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Highly selective colorimetric sensing of Hg(II) ion in aqueous medium and solid state via formation novel M-C bond

C.Parthiban, R.Manivannan and Kuppanagounder P. Elango*

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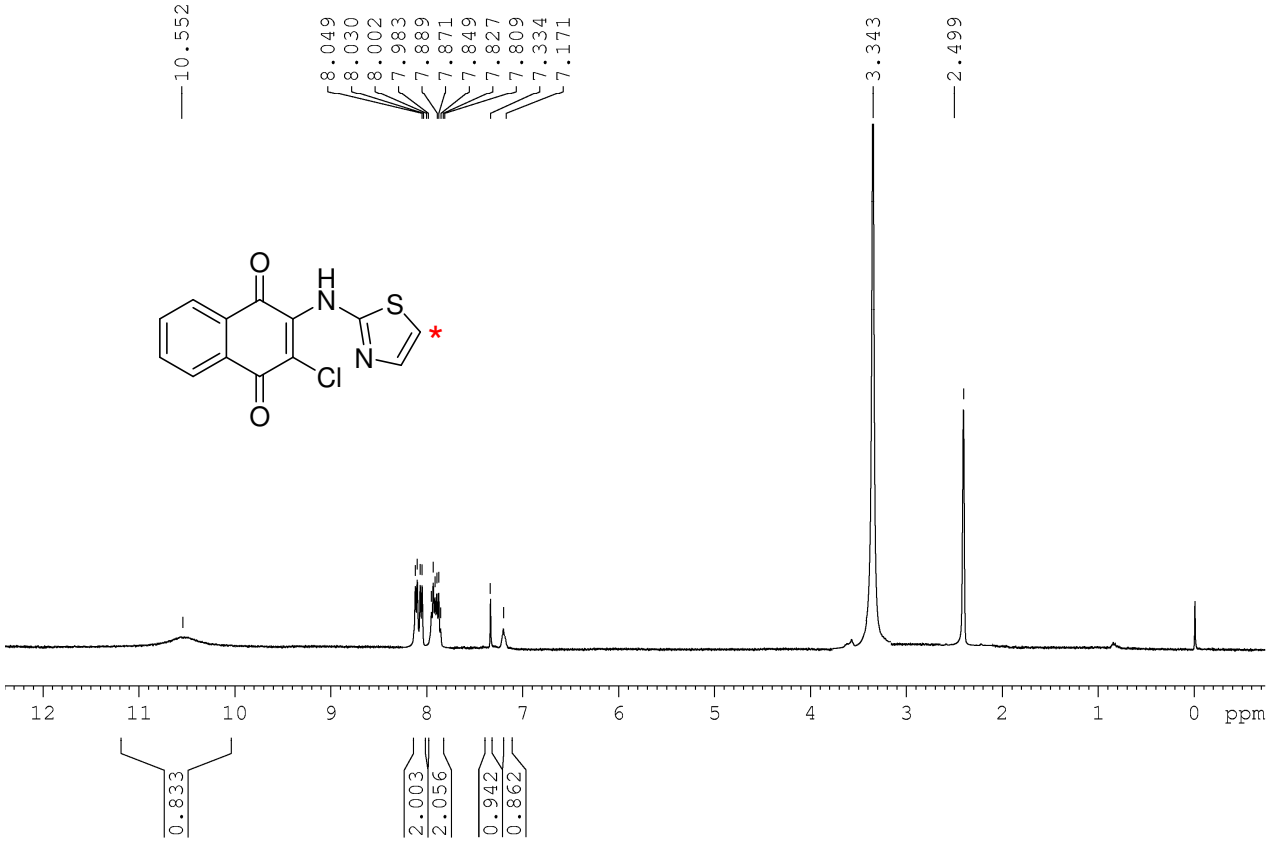

