Electronic Supplementary Information

Optical chemosensors for Hg^{2+} from terthiophene appended rhodamine derivatives : FRET based molecular and *in situ* hybrid gold nanoparticles sensors

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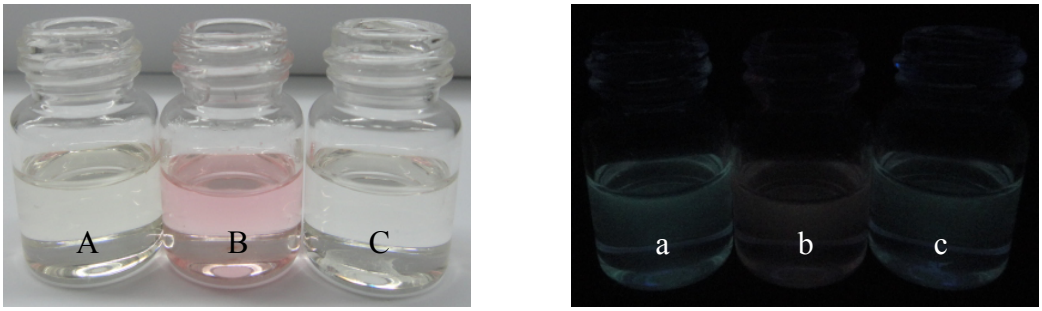

Figure S1. Color changes (A, B, C) and fluorescence changes (a, b, c) of **RhoT** (10 mM) in the presence of 10 μM of various metals. (A, a) **RhoT** only, (B, b) **RhoT** + Hg^{2+}, (C, c) **RhoT** + other metals.

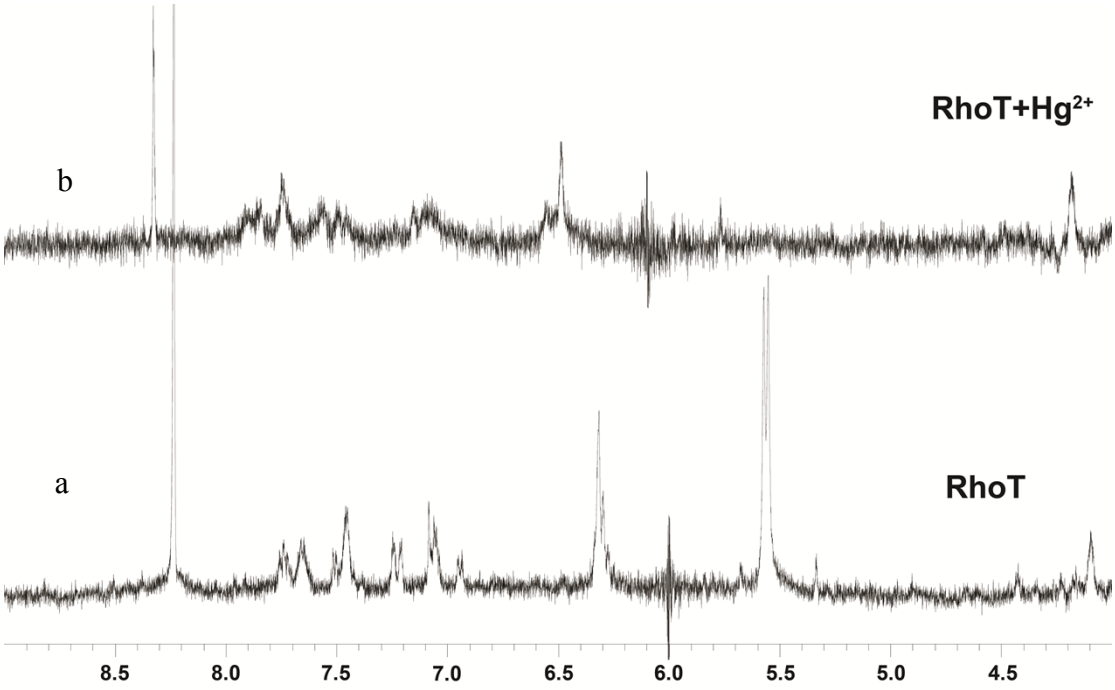

Figure S2. ^{1}H NMR spectra of RhoT in DMSO-d_6 in the absence (a) and presence (b) of Hg^{2+}.

