Supporting Information

A dual-mode turn-on fluorescent BODIPY-based probe for visualization of mercury ion in living cells

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Content

1. Additional Absorption and Emission Spectra

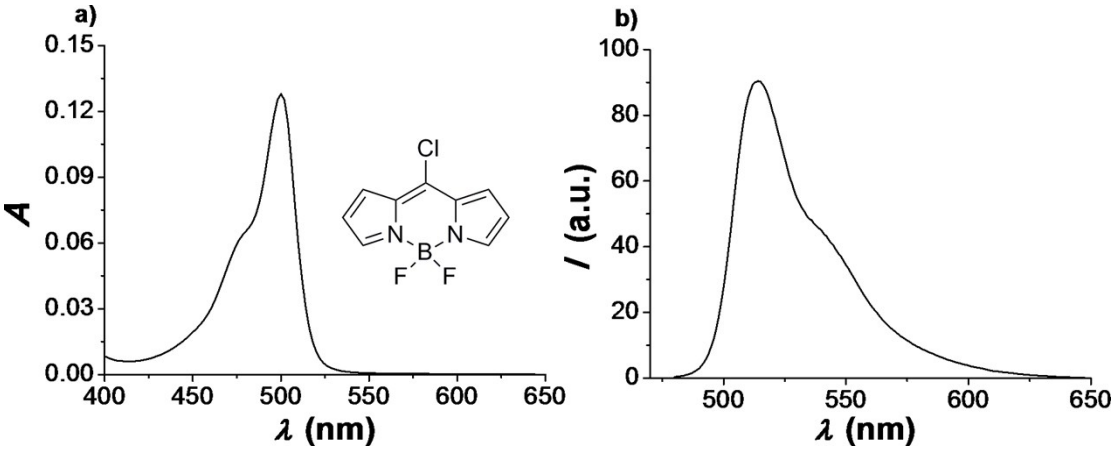

Figure S1. Absorption (**a**) and emission spectra (**b**, λ_{ex} = 470 nm) of 8-chloro-BODIPY in PBS buffer solutions (pH = 7.4, containing 0.5% DMSO) at 25 °C.

