Supporting Information

BOPHY based Fluorescent Probe for Hg^{2+} via an NTe_2 Chelation

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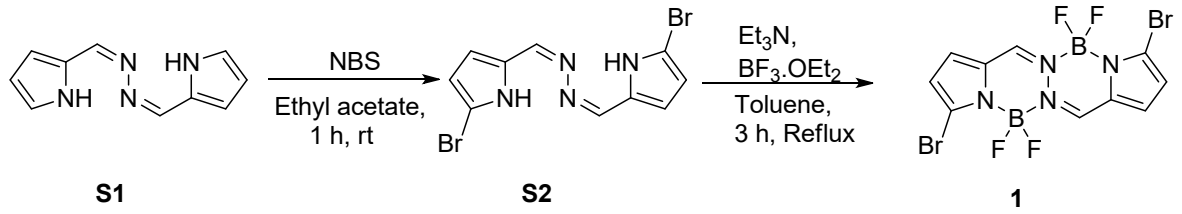
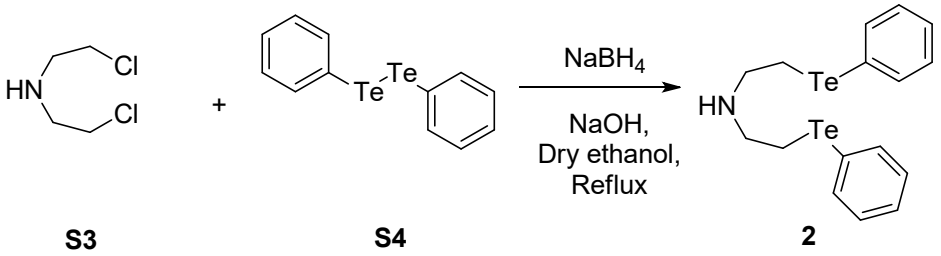
Synthesis



Scheme S1. Synthesis of compound **1**.



Scheme S2. Synthesis of compound **2**.

Characterization data

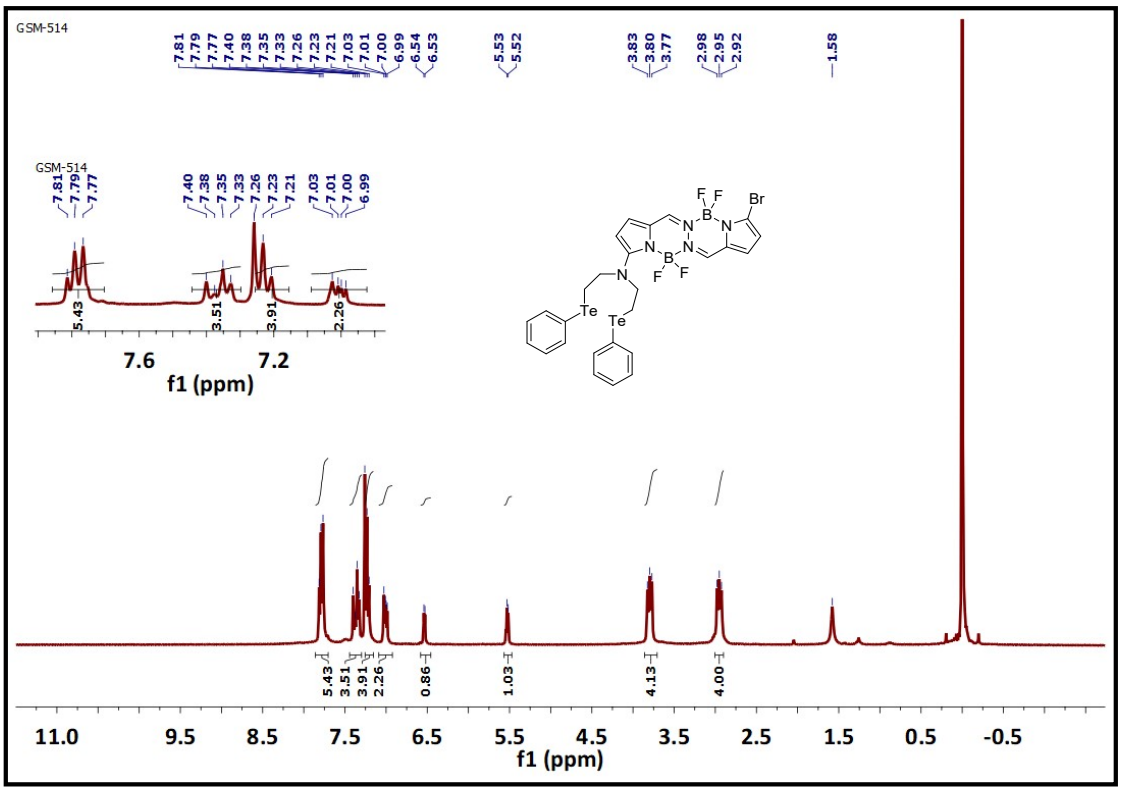


Fig. S1. ^{1}H NMR spectrum of probe **3** in $CDCl_3$.

