Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

for

Carbazole-thiosemicarbazone-Hg(II) ensamble-based colorimetric and fluorescence turn-on toward iodide in aqueous media and its application in live cell imaging

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Preparation of cells

Candida albicans cells (IMTECH No. 3018) from exponentially growing culture in yeast extract glucose broth medium (pH 6.0, incubation temperature, 37^0C) were centrifuged at 3000 rpm for 10 minutes, washed twice with 0.1 M HEPES buffer at pH 7.4. Then, it was treated with **3** (10^{-5}M) ligand for 45 minutes in 0.1 M HEPES buffer (pH 7.4) containing 0.01 % Triton X100 as permeability enhancing agent. After incubation the cells were washed again with HEPES buffer at pH 7.4. **3** (10^{-5}M) treated cells were mounted on a grease free glass slide and observed under a Leica DM 1000 fluorescence microscope equipped with UV filter. Cells without **3** treatment were used as control. Then 10^{-5}M Hg^{2+} (aqueous solution) was added to the specimen at the point of observation with the help of a micropipette. The change in fluorescence intensity was observed and recorded. After that 10^{-5}M KI was added in similar way to detect the change.

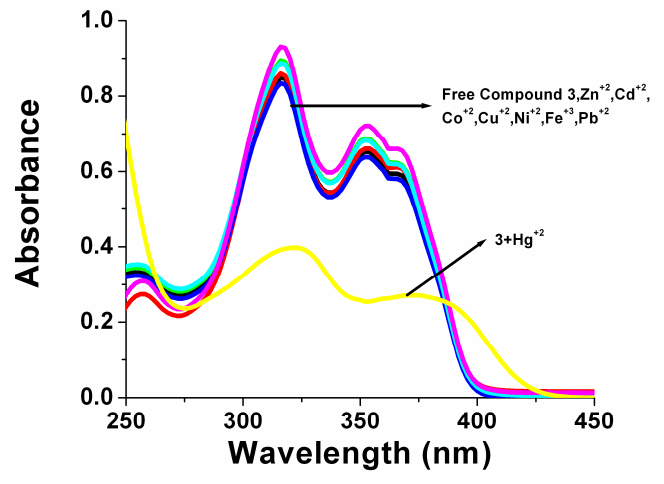


Figure S1 UV-vis spectra recorded for compound **3** (5μM) in the absence or presence of various heavy and transition metal species in pH 7.0 HEPES buffer (25 mM, pH 7.4, containing 1.0% DMSO).

Binding constant curve for receptor 3 with Hg(II) from UV-vis in pH 7.4 HEPES buffer (25 mM, pH 7.4, containing 1.0% DMSO).

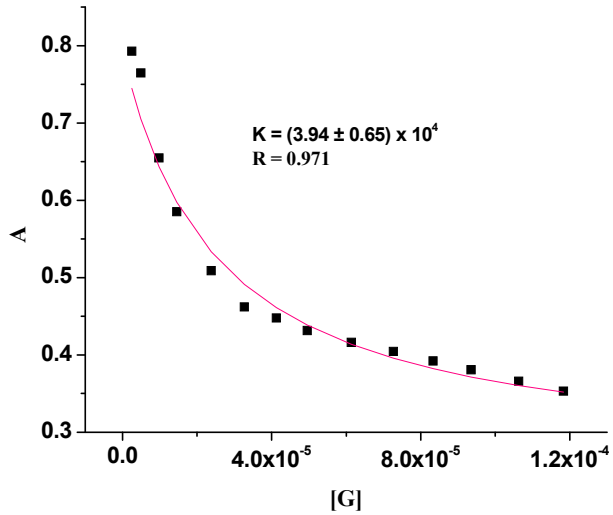
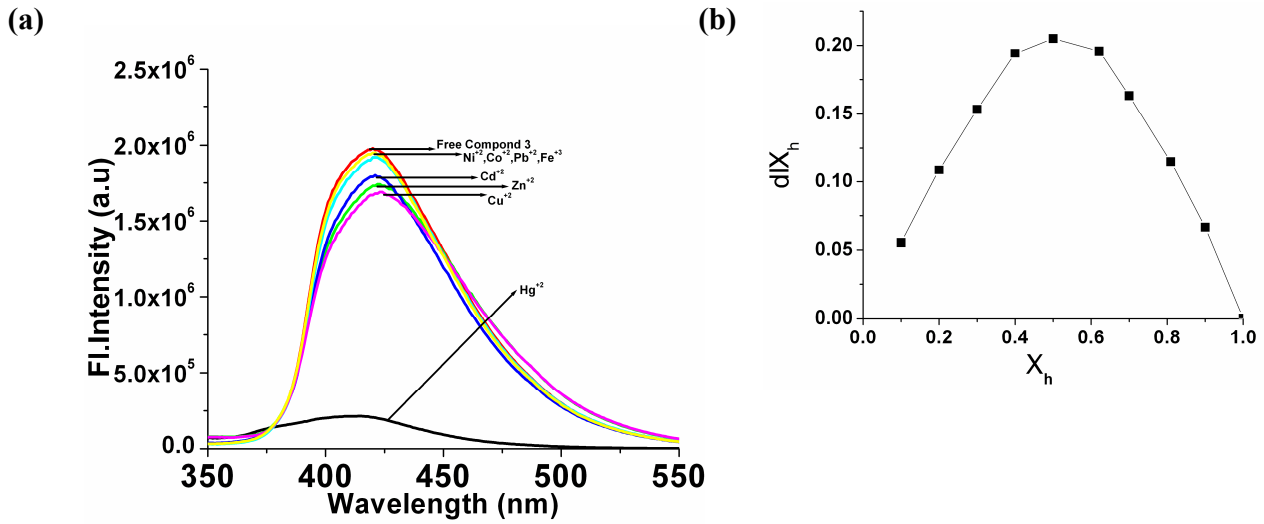


Figure S2: Binding constant curve for **3** (c = 1.00 x 10^{-5} M) with Hg(II) (c = 5.00 x 10^{-4} M) [Determined using non-linear curve fitting y= (A_0+A*K*x)/ (1+K*x). x = [G], y= absorbance in pH 7.4 HEPES buffer (25 mM, pH 7.4, containing 1.0% DMSO).



