Supporting information

Manipulation of Monomer-Dimer Transformation of a Heptamethine Cyanine Ligand: Near Infrared Chromogenic Recognition of Hg^{2+}

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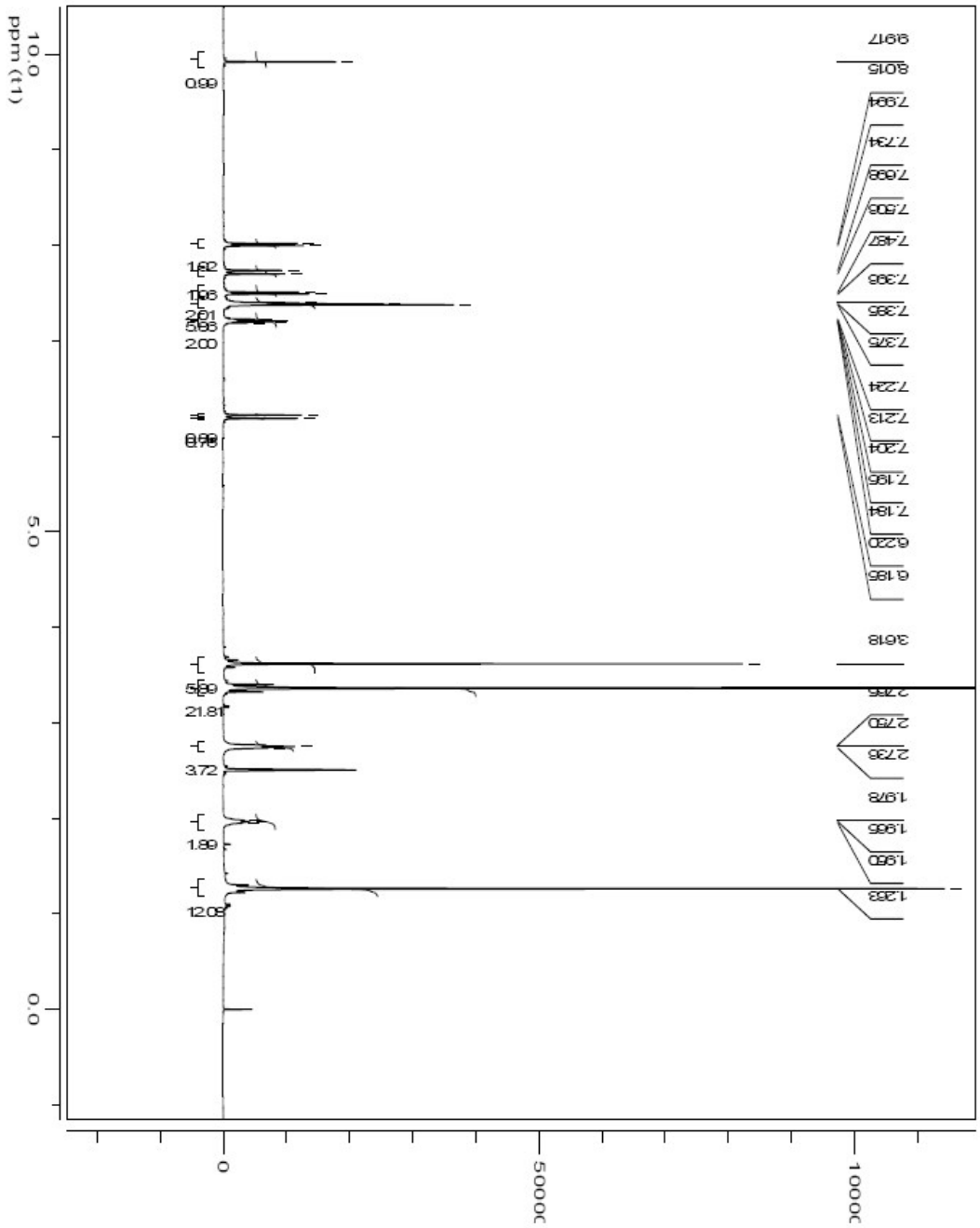

Fig. S1 ^{1}H NMR spectra of compound **2** (d_6-DMSO, 400 MHz). 3.36 (s, H_2O), 2.51(S, DMSO residual peak).