Fig. S2. ^{1}H NMR spectrum of R1

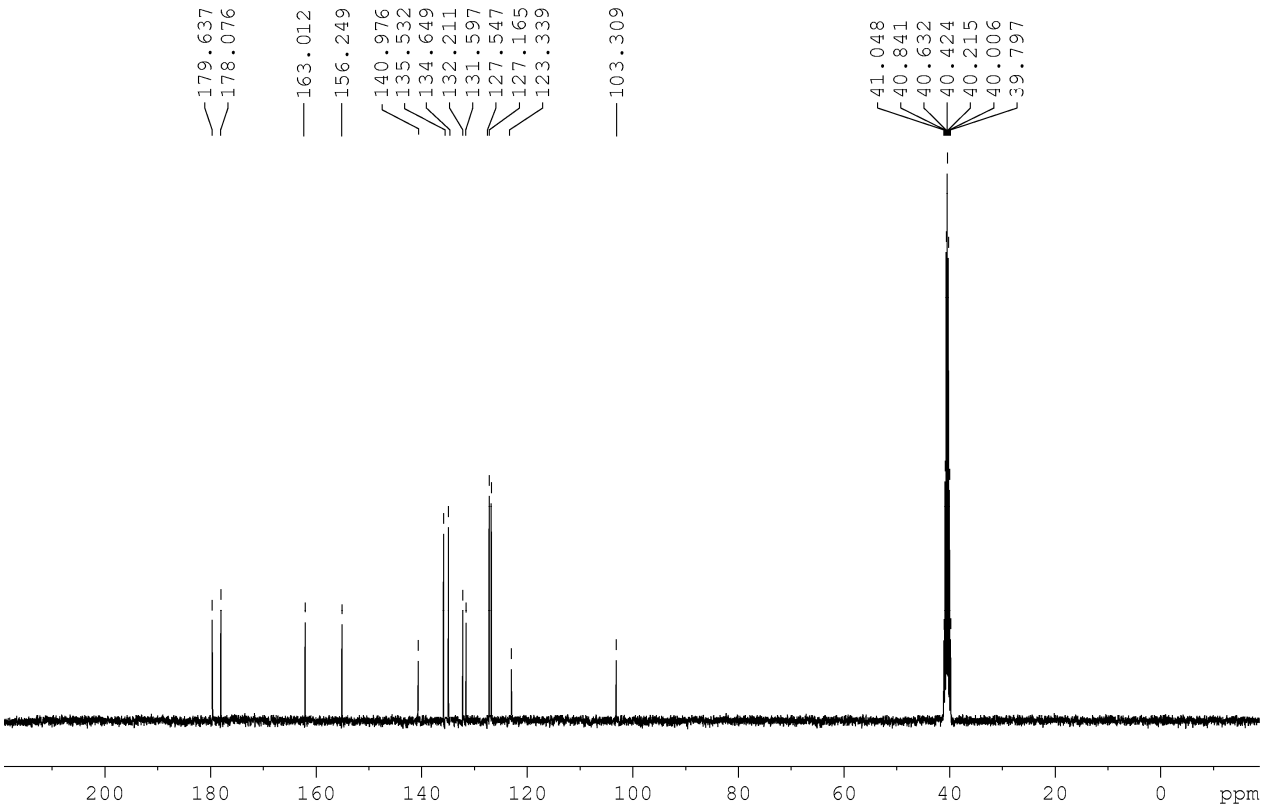

Fig. S2. ^{13}C NMR spectrum of R1

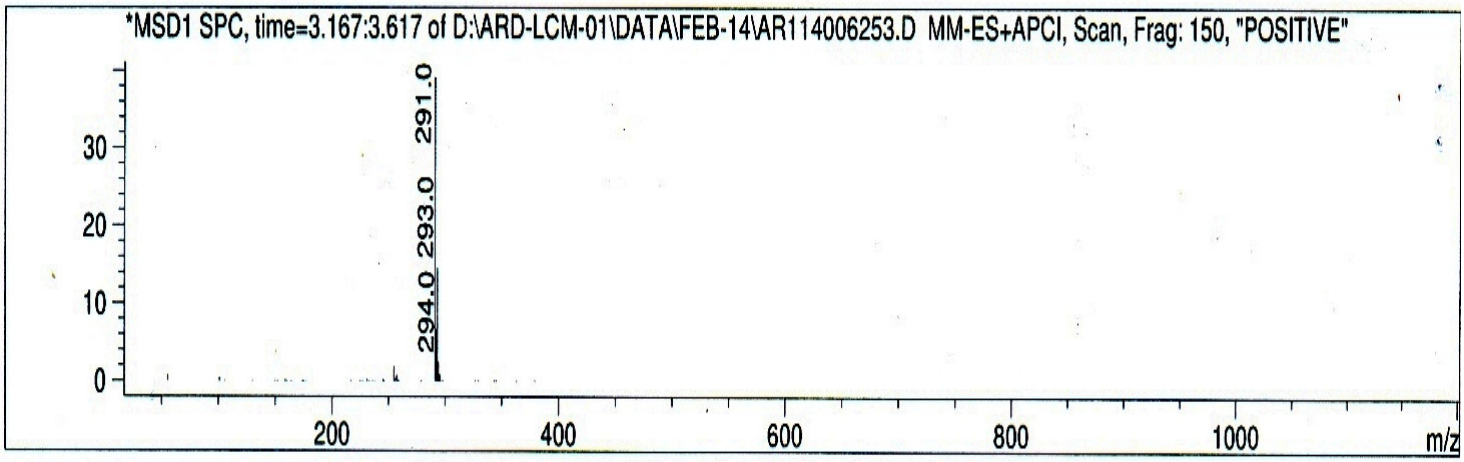

Fig. S3. LCMS spectrum of R1

Fig. S4. Colour change of receptor in aqueous solution (DMF:H_2O; 1:9 v/v) in presence of various metal ions.