Binding constant curve for receptor 3 with Hg(II) from fluorescence in pH 7.4 HEPES buffer (25 mM, pH 7.4, containing 1.0% DMSO).

(c)

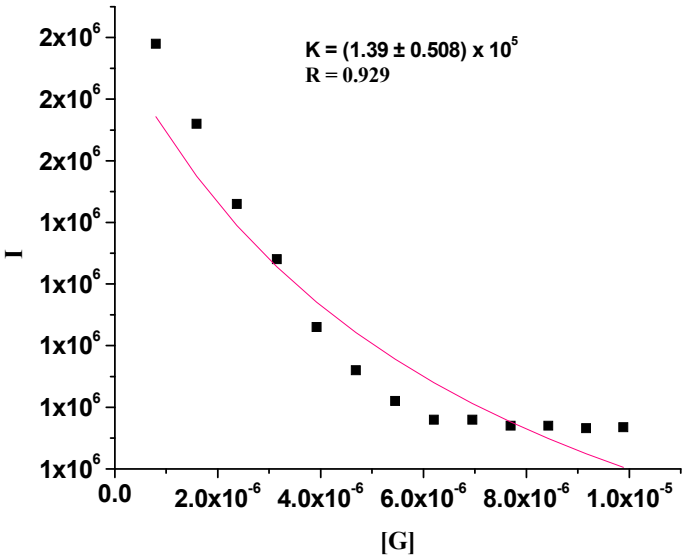


Figure S3. (a) Fluorescence spectra of compound **3** (5 μM) in the absence or presence of various heavy and transition -metal species in pH 7.4 HEPES buffer (30 mM, pH 7.4, containing 1.0% DMSO), **(b)** Job's plot of compound **3** with Hg^{+2} according to the method of continuous variations. The total concentrations of compound **4** and Hg^{+2} were kept constant at 20 μM.
(c) Binding constant curve of **3** (c = 1.00 x 10^{-5} M) with Hg(II) (c = 2.0 x 10^{-4} M) from fluorescence titration in pH 7.4 HEPES buffer (25 mM, pH 7.4, containing 1.0% DMSO). Working formula y=I_0+((I-I_0)/(2*x_2))*(x_1+x_2+1/K-((x_1+x_2+1/K)^2-4*x_1*x_2)^.5), x_1= [G], x_2 = [H], y = intensity.