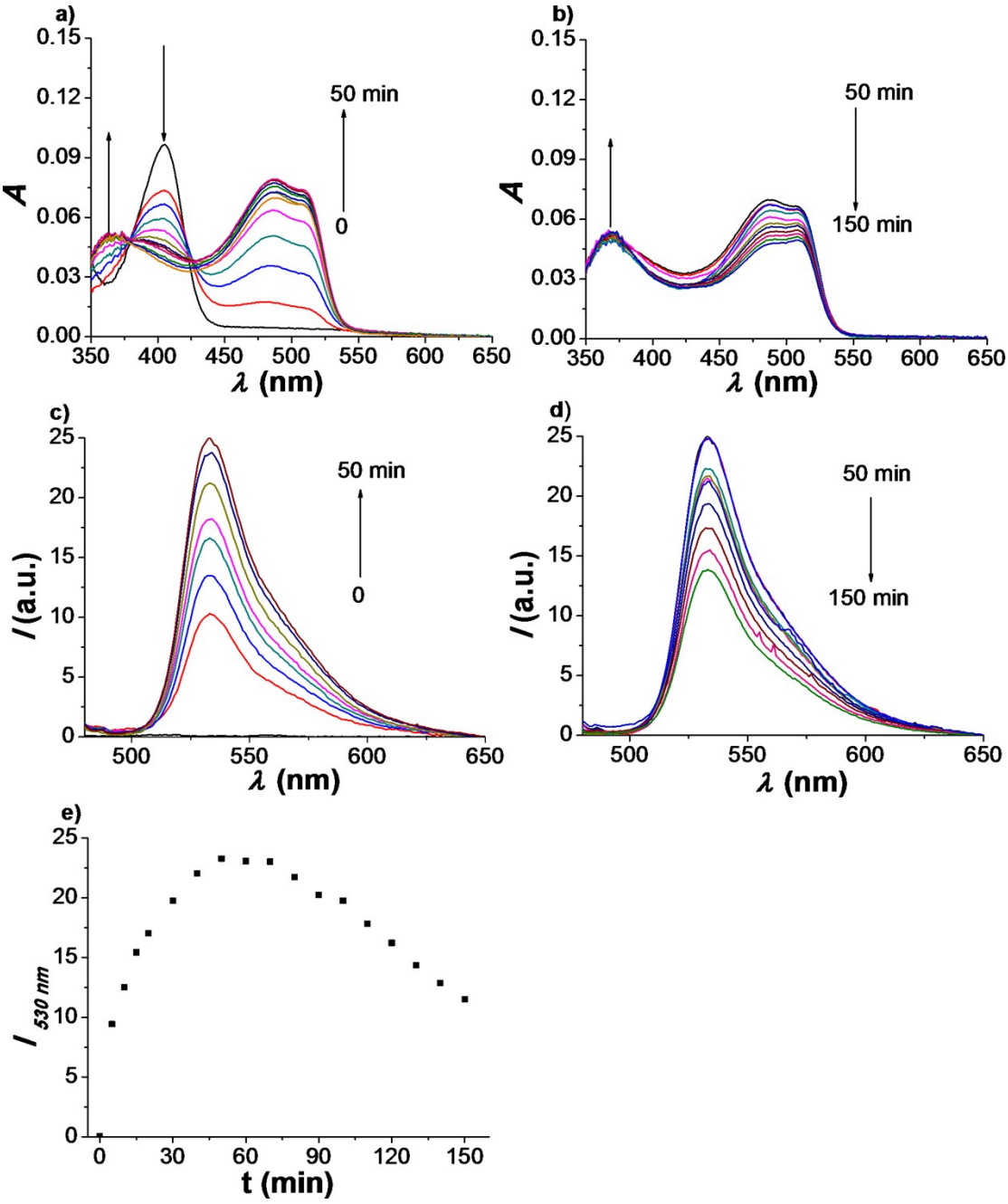

Figure S2. The time-dependent profile of probe **1** (5 μM) in PBS buffer solutions (pH = 7.4, containing 0.5% DMSO) responded to Hg^{2+} (10 μM) after the specified time periods (0-150 min) for absorption (**a**) at 0, 5, 10, 15, 20, 30, 40 and 50 min, (**b**) at 50, 60, 70, 80, 90, 100, 110, 120, 130, 140 and 150 min, and for fluorescence emission (**c**) at 0, 5, 10, 15, 20, 30, 40 and 50 min, as well as (**d**) at 50, 60, 70, 80, 90, 100, 110, 120, 130, 140 and 150 min (λ_{ex} = 470 nm). (**e**) The time-dependent emission intensities (λ_{em} = 530 nm, λ_{ex} = 470 nm).

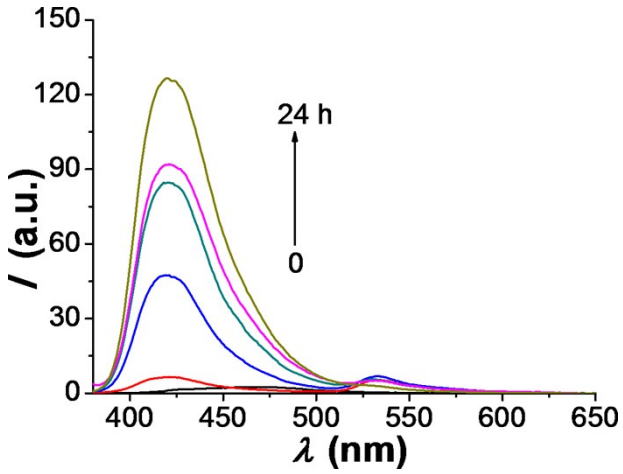

Figure S3. Fluorescence emission time profile of probe **1** (5 μM, λ_{ex} = 370 nm) in PBS buffer solutions (pH = 7.4, containing 0.5% DMSO) with Hg^{2+} (10 μM) after the specified time periods (0, 10 min, 50 min, 3 h, 6 h, and 24 h, respectively).