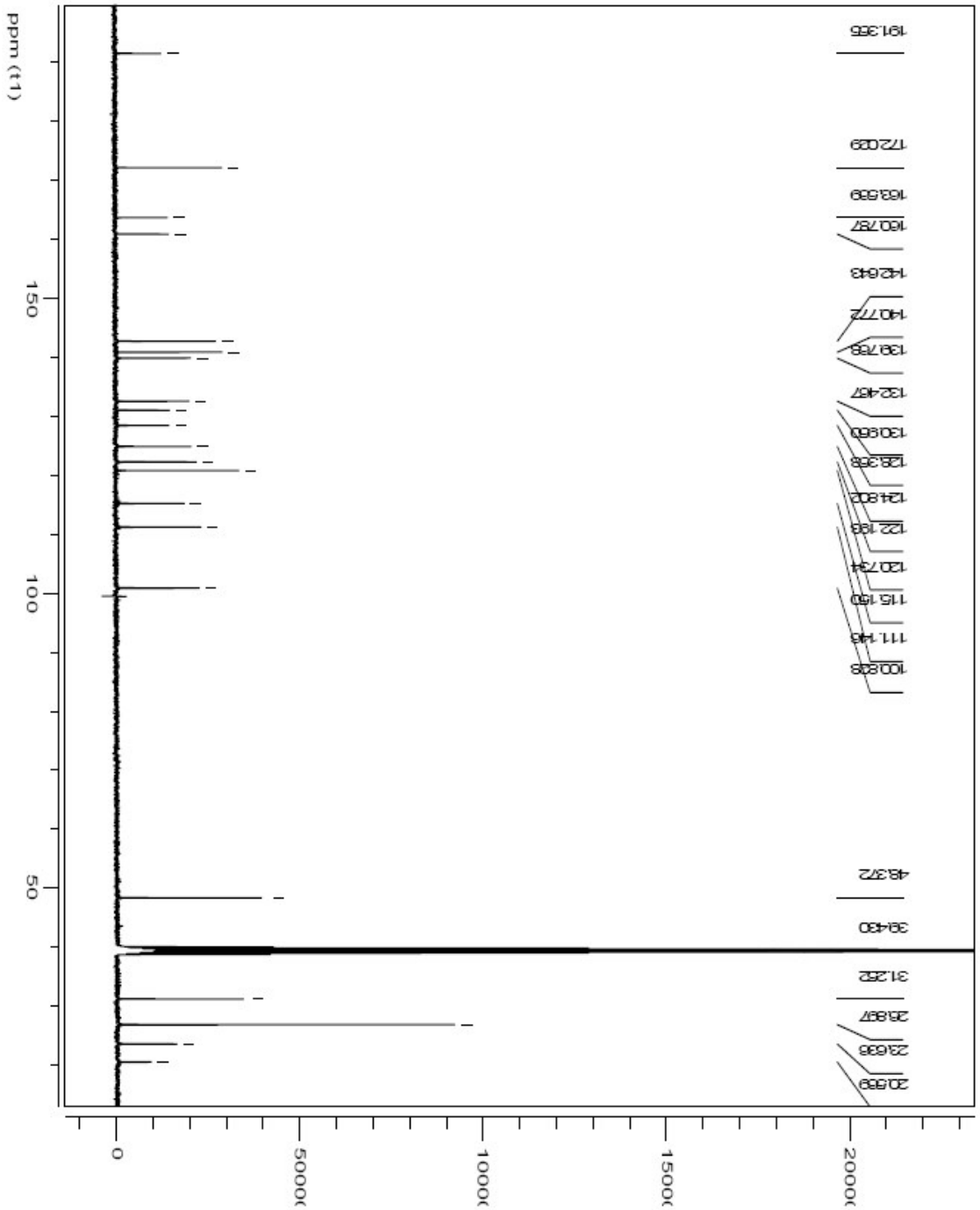

Fig. S2 ^{13}C NMR spectra of compound **2** (d_6-DMSO, 100 MHz)

