Supporting Information

New Chemodosimetric Probe for the Specific Detection of Hg^{2+} in Physiological Condition and its Utilisation for Cell Imaging Studies

Sukdeb Saha,[b,c] Hridesh Agarwalla,[a,b] Horiom Gupta,[b] Mithu Baidya,[d] Sudip Kumar Ghosh[d]* and Amitava Das[a,b]*

[a] CSIR-National Chemical Laboratory, Organic Chemistry Division, Pune: 411008, Maharashtra, India; E-Mail: a.das@ncl.res.in
[b] CSIR-Central Salt & Marine Chemicals Research Institute,Bhavnagar-364002, Gujarat, India
[c] AcSIR-Central Salt & Marine Chemicals Research Institute,Bhavnagar-364002, Gujarat, India
[d] Indian Institute Technology, Kharagapur, West Bengal-721302, India

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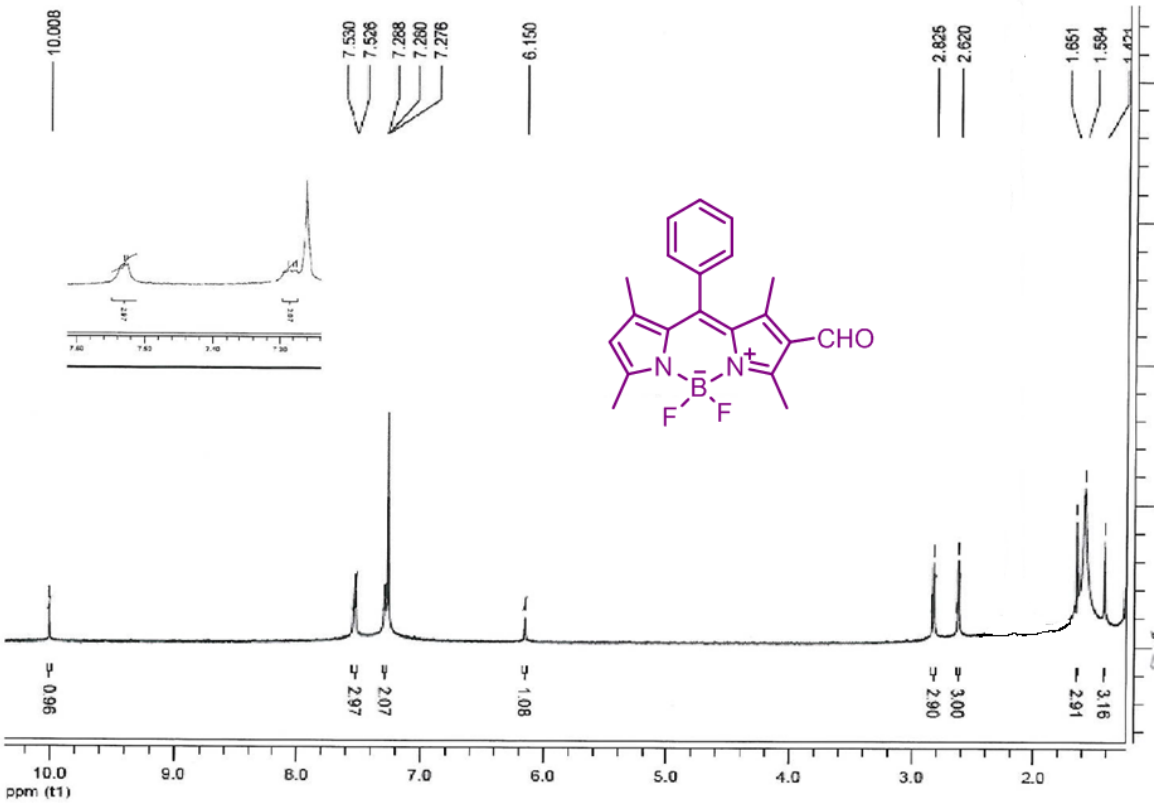
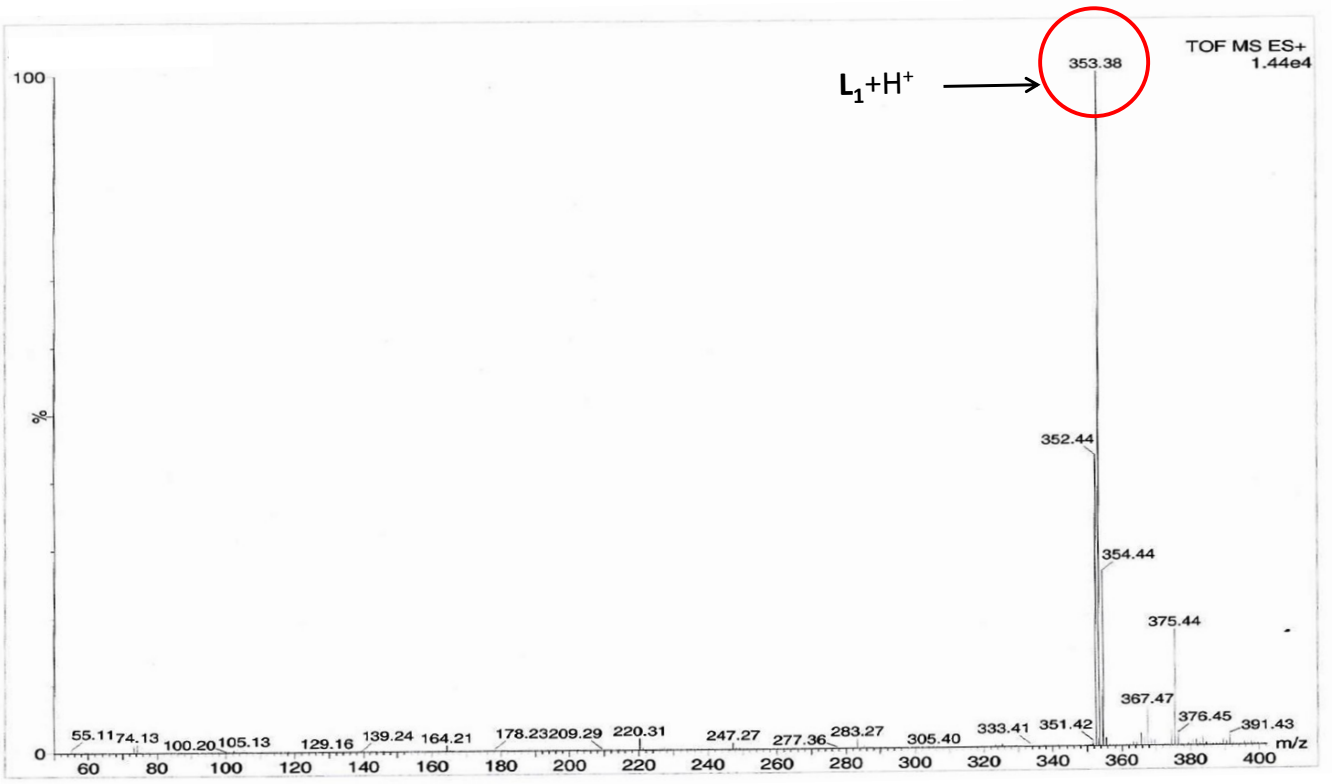
^{1}H NMR spectra of L_1 in $CDCl_3$:



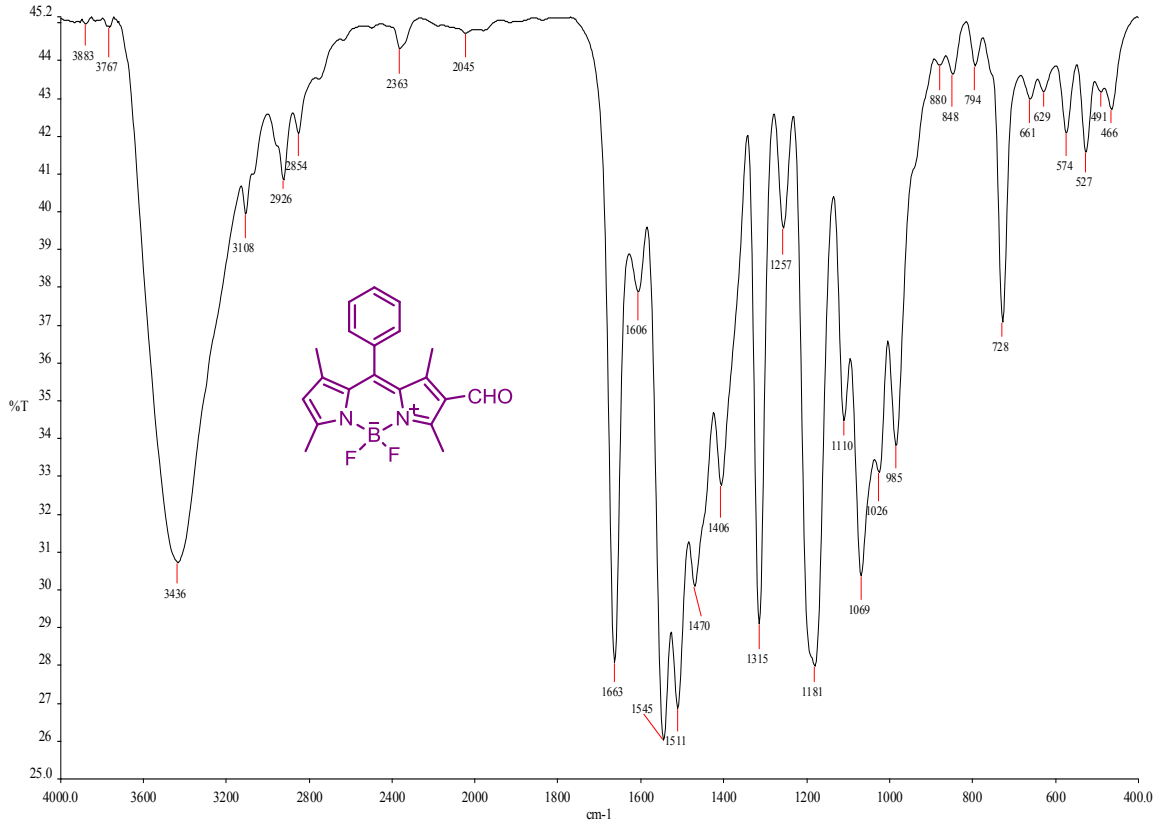
SI Figure 1: ^{1}H NMR spectra of **L_1** in $CDCl_3$.

ESI-MS spectra of L_1:



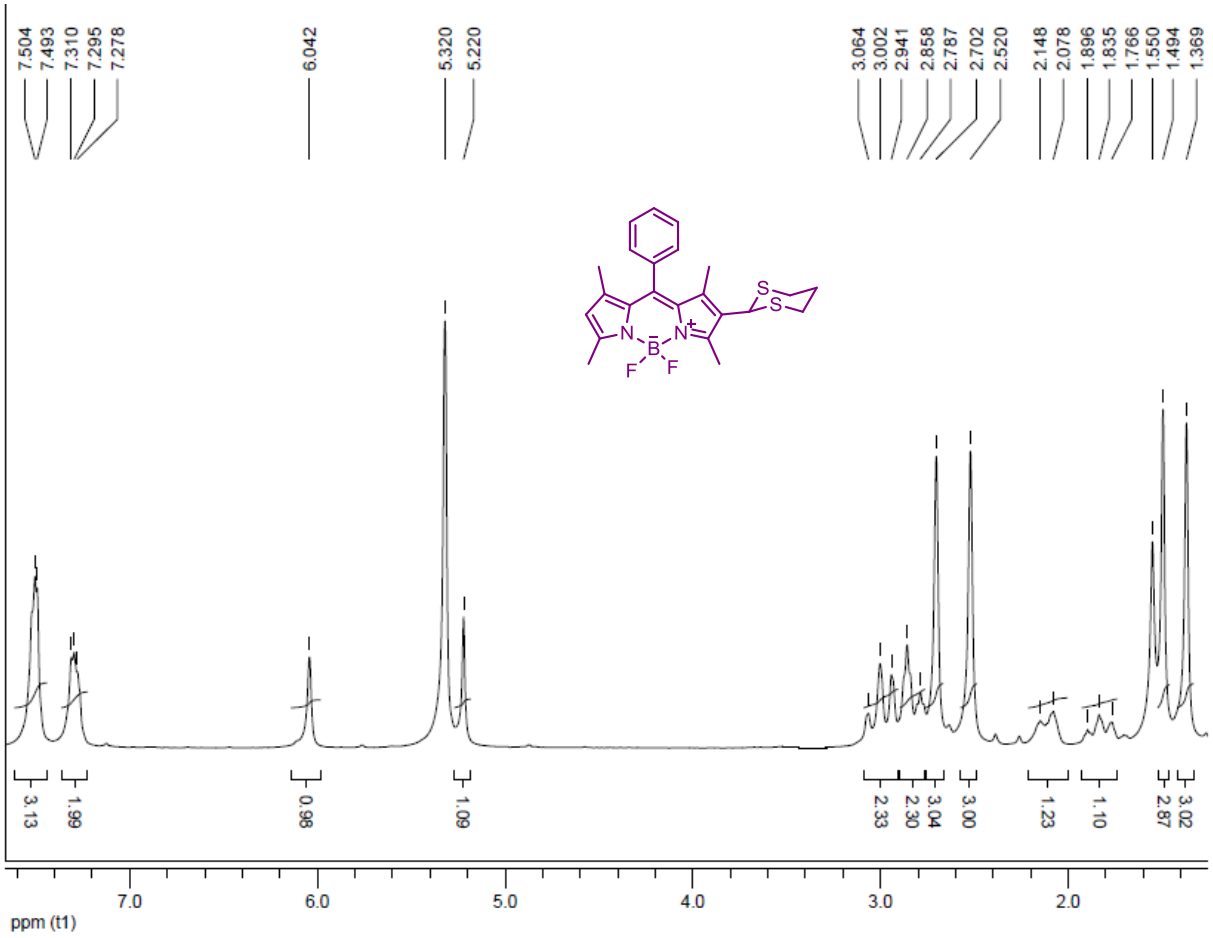
SI Figure 2: ESI-MS spectra of L_1.

FTIR spectra of L_1 :