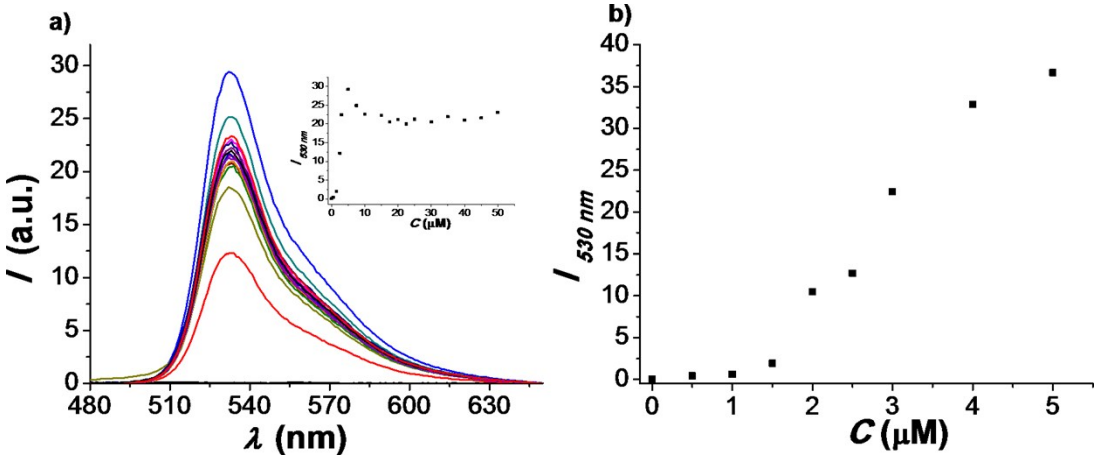

Figure S4. (**a**) Fluorescence spectra (λ_{ex} = 470 nm) of probe **1** (5 μM) in the presence of increasing concentrations of $HgCl_2$ (0-50 μM) in PBS buffer solutions (pH = 7.4, 0.5% DMSO). Insets: plot between the fluorescent intensity of probe **1** to increased concentration. (**b**) Enlarged plot between the fluorescent intensity of probe **1** to increased concentration in the range of 0-5 μM after incubation for 150 min (λ_{em} = 530 nm).

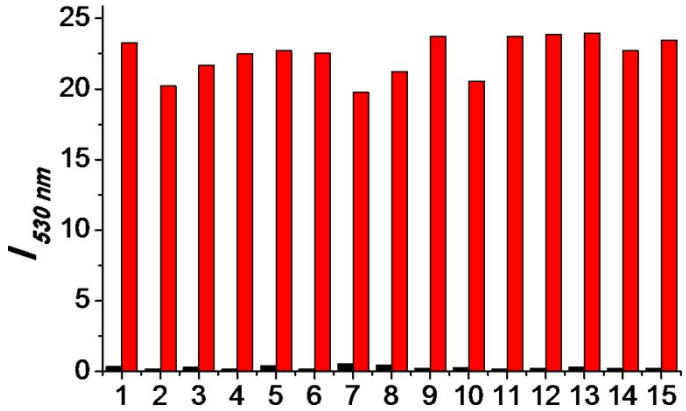

Figure S5. Selectivity of probe **1** (5 μM) toward Hg^{2+} ion (10 μM) and other various metal ions (100 μM) in PBS buffer solutions (pH = 7.4, containing 0.5% DMSO) for 150 min monitored at 530 nm (λ_{ex} = 470 nm). Black bar represents the fluorescence intensity of only a single analyte with probe **1**; Red bar represents the fluorescence intensity of mixture of analyte and $HgCl_2$ with probe **1**. (1) blank, (2) Ag^{+}, (3) Al^{3+}, (4) Ca^{2+}, (5) Cd^{2+}, (6) Co^{2+}, (7) Cu^{2+}, (8) Fe^{3+}, (9) K^{+}, (10) Mg^{2+}, (11) Na^{+}, (12) Ni^{2+}, (13) Pb^{2+}, (14) Zn^{2+}, (15) Sn^{2+}.