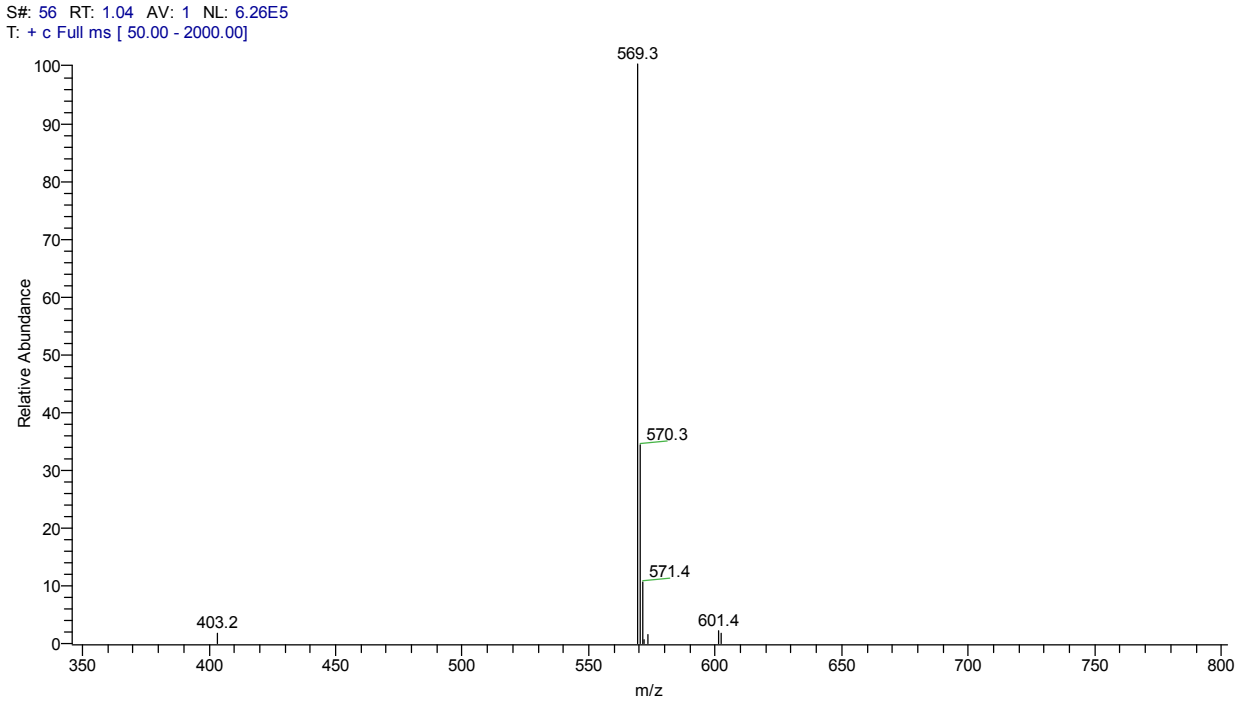

Fig. S3 ESI mass spectra of compound 2.