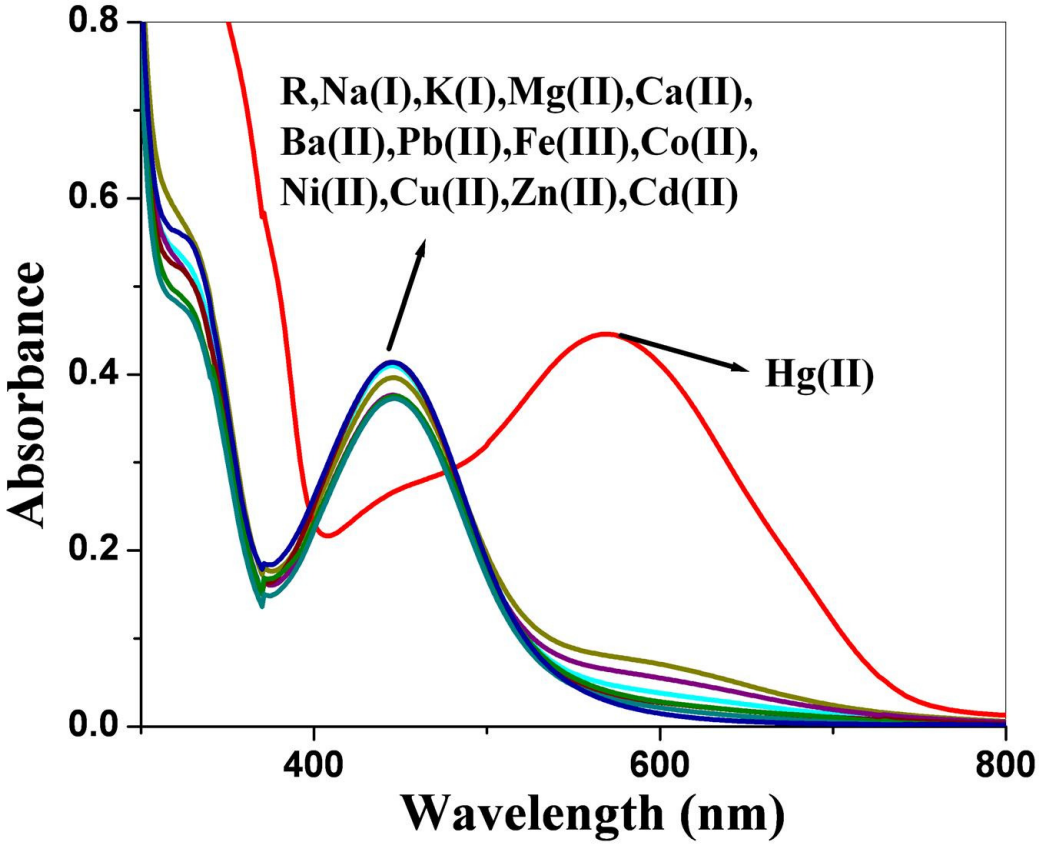

Fig. S5. UV-Vis spectral changes of the receptor upon the addition of the different cations.