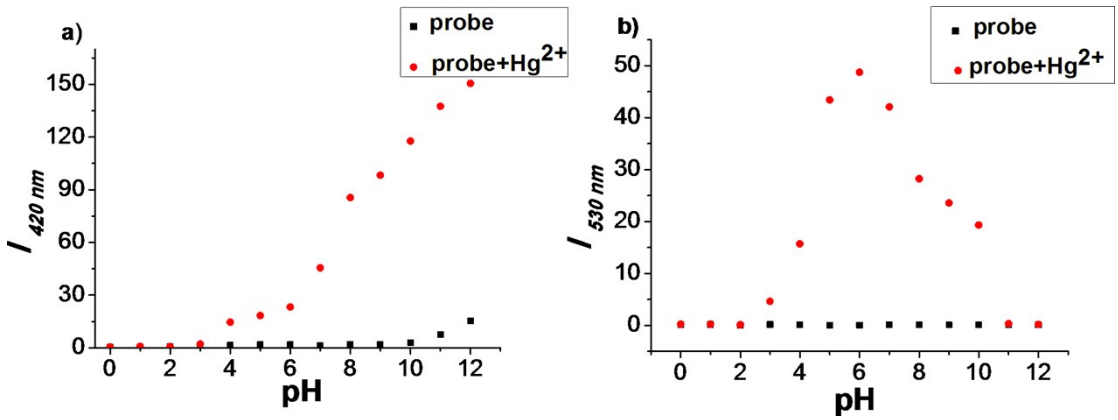

Figure S6. Fluorescence intensity profiles of probe **1** (5 μM) prior to and after addition of $HgCl_2$ (10 μM) at various pH values for 150 min incubation. (**a**) Monitored at 420 nm (λ_{ex} = 370 nm); (**b**) Monitored at 530 nm (λ_{ex} = 470 nm).

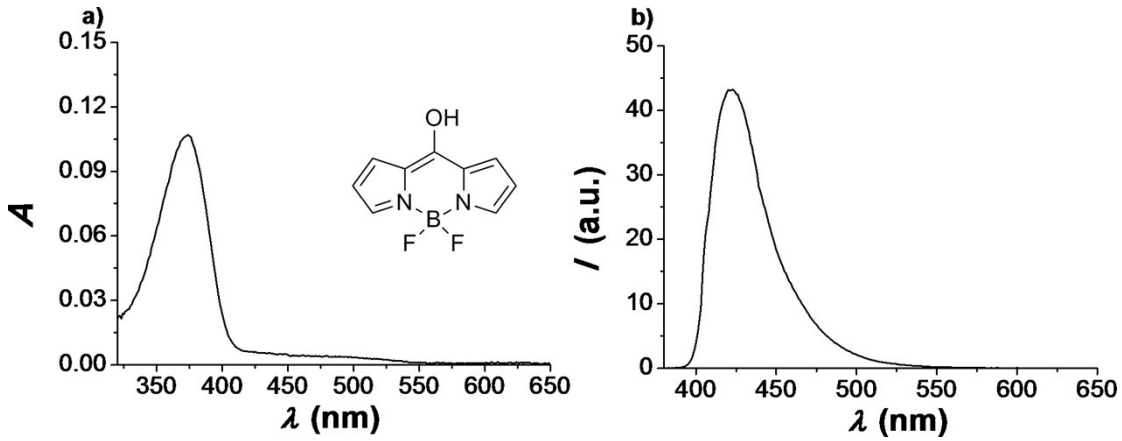

Figure S7. Absorption (**a**) and emission spectra (**b**, λ_{ex} = 370 nm) of 8-hydroxy-BODIPY measured in PBS buffer solutions (pH = 7.4, containing 0.5% DMSO) at 25 °C.