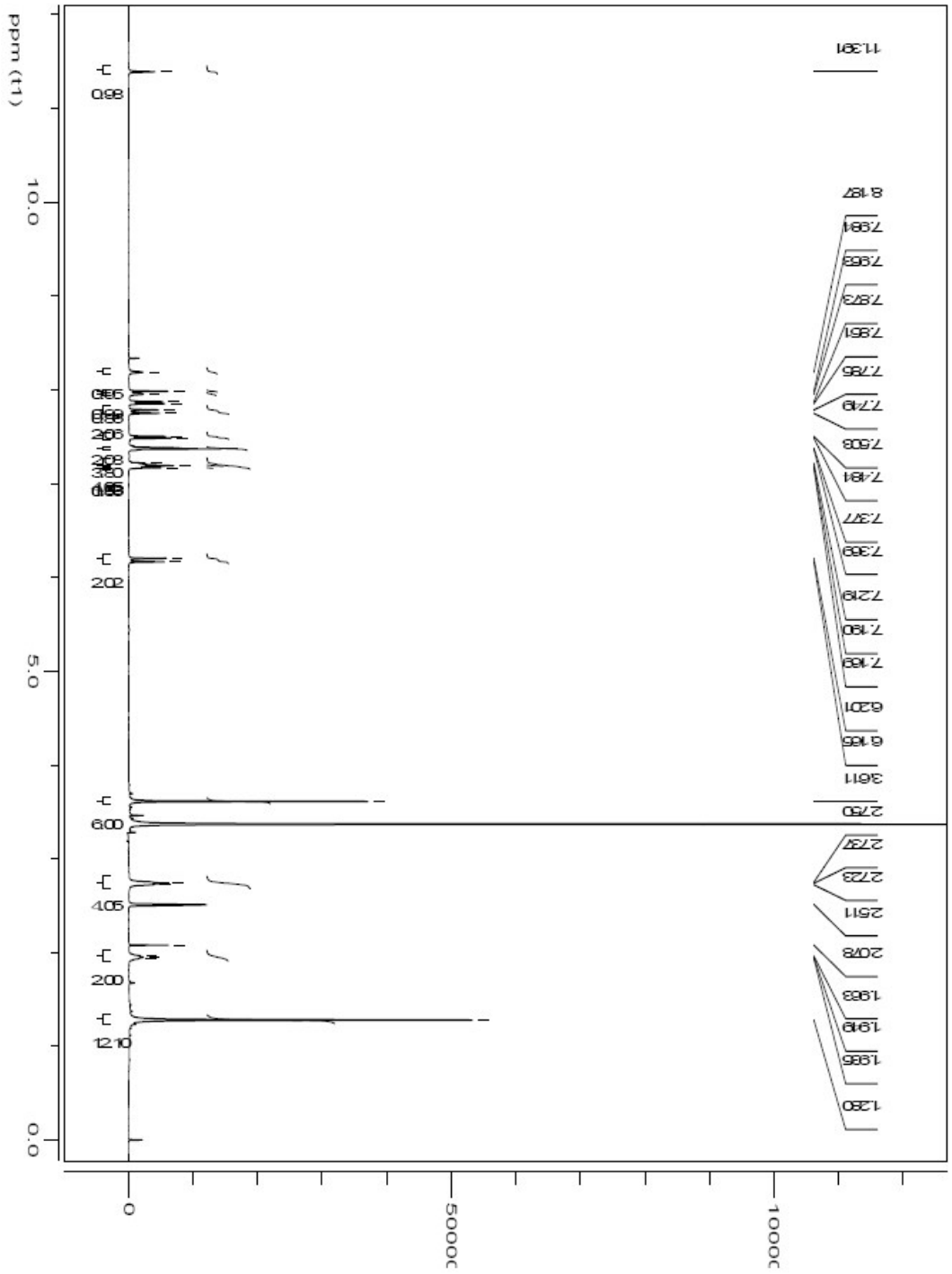

Fig. S4 ^{1}H NMR spectra of **CyL** (d_6-DMSO, 400 MHz). 3.36 (s, H_2O), 2.51(S, DMSO residual peak).

