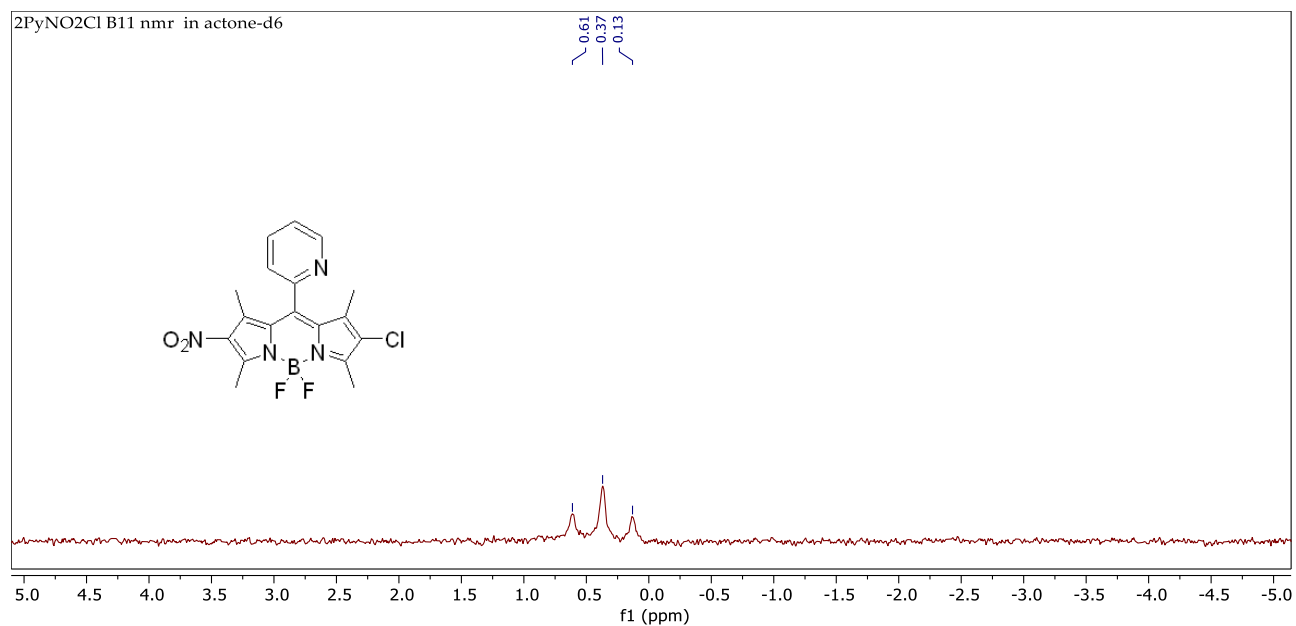


Figure S23. ¹³C of BODIPY 2PyNO₂Cl in CDCl₃



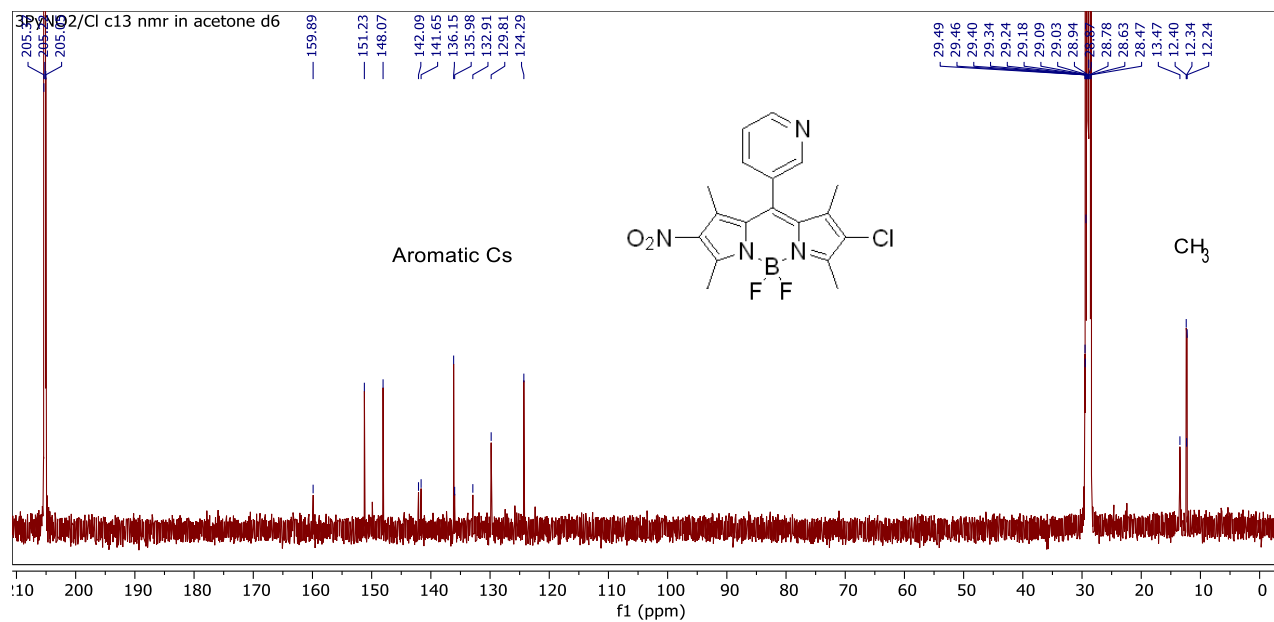


