Supporting Information

Near-infrared BODIPY two-photon ClO^- probe based on thiosemicarbazide desulfurization reaction: naked-eye detection and mitochondria imaging

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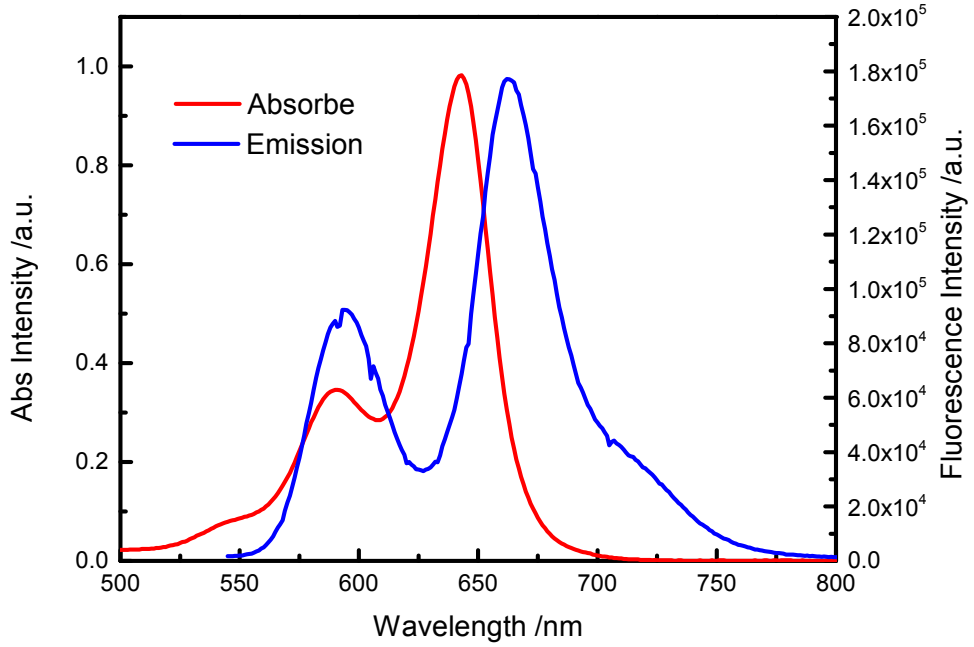


Figure S1 The absorbe and emission spectra of NCS-BOD-OCH_3 (1×10^{-5} mol/L) in solvent H_2O/THF = 1 : 1; pH = 7.4 PBS buffer.

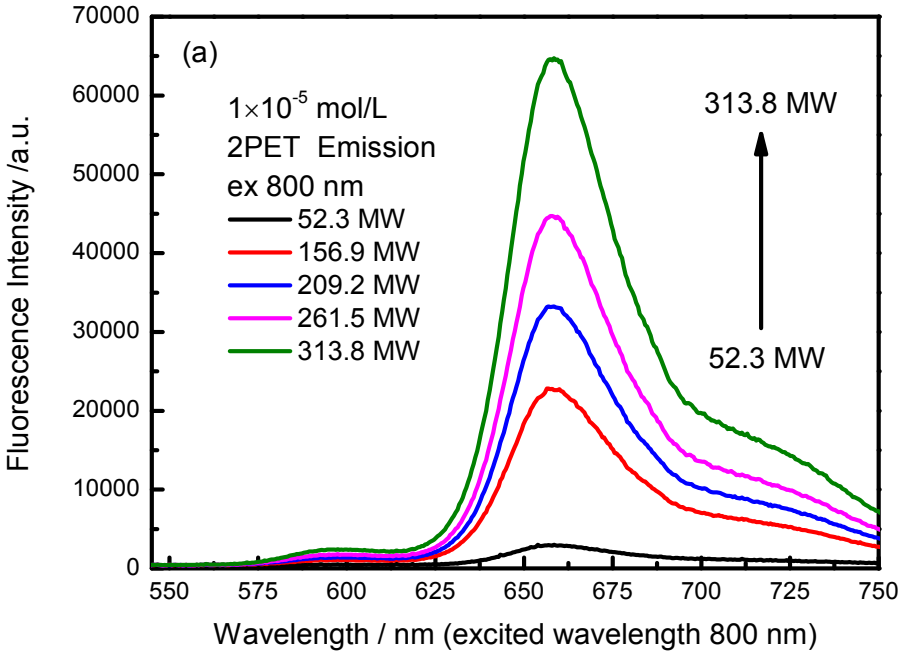


Figure S2 Up-converted fluorescence emission spectra of NCS-BOD-OCH_3 (1×10^{-5} mol/L) under different power laser in solvent H_2O/THF = 1 : 1.

