Supporting information

Rhodamine-benzothiazole conjugate as an efficient multimodal sensor for Hg^{2+} ions and its applications of imaging in living cells

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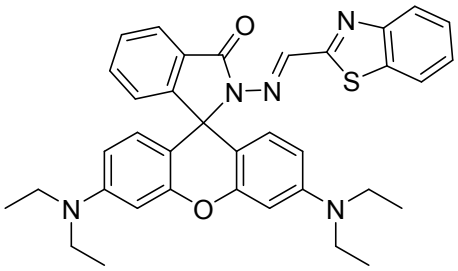
Fig. S1: The ^{1}H NMR (300 MHz, $CDCl_3$): probe RBT-1.

(E)-2-((benzo[d]thiazol-2-ylmethylene)amino)-3',6'- bis(diethylamino)spiro[isoindoline-1,9'-xanthen]-3-one



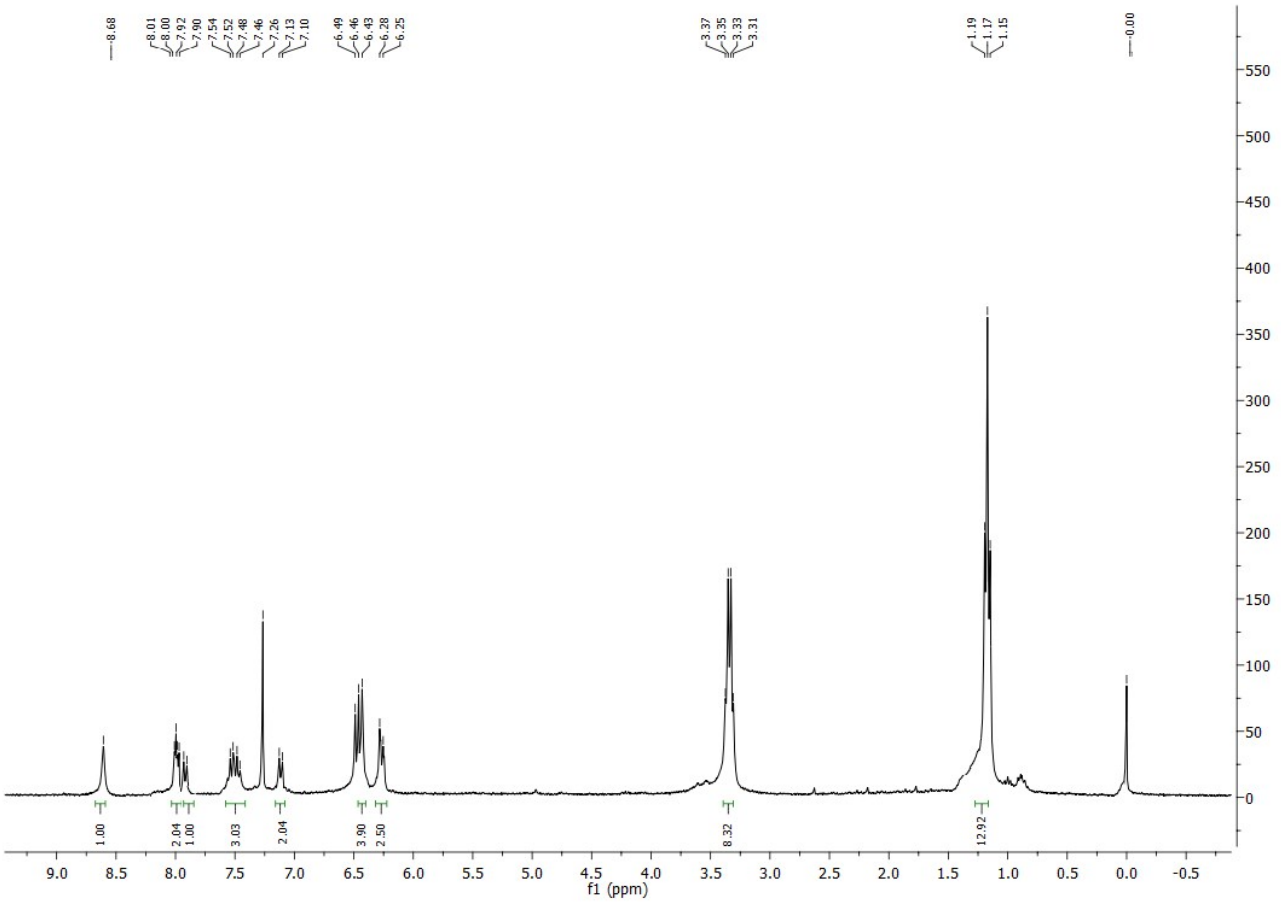
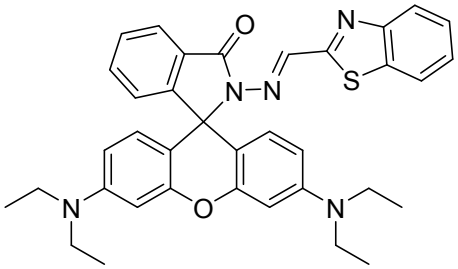


