Supplementary Information

Pyridine-2,6-dicarboxamide-based fluorescent sensor for detection of Fe^{3+} and Hg^{2+}

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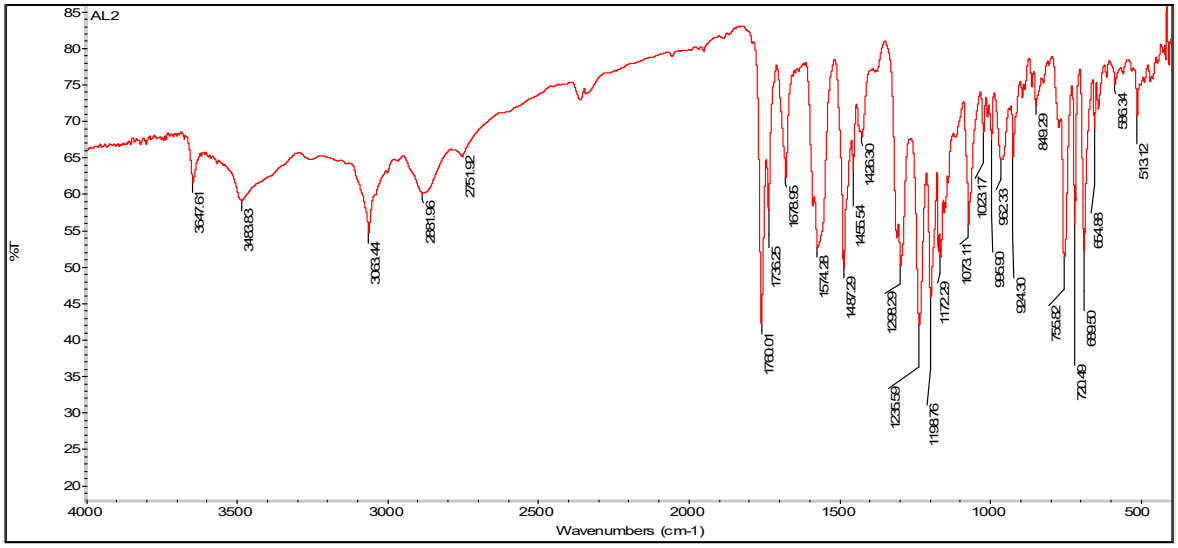

