## **Electronic Supplementary Information**

# Solvent Dependent Competition between Fluorescence Resonance Energy Transfer and Through Bond Energy Transfer in Rhodamine Appended Hexaphenylbenzene Derivatives for Sensing of Hg<sup>2+</sup> Ions

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<sup>1</sup>H NMR of compound 3 (300 MHz, CDCl<sub>3</sub>)





<sup>13</sup>C NMR spectrum of compound 3 (75 MHz, CDCl<sub>3</sub>)

#### Mass spectrum of compound 3



### <sup>1</sup>H NMR spectrum of compound 5 (300MHz, CDCl<sub>3</sub>)



#### <sup>13</sup>C NMR of compound 5 (75 MHz, CDCl<sub>3</sub>)



**MALDI-TOF of compound 5** 



#### <sup>1</sup>H NMR spectrum of compound 7 (300 MHz, CDCl<sub>3</sub>)





## <sup>13</sup>C NMR spectrum of compound 7 (100 MHz, CDCl<sub>3</sub>:DMSO; 8:2)

MALDI-TOF of compound 7



### <sup>1</sup>H NMR spectrum of compound 10 (300 MHz, CDCl<sub>3</sub>)



## <sup>13</sup>C NMR spectrum of compound 10 (75 MHz, CDCl<sub>3</sub>)



**MALDI-TOF of compound 10** 



Mass (m/z)



#### <sup>1</sup>H NMR spectrum of compound 11 (300 MHz, CDCl<sub>3</sub>)

### <sup>13</sup>C NMR spectrum of compound 11 (75 MHz, CDCl<sub>3</sub>)



Mass spectrum of compound 11









**Figure S2.** Fluorescence response of receptor **5** (1  $\mu$ M) on addition of Hg<sup>2+</sup> (50 eq) in THF,  $\lambda_{ex} = 290$  nm. Inset shows the change in the fluorescence of compound **5** on addition of Hg<sup>2+</sup> ions.



**Figure S3.** Fluorescence response of receptor **7** (1  $\mu$ M) on addition of Hg<sup>2+</sup> (0-20 eq) in THF,  $\lambda_{ex} = 290$  nm. Inset shows the change in the fluorescence of compound **7** on addition of Hg<sup>2+</sup> ions.



**Figure S4** Spectral overlap of the absorption spectrum of rhodamine B (2.0  $\mu$ M in THF) and emission spectrum of diamine **3** (2.0  $\mu$ M in THF)



**Figure S5** The spectral overlay of the absorption spectrum of rhodamine B,  $(2.0 \ \mu\text{M} \text{ in acetonitrile})$  and fluorescence spectrum of compound **6** (2.0  $\mu\text{M}$  in acetonitrile).



Figure S6 The fluorescence spectrum of compound 5 (1  $\mu$ M) in different ratios of THF and methanol



**Figure S7**. The selectivity graph of derivative **5** (1  $\mu$ M) and **7** (1  $\mu$ M) towards Hg<sup>2+</sup> ions at 585 nm; A = Hg<sup>2+</sup>, B = Pb<sup>2+</sup>, C = Ba<sup>2+</sup>, D = Ag<sup>+</sup>, E = Cd<sup>2+</sup>, F = Zn<sup>2+</sup>, G = Cu<sup>2+</sup>, H = Ni<sup>2+</sup>, I = Co<sup>2+</sup>, J = Fe<sup>2+</sup>, K = Fe<sup>3+</sup>, L = Mn<sup>2+</sup>, M = Ca<sup>2+</sup>, N = K<sup>+</sup>, O = Mg<sup>2+</sup>, P = Na<sup>+</sup>, Q = Li<sup>+</sup> in THF.