Fig. S2: The ^{13}C NMR (75 MHz, $CDCl_3$): probe RBT-1.

(E)-2-((benzo[d]thiazol-2-ylmethylene)amino)-3',6'- bis(diethylamino)spiro[isoindoline-1,9'-xanthen]-3-one



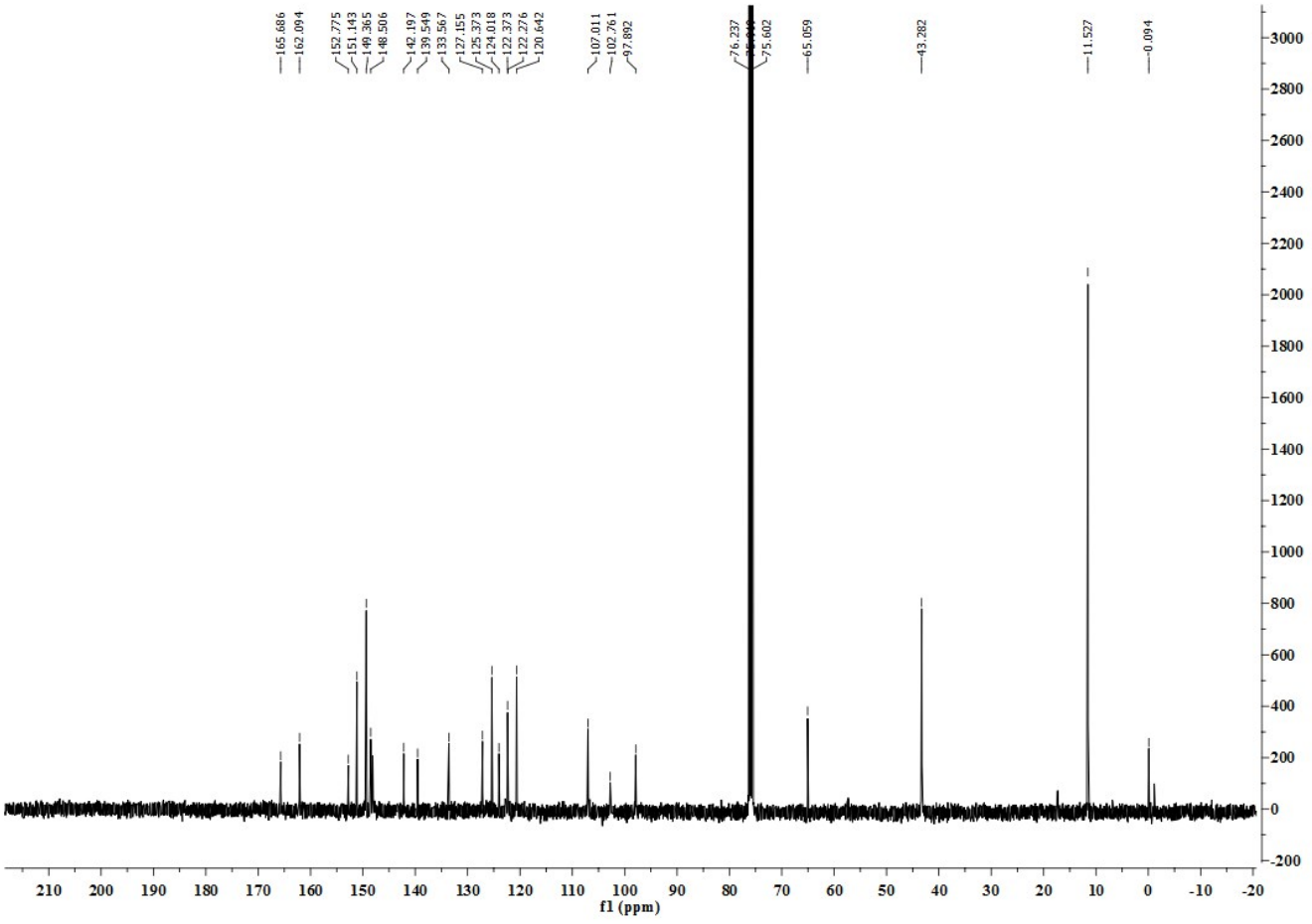
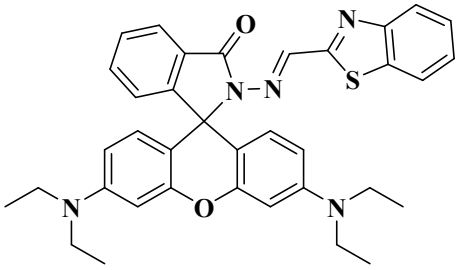