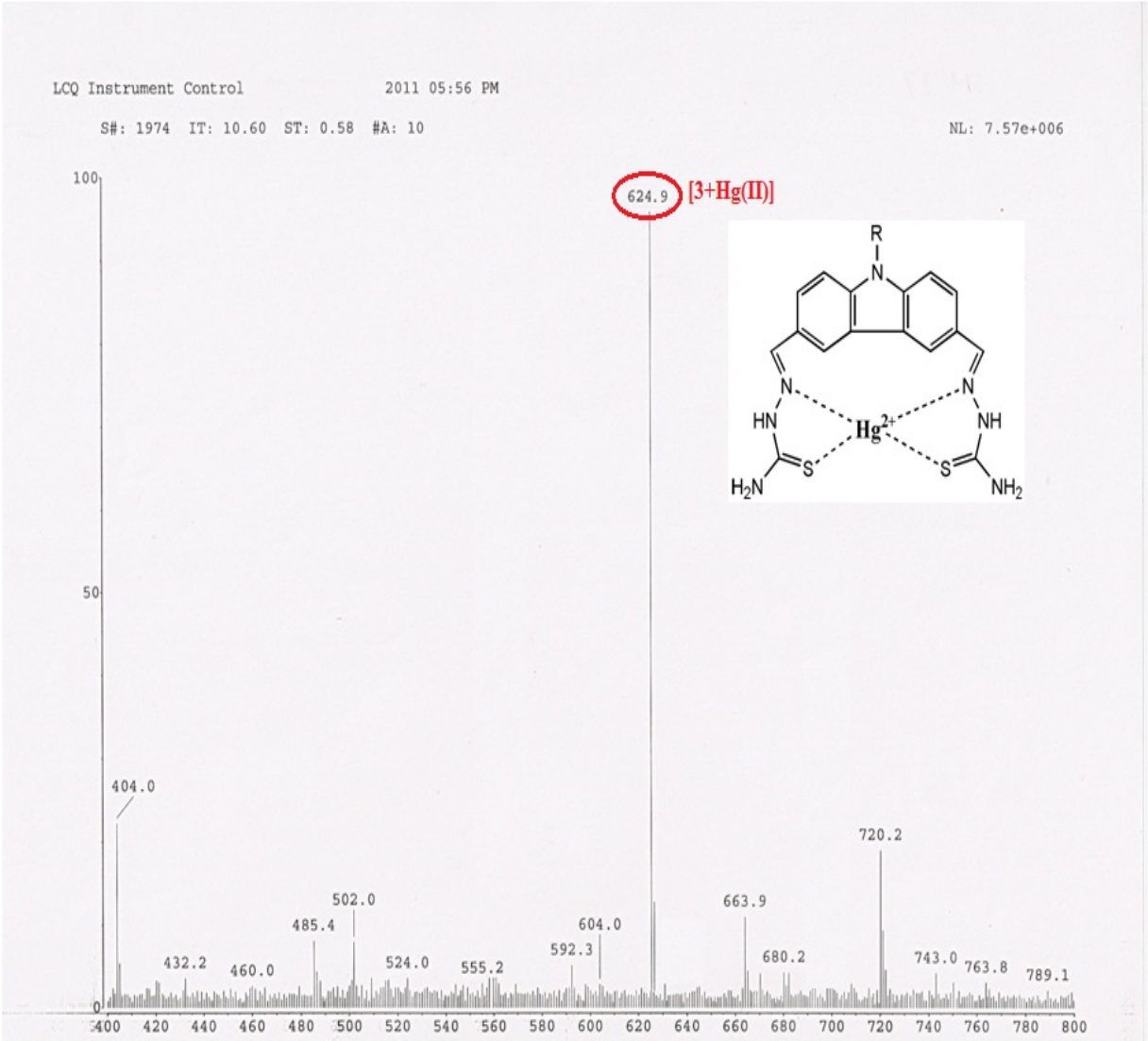


Figure S4. ESI-MS spectrum of Compound **3** +Hg^{+2}

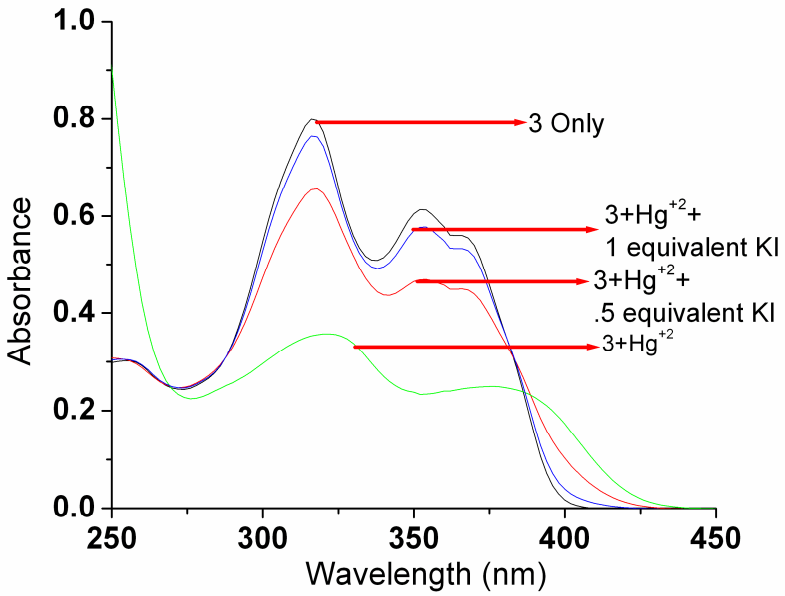


Figure S5. The absorption spectra of the **3-** Hg^{+2} ensemble (10μM) in pH 7.4 HEPES buffer (30 mM, pH 7.4, containing 1.0% DMSO) in the presence of Iodide anions .

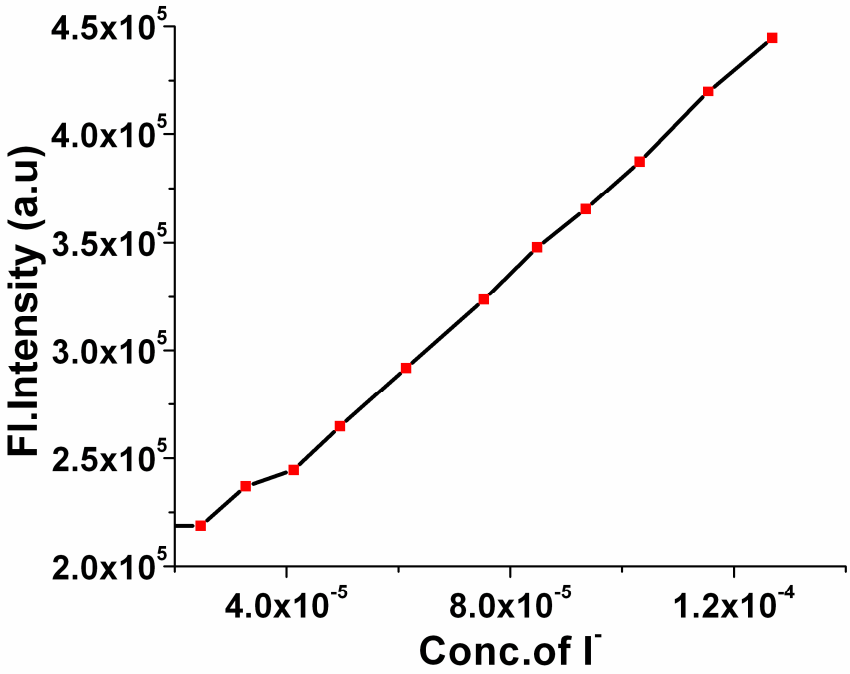


Figure S6. Plot of the fluorescence intensity (at 425 nm) as a function of the concentrations of Iodide anions. The concentration of the 3-Hg ensemble was 5 μM.