2. NMR Spectra

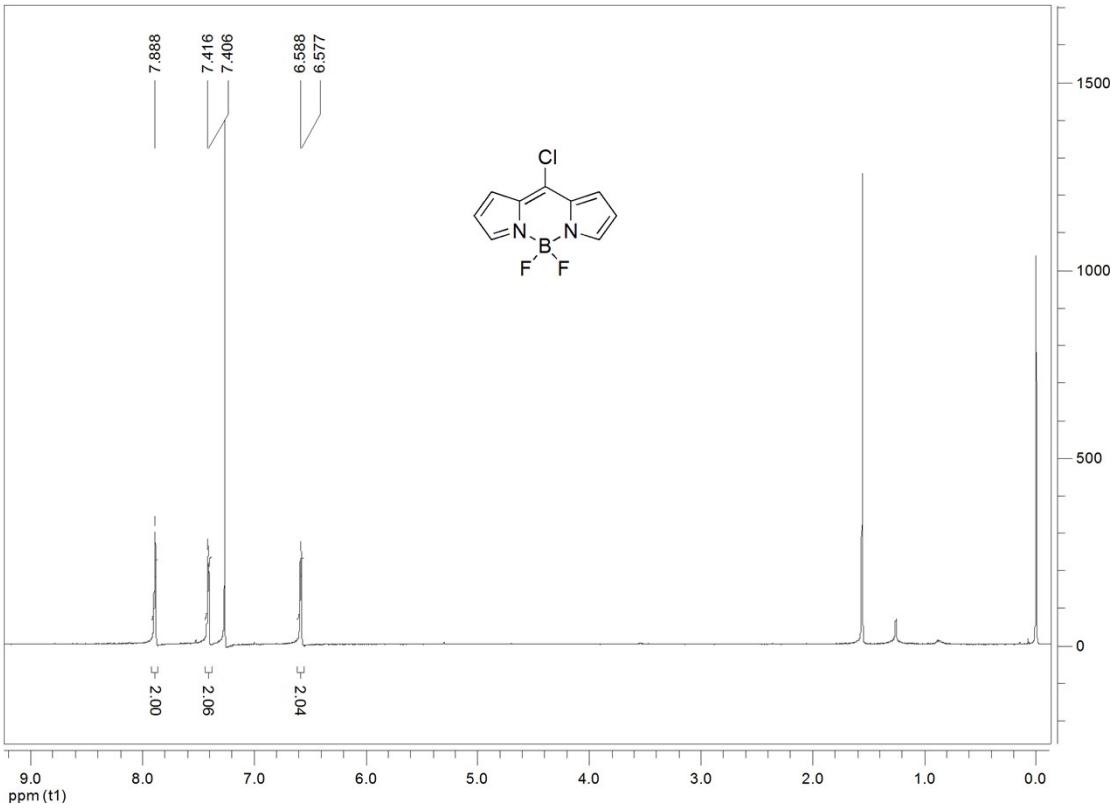

Figure S8. ^{1}H NMR spectra of 8-chloro-BODIPY in $CDCl_3$.