Fig. S3. The ESI-Mass spectrum of probe **RBT-1**.



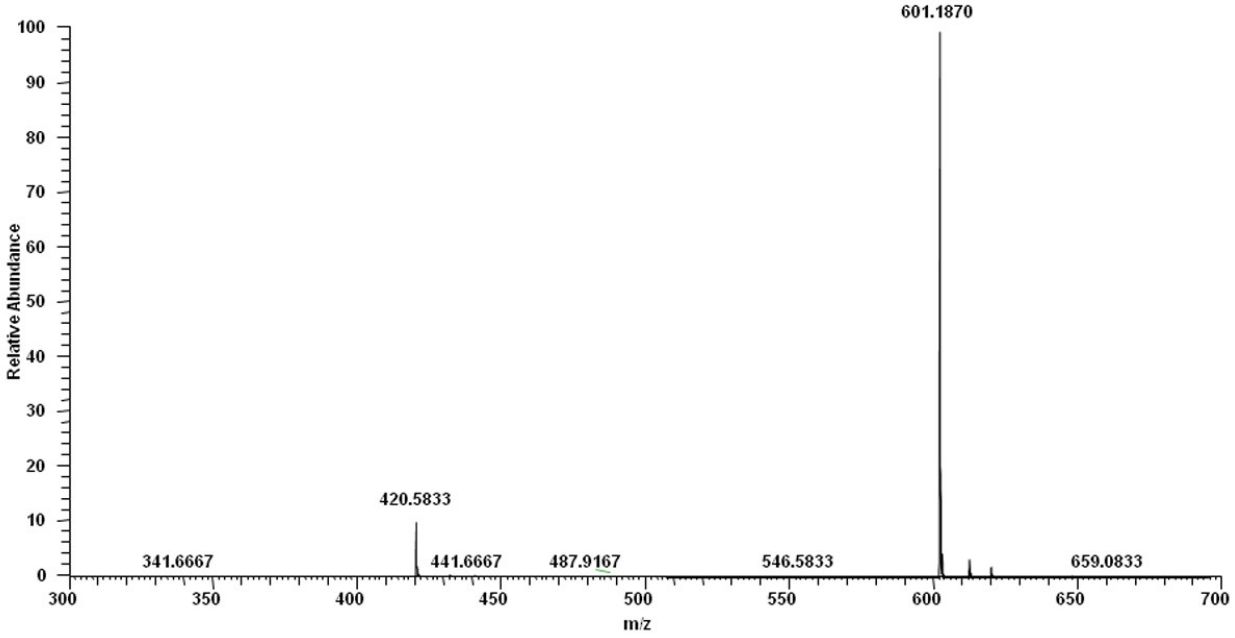
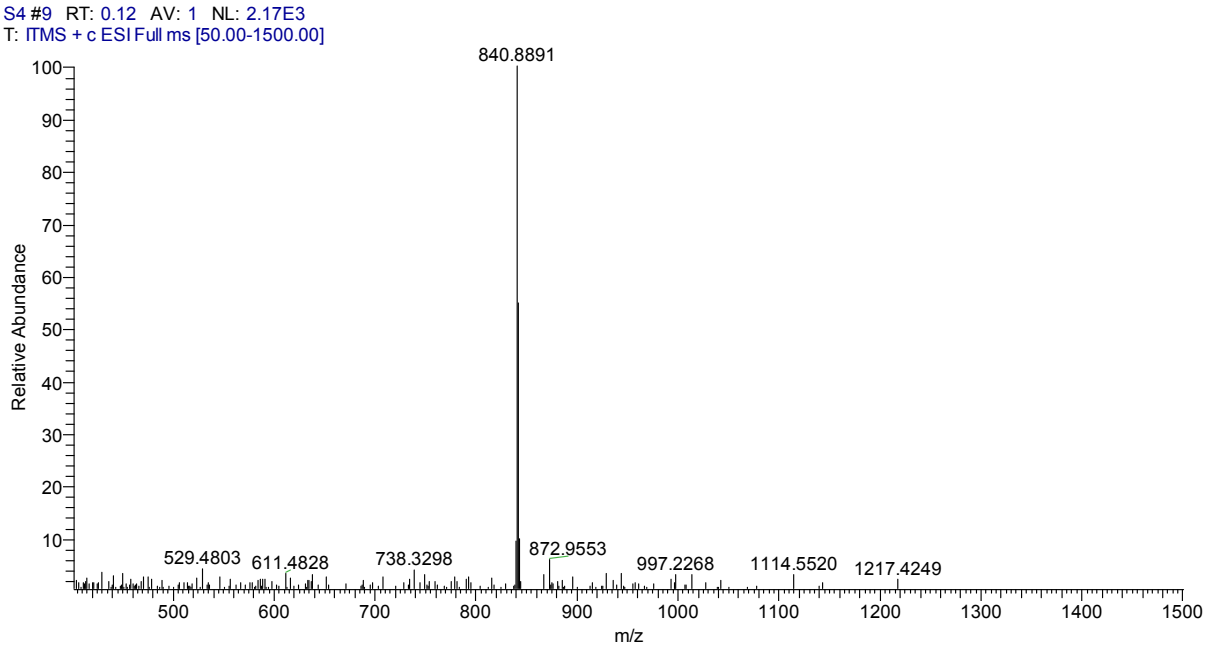