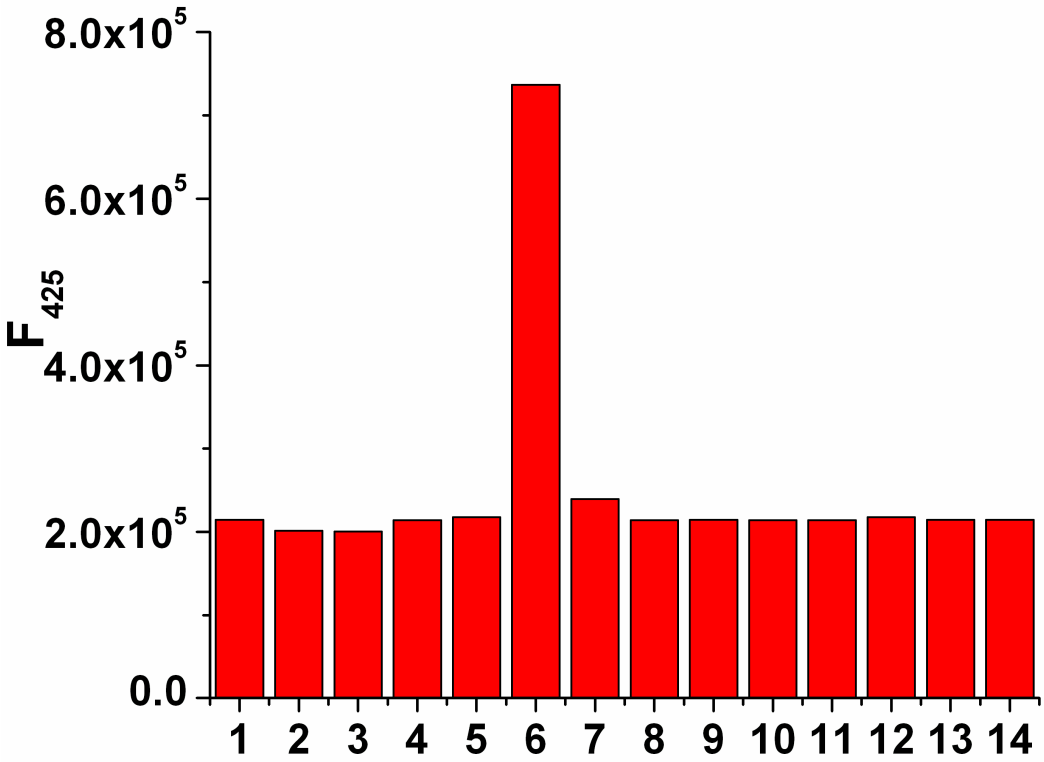
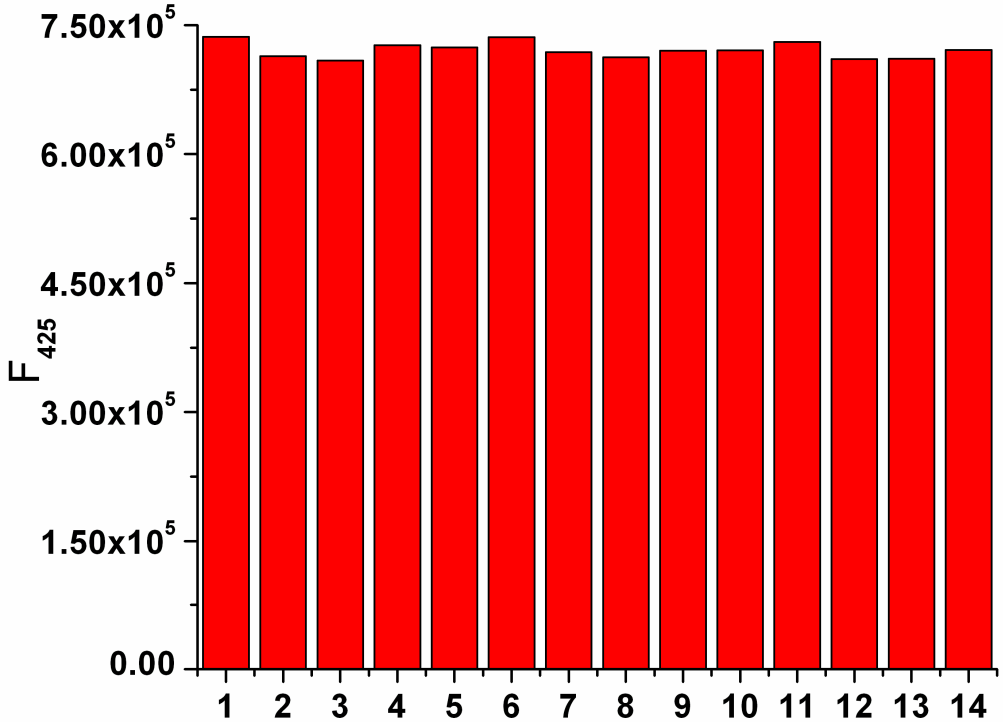


Figure S7. Fluorescence intensity response of **3**–Hg ensemble toward various anions. 1. **3**–Hg^{+2}, 2. F^-, 3.Cl^-, 4.Br^-, 5.NO_3^-, 6. I^-, 7.NO_2^-, 8.SO_4^-2, 9.SO_3^{-2} 10.CO_3^{-2}, 11.PO_4^{-3}, 12. CH_3COO^-, 13.N_3^-, 14.CN^-.