Figure S8. Competitive selectivity of receptor 5 (1.0  $\mu$ M) and 7 towards Hg<sup>2+</sup> ions (20 eq and 60 eq , respectively) in the presence of other metal ions (100 eq) A = none, B = Pb<sup>+</sup>, C = Ba<sup>+</sup>, D = Ag<sup>+</sup>, E = Cd<sup>2+</sup>, F = Zn<sup>2+</sup>, G = Cu<sup>2+</sup>, H = Ni<sup>2+</sup>, I = Co<sup>2+</sup>, J = Fe<sup>2+</sup>, K = Fe<sup>3+</sup>, L = Mn<sup>2+</sup>, M = Ca<sup>2+</sup>, N = K<sup>+</sup>, O = Mg<sup>2+</sup>, P = Na<sup>+</sup>, Q = Li<sup>+</sup> in methanol.



**Figure S9.** Fluorescence response of receptor **5** (1  $\mu$ M) on addition of Hg<sup>2+</sup> (0-20 eq) in n-butanol,  $\lambda_{ex} = 290$  nm.



Wavelength

Figure S10. Fluorescence response of receptor 5 (1  $\mu$ M) on addition of Hg<sup>2+</sup> (0-20 eq) in n-propanol,  $\lambda_{ex}$  = 290 nm.



Figure S11. Fluorescence response of receptor 5 (1  $\mu$ M) on addition of Hg<sup>2+</sup> (0-20 eq) in ethanol,  $\lambda_{ex} = 290$  nm.



**Figure S12.** Fluorescence response of receptor 7 (1  $\mu$ M) on addition of Hg<sup>2+</sup> (0-60 eq) in n-butanol,  $\lambda_{ex} = 290$  nm.



Figure S13. Fluorescence response of receptor 7 (1  $\mu$ M) on addition of Hg<sup>2+</sup> (0-60 eq) in n-propanol,  $\lambda_{ex} = 290$  nm.







**Figure S15**. The change in relative intensity on subsequent addition of  $Hg^{2+}$  ions in compound 5 (0.5  $\mu$ M in THF) and 7 (0.5  $\mu$ M in THF).



**Figure S16.** Fluorescence spectra showing reversibility of  $Hg^{2+}$  coordination to receptor **5** (1  $\mu$ M in methanol) by TBAI (100 eq)



**Figure S17** Fluorescence spectra showing reversibility of  $Hg^{2+}$  coordination to receptor **7** (1 µM in methanol) by TBAI (100 eq).



**Figure S18.** Partial <sup>1</sup>H NMR spectrum of receptor **5** before (a), after addition of 0.5 equiv. (b), 1.0 equiv. (c) and 2 equiv. (d) of  $Hg^{2+}$  ions in CDCl<sub>3</sub>:CD<sub>3</sub>CN (8:2)



Figure S19. Job's plot for determining the stoichiometry of receptor 5 and  $Hg^{2+}$  ion in THF



**Figure S20** The cyclic voltammograms for derivative **5** before (A) and after (B) addition of  $Hg^{2+}$  ions in 1,2dichloromethane (10<sup>-3</sup> M solution) using ferrocene as internal standard.



**Figure S21.** The fluorescence spectrum of compound **6** and equimolar (1  $\mu$ M) solution of compound **6** + rhodamine B in methanol at excitation wavelength of  $\lambda_{eq} = 290$  nm.



Figure S22 Fluorescence response of receptor 11 (1  $\mu$ M) on addition of Hg<sup>2+</sup> (0-50 eq) in THF,  $\lambda_{ex} = 290$  nm.

Resonance energy transfer efficiency  $E = [1 - F_D'/F_D]$ 

 $F_D$  = Fluorescence intensity of free ligand;

 $F_D'$  = Fluorescence intensity of corresponding amine

#### **Equation 1**

$$\phi_{fs} = \phi_{fr} \times \frac{1 - 10^{-\text{ArLr}}}{1 - 10^{-\text{AsLs}}} \times \frac{N_s^2}{N_r^2} \times \frac{D_s}{D_r}$$

 $\phi_{fs}$  = quantum yield of sample;  $\phi_{fr}$  = quantum yield of reference;  $A_r$  = Absorbance of reference;  $A_s$  = Absorbance of sample;  $N_R$  = refractive index of reference;  $N_S$  = refractive index of sample;  $D_s$  = area under the curve of fluorescence graph of sample;  $D_R$  = area under the curve of fluorescence graph of sample;  $L_R$  = length of reference.

#### **Equation 2**