

Optical Properties and Mechanofluorochromism of New BODIPY

Dyes Based on Pyridine-Pyrimidine-Hybrid Structure

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Table S1. Crystal data for **PPB1–3**.

Compound	PPB1	PPB2	PPB3
Empirical formula	C ₁₁ H ₆ BClF ₂ N ₄	C ₁₃ H ₁₂ BF ₂ N ₅	C ₁₂ H ₉ BF ₂ N ₄
Formula weight	278.46	287.09	274.04
Crystal system	Monoclinic	Monoclinic	Triclinic
space group	P2(1)/n	P2(1)/c	P-1
	a = 10.4083(9) Å	a = 7.2050(6) Å	a = 7.2996(6) Å
	α = 90°	α = 90°	α = 84.089(2)°
Unit cell dimensions	b = 5.5521(17) Å	b = 18.0229(15) Å	b = 9.5435(7) Å
	β = 93.8410 (10)°	β = 118.152(3)°	β = 80.1410 (10)°
	c = 19.6438(17) Å	c = 11.3751(9) Å	c = 17.2754(15) Å
	γ = 90°	γ = 90°	γ = 84.539(2)°
Volume	1113(2) Å ³	1302.37(18) Å ³	1175.69(16) Å ³
Z	4	4	4
Cal. density	1.633 mg/m ⁻³	1.464 mg/m ⁻³	1.548 mg/m ⁻³
F(000)	560	592	560
Crystal size	0.22 × 0.20 × 0.18 mm ³	0.22 × 0.20 × 0.18 mm ³	0.22 × 0.20 × 0.18 mm ³
GOF	1.006	0.672	0.929
R indices	R ₁ = 0.0597, wR ₂ = 0.0970	R ₁ = 0.0871, wR ₂ = 0.2006	R ₁ = 0.1031, wR ₂ = 0.1275
CCDC No.	1554080	1554081	1554082

Table S2 Calculated electronic excitation energies, oscillator strengths, and related wave functions

Dye	State ^[a]	Energy (eV)	λ (nm)	F ^[b]	Orbitals (coefficient) ^[c]
PPB1	S_1	3.64	340	0.448	H-L (0.694)
	S_2	4.08	303	0.045	H-L+1 (0.692)
	S_3	4.71	263	0.250	H-L+2 (0.689)
PPB2	S_1	3.63	340	0.437	H-L (0.693)
	S_2	4.23	292	0.250	H-L+1 (0.690)
	S_3	4.64	266	0.137	H-L+2 (0.694)
PPB3	S_1	3.66	338	0.428	H-L (0.694)
	S_2	4.11	301	0.084	H-L+1 (0.696)
	S_3	4.62	268	0.258	H-L+2 (0.693)
PPB4	S_1	3.58	346	0.588	H-L (0.693)
	S_2	4.01	308	0.054	H-L+1 (0.690)
	S_3	4.56	271	0.099	H-1-L (0.510), H-1-L+1 (0.415), H-1-L+2 (-0.102), H-1-L+3 (0.109)

[a] Excited state. [b] Oscillator strength. [c] MOs involved in the transitions.