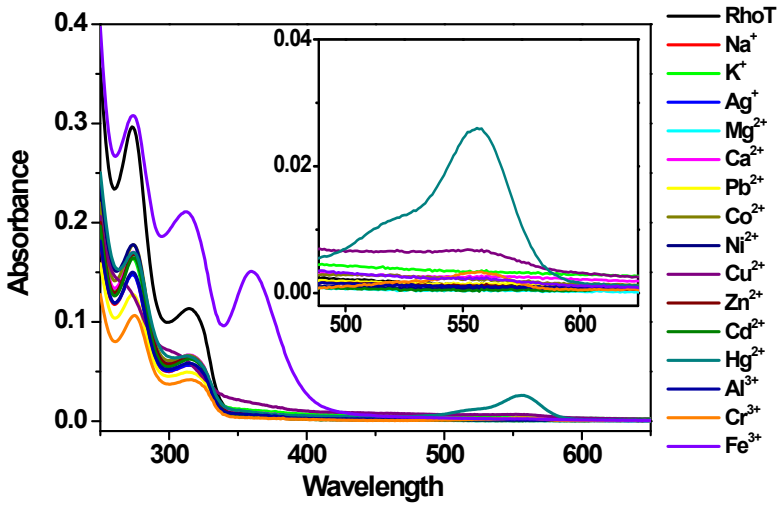

Figure S3. Absorption spectra changes of **RhoT** (10 μM) in 0.01 mol/L of $TBAPF_6$ in DMSO to 10 μM of various cations.

Table S1. Complexation energies obtained at the B3LYP/LanL2DZ level of theory.

Complexation	ΔE (kcal/mol)
RhoT + Hg^{2+} → **RhoT**•Hg^{2+}	-276.28
2**RhoT** + Hg^{2+} → 2**RhoT**•Hg^{2+}	-350.47

Table S2. Energy gaps (E_{gap}, in eV) of ligand and its complexes obtained at the B3LYP/LanL2DZ level of theory.

	E_{HOMO}	E_{LUMO}	E_{gap}
RhoT	-5.306	-1.769	3.537
RhoT-Hg^{2+}	-9.497	-9.089	0.408
2**RhoT**-Hg^{2+}	-8.626	-5.769	2.857

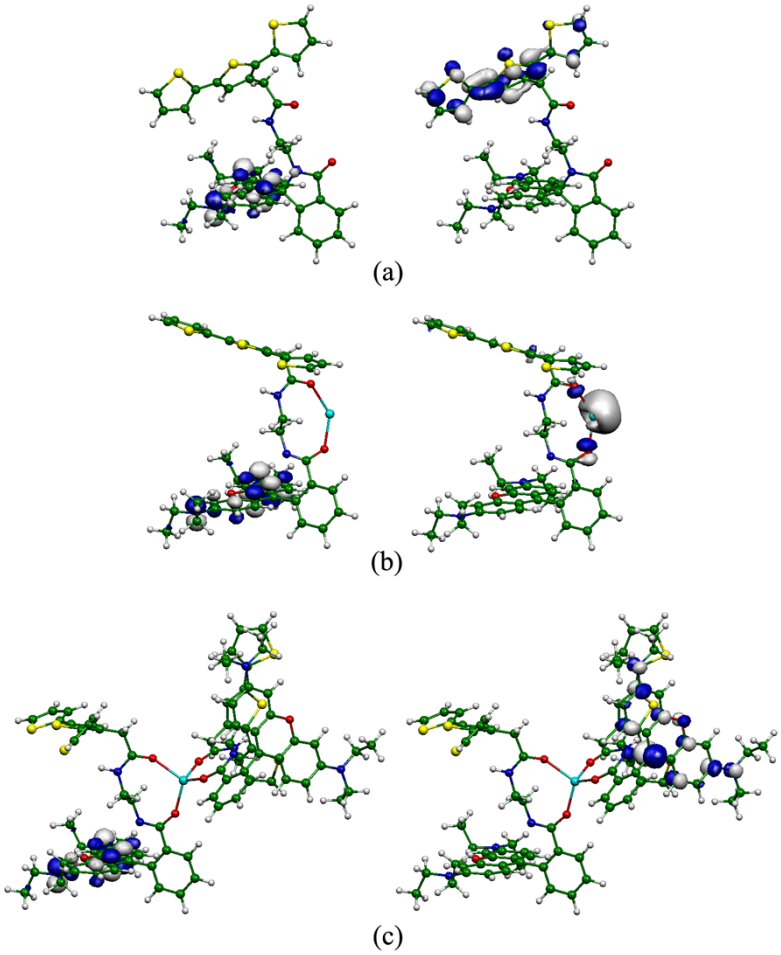

Figure S4. Plots of HOMO (left) and LUMO (right) orbitals of (a) **L**, (b) **L**-Hg^{2+} (1:1) and (c) 2**L**-Hg^{2+} (2:1) obtained at the B3LYP/LanL2DZ level of theory, the O-Hg bond distances are in Å.