Figure S26. ¹³C of BODIPY 3PyNO₂Cl in Acetone-d₆

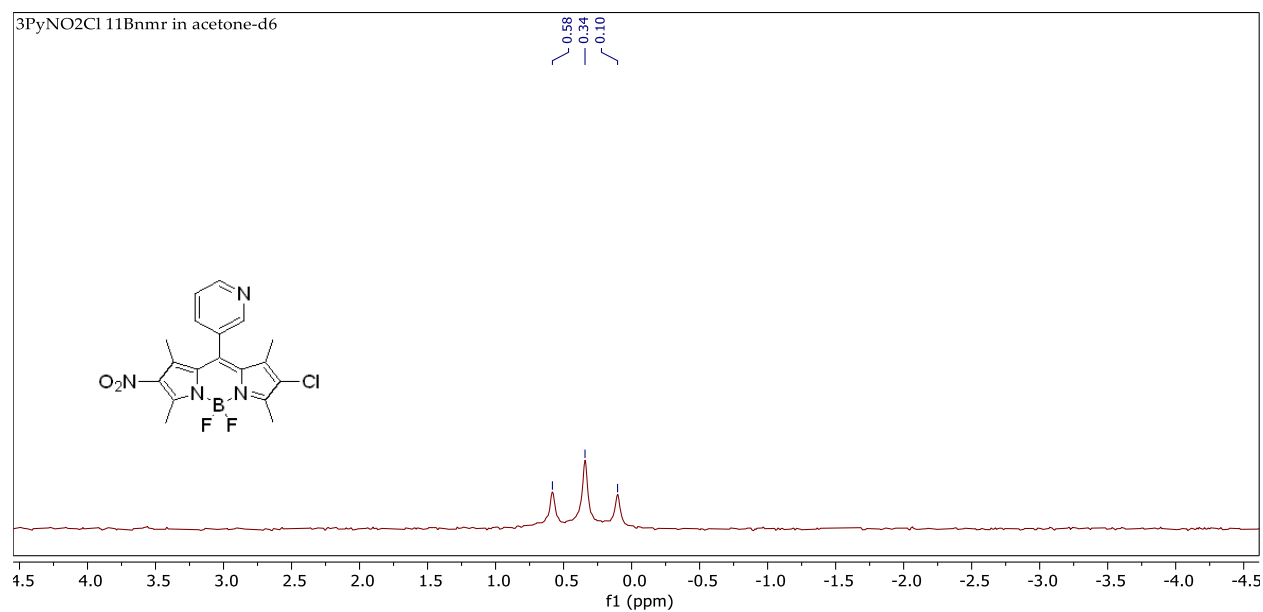


Figure S27. ¹¹B of BODIPY 3PyNO₂Cl in acetone-d₆