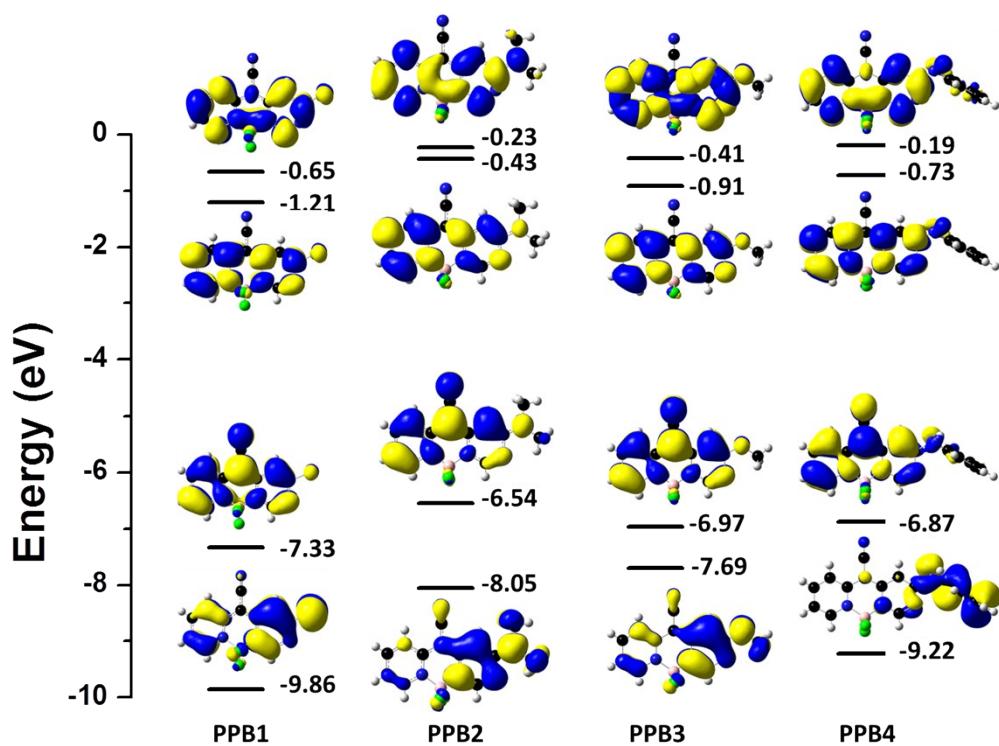


Fig. S1. Molecular orbital energy plots of HOMOs and LUMOs of **PPB1–4** calculated by using CAM-B3LYP/6-31G(d) basis set with Go3 program.

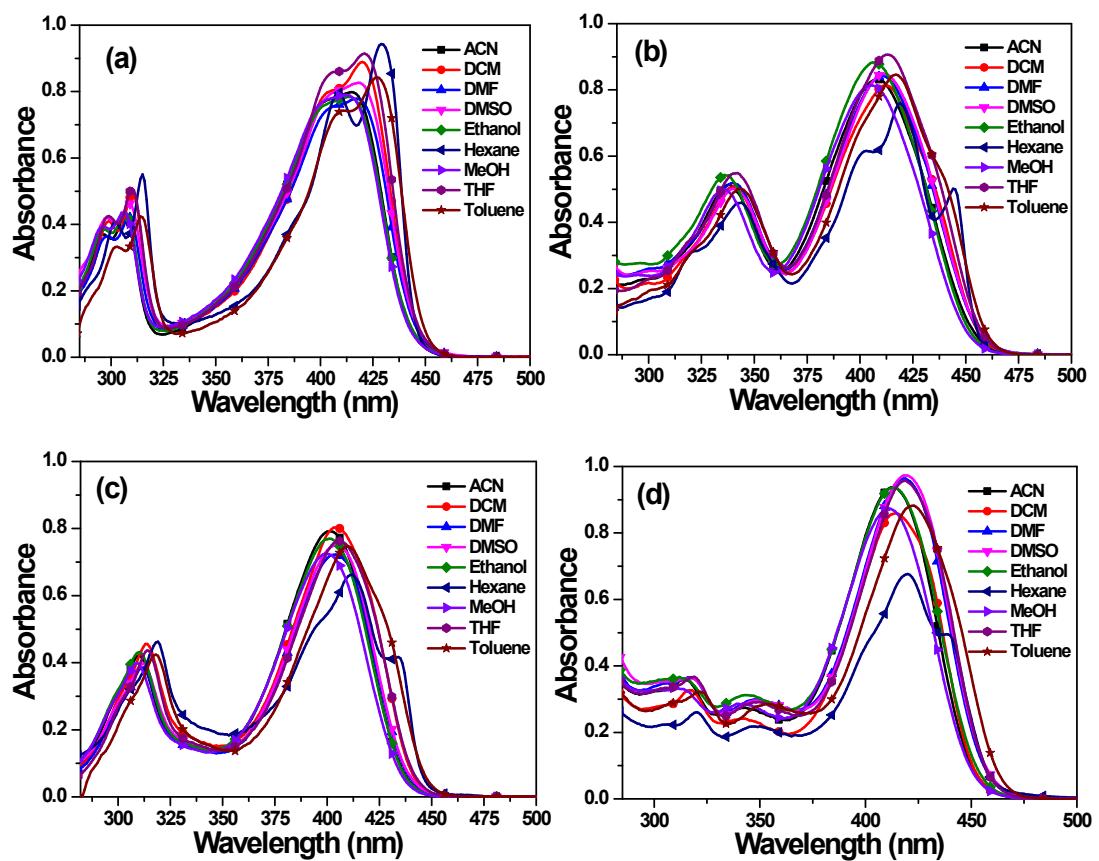


Figure S2. Absorption spectra of **PPB1** (a), **PPB2** (b), **PPB3** (c) and **PPB4** (d) in different solvents ($30 \mu\text{M}$).