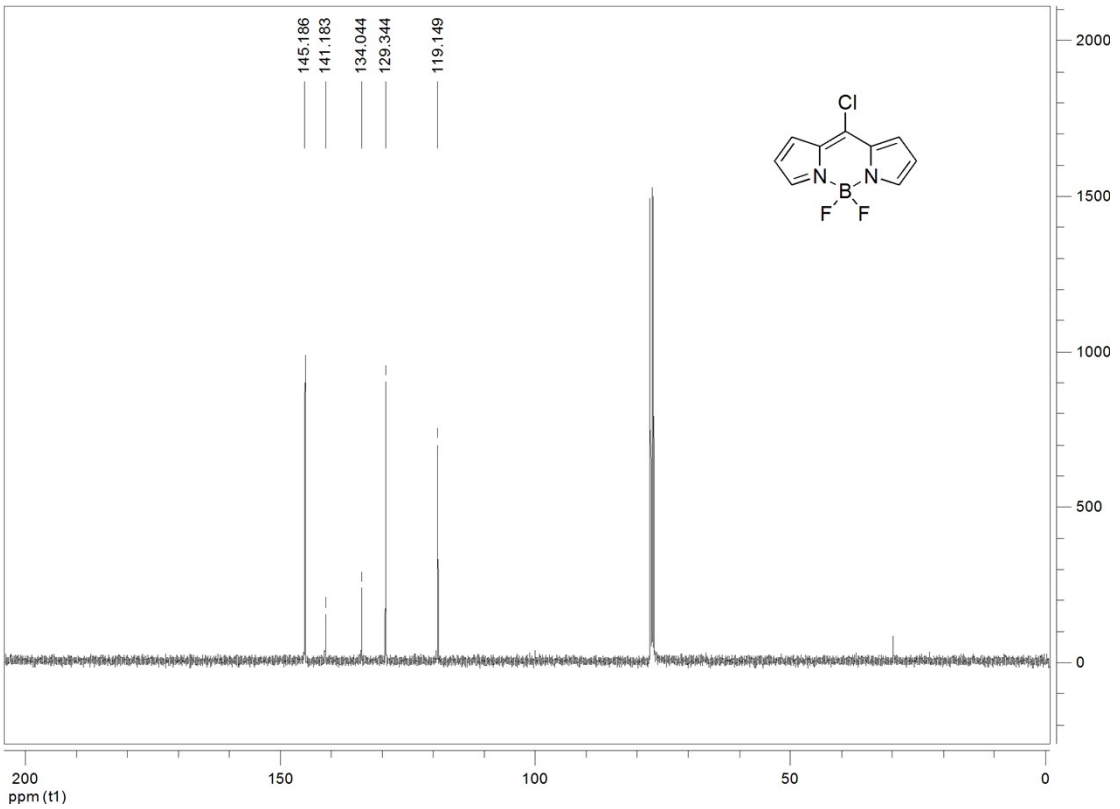

Figure S9. ^{13}C NMR spectra of 8-chloro-BODIPY in $CDCl_3$.