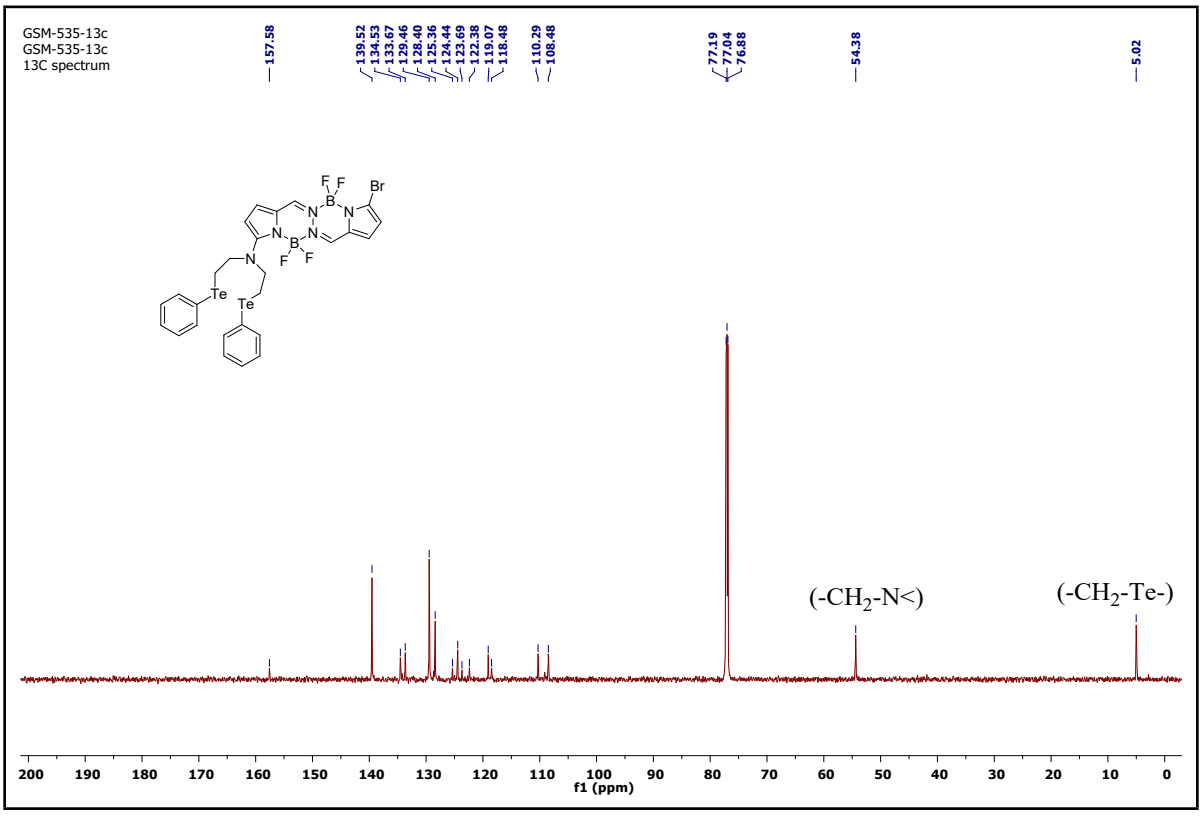


Fig. S2. ^{13}C NMR spectrum of probe **3** in $CDCl_3$.

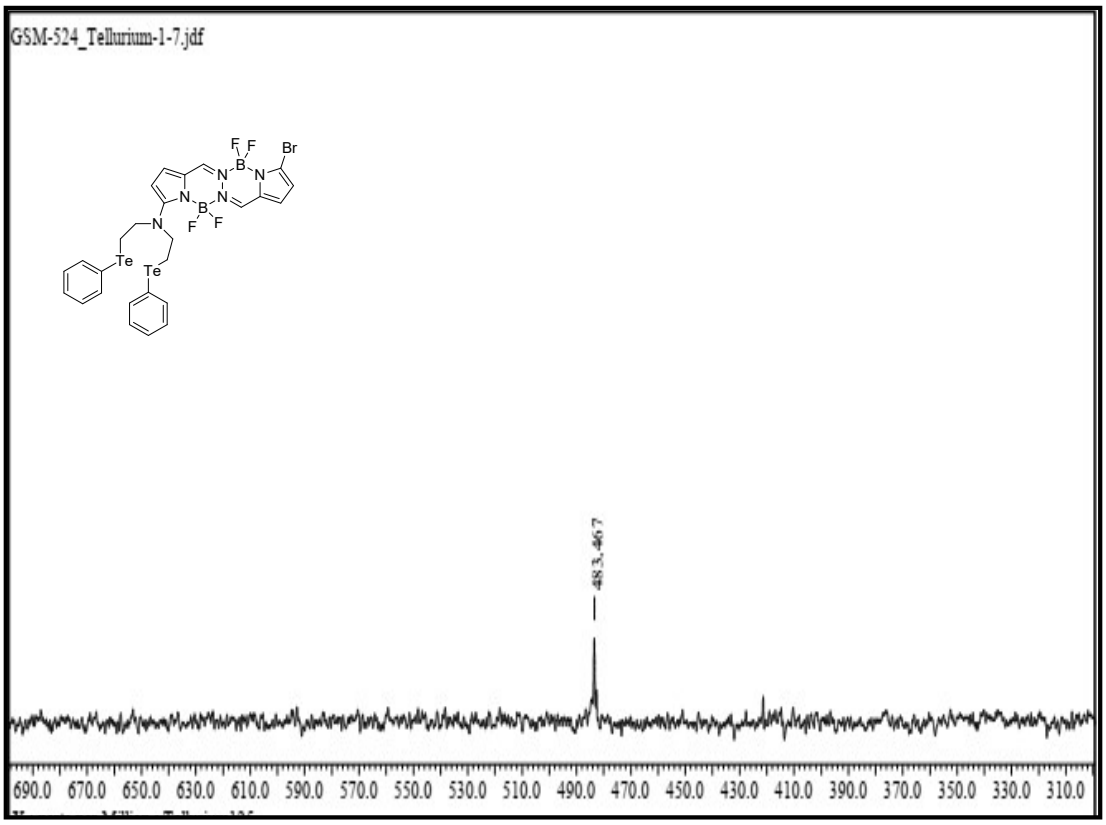


Fig. S3. ^{125}Te NMR spectrum of probe **3** in $CDCl_3$.