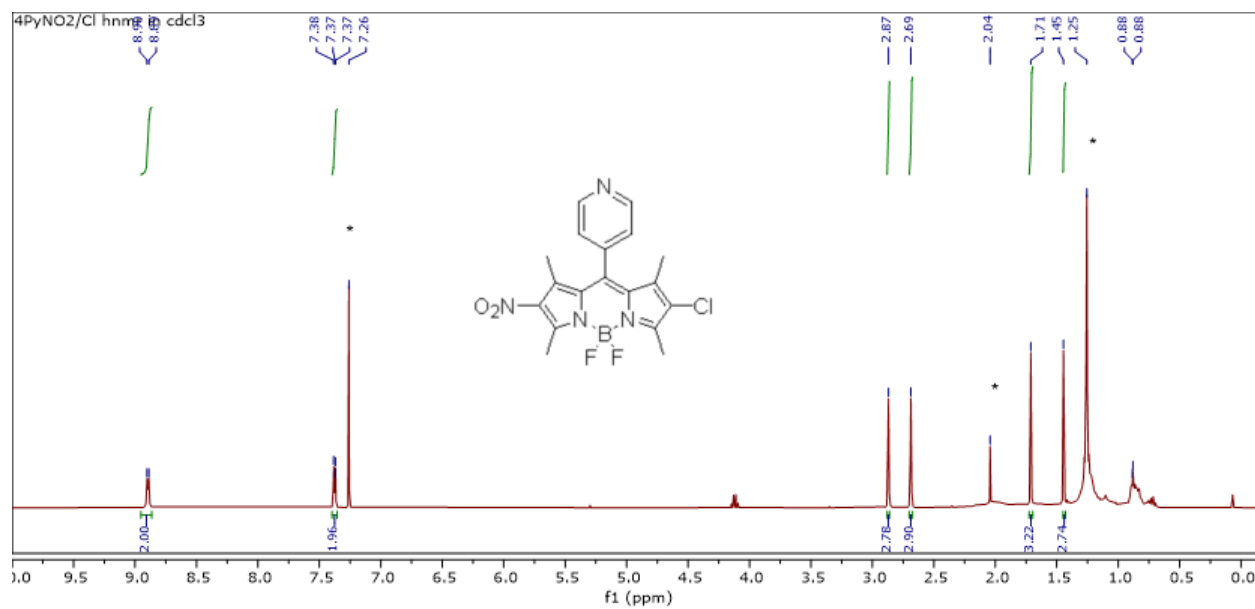


Figure S28. ¹H of BODIPY 4PyNO₂Cl in CDCl₃

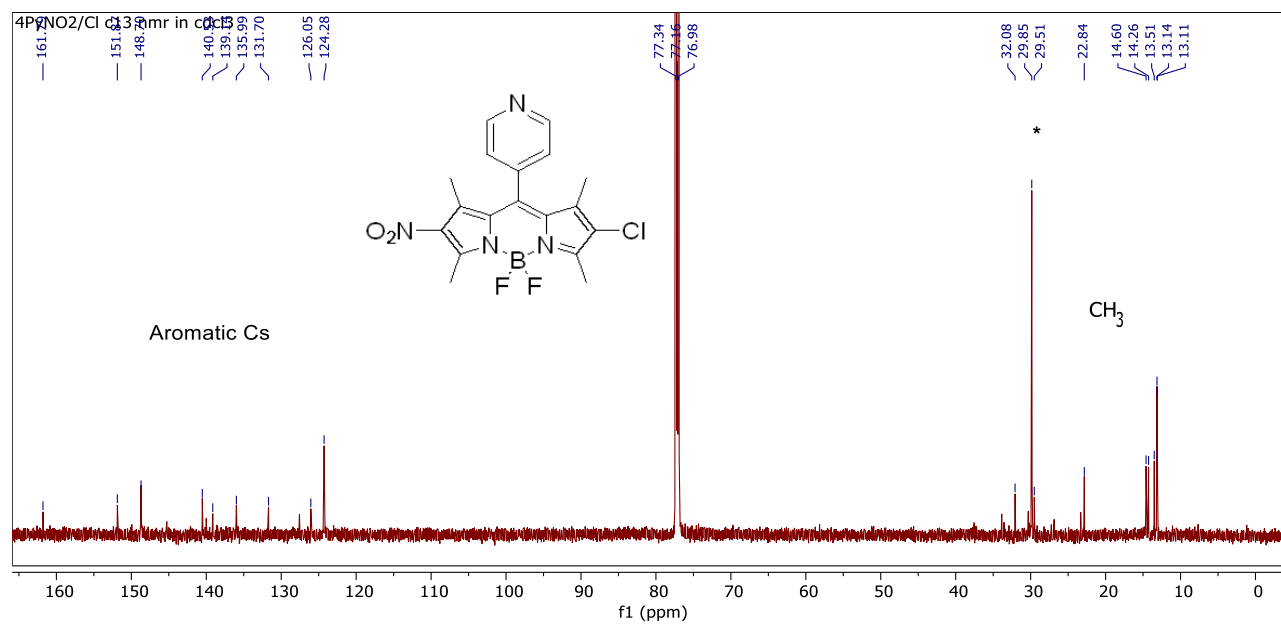