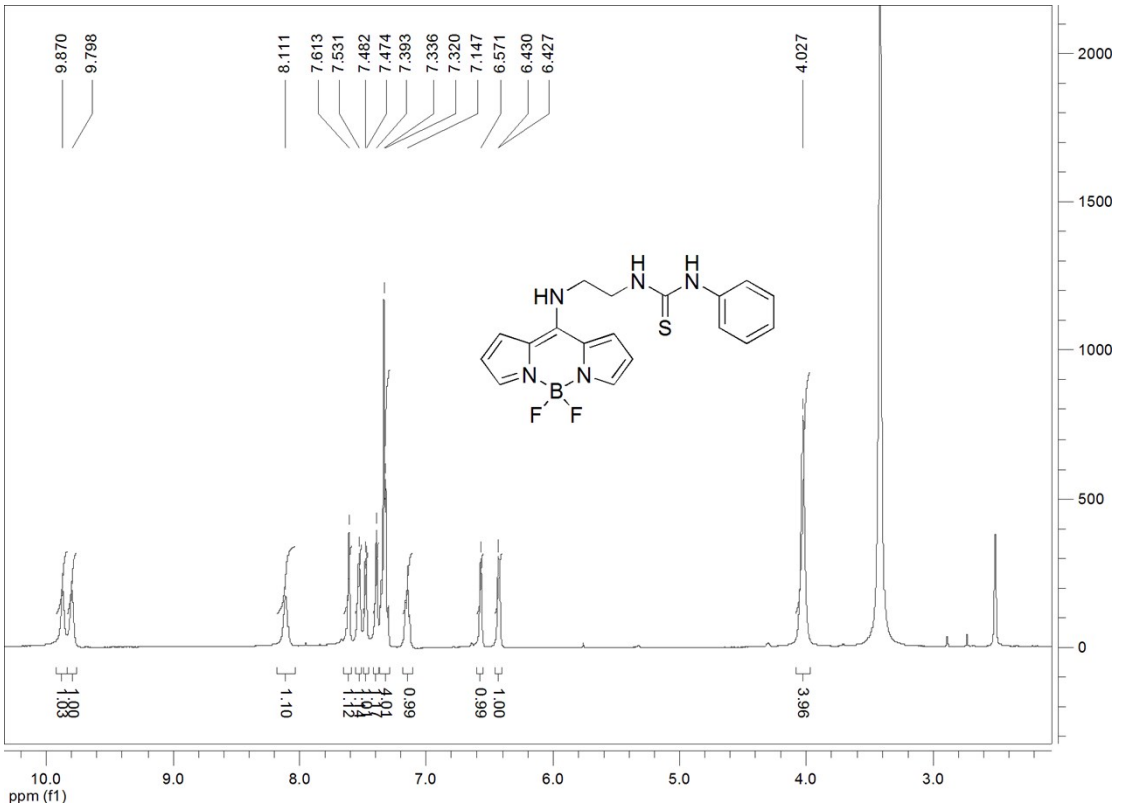

Figure S10. ^{1}H NMR spectra of **1** in DMSO.