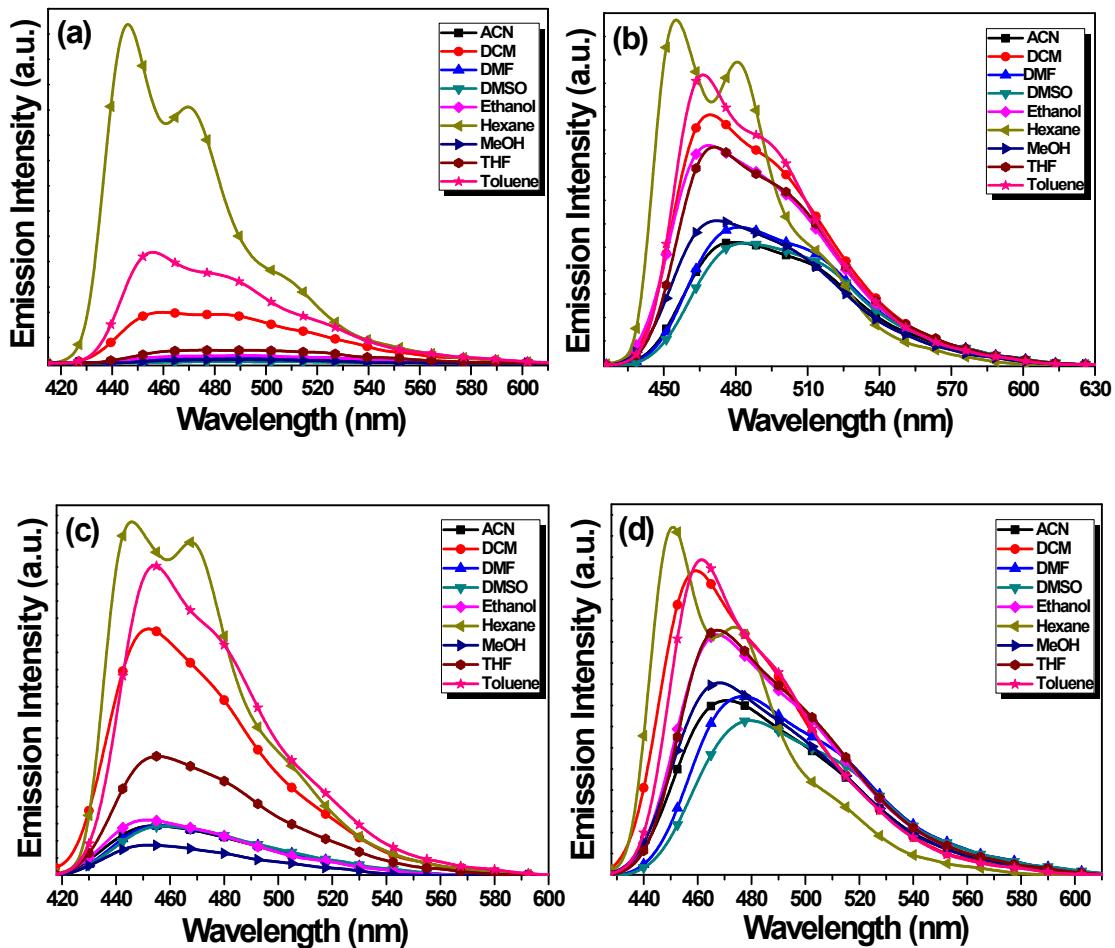


Figure S3. Emission spectra of **PPB1** (a), **PPB2** (b), **PPB3** (c) and **PPB4** (d) in different solvents ($10 \mu\text{M}$).

