Supporting Information

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

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1. Additional Absorption and Emission Spectra

Figure S1. Absorption (a) and emission spectra (b, $\lambda_{ex} = 470$ 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, $\lambda_{ex} = 370$ 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 ($\lambda_{ex} = 470$ 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 ($\lambda_{em} = 530$ nm).
Figure S5. Selectivity of probe 1 (5 µM) toward Hg²⁺ 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<sub>ex</sub> = 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<sub>2</sub> with probe 1. (1) blank, (2) Ag⁺, (3) Al³⁺, (4) Ca²⁺, (5) Cd²⁺, (6) Co²⁺, (7) Cu²⁺, (8) Fe³⁺, (9) K⁺, (10) Mg²⁺, (11) Na⁺, (12) Ni²⁺, (13) Pb²⁺, (14) Zn²⁺, (15) Sn²⁺.

Figure S6. Fluorescence intensity profiles of probe 1 (5 µM) prior to and after addition of HgCl<sub>2</sub> (10 µM) at various pH values for 150 min incubation. (a) Monitored at 420 nm (λ<sub>ex</sub> = 370 nm); (b) Monitored at 530 nm (λ<sub>ex</sub> = 470 nm).
Figure S7. Absorption (a) and emission spectra (b, $\lambda_{\text{ex}} = 370$ 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$_3$. 