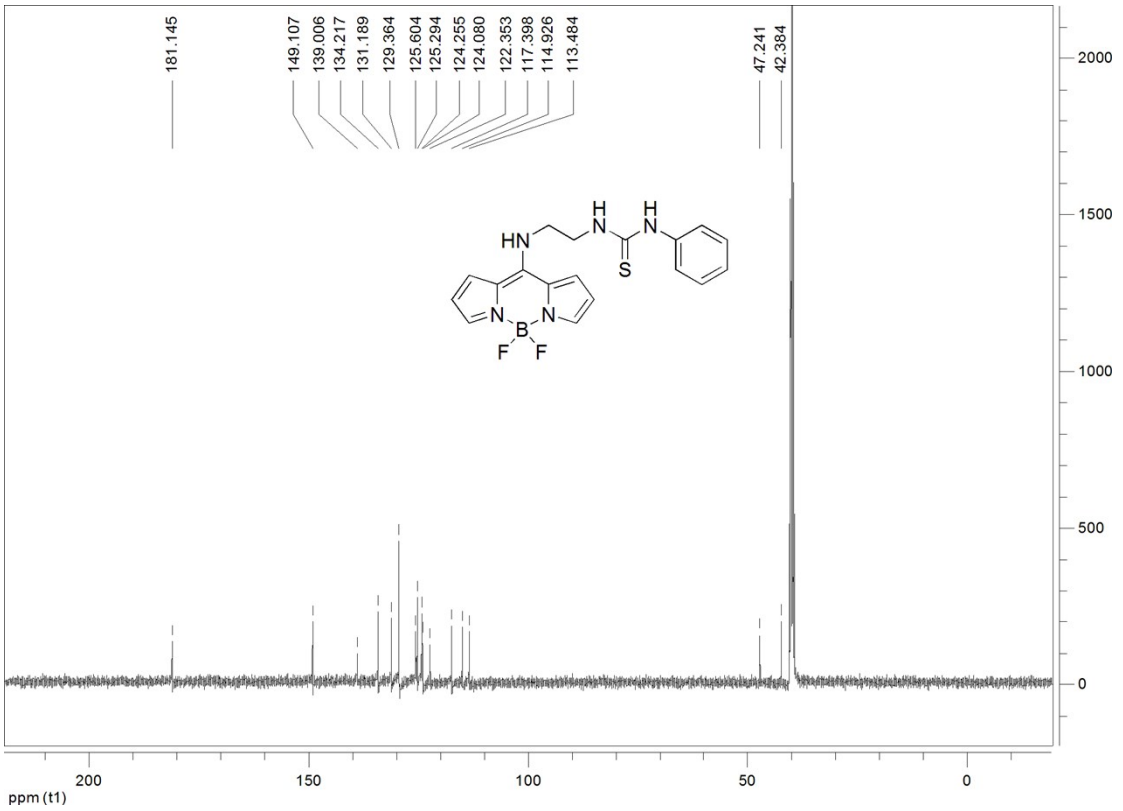

Figure S11. ^{13}C NMR spectra of **1** in DMSO.

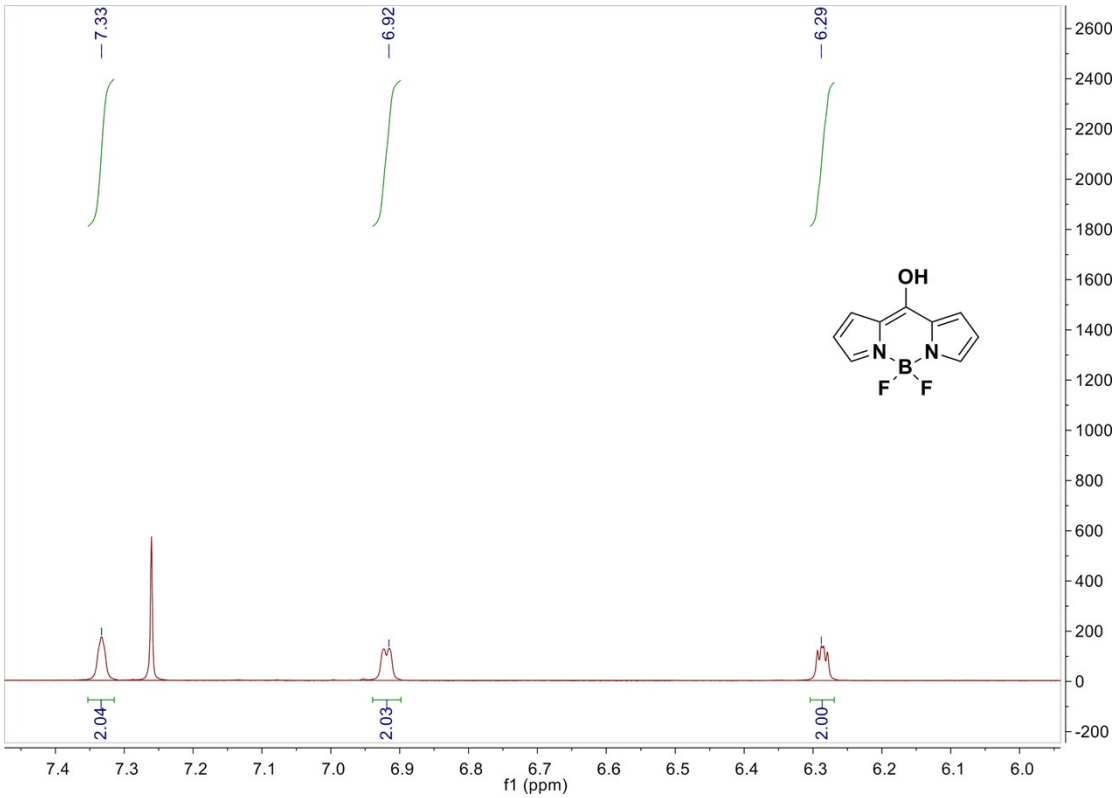

Figure S12. ^{1}H NMR spectra of 8-hydroxy-BODIPY in $CDCl_3$.