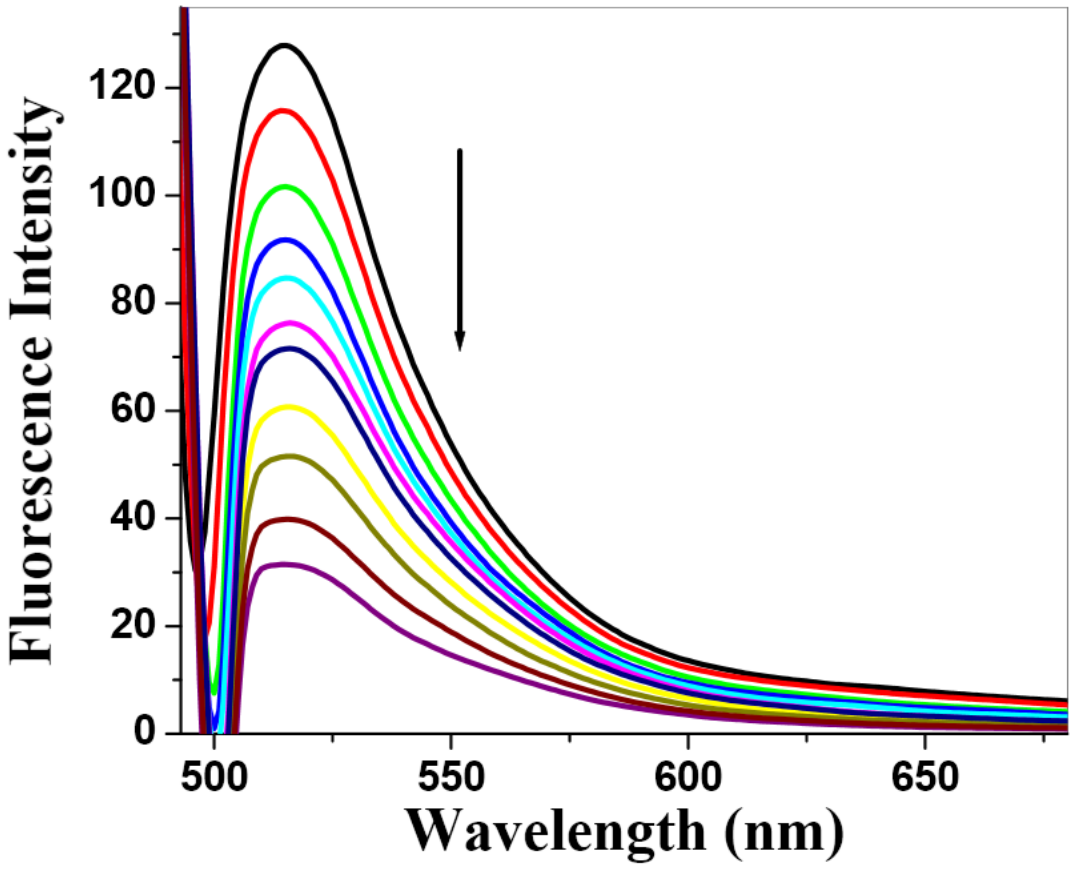

Fig. S6. Fluorescence changes of R1(6.5 x 10^{-4} M) upon addition of Hg(II) (0-2.5 x 10^{-3} M) in DMF: H_2O (1:9 v/v).

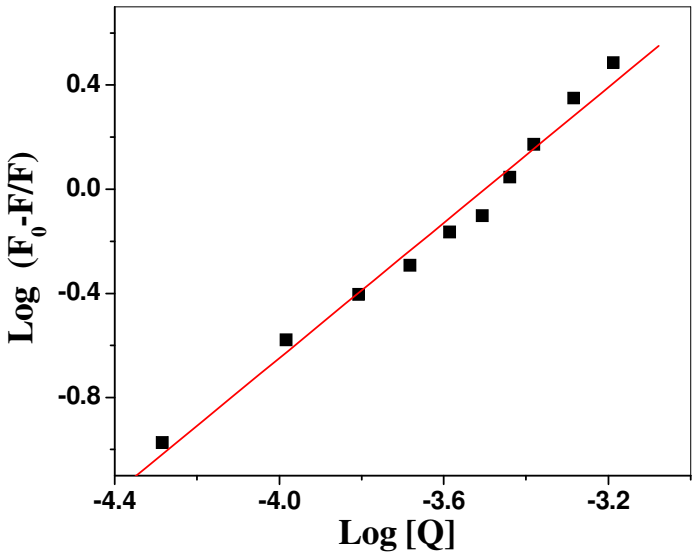