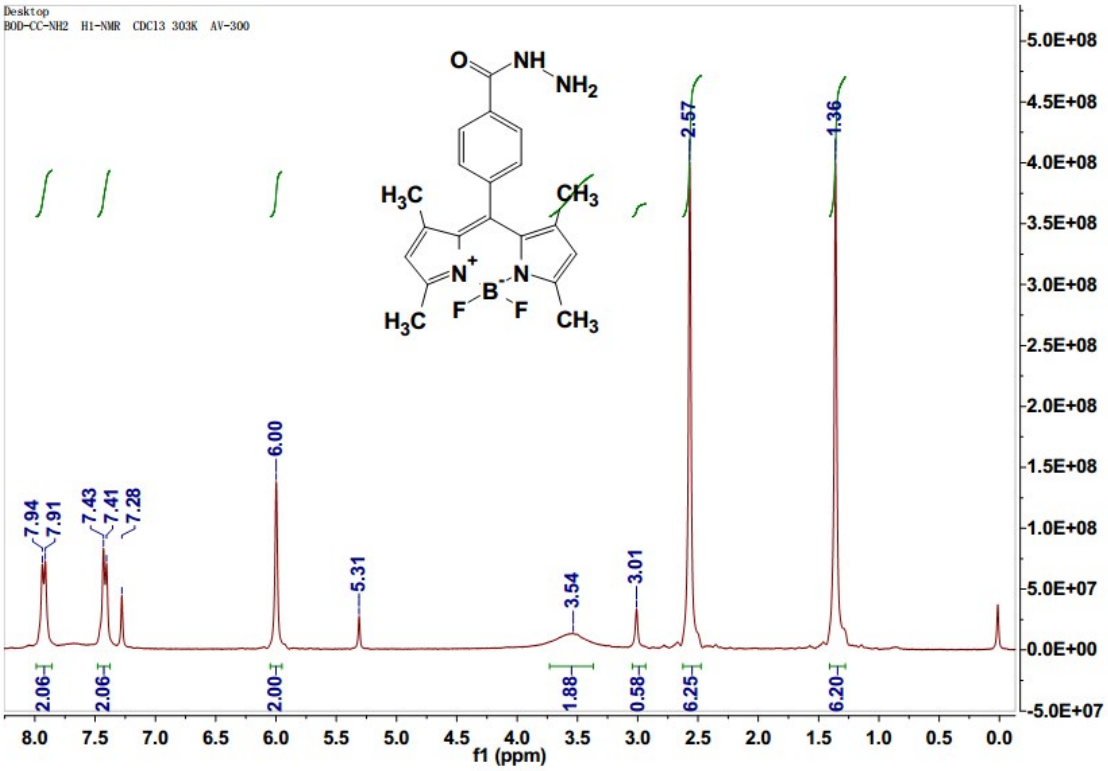


Figure S3. [1]H NMR spectra of compound **NH_2-BODIPY**

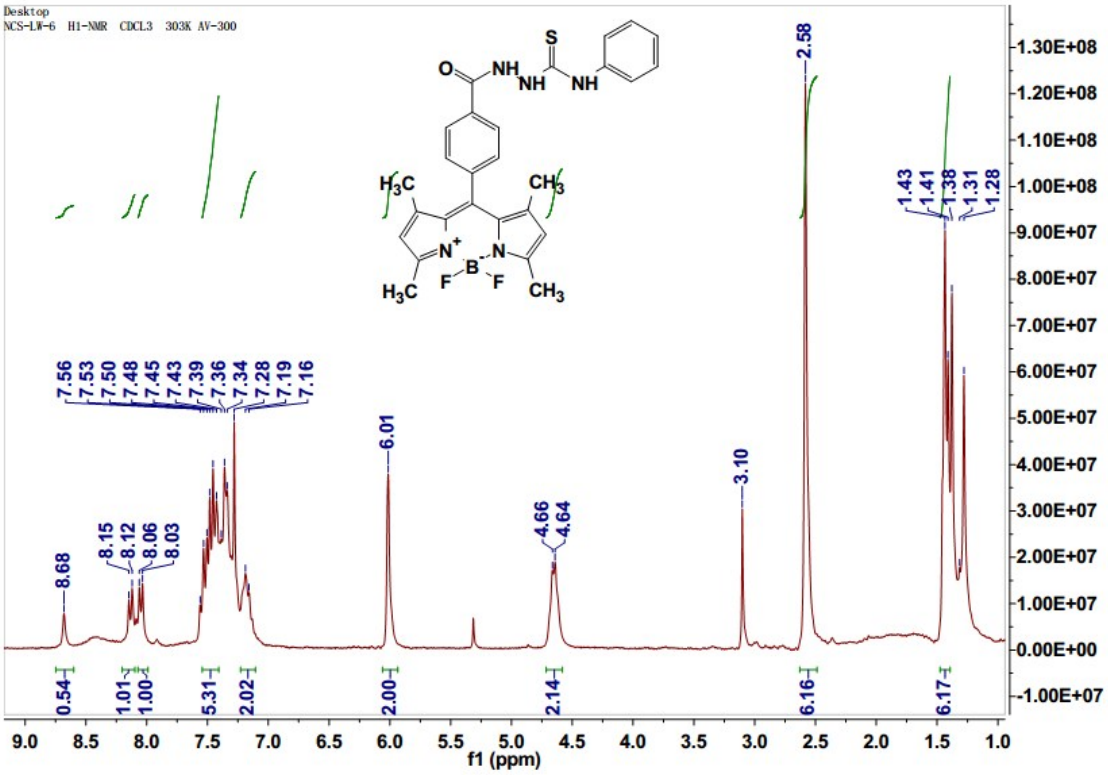