(b)

Figure S8 The fluorescence intensity changes of the **3**–Hg ensemble to Iodide anions in the presence of various test anions.1. I^-, 2. I^-+ F^-, 3.I^-+Cl^-, 4. I^-+Br^-, 5. I^-+NO_3^-, 6.I^-,7. I^-+ NO_2^-,8. I^-+SO_4^{-2},9. I+SO_3^{-2}10. I^-+CO_3^{-2},11. I^-+PO_4^{-3},12. I^-+CH_3COO^-,13. I^-+N_3^-,14. I^-+CN^-.

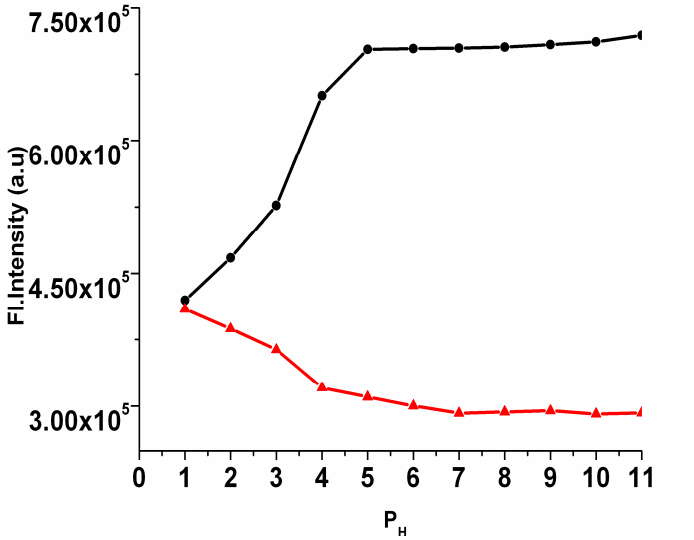


Figure S9. The pH effects on the fluorescence intensity at 425nm of the 3-Hg^{+2}ensemble (5 μM) (▶), and the ensemble (5 μM) toward iodide anions (10 μM) (●).

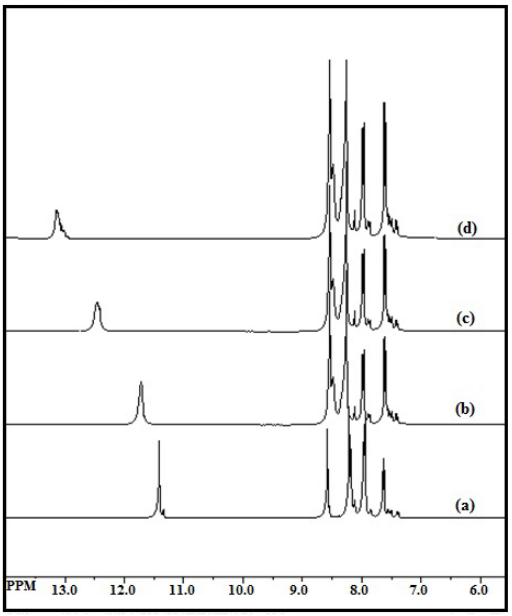


Figure S10. 1H NMR (400 MHz) spectra of Compound **3** (a), **3** + .5 equivalent Hg^{+2}(b), **3**+ 1 equivalent Hg^{+2} (c), and **3**+ 1.5 equivalent Hg^{+2} in d_6 DMSO-$D_2$0 (d).