Fig. S7. Benesi-Hildebrand plot of the R1 with Hg(II).

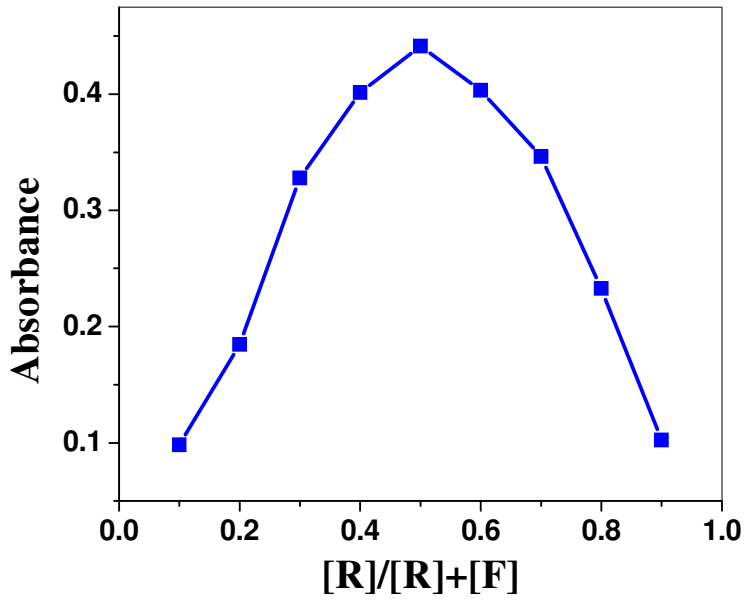

Fig. S8. Job's plot of R1 (2.5 x 10^{-4} M) upon addition of Hg(II).