Figure S4. [1]H NMR spectra of compound **NCS-BODIPY**

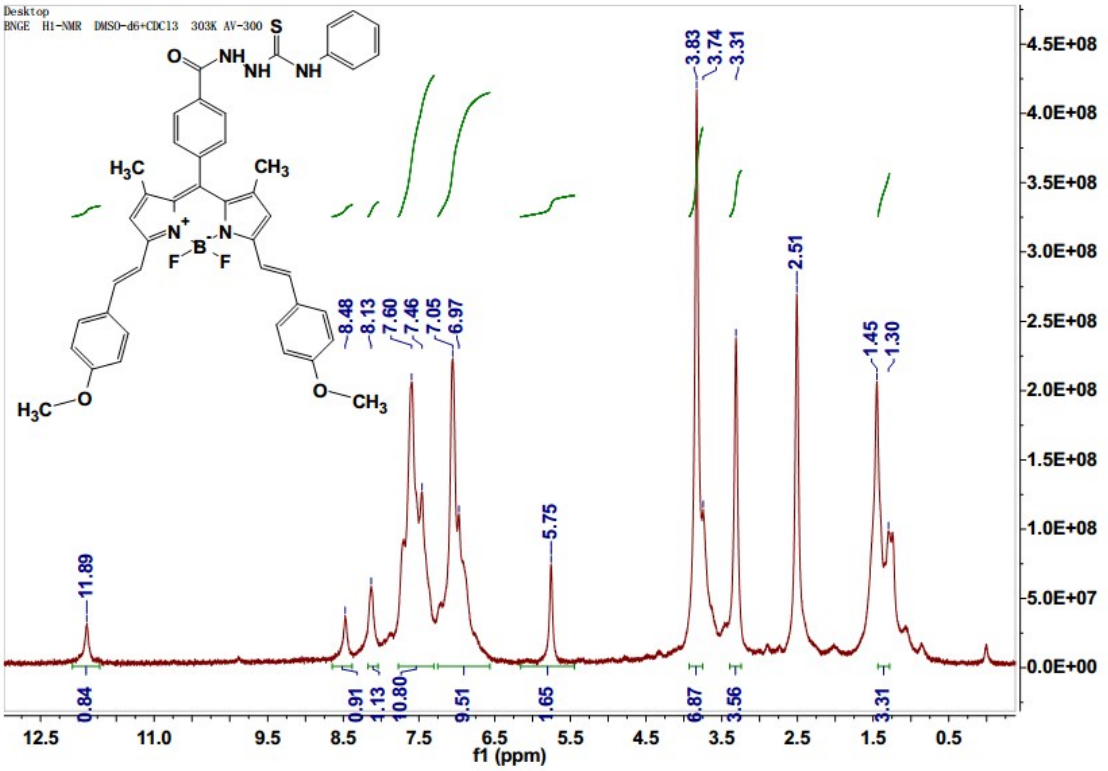


Figure S5. ^{1}H NMR spectra of compound **NCS-BOD-OCH$_3$**

