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Electronic Supplementary Information

Optical chemosensors for Hg²⁺ from terthiophene appended rhodamine derivatives : FRET based molecular and *in situ* hybrid gold nanoparticles sensors

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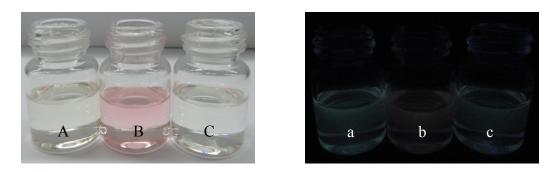


Figure S1. Color changes (A, B, C) and fluorescence changes (a, b, c) of **RhoT** (10 mM) in the presence of 10 μ M of various metals. (A, a) **RhoT** only, (B, b) **RhoT** + Hg²⁺, (C, c) **RhoT** + other metals.

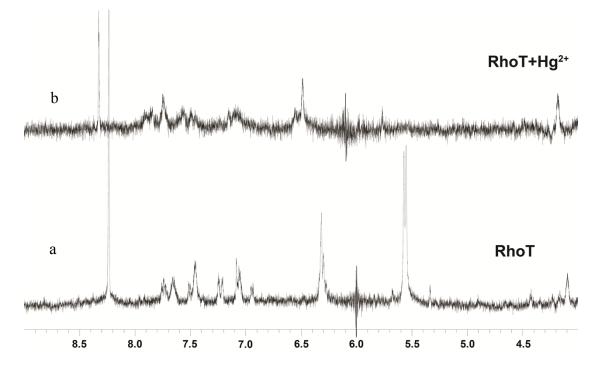


Figure S2.¹H NMR spectra of RhoT in DMSO-d₆ in the absence (a) and presence (b) of Hg^{2+} .

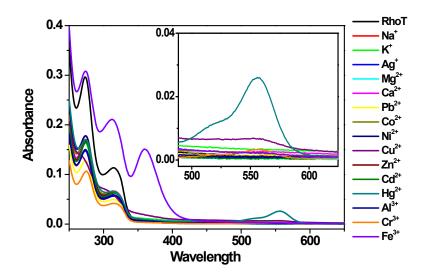


Figure S3. Absorption spectra changes of RhoT (10 μ M) in 0.01 mol/L of TBAPF₆ in DMSO to 10 μ M of various cations.

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

Complexation	ΔE (kcal/mol)		
RhoT + Hg ²⁺ \rightarrow RhoT •Hg ²⁺	-276.28		
2 RhoT + Hg ²⁺ \rightarrow 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.

	$E_{ m HOMO}$	$E_{\rm LUMO}$	$E_{\rm gap}$
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
2 RhoT- Hg ²⁺	-8.626	-5.769	2.85

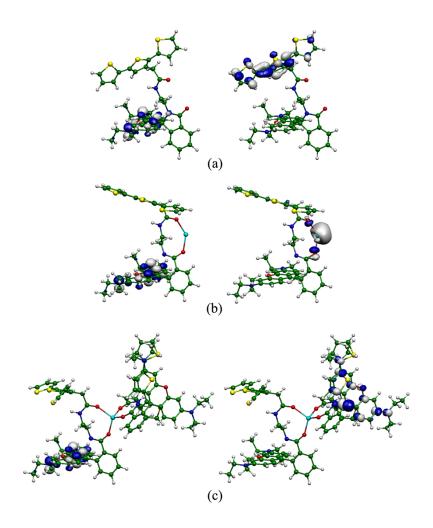


Figure S4. Plots of HOMO (left) and LUMO (right) orbitals of (a) L, (b) L-Hg²⁺ (1:1) and (c) 2L-Hg²⁺ (2:1) obtained at the B3LYP/LanL2DZ level of theory, the O-Hg bond distances are in Å.

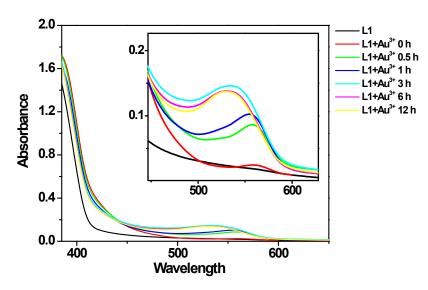


Figure S5. UV-vis absorption spectra of rhodamine functionalized with terthiophene (**RhoT**) 10^{-3} M before and after treated with AuCl₃ at different time (0–12 hour). AuNPs showed their characteristic absorption bands at 570 nm.

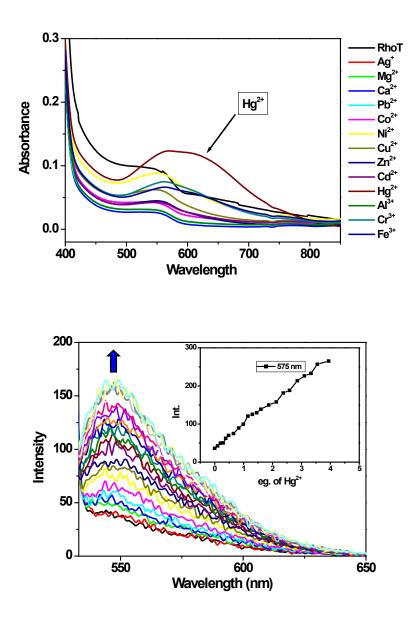


Figure S6 (a) Absorption spectra and (b) fluorescence spectra **AuNPs-RhoT** in 50:50, DMSO:H₂O in the presence of different amounts of Hg²⁺, E_x =520 nm.

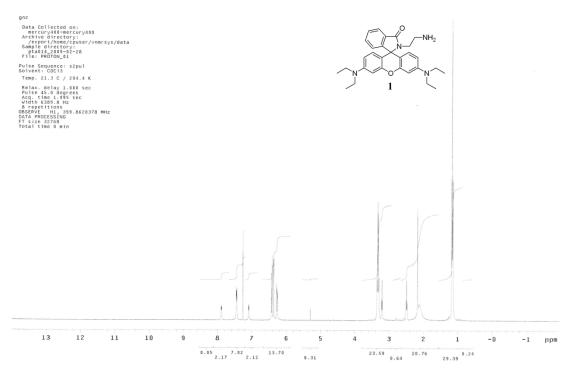


Figure S7. ¹H NMR spectrum of N-(rhodamine B)lactam-ethylenediamine (Rho).

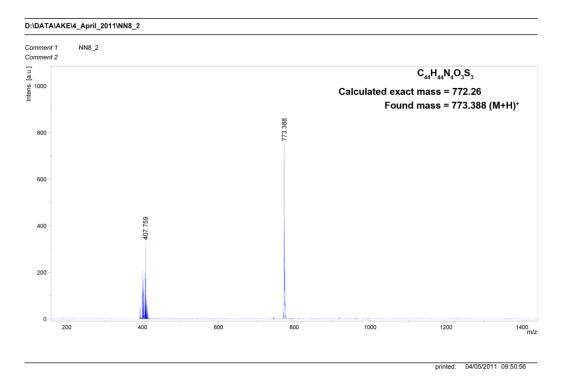


Figure S8. Mass spectrum of fluorescent chemosensor (RhoT).