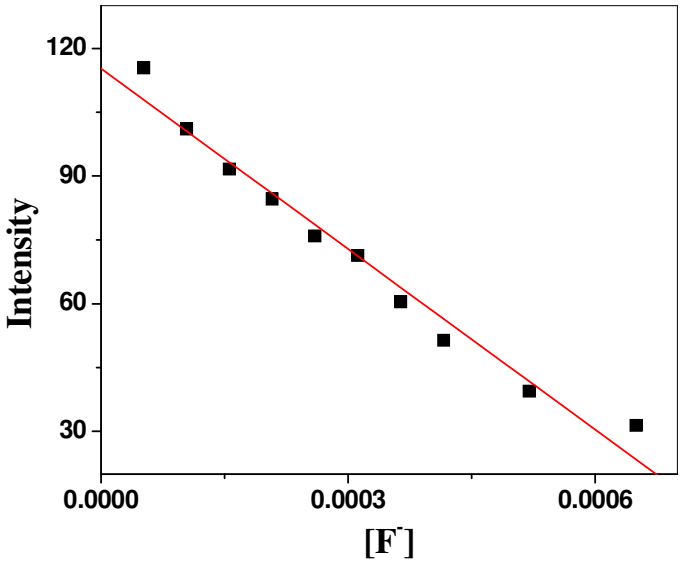

Fig. S9. Detection limits plot of the receptor.

Table S1. Crystal data and structure refinement for the Hg(II) complex.

Empirical formula	$C_{16}H_{13}Cl_2HgN_3O_3S$
Formula weight	598.84
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 12.9121(5) A alpha = 90 deg.
	b = 7.7803(3) A beta = 94.4640(10) deg.
	c = 18.6223(8) A gamma = 90 deg.
Volume	1865.12(13) A^3
Z, Calculated density	4, 2.133 Mg/m^3
Absorption coefficient	8.672 mm^-1
Crystal size	0.35 x 0.30 x 0.25 mm
Theta range for data collection	2.19 to 26.00 deg.
Limiting indices	-15<=h<=15, -9<=k<=9, -22<=l<=22
Reflections collected / unique	26561 / 3661 [R(int) = 0.0471]
Completeness to theta = 26.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.2294 and 0.1503
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3661 / 1 / 239
Goodness-of-fit on F^2	1.187
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0899
R indices (all data)	R1 = 0.0500, wR2 = 0.0970
Largest diff. peak and hole	0.765 and -0.942 e.A^-3