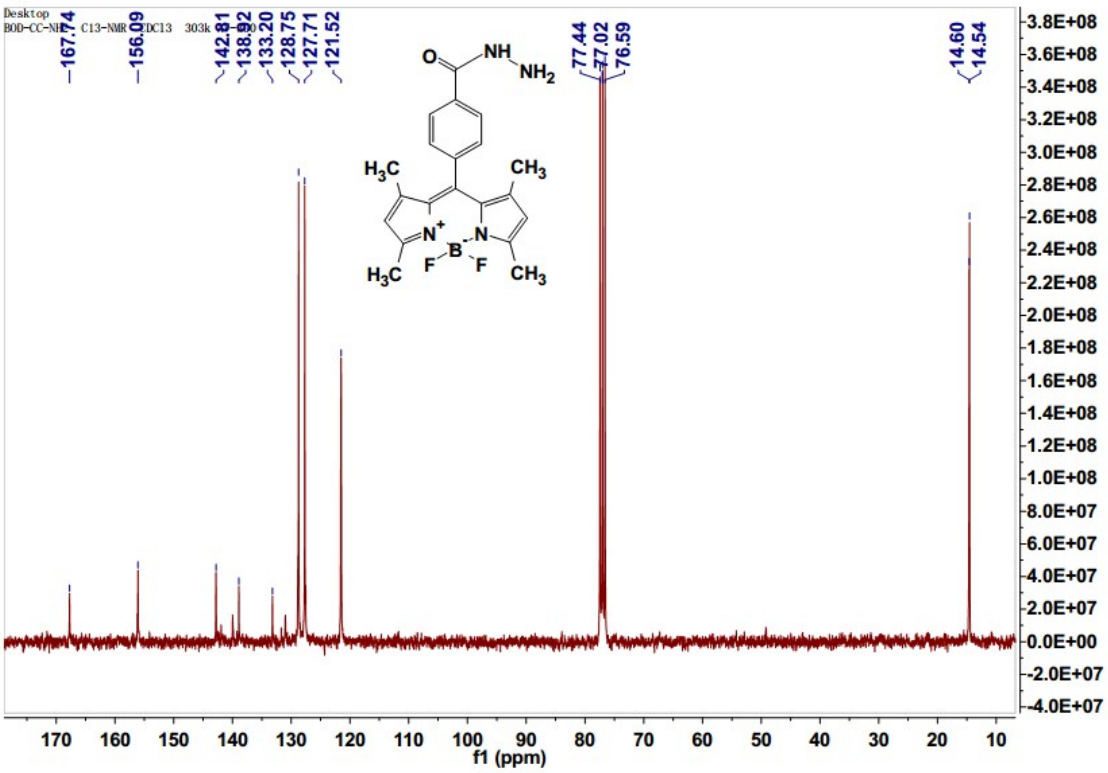


Figure S6. ^{13}C NMR spectra of compound **NH$_2$-BODIPY**

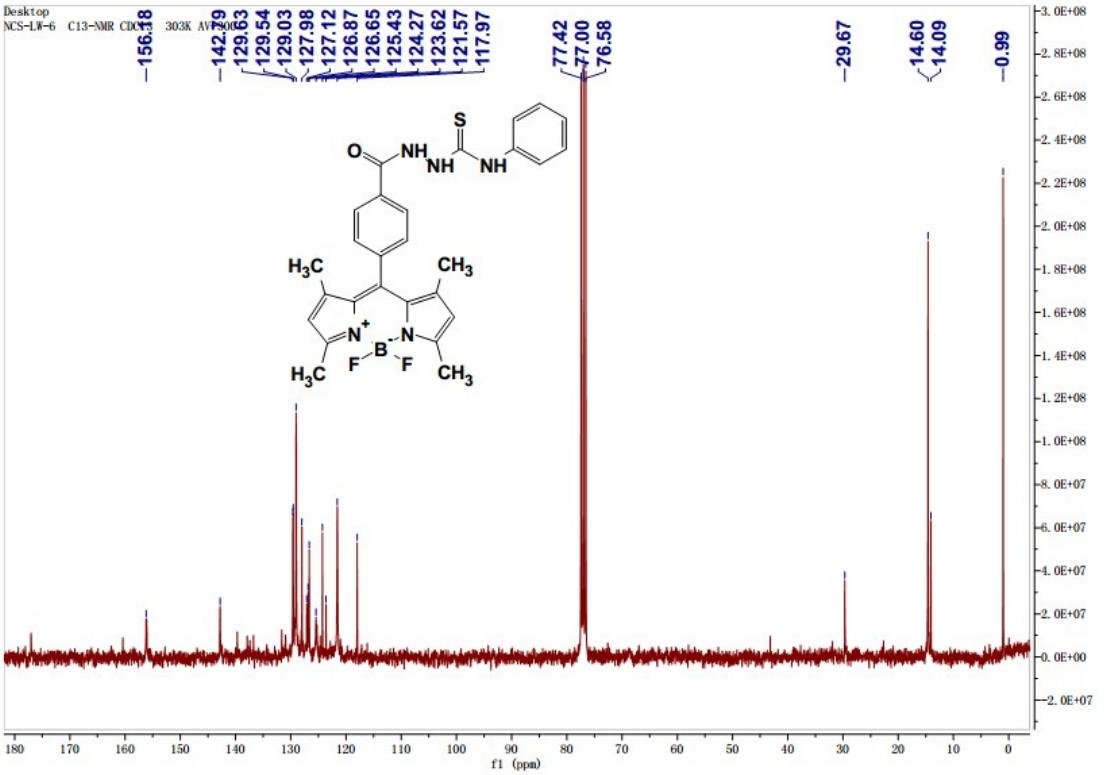


Figure S7. ^{13}C NMR spectra