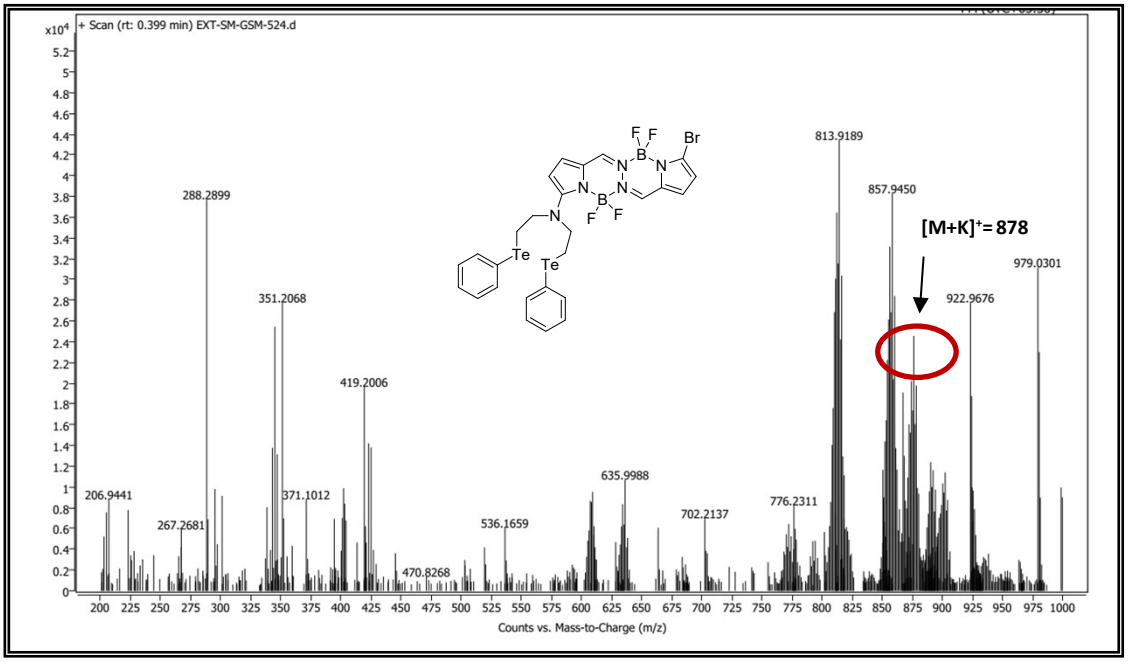


Fig. S4. Mass spectrum of probe **3**.

Table S1. Refinement details of X-ray structure of probe **3**.

Compound	**Probe 3 (CCDC# 2150059)**
Formula	$C_{26}H_{23.77}B_2Br_{1.23}F_4N_5Te_2$
Crystal System	Triclinic
Space Group	P -1
T/K	100(2)
a [A^0]	12.0491(9)
b [A^0]	12.3467(9)
c [A^0]	12.4561(9)
α [^{0}]	61.172(3)
β [^{0}]	62.951(2)
γ [^{0}]	81.418(3)
V [Å3]	1440.00(19)
Z	2
ρ_{cal}Mg/m^3	1.978
μ(mm^{-1})	3.788
F(000)	816
Crystal Size [mm^3]	0.23 x 0.16 x 0.11
GOF	1.044
***2Θ* range (deg)**	1.905 to 26.372
Reflections collected	5885
Independent reflections	5885
Parameters	371
R_{int}	0.1410
R_1,wR2[I>2σ(I)]	R1 = 0.0523, wR2 = 0.1174
R_1,wR2[I>2σ(I)]	R1 = 0.0072, wR2 = 0.1287

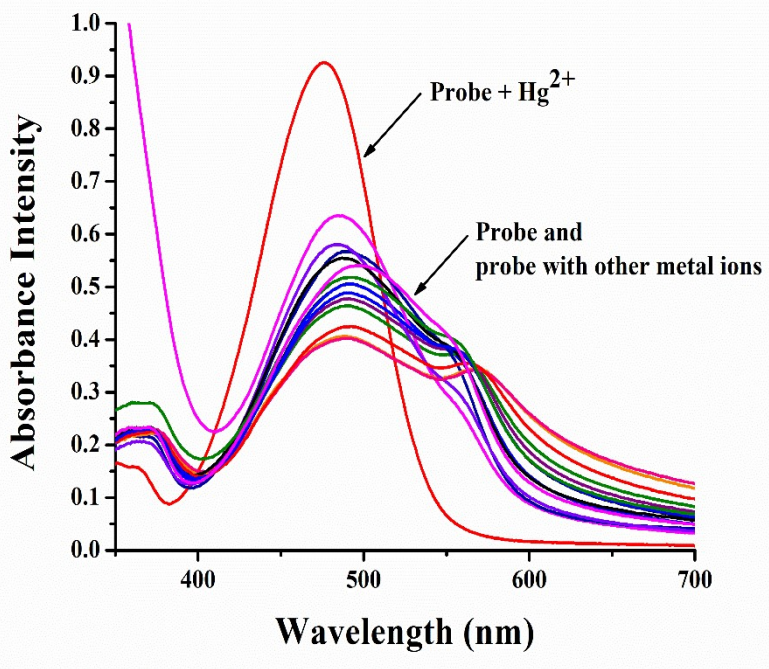


Fig. **S5.** Absorption spectra of probe **3** (20 μM) with metal ions (Hg^{2+}, Hg^{+}, Cu^{2+}, Ca^{2+}, Na^{+}, Co^{2+}, K^{+}, Zn^{2+}, Al^{3+}, Fe^{2+}, Cd^{2+}, Mn^{2+}, Ag^{+}, Fe^{3+}, Pb^{2+}, Hg^{+}, Cu^{+}, 6 equiv) in the solution (DMSO/water, 1:1 v/v) incubated for 20 min at rt.