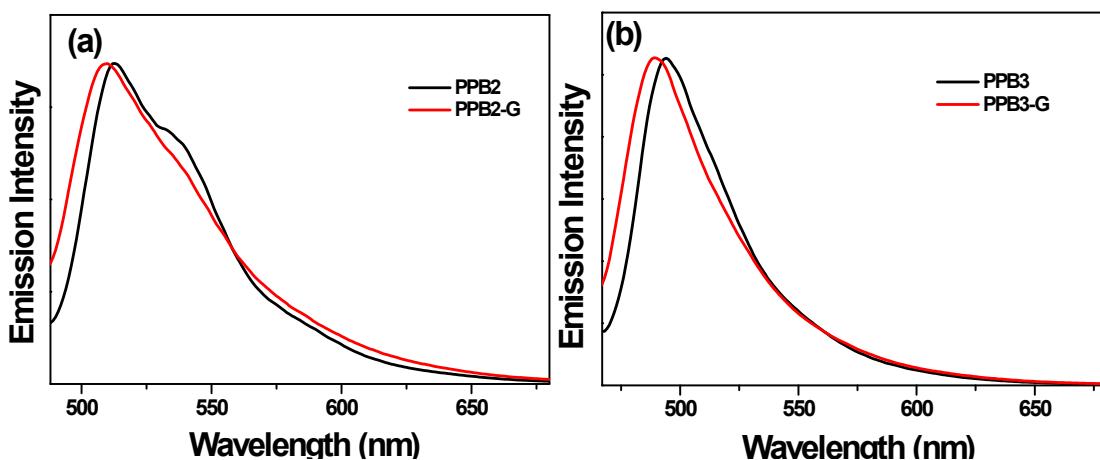


Fig. S4. Solid-state emission spectra of **PPB2** (a) and **PPB3** (b) under different conditions.

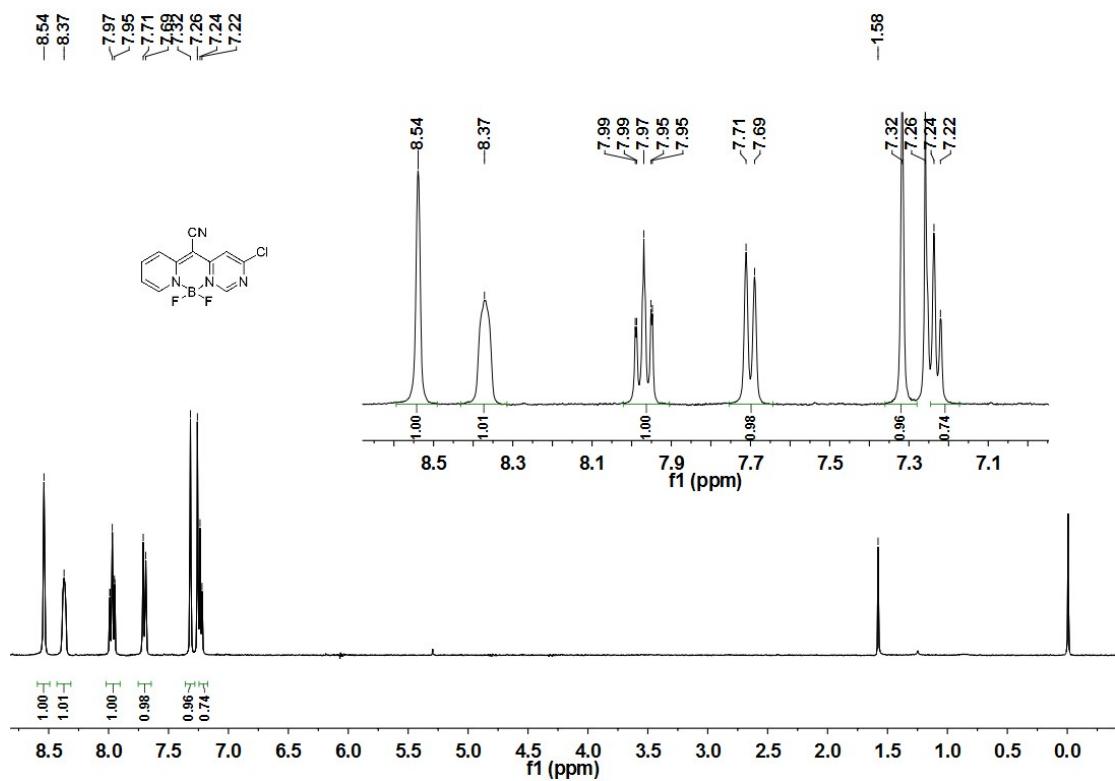


Figure S5. ^1H NMR of **PPB1** in CDCl_3 .