of compound **NCS-BODIPY**

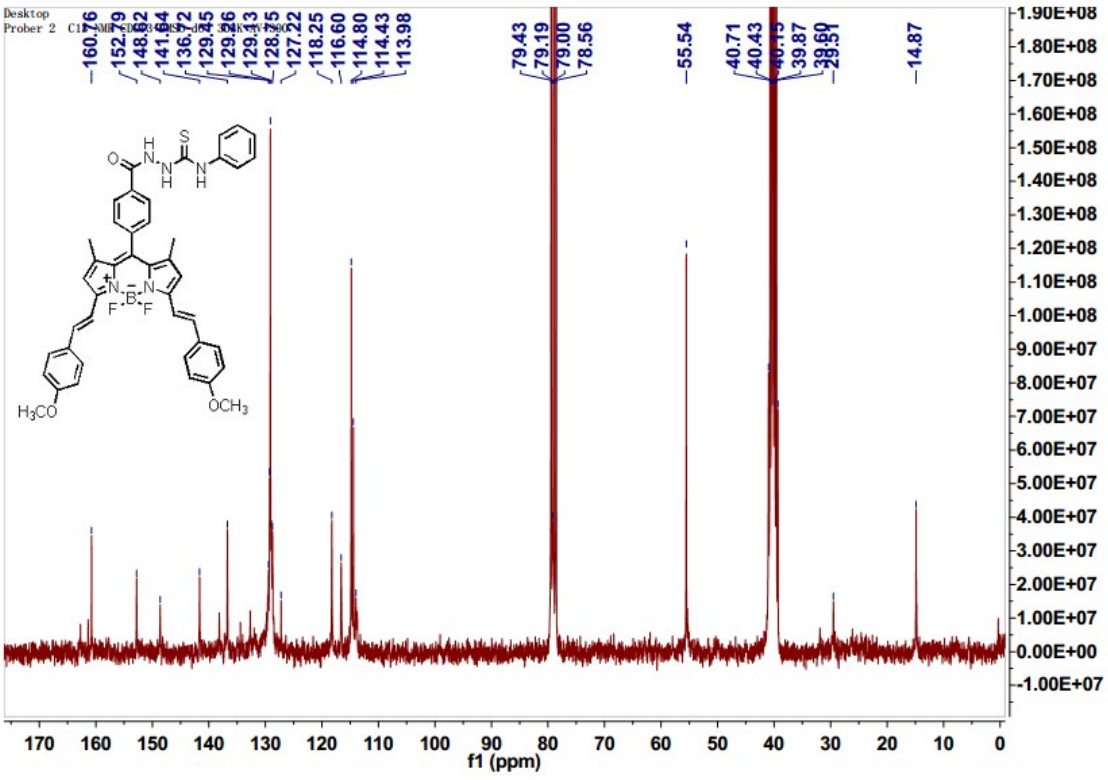


Figure S8. ^{13}C NMR spectra of compound **NCS-BOD-OCH$_3$**

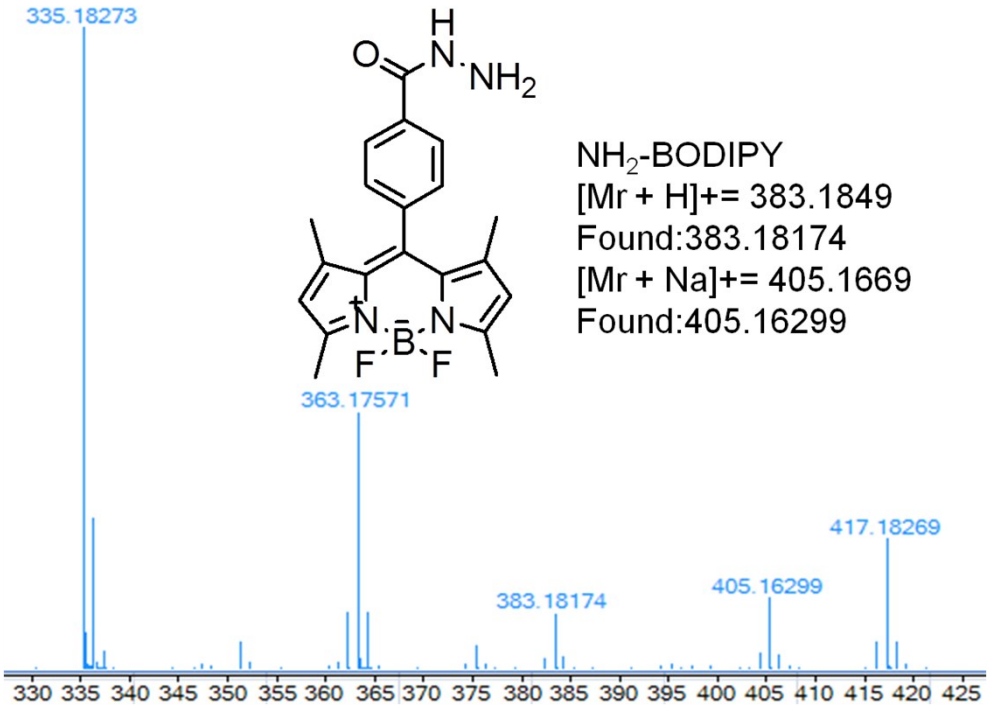