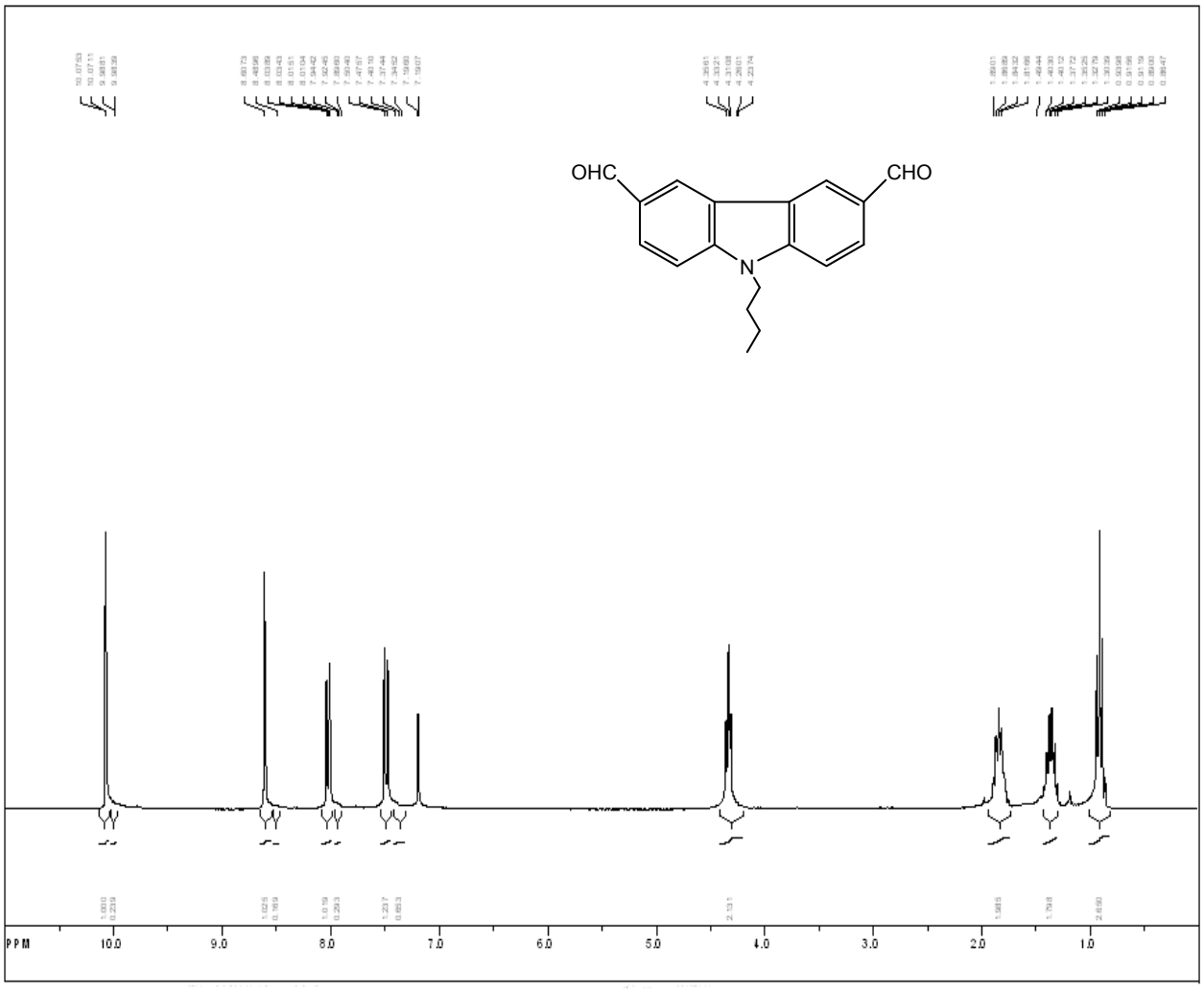


Figure S11. ^{1}H NMR spectrum of compound **2**.