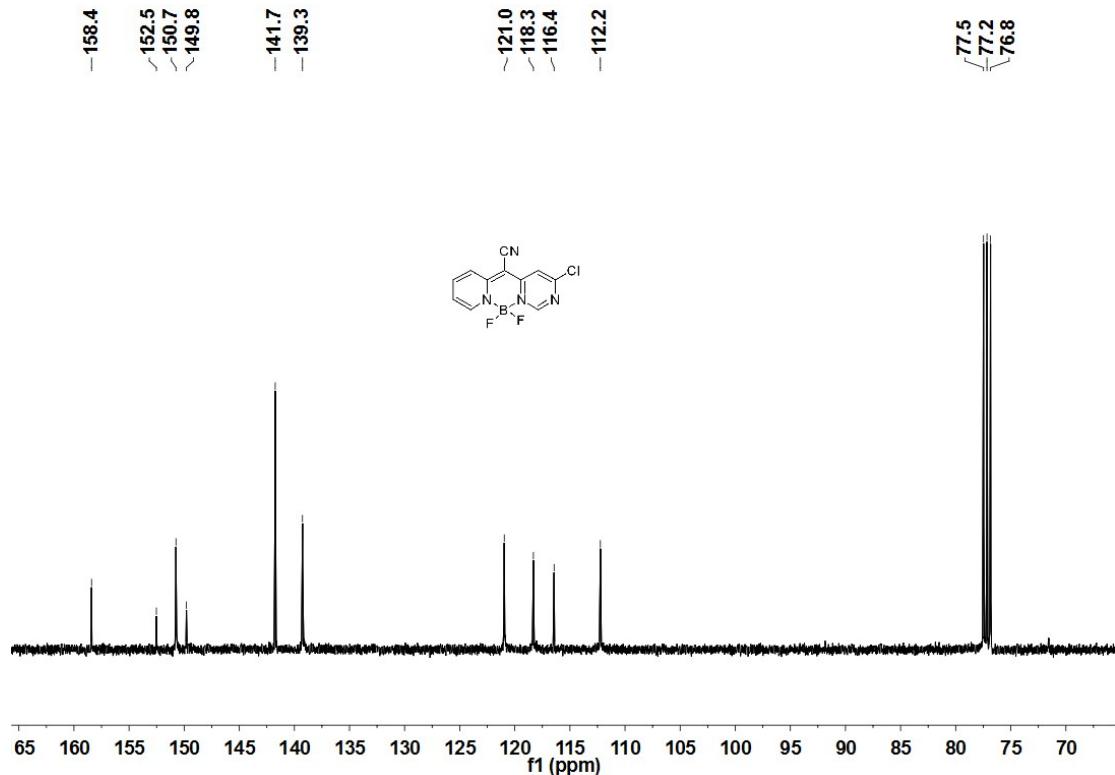


Figure S6. ^{13}C NMR of PPB1 in CDCl_3 .