Figure S29. ¹³C of BODIPY 4PyNO₂Cl in CDCl₃

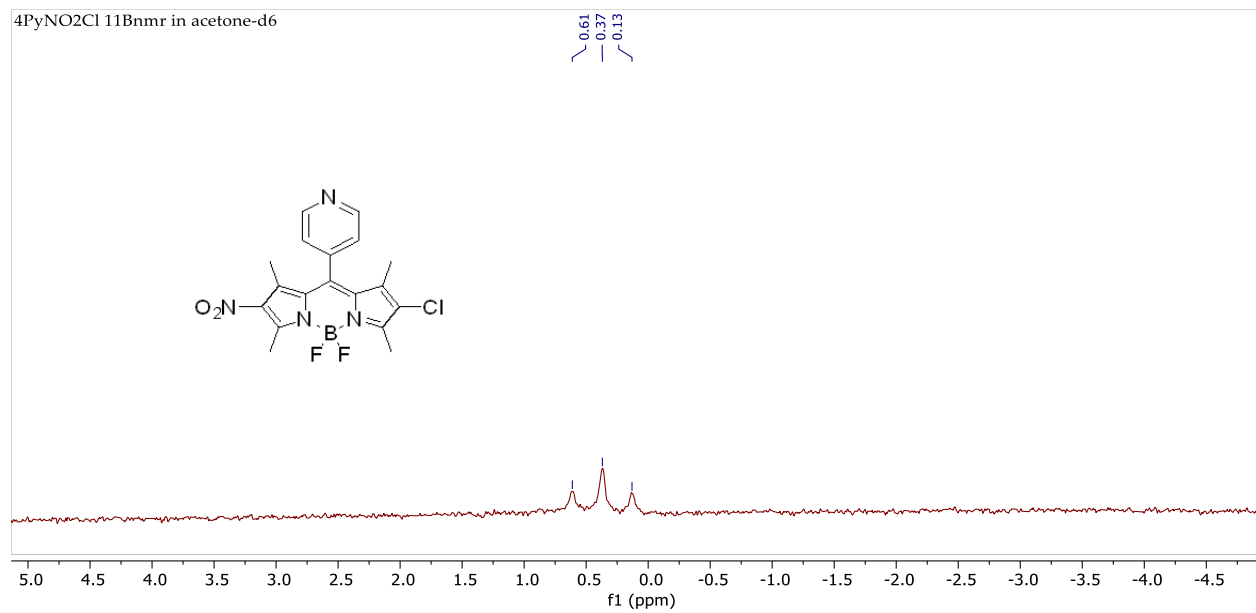


Figure S30. ¹¹B of BODIPY 4PyNO₂Cl in acetone-d₆