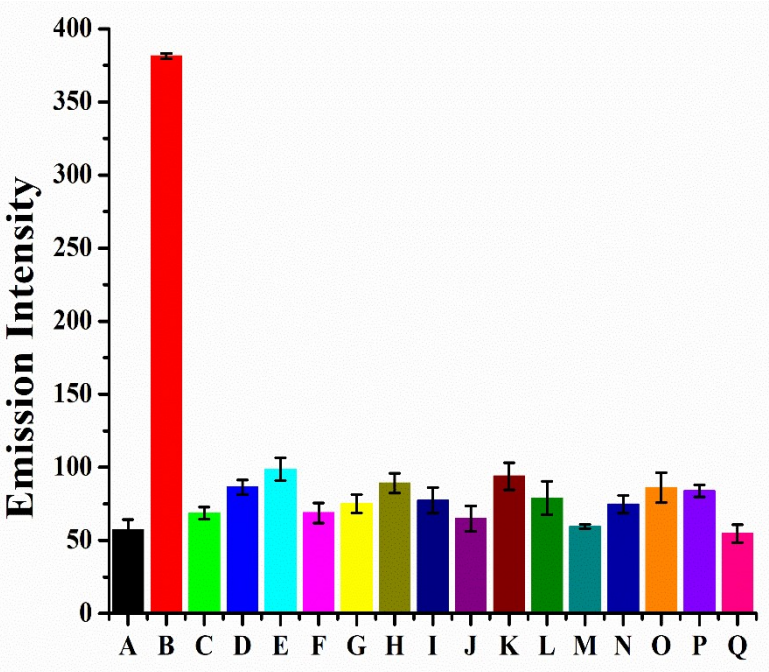


Fig. S6. Selectivity study bar graph for emission of probe **3** (20 μM) with metal ions (Hg^{2+}, Cu^{2+}, Ca^{2+}, Na^{+}, Co^{2+}, K^{+}, Zn^{2+}, Al^{3+}, Fe^{2+}, Cd^{2+}, Mn^{2+}, Ag^{+}, Fe^{3+}, Pb^{2+}, Cu^{+}, 6 equiv).(A = probe **3**, B = probe **3** + Hg^{2+}, C = probe **3** + Cu^{2+}, D = probe **3** + Ca^{2+}, E = probe **3** + Na^{+}, F = probe **3** + Co^{2+}, G = probe **3** + K^{+}, H = probe **3** + Zn^{2+}, I = probe **3** + Al^{3+}, J = probe **3** + Fe^{2+},

K = probe **3** + Cd^{2+}, L = probe **3** + Mn^{2+}, M = probe **3** + Ag^{+}, N = probe **3** + Fe^{3+}, O = probe **3** + Pb^{2+}, P = probe **3** + Hg^{+}, Q = probe **3** + Cu^{+} in the solution (DMSO/water, 1:1 v/v) incubated for 20 min. λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm.

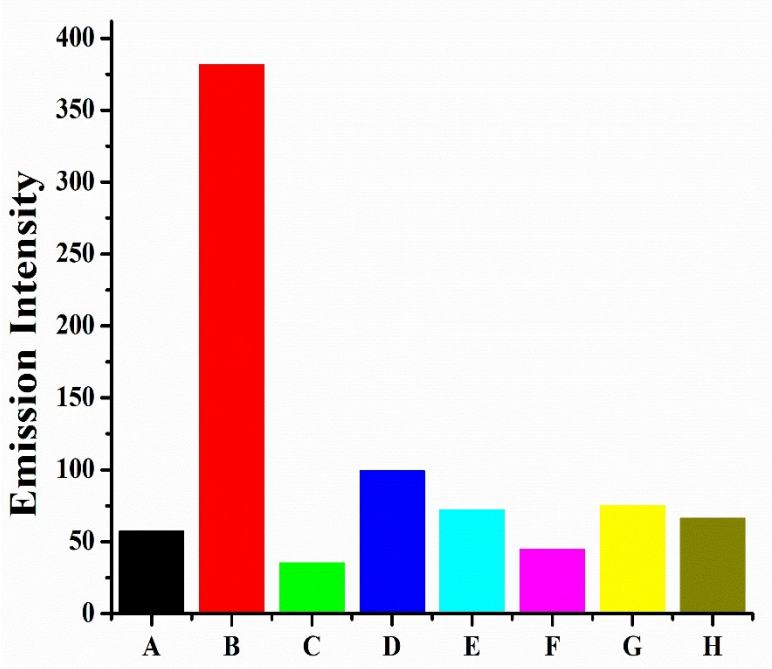


Fig. S7. Selectivity study bar graph for emission of probe **3** (20 μM) with ROS ($O_2^{\cdot-}$, H_2O_2, NaOCl, *t*BuO_2H, $^{\bullet}OH$, *t*$BuO^{\bullet}$, 6 equiv). (A = probe **3**, B = probe **3** + Hg^{2+}, C = probe **3** + $O_2^{\cdot-}$, D = probe **3** + H_2O_2, E = probe **3** + NaOCl, F = probe **3** + *t*BuO_2H, G = probe **3** + $^{\bullet}OH$, H = probe **3** + *t*$BuO^{\bullet}$) in the solution (DMSO/water, 1:1 v/v) incubated for 20 min. λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm.