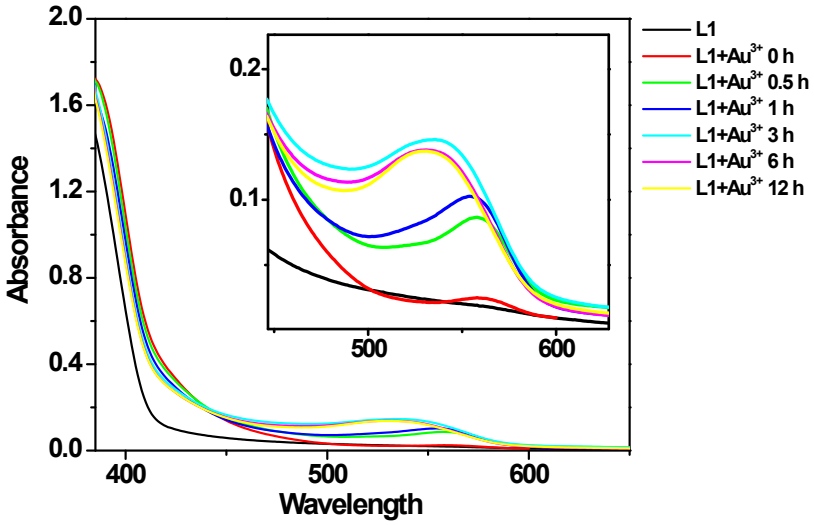

Figure S5. UV-vis absorption spectra of rhodamine functionalized with terthiophene (**RhoT**) 10^{-3} M before and after treated with $AuCl_3$ at different time (0–12 hour). AuNPs showed their characteristic absorption bands at 570 nm.

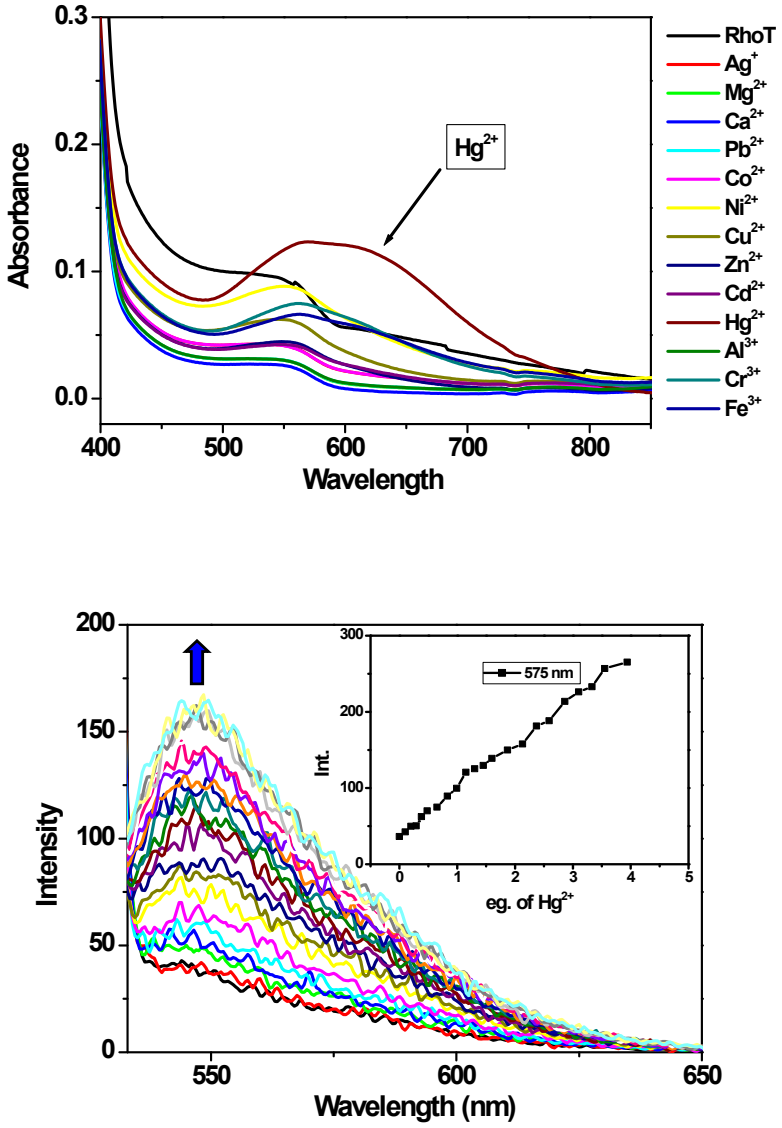

Figure S6 (a) Absorption spectra and (b) fluorescence spectra **AuNPs-RhoT** in 50:50, DMSO:H_2O in the presence of different amounts of Hg^{2+}, E_x=520 nm.