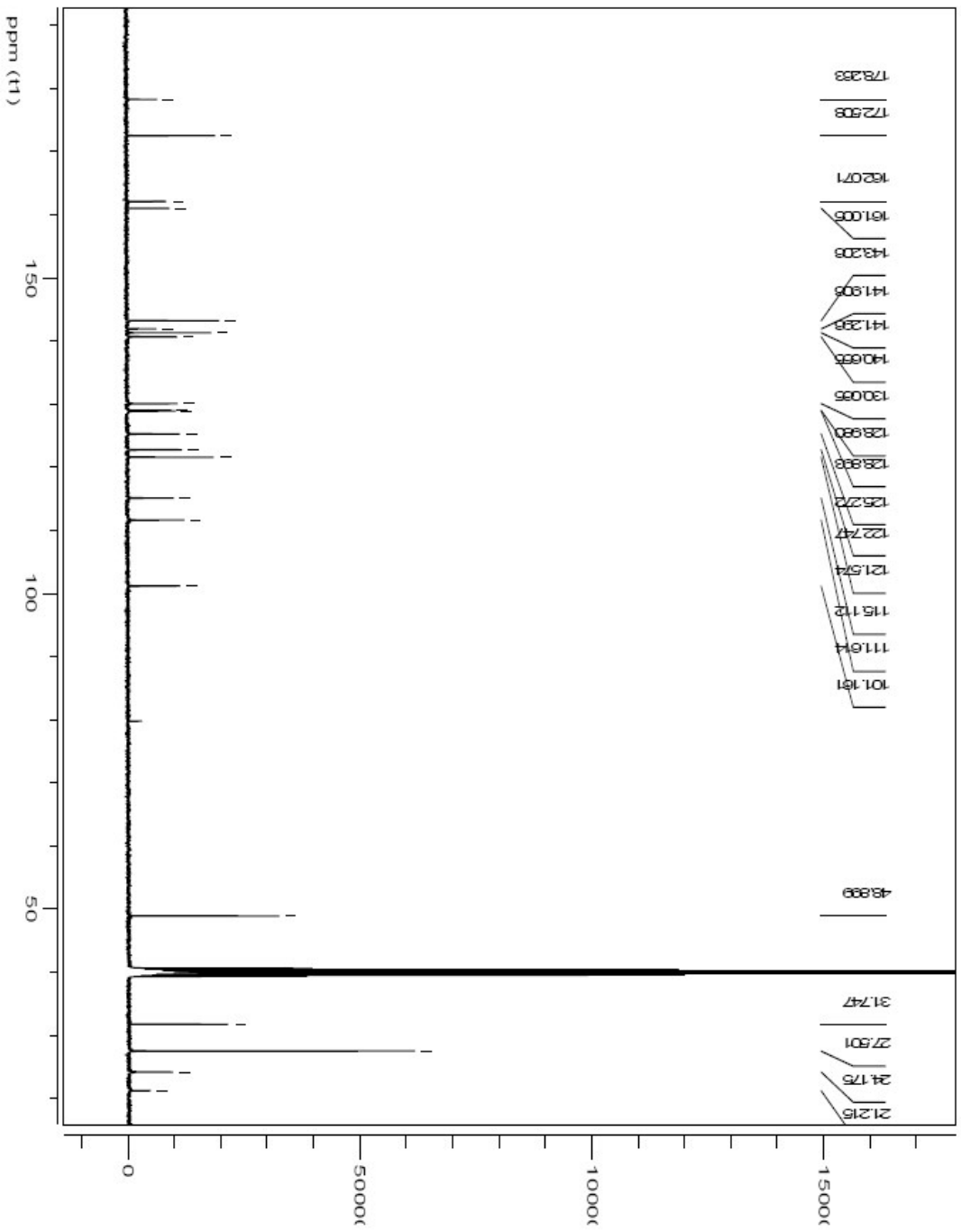

Fig. S5 ^{13}C NMR spectra of **CyL** (d_6-DMSO, 100 MHz)