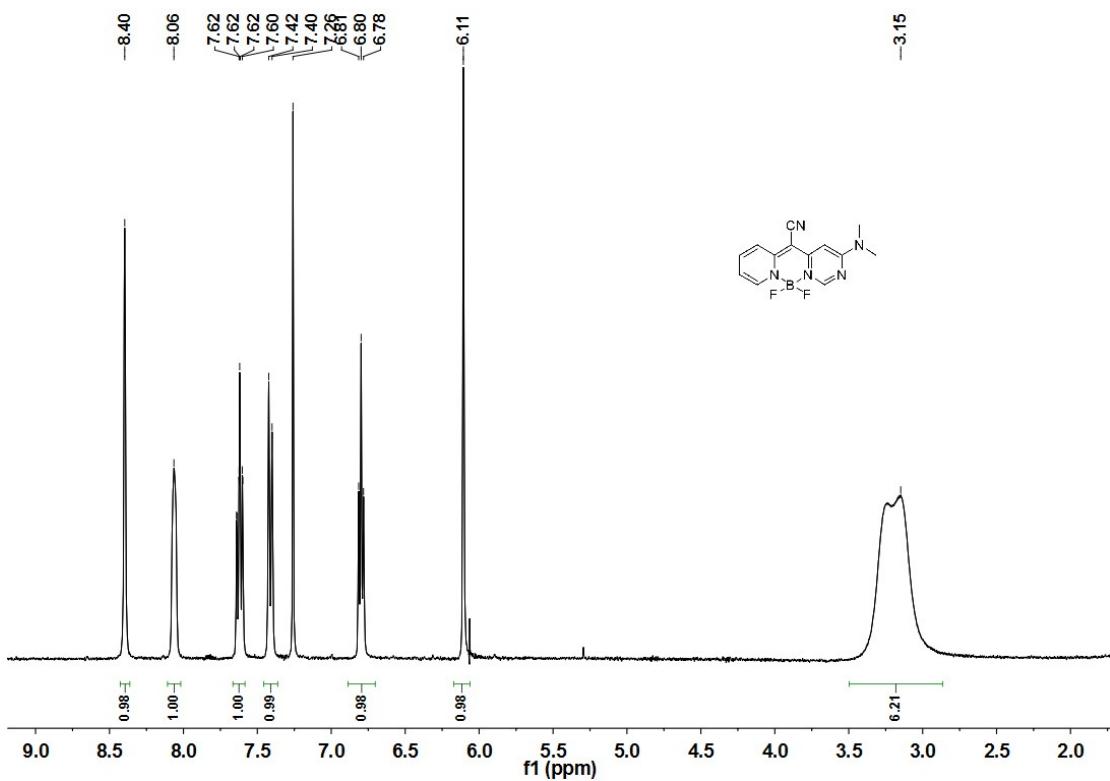


Figure S7. ^1H NMR of **PPB2** in CDCl_3 .

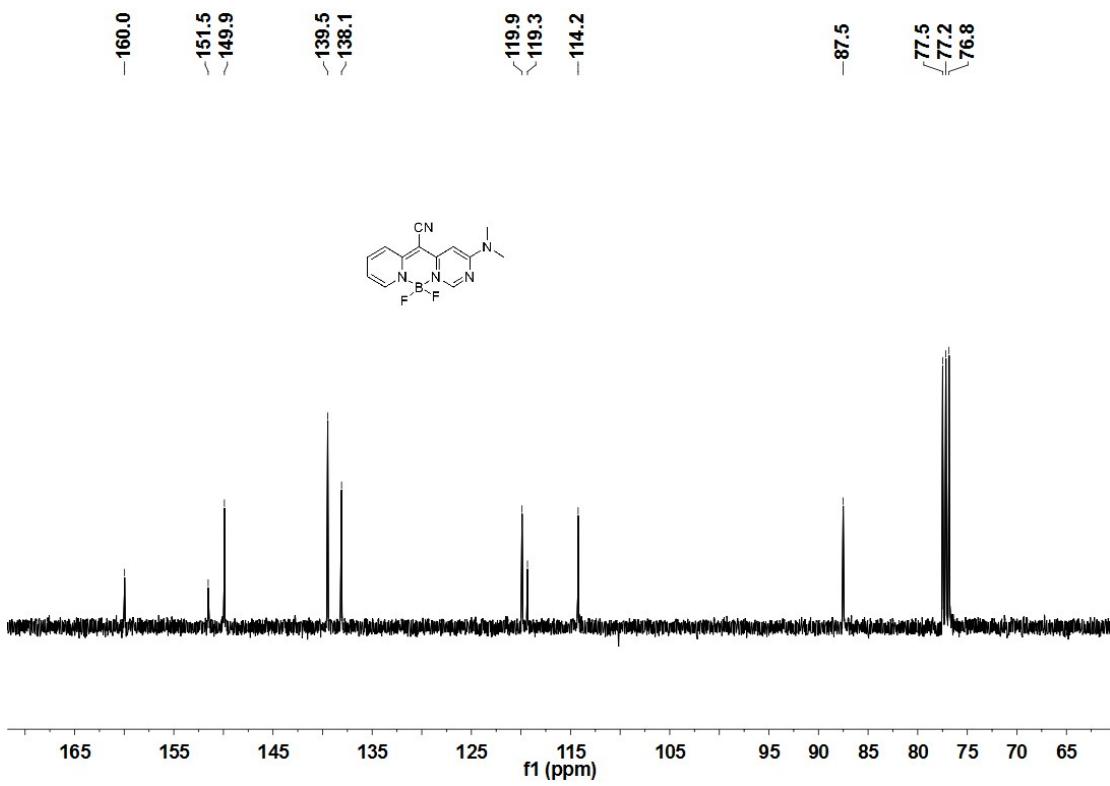


Figure S8. ^{13}C NMR of **PPB2** in CDCl_3 .