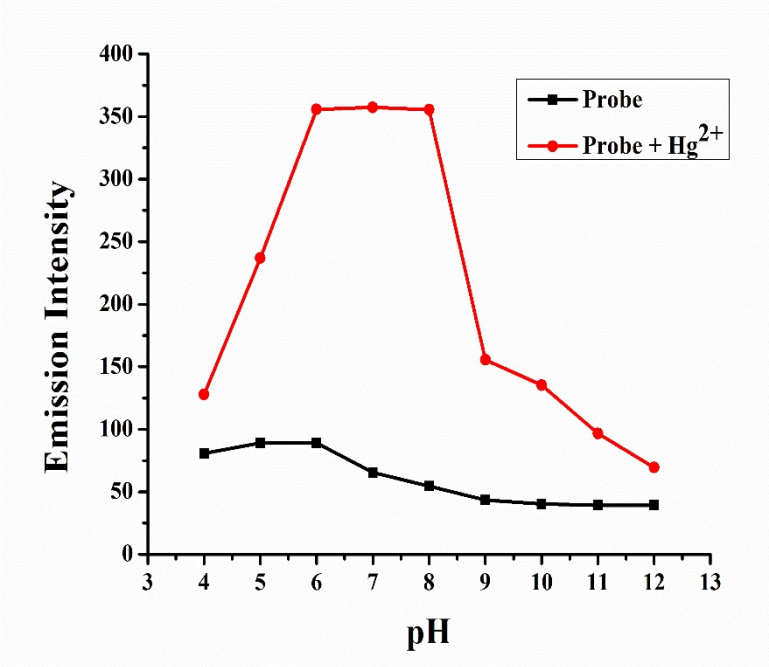


Fig. S8. Fluorescence intensity change of probe **3** (20 μM, black) and probe (20 μM) with 6 equiv of Hg^{2+} (red), in the solution (DMSO/1 mM PBS, 1:1 v/v) incubated for 20 min. λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm, under different pH range.

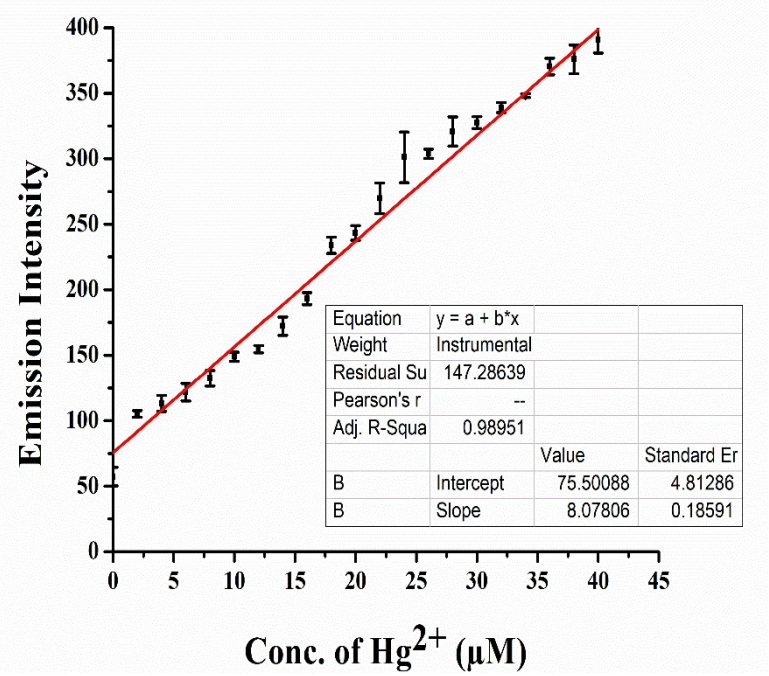


Fig. S9. Plot for the calculation of limit of detection from the emission of probe **3** (20 μM, DMSO/water, 1:1 v/v) with increasing concentration of Hg^{2+} (0 to 2 equiv) incubated for 20 min at rt. λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm (average of three experiments).

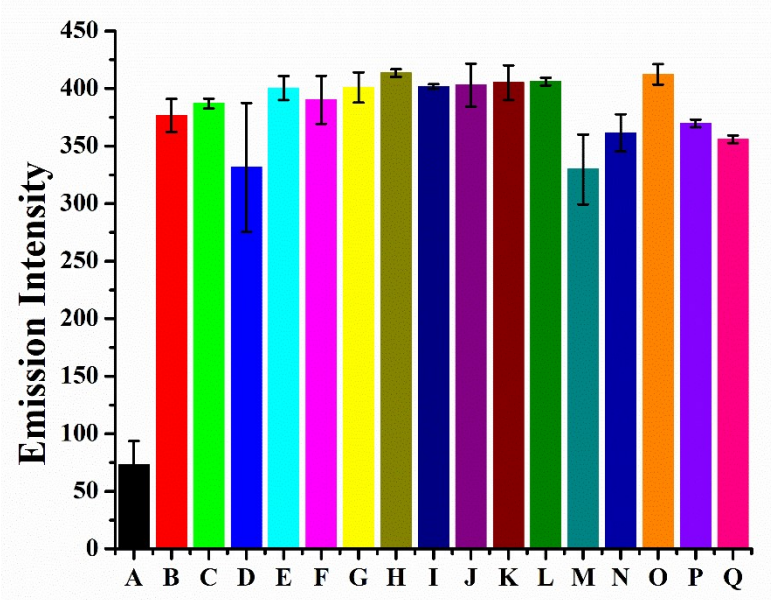


Fig. S10. Fluorescence intensity of probe **3** (20 μM) and Hg^{2+} (6 equiv) with metal ions (Hg^{2+}, Cu^{2+}, Ca^{2+}, Na^{+}, Co^{2+}, K^{+}, Zn^{2+}, Al^{3+}, Fe^{2+}, Cd^{2+}, Mn^{2+}, Ag^{+}, Fe^{3+}, Pb^{2+}, 6 equiv). (A = probe **3**, B = probe **3** + Hg^{2+}, C = probe **3** + Hg^{2+} + Cu^{2+}, D = probe **3** + Hg^{2+} + Ca^{2+}, E = probe **3** + Hg^{2+} + Na^{+}, F = probe **3** + Hg^{2+} + Co^{2+}, G = probe **3** + Hg^{2+} + K^{+}, H = probe **3** + Hg^{2+} + Zn^{2+}, I = probe **3** + Hg^{2+} + Al^{3+}, J = probe **3** + Hg^{2+} + Fe^{2+}, K = probe **3** + Hg^{2+} + Cd^{2+}, L = probe **3** + Hg^{2+} + Mn^{2+}, M = probe **3** + Hg^{2+} + Ag^{+}, N = probe **3** + Hg^{2+}+ Fe^{3+}, O = probe **3** + Hg^{2+} + Pb^{2+}, P = probe **3** + Hg^{2+} + Hg^{+}, Q = probe **3** + Hg^{2+} + Cu^{+}) in solution (DMSO/water, 1:1 v/v) incubated for 20 min. λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm.