Figure S9. HRMS spectra of **NH_2-BODIPY**

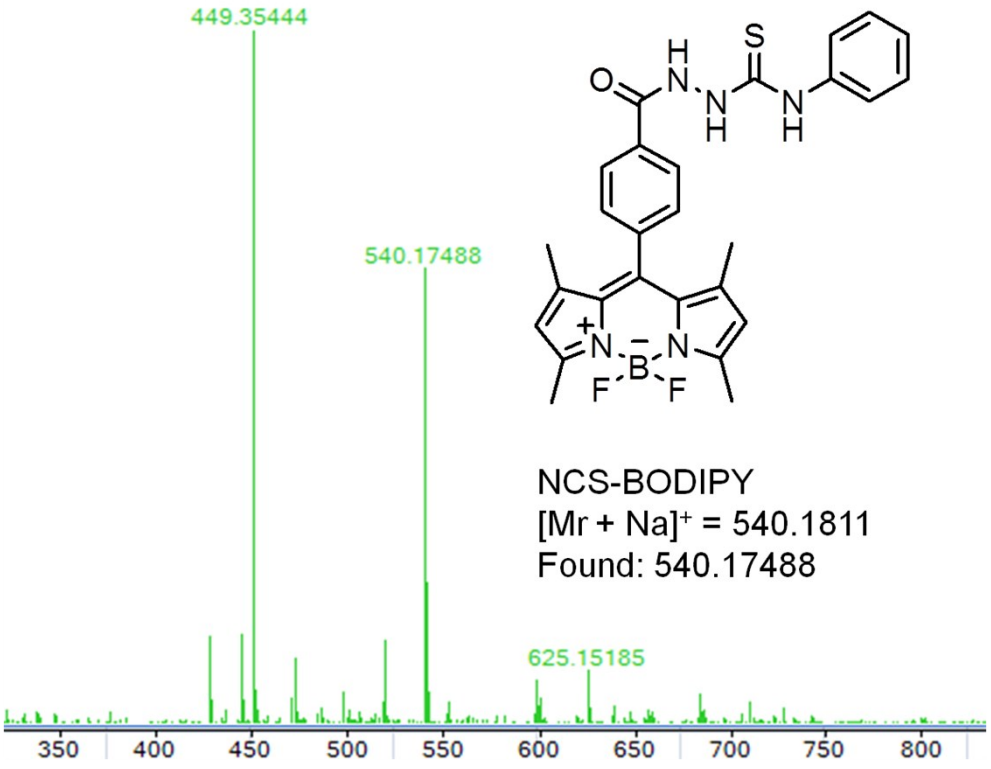
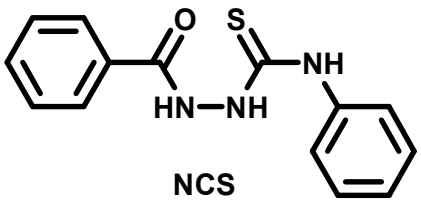
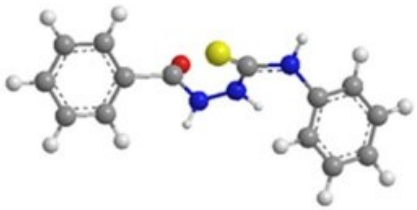
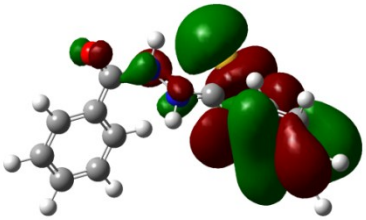


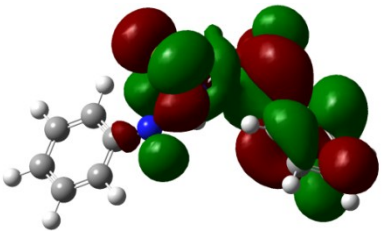
Figure S10. HRMS spectra of **NCS-BODIPY**