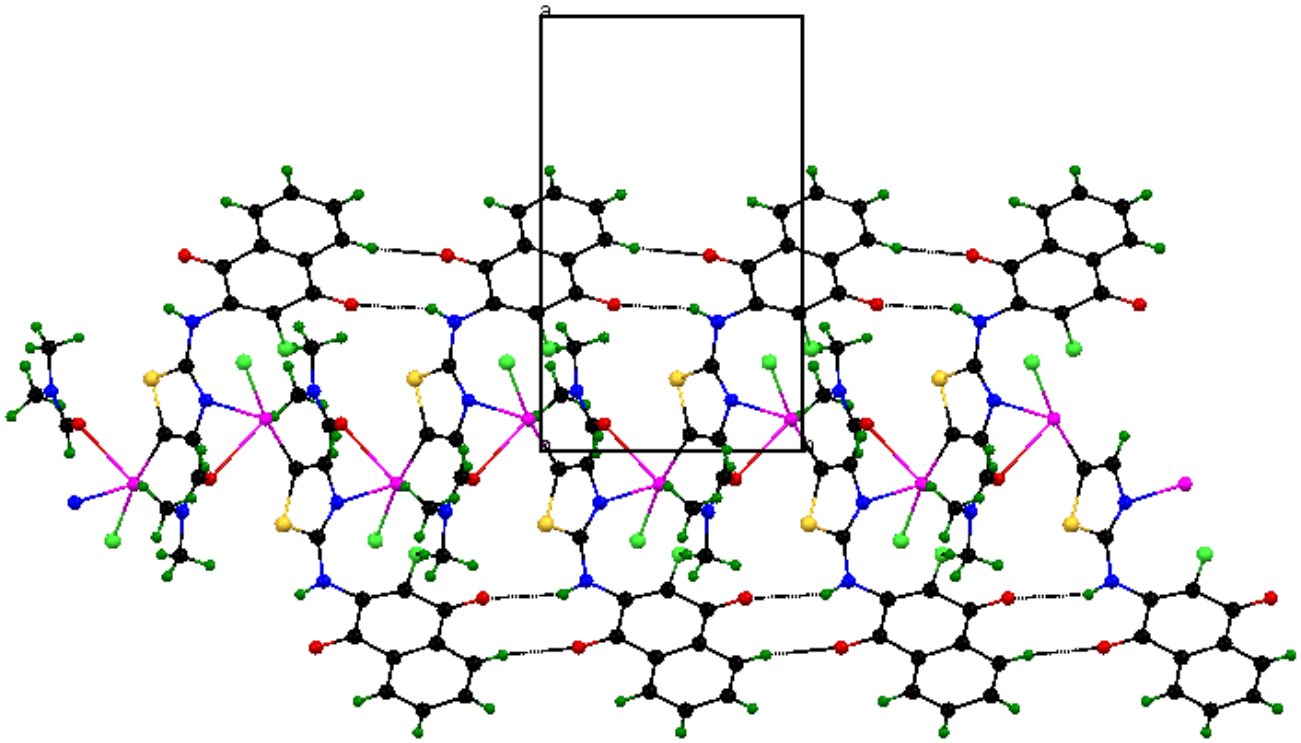

Fig. S10. Packing diagram of the Hg(II) complex.

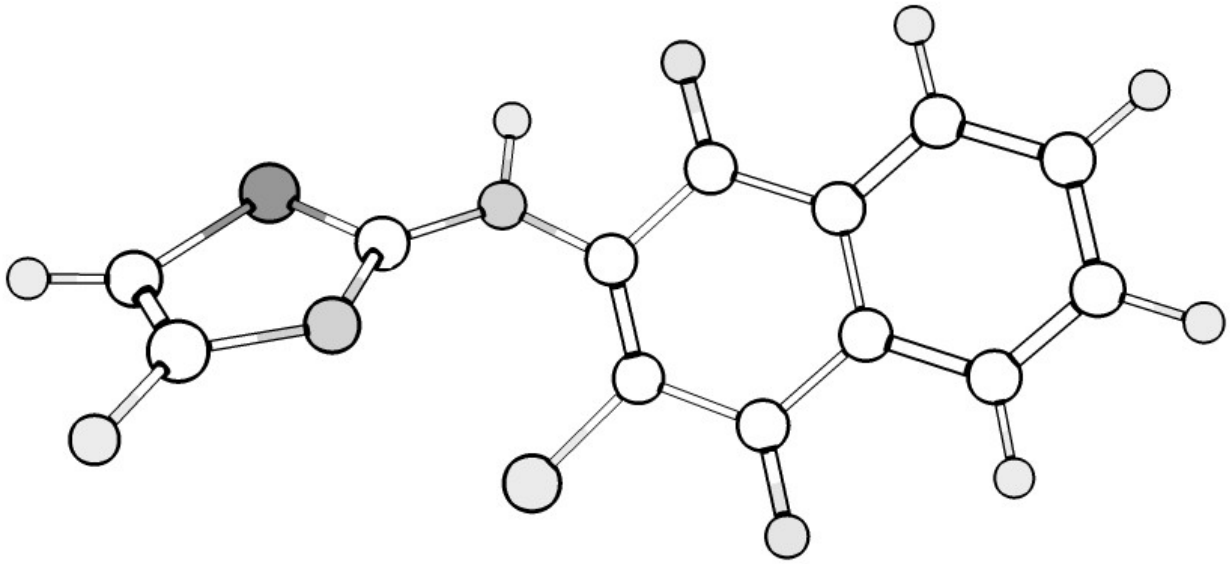

Fig. S11. Optimized geometry of the receptor R1.