Figure- S1.FT-IR spectra of Ligand

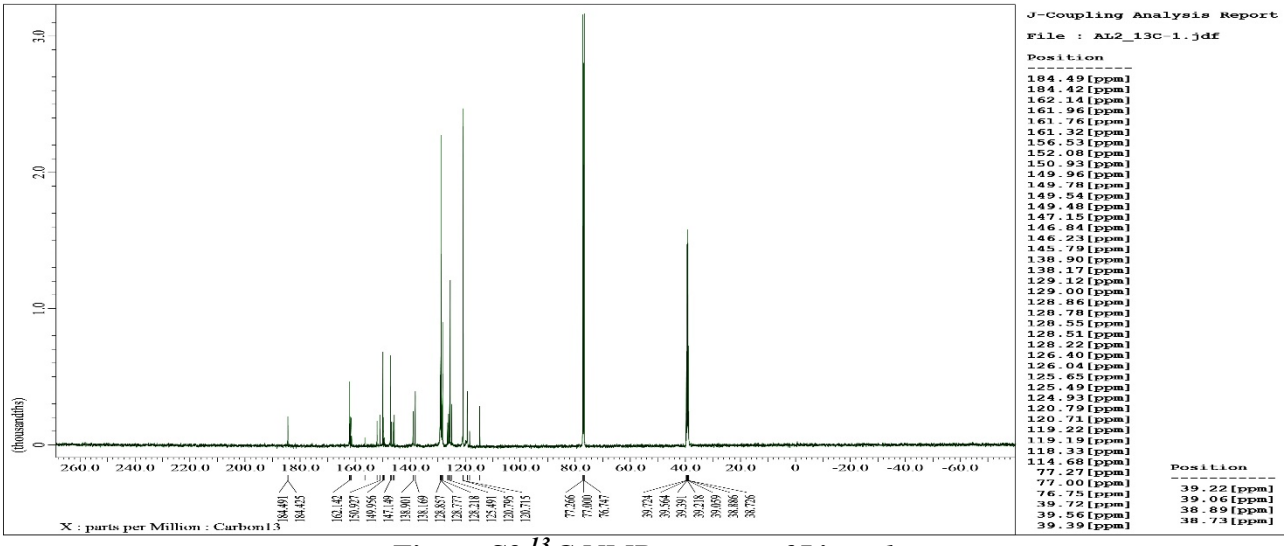

Figure S2.^{13}C NMR spectra of Ligand

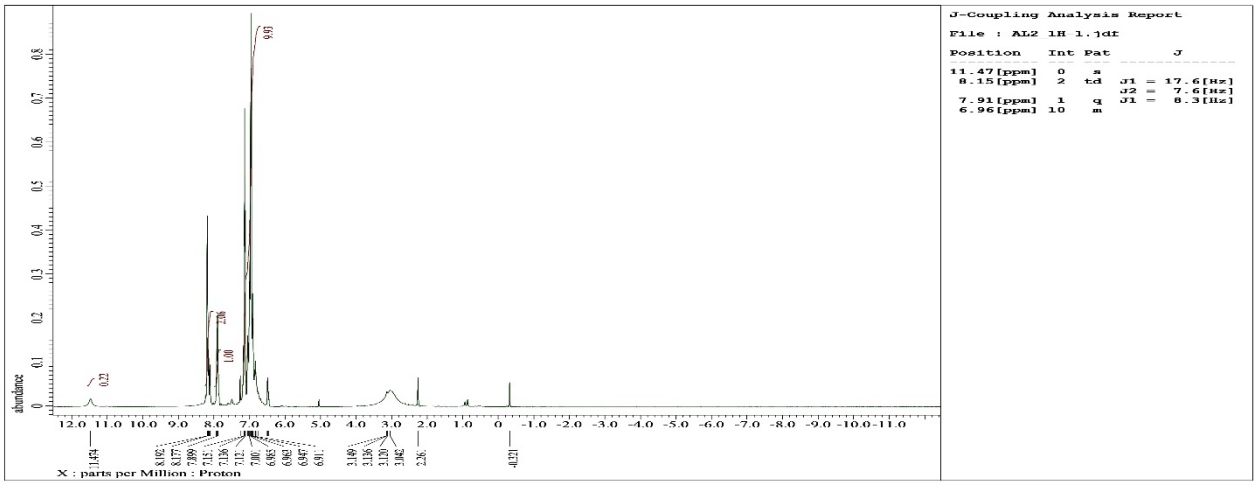

Figure S3. ^{1}H NMR spectra of Ligand

General procedure for drawing Job's plot by fluorescence method:

Stock solution of same concentration of sensor and Fe and Hg were prepared in the order of ≈ 1.0 x 10^{-5} ML^{-1} CH_3OH-H_2O (7:3, v/v, at pH 7.0) media. The fluorescence in each case with different *host–guest* ratio but equal in volume was recorded. Job's plots were drawn by plotting $\Delta I.X_{host}$*vs*. X_{host} (ΔI = change of fluorescence intensity of the spectrum during titration and X_{host} is the mole fraction of the host in each case, respectively).

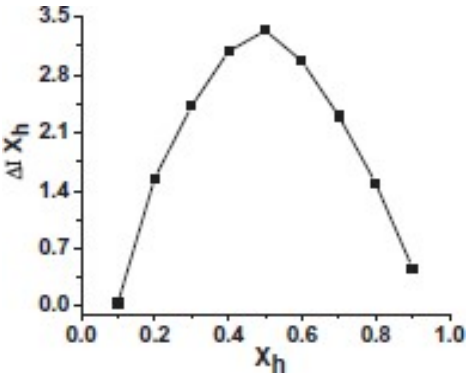

Figure-S4

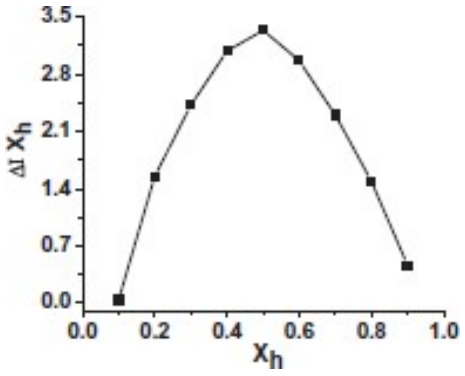

Figure-S5

Figure S4,S5: Job's plot diagram of the (a): Hg^{2+} complex for Ligand; (b): Fe^{+3} complex for ligand determined by fluorescence method in CH_3OH (where X_h is the mole fraction of the host and DI is the change of emission intensity)

1. Determination of Detection Limit:

The detection limit DL of **L** for Fe^{+3} and Hg^{+2} was determined from the following equation[1]:

DL = K* Sb1/S Where K = 2 or ; Sb1 is the standard deviation of the blank solution; Sistheslope of the calibration curve. From the first graph we get slope = -76.38759,and Sb1valueis 12.61. Thus using the formula we get the Detection Limit = 0.49 μM i.e. L can detect Fe^{3+} in this minimum concentration.