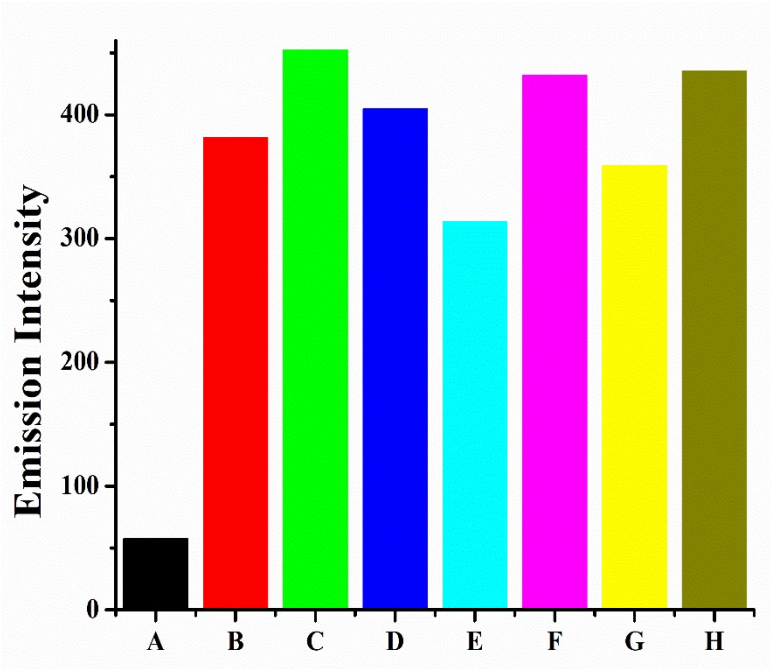


Fig. S11. Fluorescence intensity of probe **3** (20 μM) and Hg^{2+} (6 equiv) with ROS ($O_2^{\cdot-}$, H_2O_2, NaOCl, *t*BuO_2H, $^{\cdot}OH$, *t*$BuO^{\cdot}$, 6 equiv). (A = probe **3**, B = probe **3** + Hg^{2+}, C = probe **3** + Hg^{2+} + $O_2^{\cdot-}$, D = probe **3** + Hg^{2+} + H_2O_2 , E = probe **3** + Hg^{2+} + NaOCl, F = probe **3** + Hg^{2+} + *t*BuO_2H, G = probe **3** + Hg^{2+} + $^{\cdot}OH$, H = probe **3** + Hg^{2+} + *t*$BuO^{\cdot}$) in solution (DMSO/water, 1:1 v/v) incubated for 20 min. λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm.

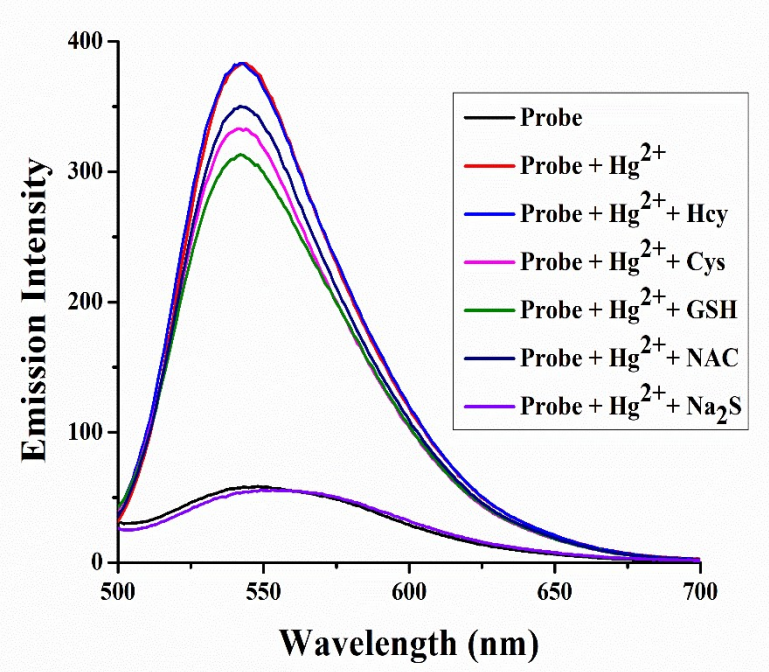


Fig. S12. Fluorescence response of probe **3** (20 μM) with Hg^{2+} (6 equiv) in solution (DMSO/water, 1:1, v/v) incubated for 20 min and after addition of biothiols (DL-homocysteine, L-cysteine, glutathione, N-acetyl-L-cysteine, Na_2S, 6 equiv) incubated for 30 min at rt, λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm.