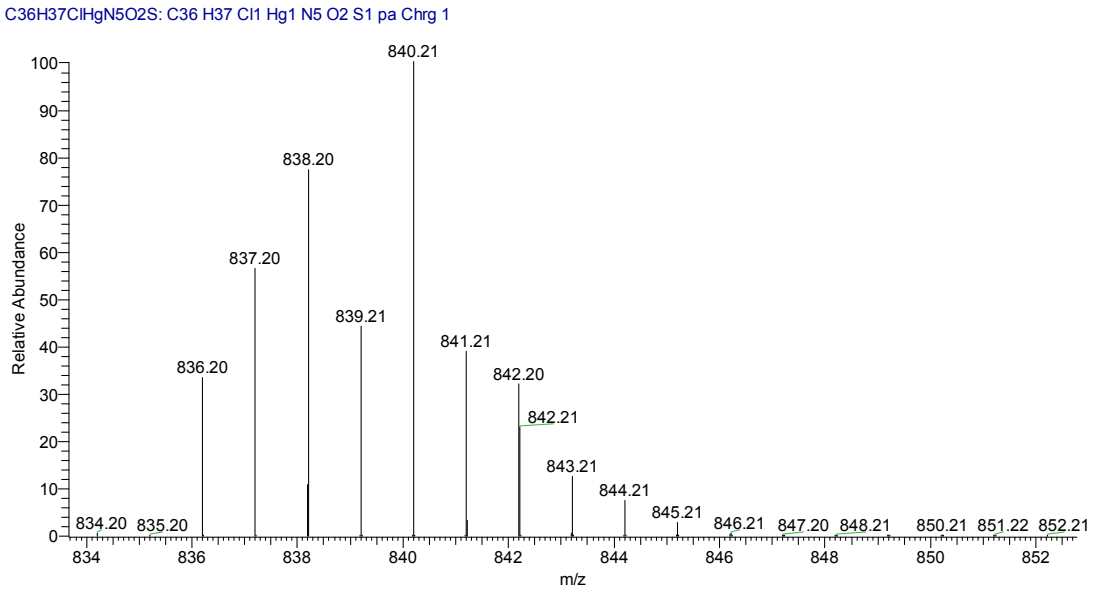


Fig. S4. The ESI-Mass spectrum of Compound **RBT-1+Hg^{2+}.**



Stimulated.