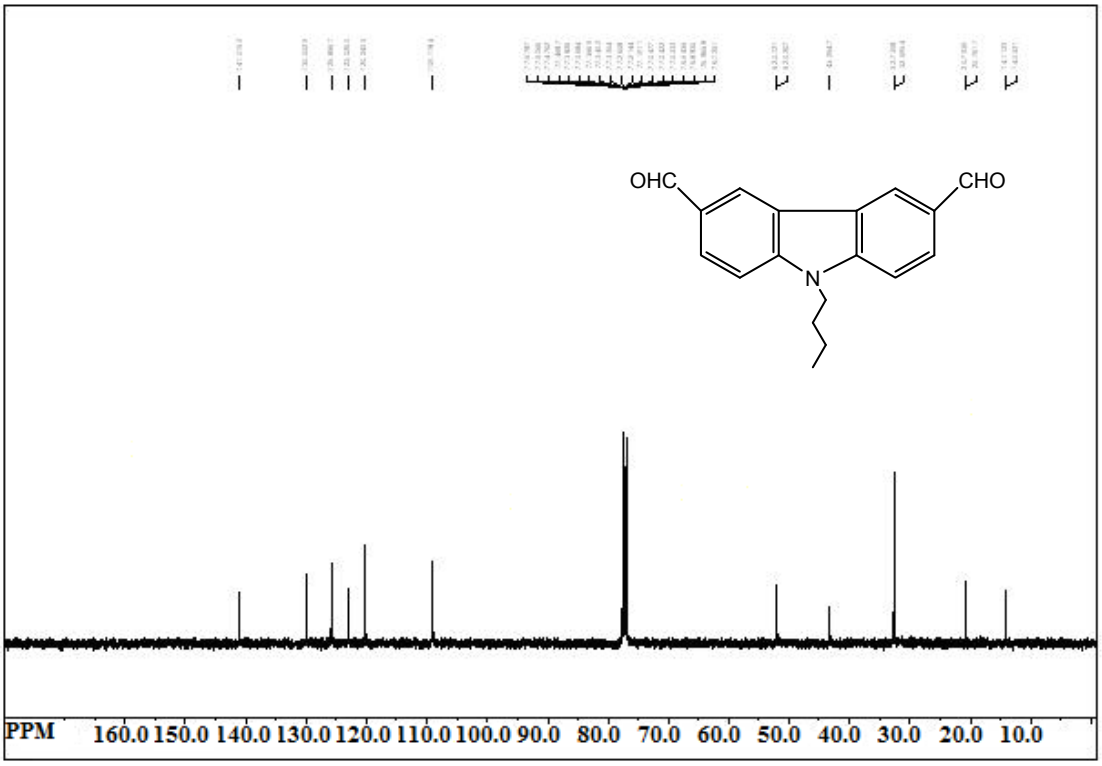


Figure S12. ^{13}C NMR spectrum of compound **2.**

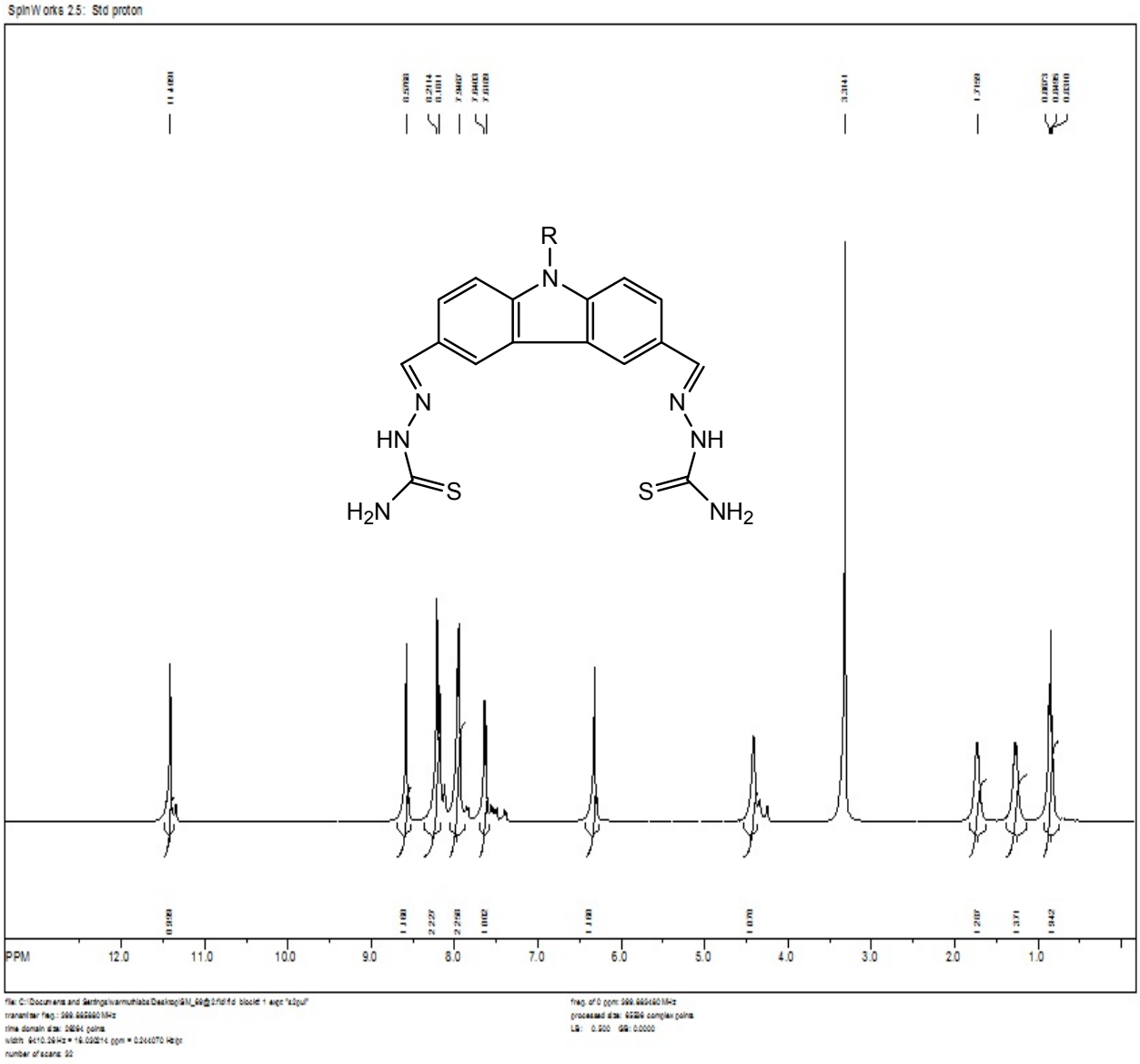


Figure S13. ^{1}H NMR spectrum of compound **3**