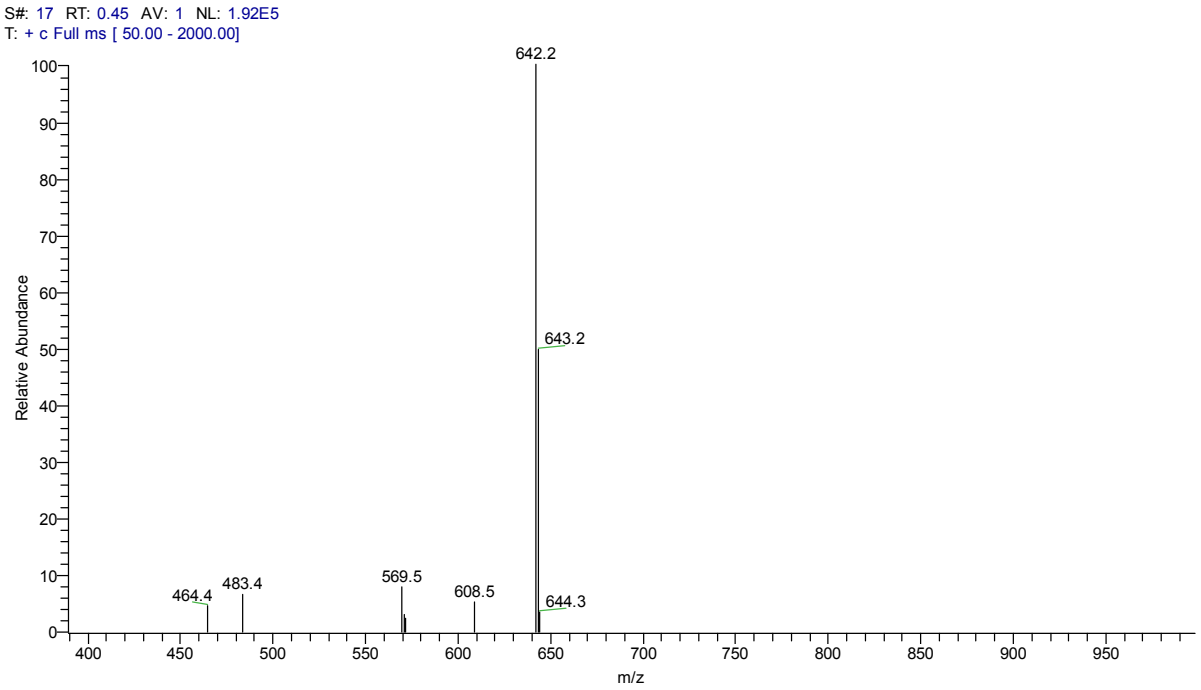

Fig. S6 ESI mass spectra of compound CyL.

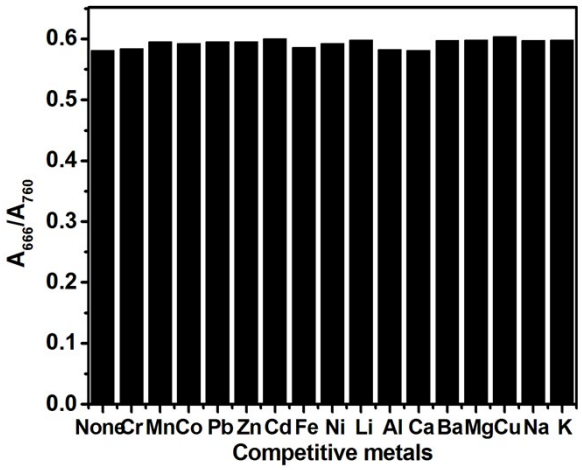

Fig. S7 The absorbance response of **CyL** to Hg^{2+} (1.0×10^{-5} M) in the presence of competitive metal ions (From left to right: no competitive cation(none), Li^{+}(100 equiv.), Na^{+}(100 equiv.), K^{+}(100 equiv.), Cr^{3+}(40 equiv.), Mn^{2+}(40 equiv.), Co^{2+}(40 equiv.), Pb^{2+}(40 equiv.), Zn^{2+}(40 equiv.), Cd^{2+}(40 equiv.), Fe^{3+}(40 equiv.), Ni^{2+}(40 equiv.), Al^{3+}(40 equiv.), Ca^{2+}(100 equiv.), Ba^{2+}(100 equiv.), Mg^{2+}(100 equiv.), Cu^{2+}(20 equiv.).