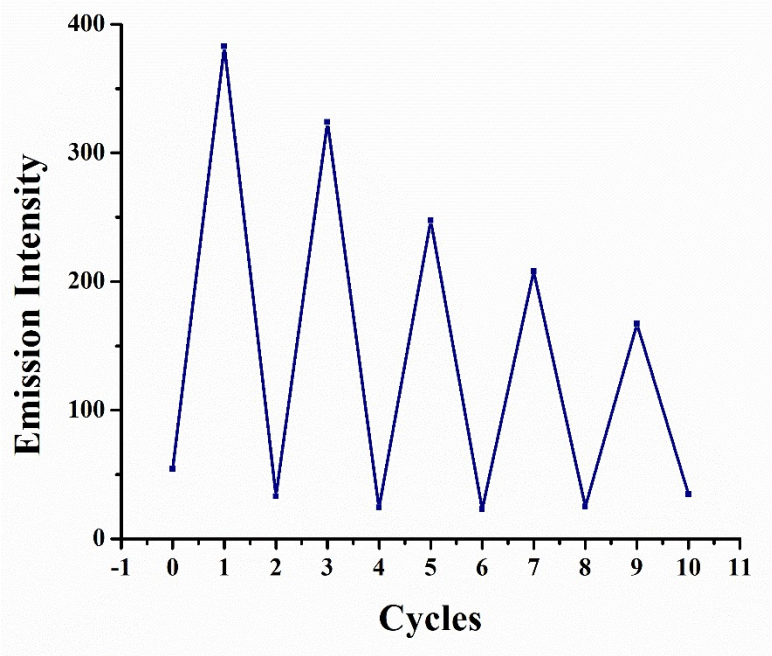


Fig. S13. Redox cycles of probe **3** (20 μM) with 6 equiv of Hg^{2+} and Na_2S in solution (DMSO/water, 1:1, v/v) λ_{ex} = 486 nm, λ_{em} = 547 nm, slit width 5 nm/5 nm.

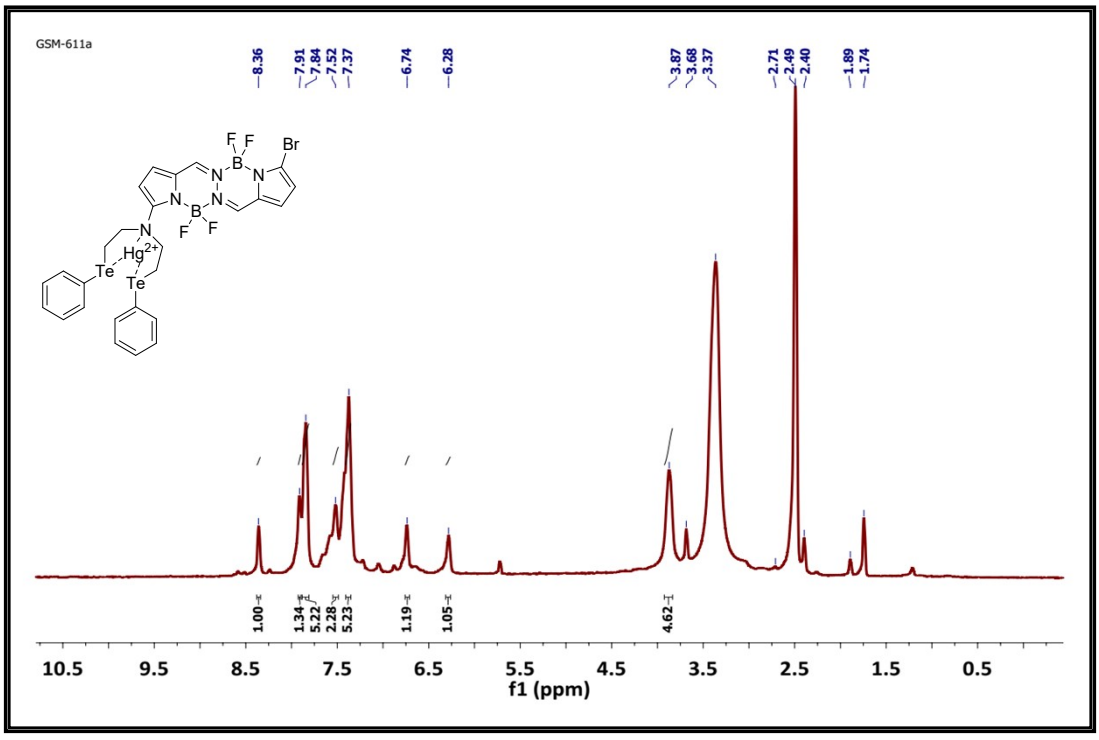


Fig. S14. ^1H NMR spectrum of compound **4** in DMSO-d_6.