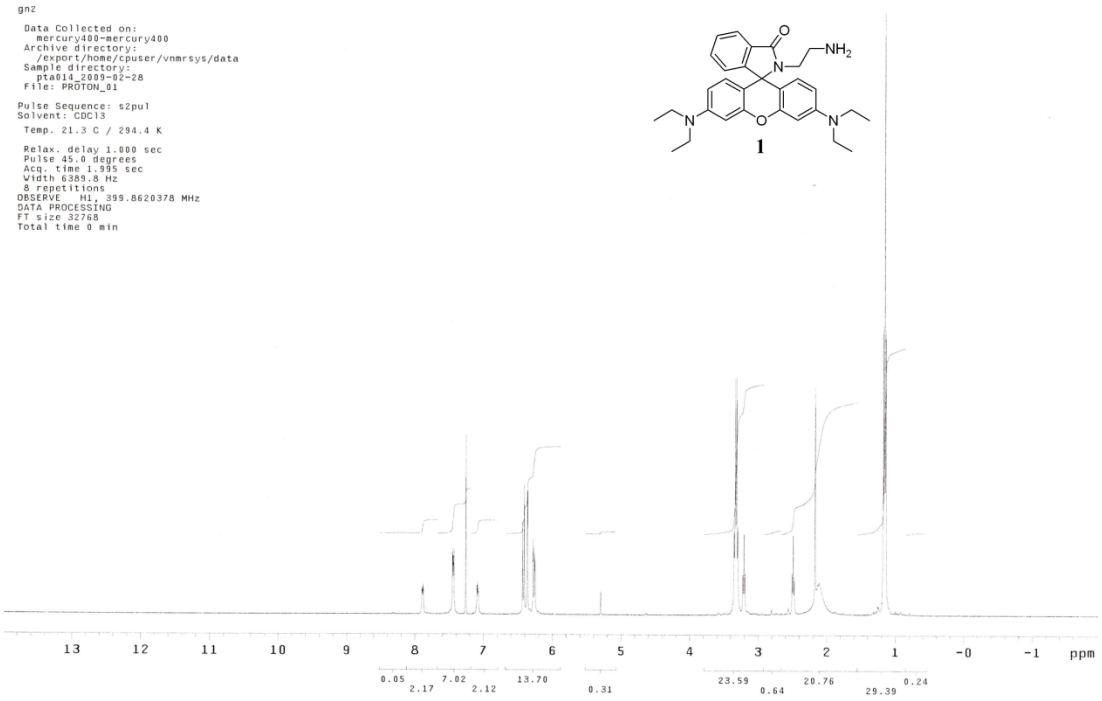

Figure S7. ^{1}H NMR spectrum of N-(rhodamine B)lactam-ethylenediamine (**Rho**).