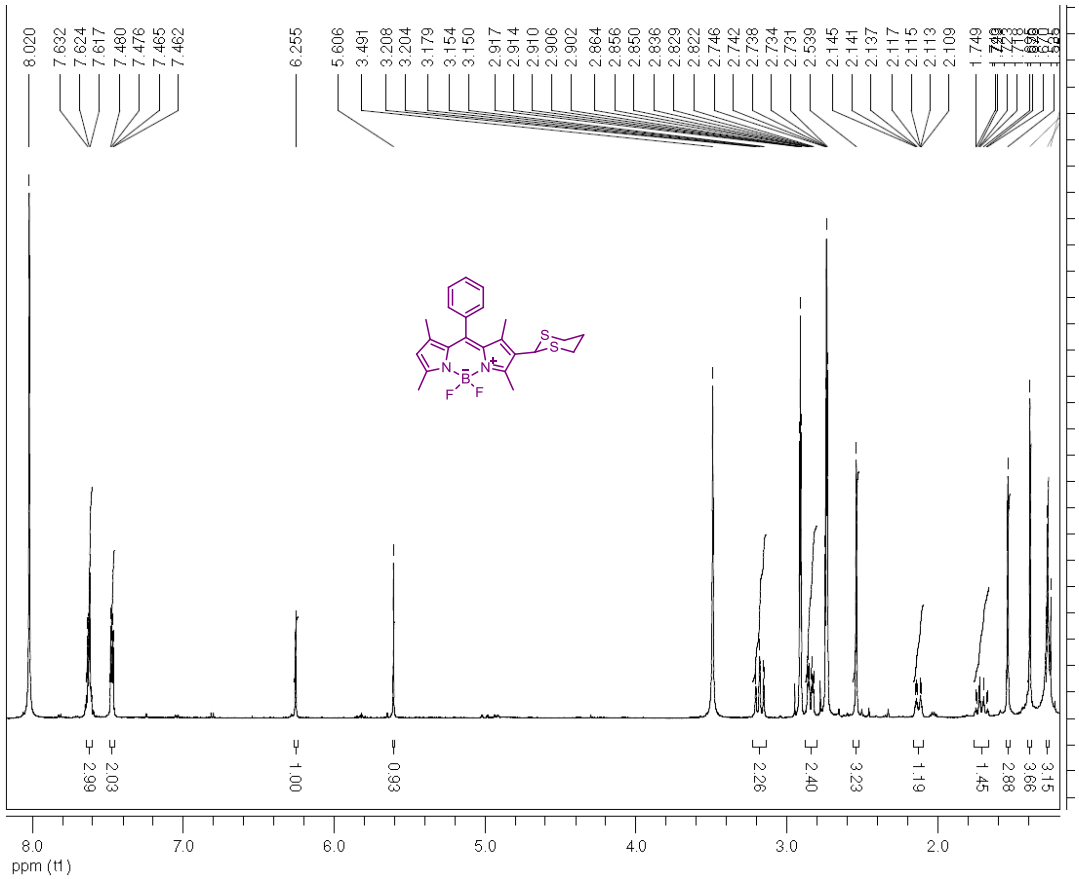
SI Figure 3: FTIR spectra of L_1.

^{1}H NMR spectra of L_2 in CD_2Cl_2:



SI Figure 4: ^{1}H NMR spectra of **L_2** in CD_2Cl_2.

^{1}H NMR spectra of L_2 in DMF-d_7:



SI Figure 5: ^{1}H NMR spectra of **L_2** in DMF-d_7.

^{13}C NMR spectra of L_2 in $CDCl_3$:

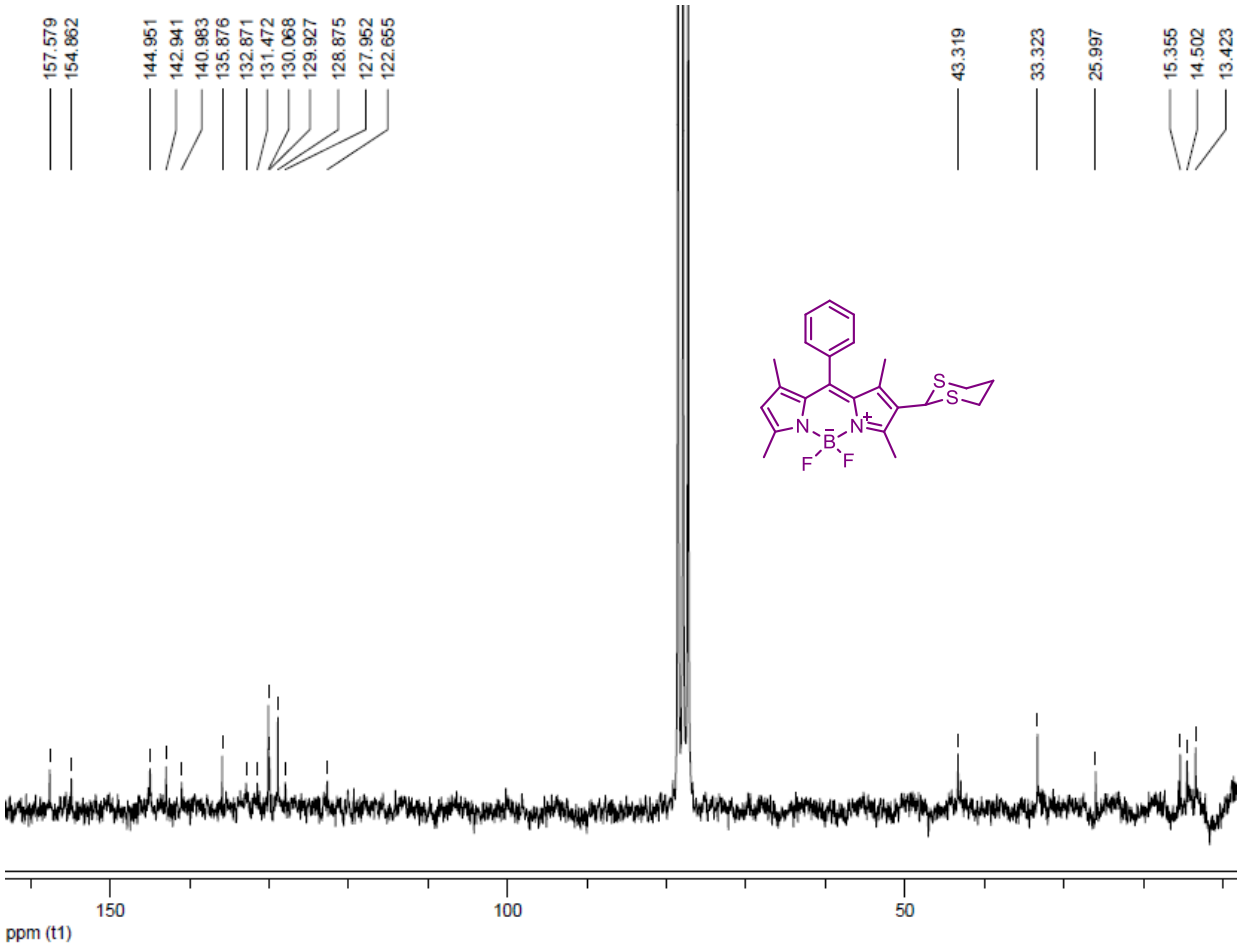
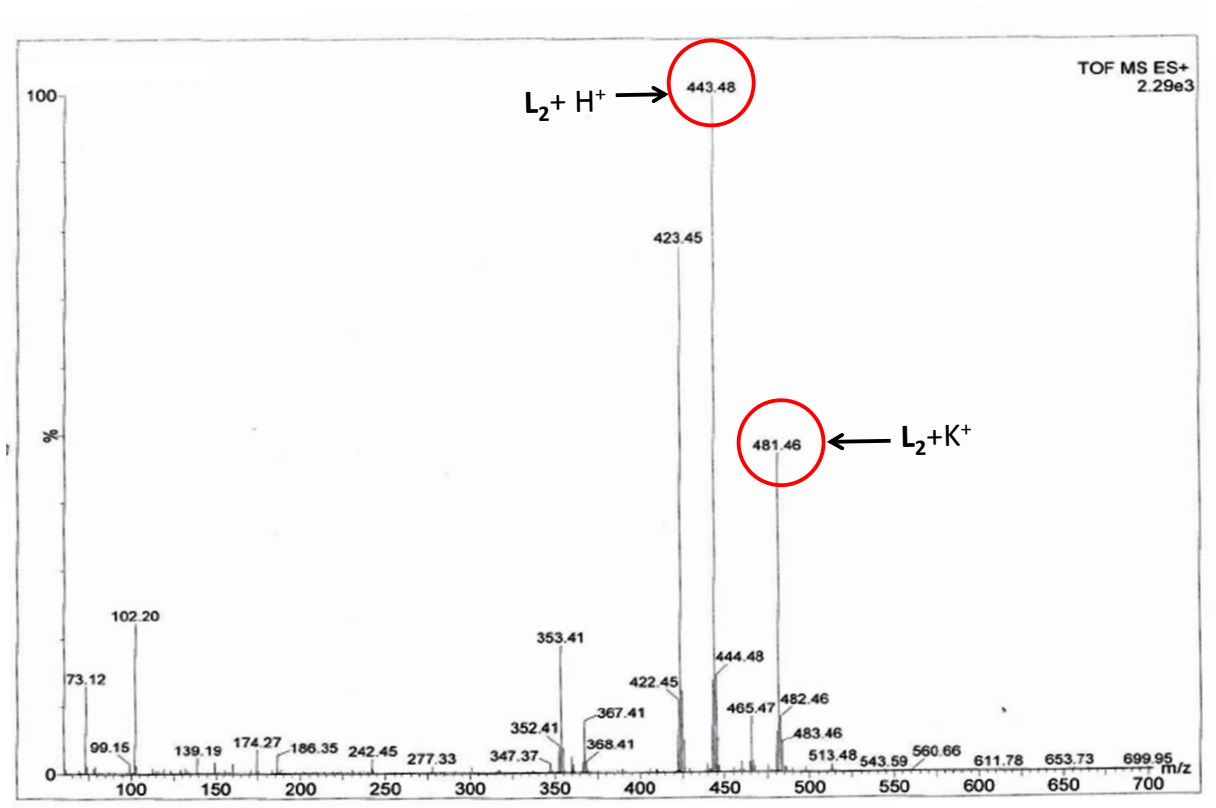