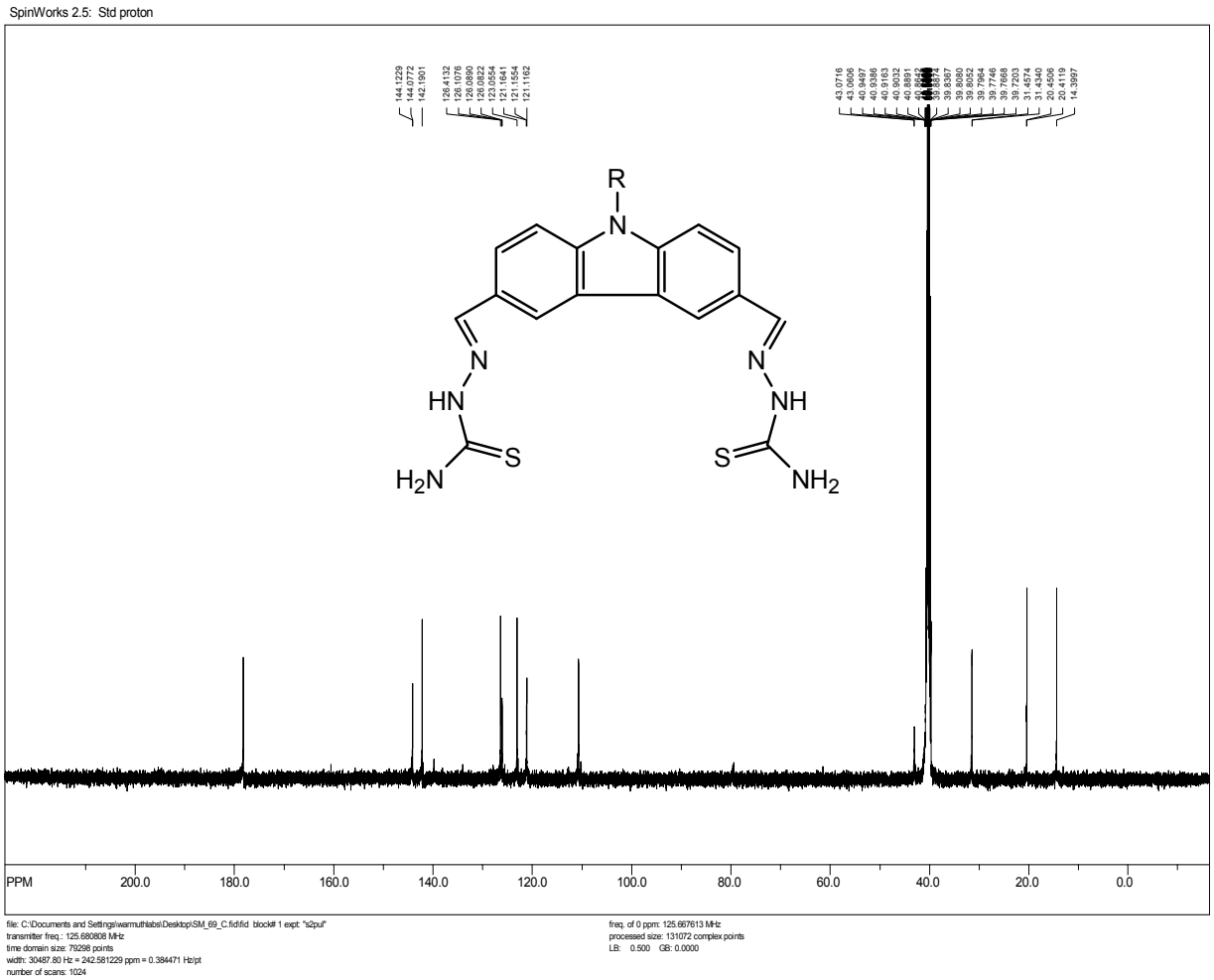


Figure S14. ^{13}C NMR spectrum of compound **3.**

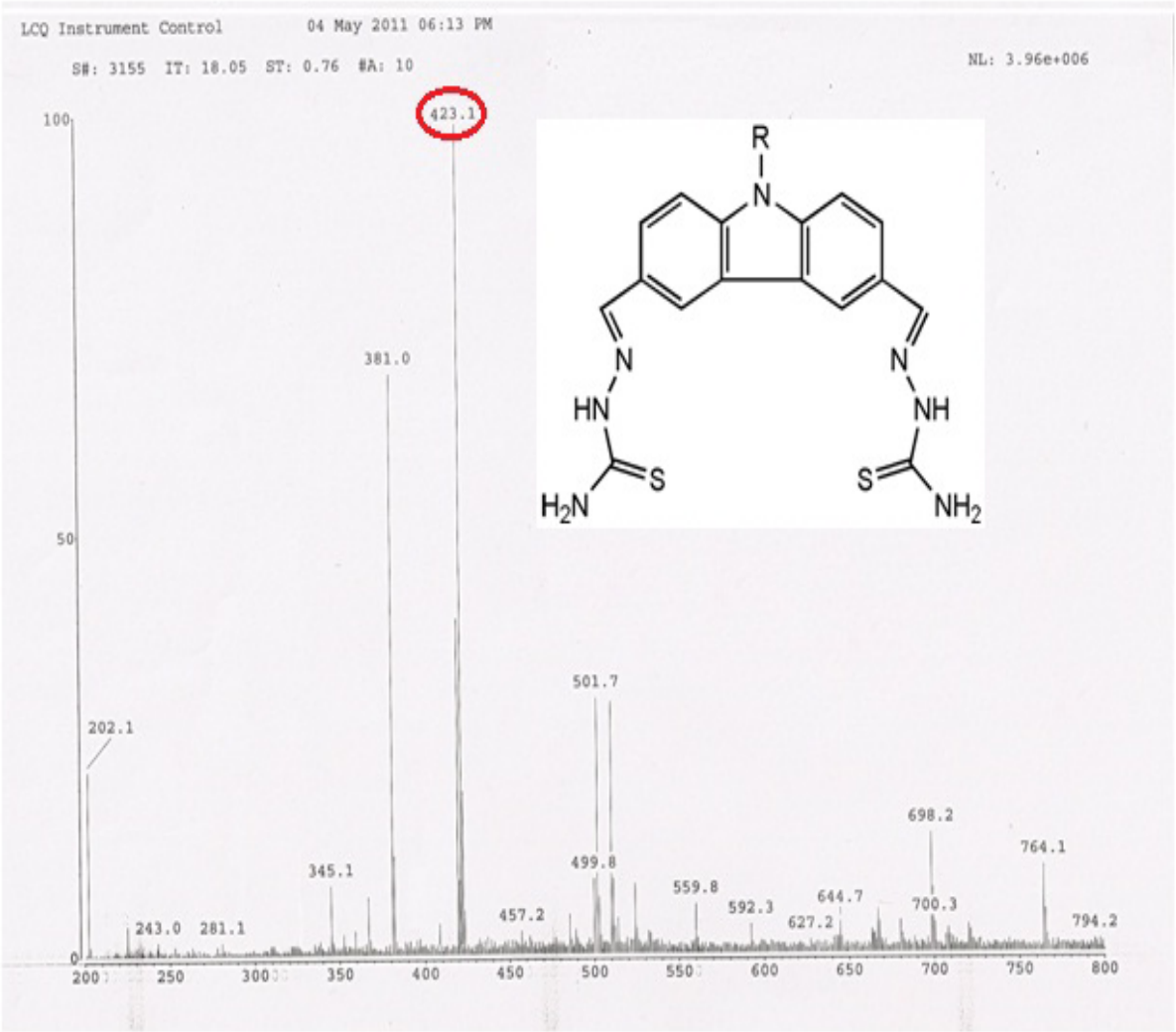


Figure S15. ESI-MS spectrum of Compound **3.**