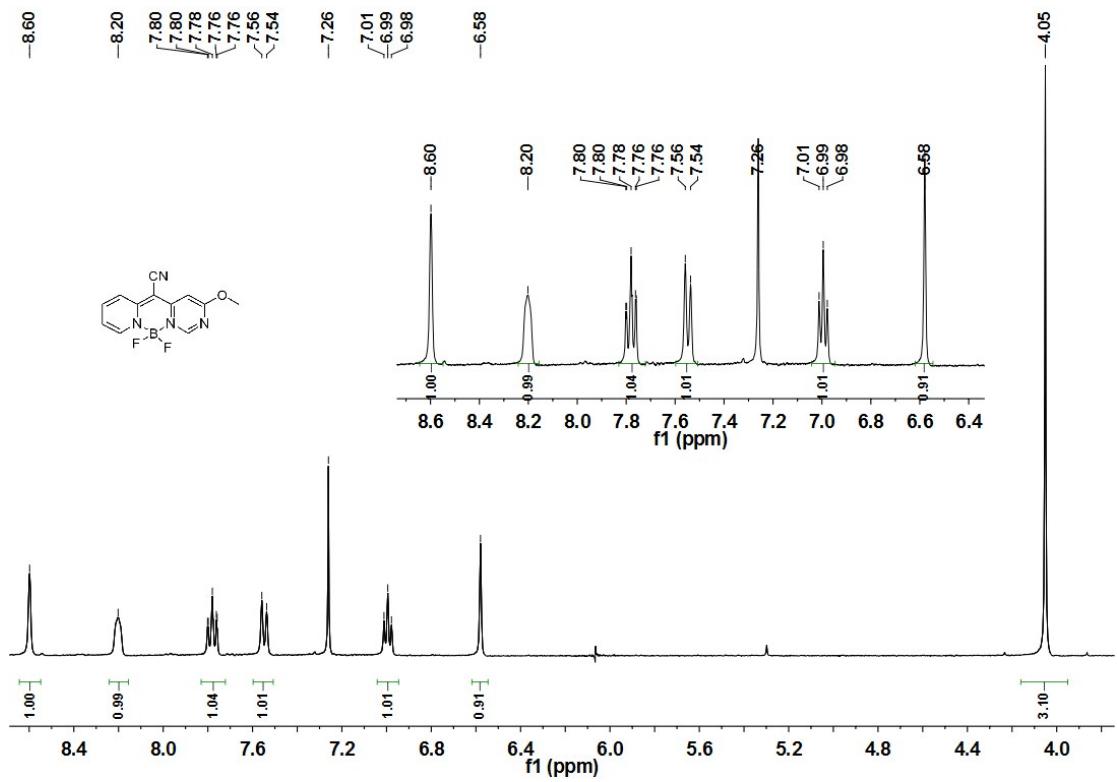


Figure S9. ^1H NMR of **PPB3** in CDCl_3 .