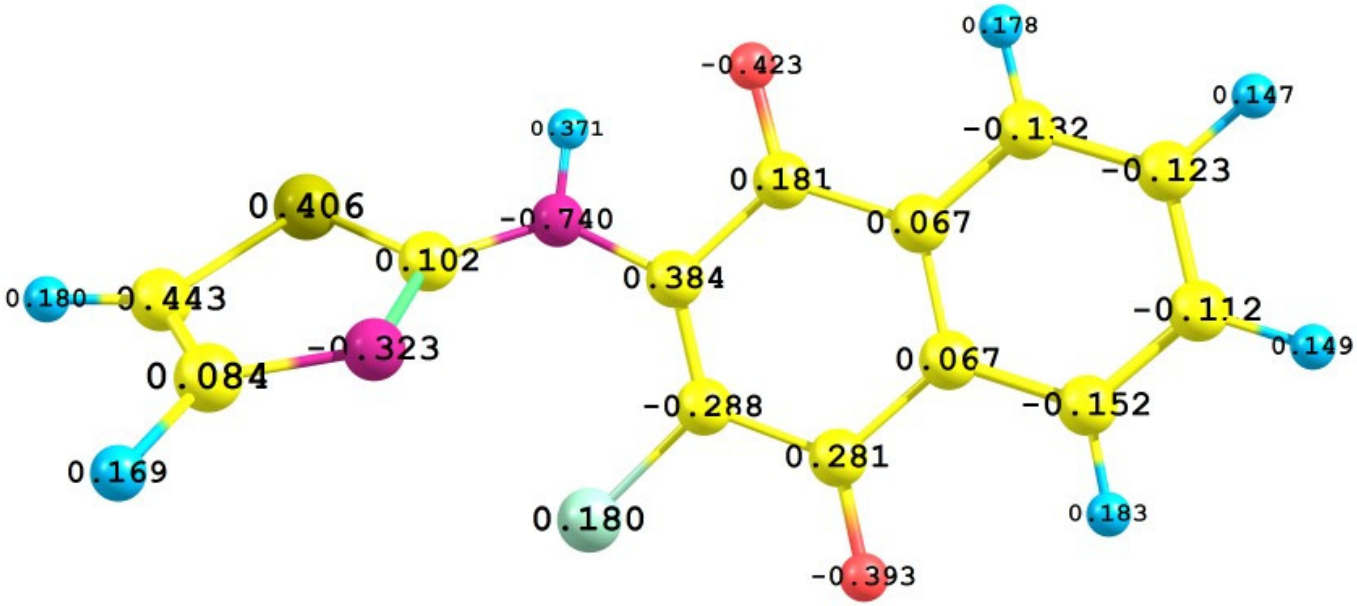

Fig. S12. Mullikan Chagres of the receptor R1.

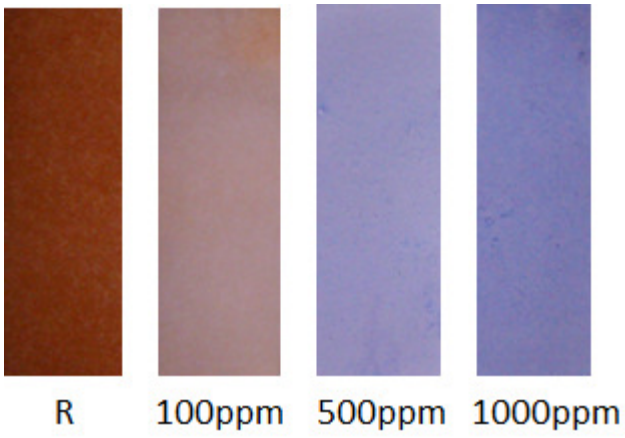

Fig. S13. Color changes of the test papers for detecting Hg(II) in aqueous solution with different concentrations.