NCS

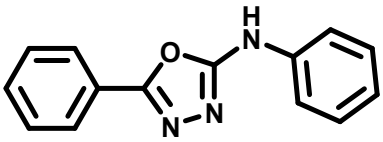




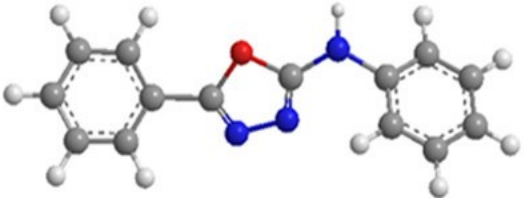


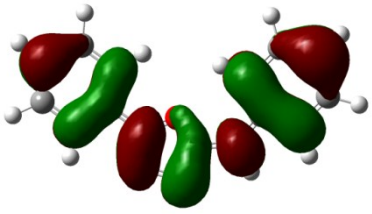
HOMO (-5.3 eV) LUMO (-1.823 eV)

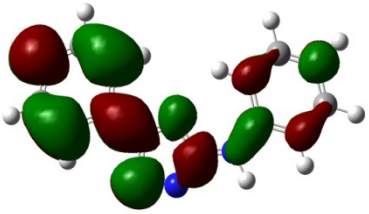
DFT calculations of NCS structure



NCS/ClO$^-$

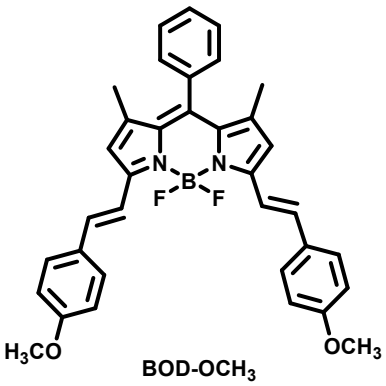




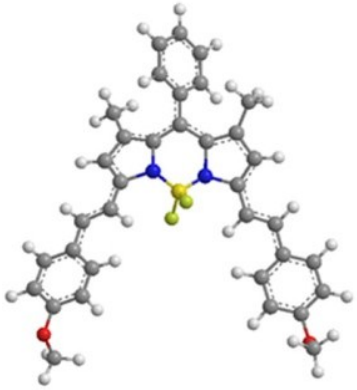


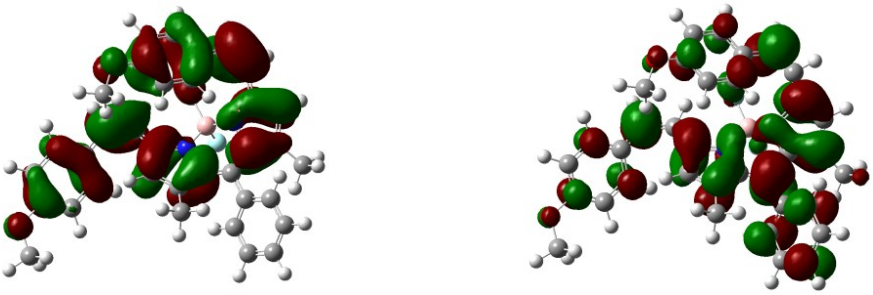
HOMO (-5.39 eV) LUMO (-0.87) eV

DFT calculations of NCS after reacting with ClO$^-$



BOD-OCH$_3$



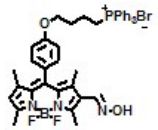
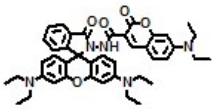
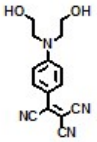
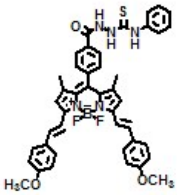


HOMO -4.79 eV LUMO -2.72 eV

DFT calculations of BOD-OCH_3 structure

Figure S11 The DFT calculations of different parts of NCS-BOD-OCH_3 based on B3LYP/6-31G(d) basis set.

Table 1 Comparison with some published research work

Compounds	λ_{em} (nm)	LOD	Detection time
	529	2.5×10^{-7} M	Within 125 s
	501/578	2.4×10^{-8} M	60 s
	527	4×10^{-6} M	600 s
	595/665	1.15×10^{-6} M	540 s