From the graph 2 we get slope = 5694.78535, and Sb1 value is 12.61 Thus using the formula we get the Detection Limit = 0.0066 μM i.e. L can detect Hg^{2+} in this minimum concentration

2. Determination of Binding and Association constant:

The spectra of these solutions were recorded by means of fluorescence methods. Binding constant was calculated according to the Benesi-Hildebrand equation. *Ka*was calculated following the equation stated below.

$1/(F-Fo) = 1/\{K(Fmax–Fo)\ [Cu^{2+}]n\} + 1/[Fmax-Fo]$

$1/(F-Fo) = 1/\{K(Fmax–Fo)\ [F^{-}]n\} + 1/[Fmax-Fo]$

Here Fo is the fluorescence of ligand in the absence of metal ions, F is the fluorescence recorded in the presence of added metal ions, Fmax is fluorescence in the presence of added $[Fe^{3+}]$ max, and $[Hg^{+2}]$max, K is the association constant (M-1). The association constant (Ka) could be determined from the slope of the straight line of the plot of 1/(F-Fo) against $1/[Fe^{3+}]n$ and $1/[Hg^{+3}]n$ respectively. The association constant (*Ka*) as determined by the Fluorescence titration method for sensors with Fe^{3+} and Hg^{+2} is found to be 2.54×10^{1} M^{-1} and $0.18x10^{2}$ M^{-1} respectively.

Table-S1 XRD peaks data of Ligand

Peak position(2 theta)	Theta(radian)	FWHM	FWHM(radians)	β cosθ	4 sin θ
10	0.087266	0.0648	0.001130973	0.001127	0.348623
17	0.148353	0.0611	0.001066396	0.001055	0.5912376
18	0.15708	0.0606	0.00105767	0.001045	0.6257379
19	0.165806	0.0601	0.001048943	0.001035	0.6601904
21	0.18326	0.0591	0.00103149	0.001014	0.7289421
25	0.218166	0.0572	0.000998328	0.000975	0.8657585
26	0.226893	0.0568	0.000991347	0.000966	0.8998042
28	0.244346	0.0559	0.000975639	0.000947	0.9676876
29	0.253073	0.0555	0.000968658	0.000938	1.00152
40	0.349066	0.0518	0.000904081	0.00085	1.3680806
80	0.698132	0.0604	0.001054179	0.000808	2.5711504

Table -S2 P-XRD peaks data of Complexes

2 theta	Theta (radian)	FWHM	FWHM (Radian)	B Cos theta	4 sin theta
14.9986	0.130887477	0.8757	0.015283848	0.015153117	0.522056318
16.1593	0.141016495	1.1404	0.019903735	0.019706163	0.562198368
18.2975	0.15967581	0.81252	0.014181149	0.014000749	0.635992596
18.4604	0.161097381	0.1426	0.00248884	0.002456614	0.641605898
22.7164	0.198237987	4.2357	0.073926911	0.072479061	0.787768533
22.859	0.199482407	0.1222	0.002132792	0.002090498	0.792648114
26.4837	0.231113882	0.57686	0.010068106	0.009800414	0.916247724
27.339	0.238577782	0.8349	0.014571754	0.01415901	0.945283729
29.0495	0.253504711	1.52192	0.026562515	0.025713561	1.003192762
32.2873	0.281759846	3.2175	0.056155969	0.053941604	1.112186116
34.2626	0.29899759	1.9549	0.034119442	0.032605638	1.178249679
35.9324	0.313569344	1.6494	0.028787461	0.027383745	1.233823569
38.7018	0.337736918	2.7491	0.047980846	0.045270263	1.325410836
46.1753	0.402955509	6.99819	0.122141457	0.112358665	1.568555367
50.7775	0.44311728	4.49848	0.078513287	0.070930435	1.715031023
77.4741	0.676089065	2.72566	0.047571741	0.037107192	2.502988746
82.2799	0.718027582	0.14234	0.002484302	0.00187094	2.631602059