Quantum yield Calculation.

Determination of fluorescence quantum yield:

Fluorescence quantum yield was determined using the standard solutions of Rhodamine 6G (ΦF = 0.94 in acidified CH_3OH) as a reference. The quantum yield was calculated using the following equation:

$$\Phi F\ s = (O.D_{(ref)}/O.D_{(s)}) * (I\ s / I\ ref) * (\eta_{S(sol)}/\eta_X\ (ref))^2 * \Phi F\ (ref)$$

Where ΦF is the fluorescence quantum yield, *OD* is the absorbance at the excitation wavelength, *I* is the emission intensity maximum wavelength, and η is the refractive index of the solvents used. Subscripts 'S' is sample and 'X' reference to the standard and to the unknown sample respectively.

Solid state quantum yield (Φ) was measured on a ELCO-SL-174 spectrofluorometer by Absolute PL Quantum Yield Measurement System.

Figure S5. Solid state fluorescence images using **TLC plate**

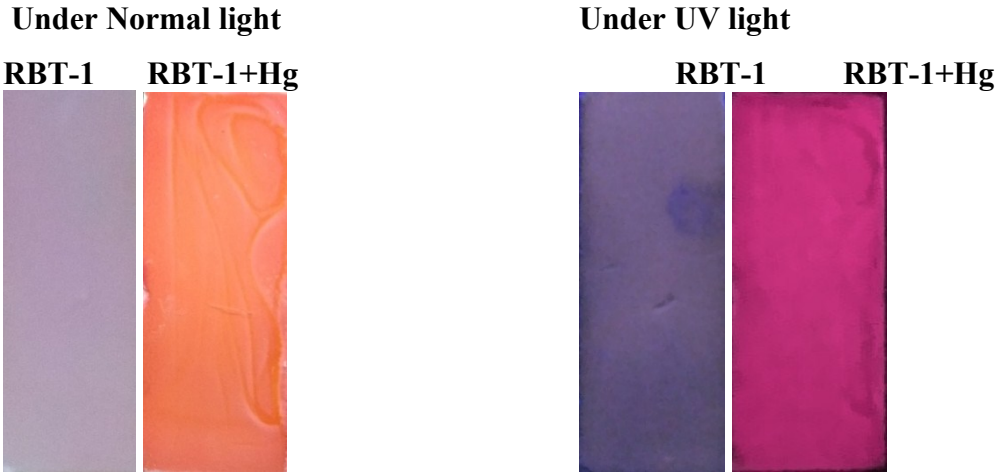
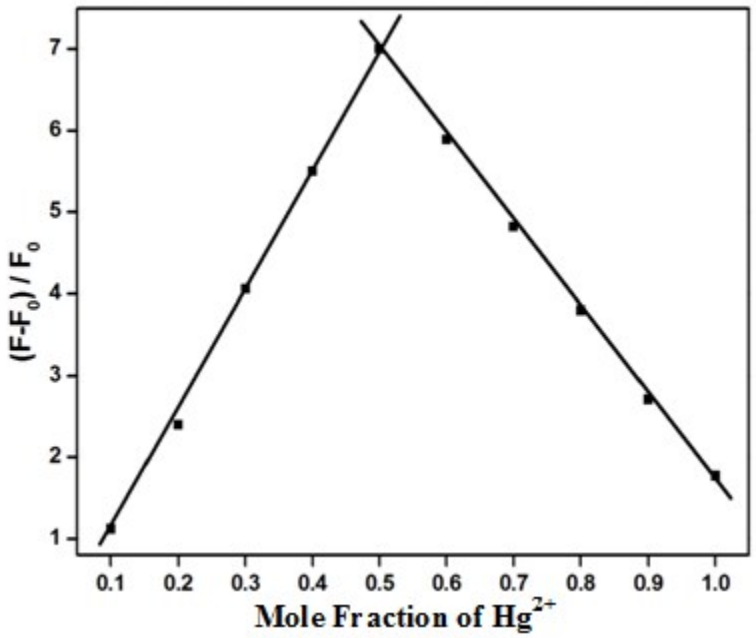


Figure S6: The Jobs plot between **RBT-1** and **Hg^{2+}**



Calculation of Binding constant:

The binding constant K was determined from the plot of the linear regression of log [(F - F0) / (Fm - F)] vs. log [M] in equation to obtain the intercept as log K and the slope as n. F - Fluorescence Intensity, F_o - Fluorescence Intensity at initial concentration, Fm- Fluorescence Intensity at maximum

Log $F-F_o/F_m-F$ = log k + n log (M)

Figure S7: The effect of pH on the fluorescence of **RBT-1** and **RBT-1+Hg^{2+}.**

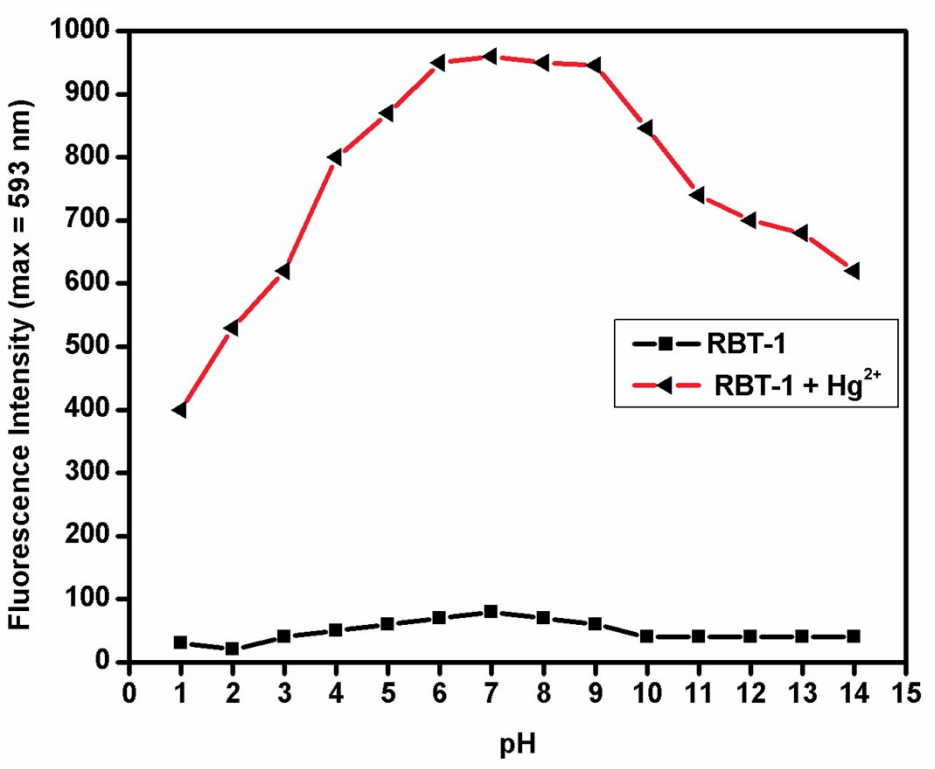


Figure S8: The plausible mechanism of probe RBT-1 and Hg^{2+} complex.

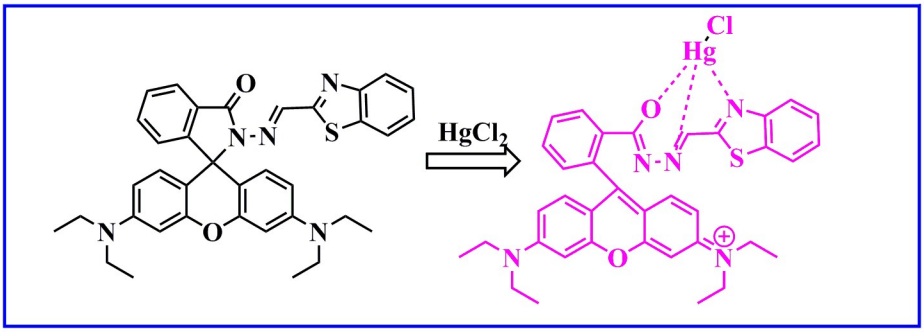
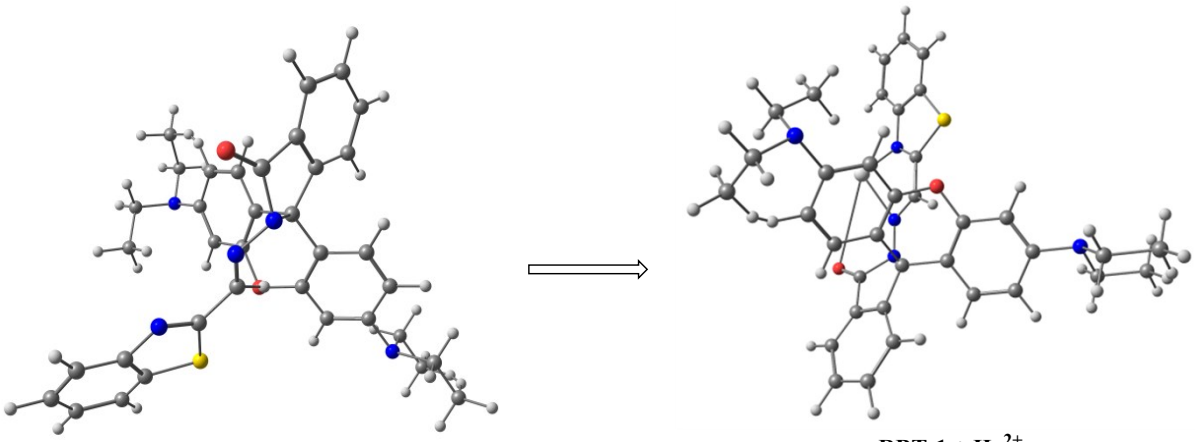