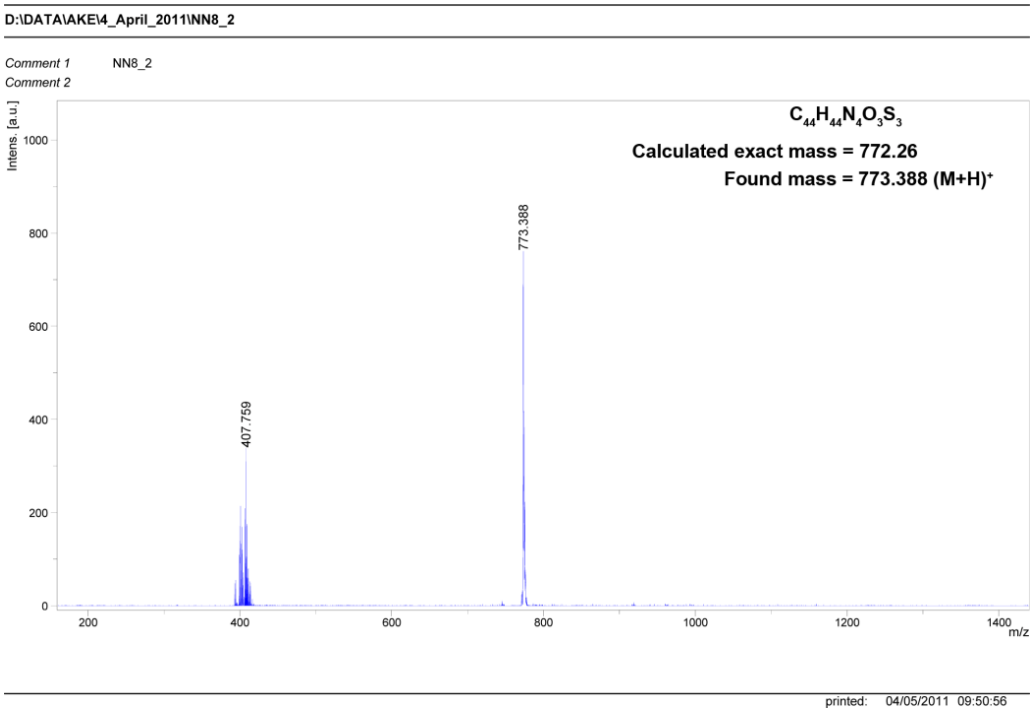

Figure S8. Mass spectrum of fluorescent chemosensor (**RhoT**).

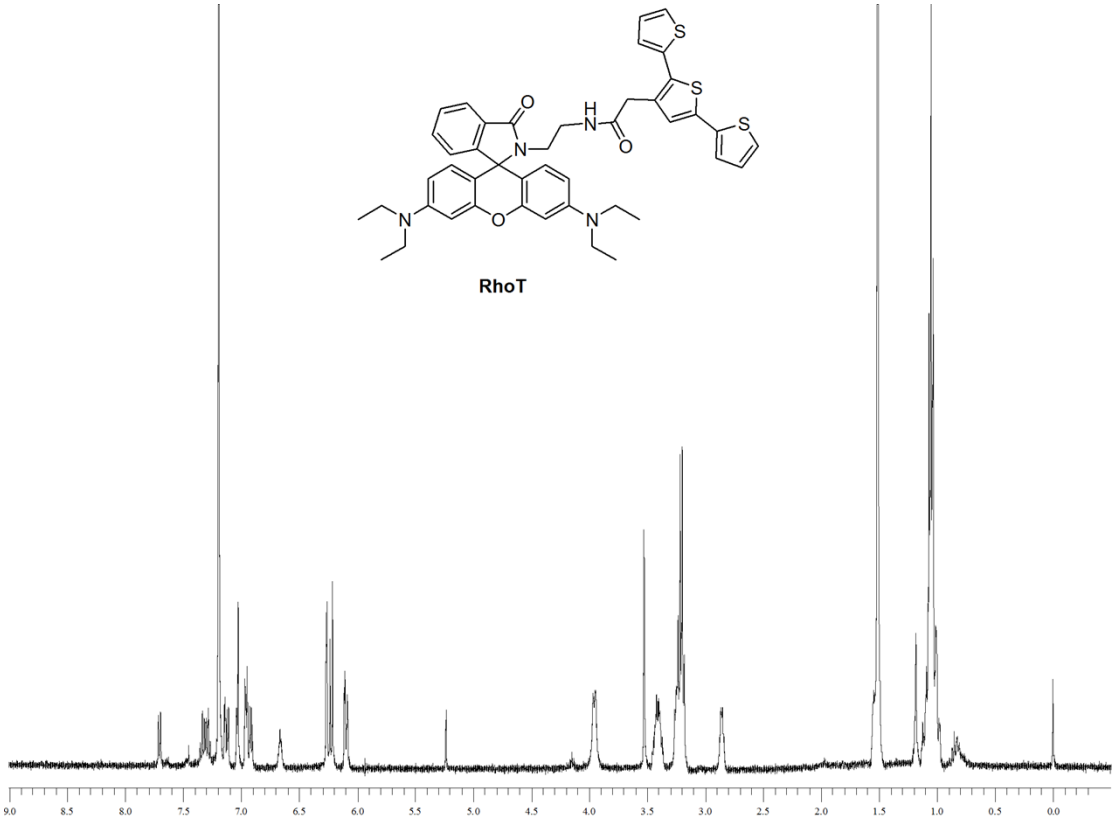

Figure S9. ^{1}H NMR of fluorescent chemosensor (**RhoT**).