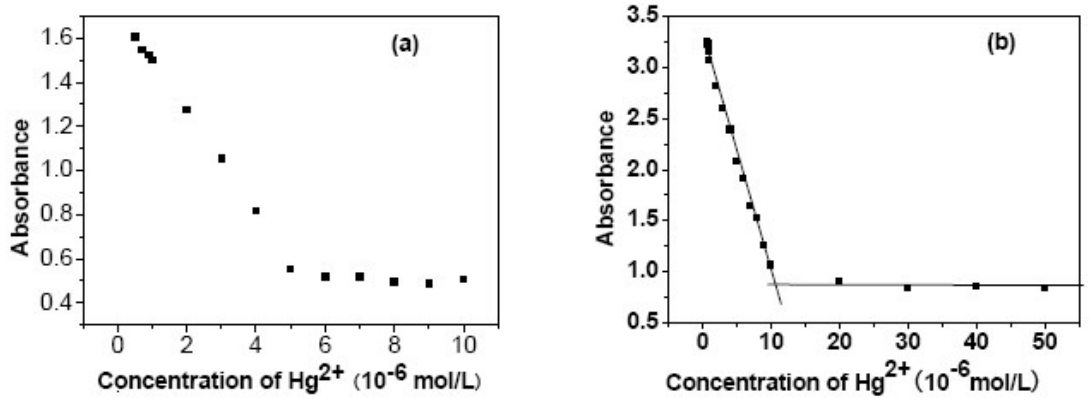

Fig S8 Absorbance titrations of **CyL** with Hg^{2+} in aqueous solution of pH 4.00 at 760 nm. (a) [**CyL**] = 1.0×10^{-5} M ; (b) [CyL] = 2.0×10^{-5} M

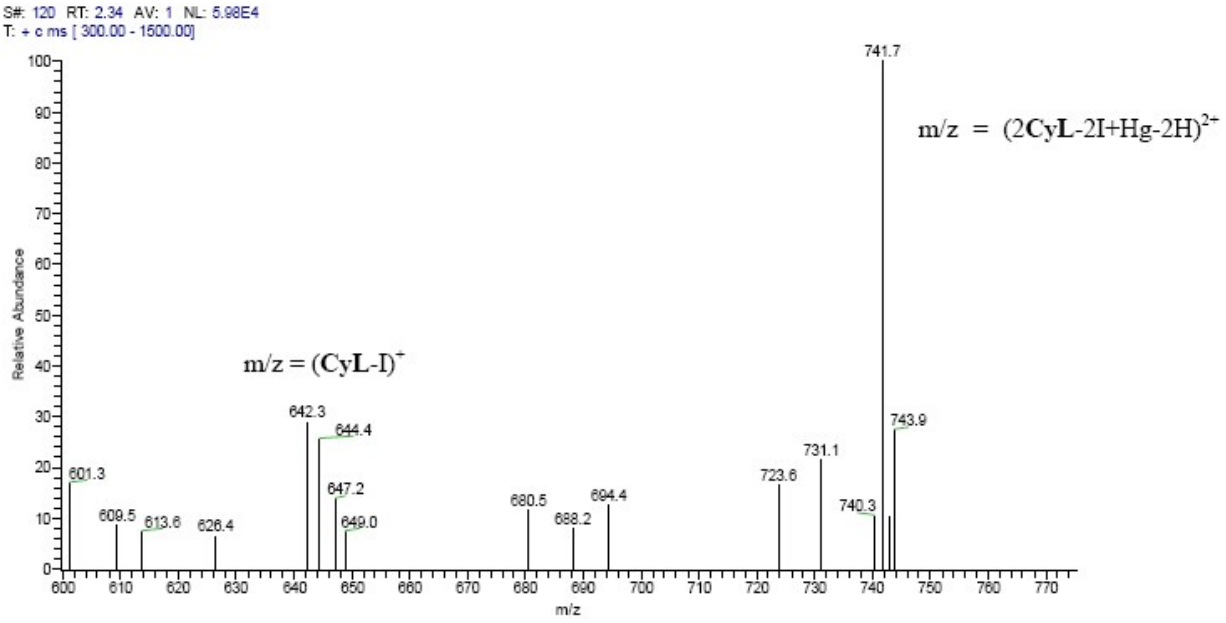

Fig. S9 ESI mass spectra of the reaction products of **CyL** with Hg^{2+} in pH 4.00 acetate buffer solution. m/z (741.7): $[2\mathbf{CyL}\text{-}2I+Hg-2H]^{2+}$ for $Hg(\mathbf{CyL})_2$ complex; m/z (642.3): $[\mathbf{CyL}\text{-}I]^{+}$ for **CyL** monomer.