Figure S9: The Optimized Geometry of plausible structure of probe **RBT-1 + Hg^{2+}**.



RBT-1 **RBT-1 + Hg^{2+}**

Figure S10: The cytotoxicity of the probe **RBT-1** at varying concentration dependent assay.

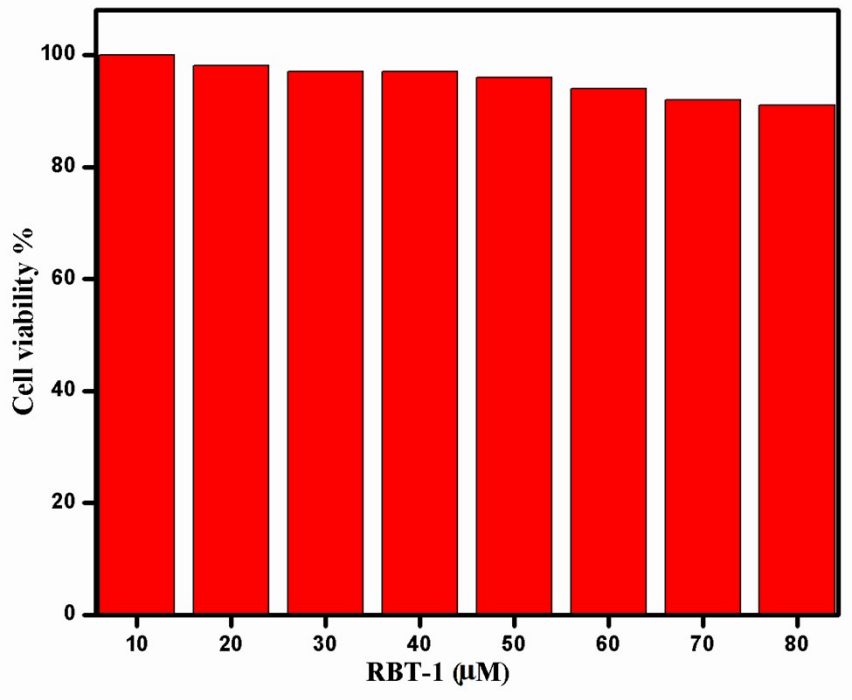


Table-S1: The quantification of **Hg^{2+}** in water samples with **RBT-1.**

Sample	Hg^{2+} added (μgL^{-1})	Hg^{2+} found (μgL^{-1})	Recovery (%)
Drinking water			
A	0	-	-
B	50	$50.01^{a} \pm 0.02^{b}$	99.12
C	100	$100.03^{a} \pm 0.03^{b}$	99.07
Tap water			
A	0	-	-
B	50	$50.04^{a} \pm 0.03^{b}$	99.29
C	100	$100.00^{a} \pm 0.06^{b}$	99.06
River water			
A	0	-	-
B	50	$50.06^{a} \pm 0.05^{b}$	99.02
C	100	$100.04^{a} \pm 0.06^{b}$	98.88

[a] Average of 3 measurements. [b] Standard deviation.