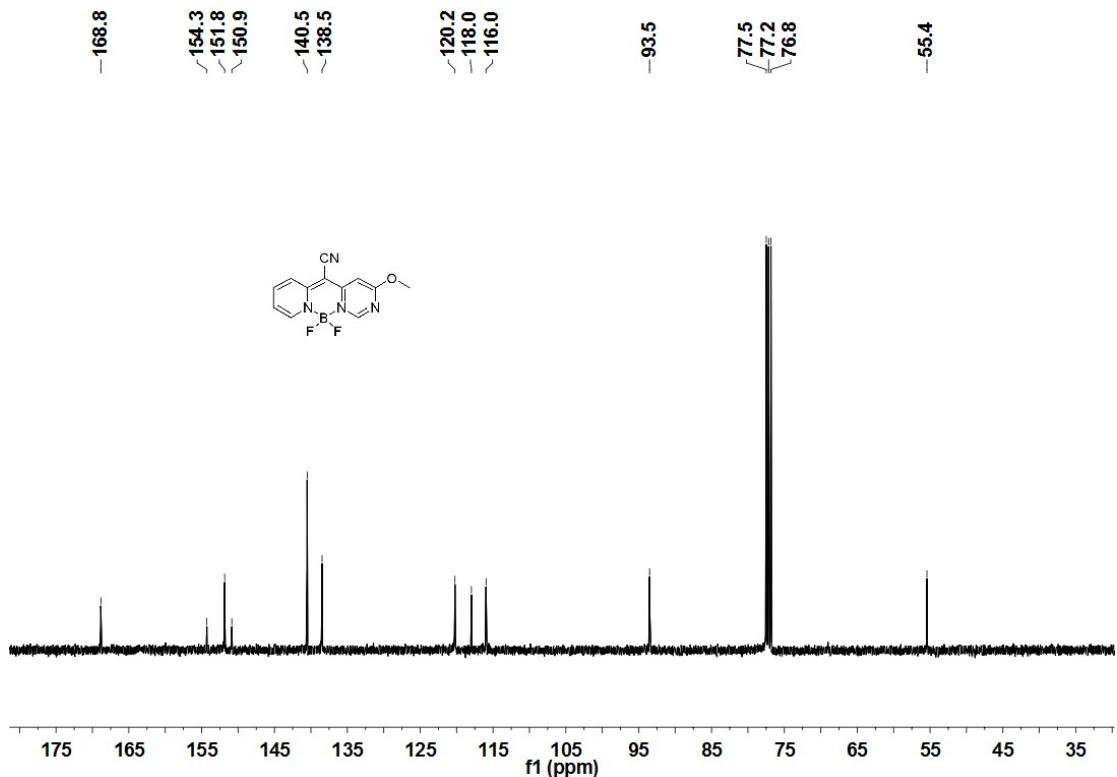


Figure S10. ^{13}C NMR of **PPB3** in CDCl_3 .

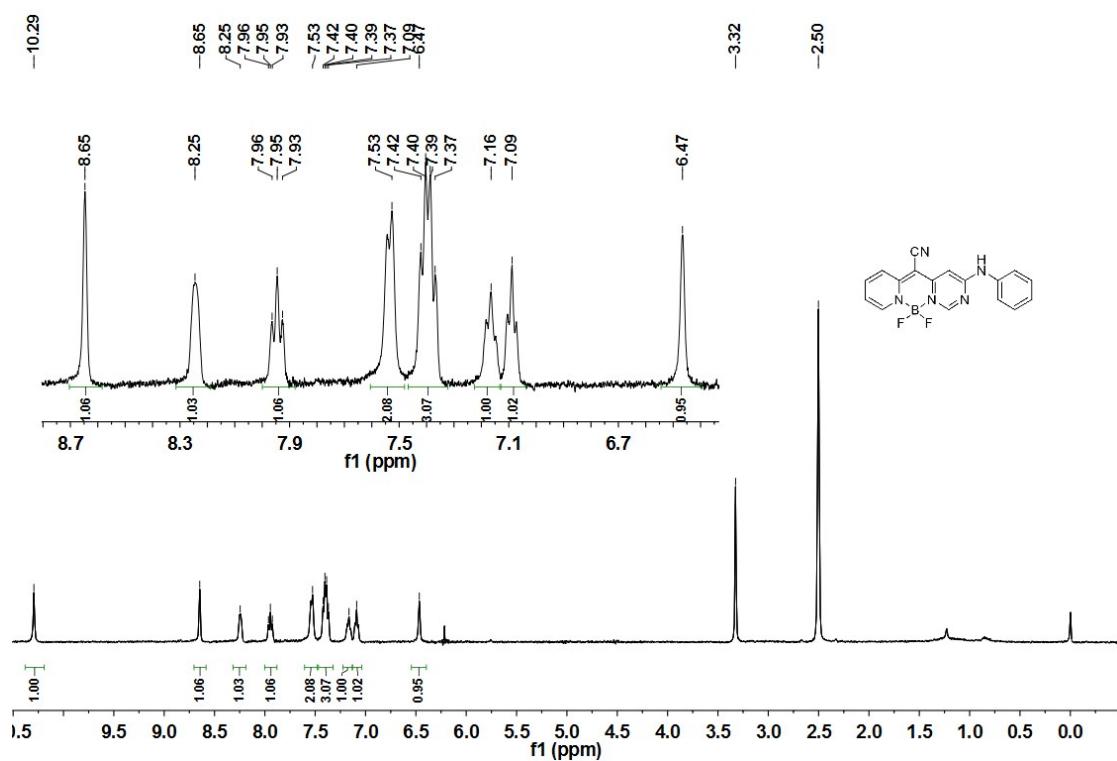


Figure S11. ^1H NMR of PPB4 in DMSO.