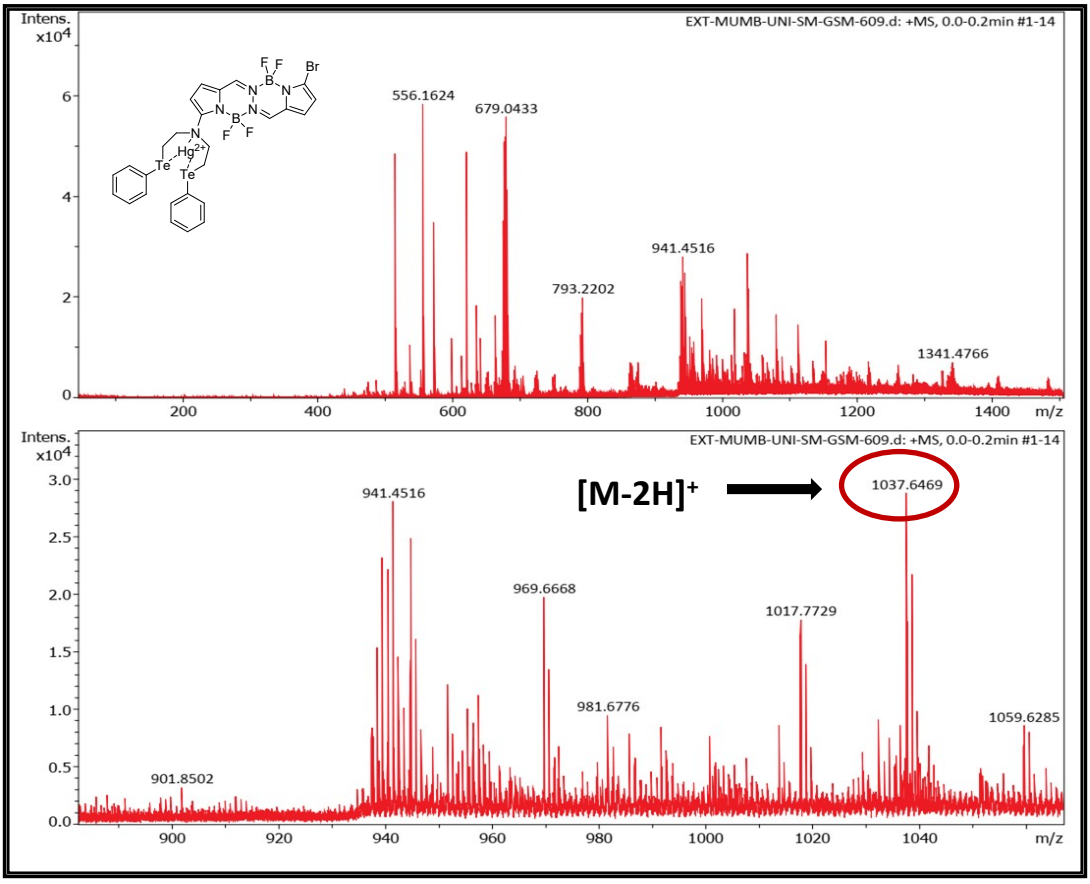


Fig. S15. Mass spectrum of compound **4**.

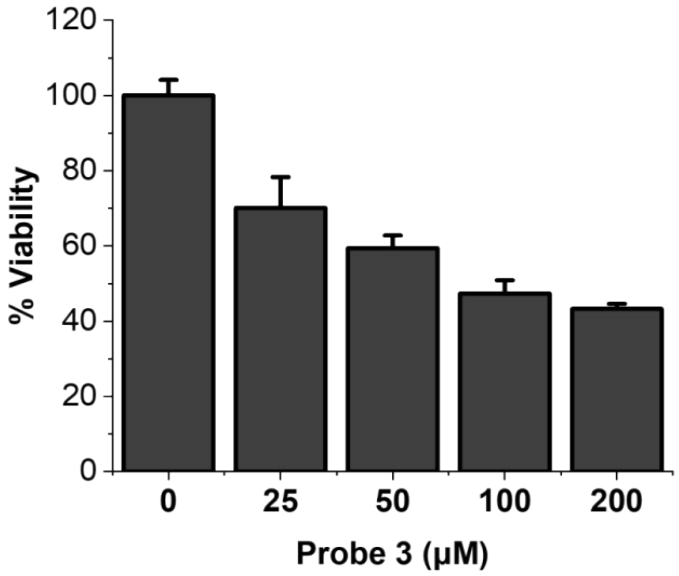


Fig. S16. Concentration-dependent cell viability assay of probe 3 in HeLa cells for 1 h.

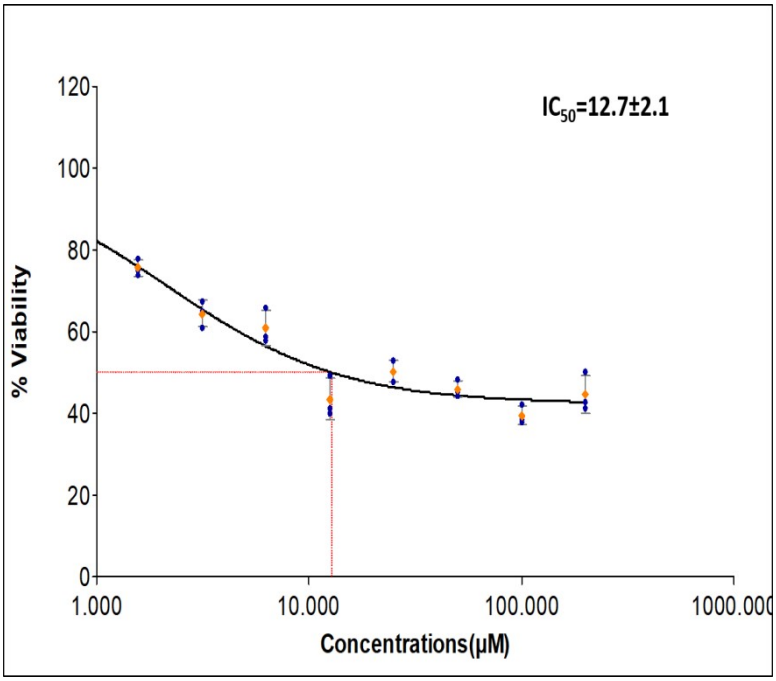


Fig. S17. Concentration-dependent cell viability assay of probe **3** in HeLa cells for 24 h.

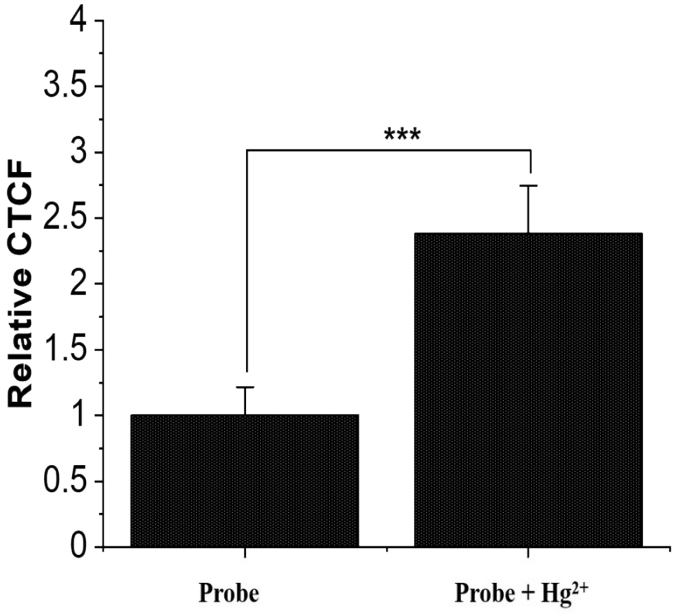


Fig. S18. Fluorescence intensity quantification of probe **3**.