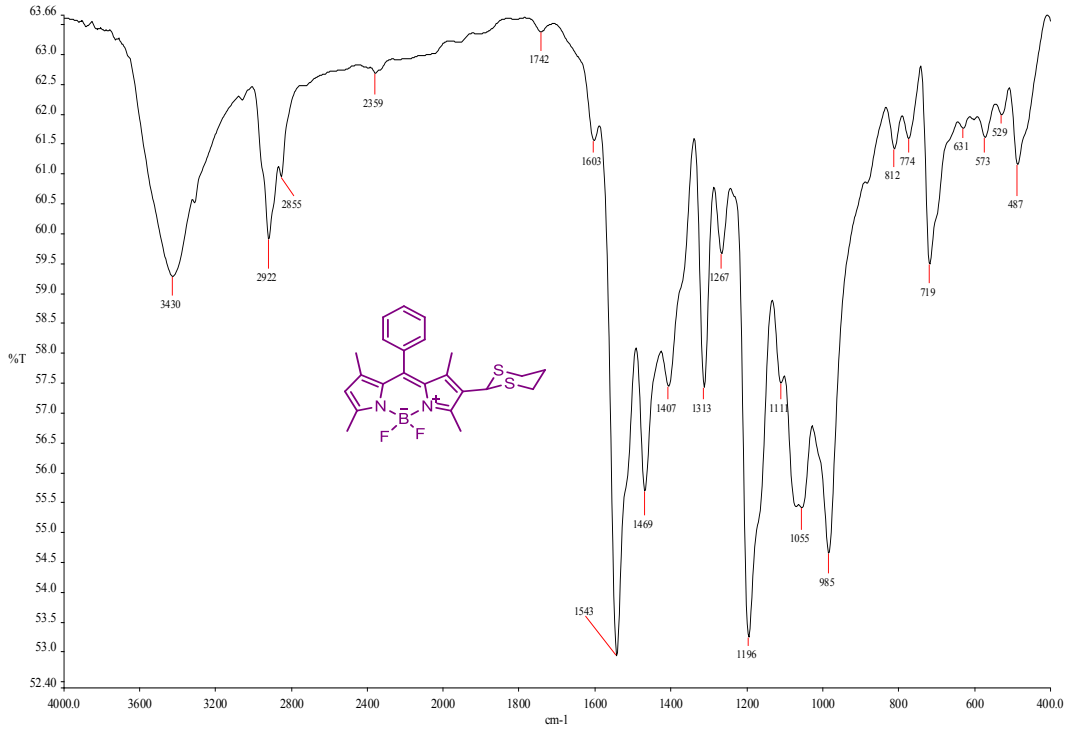
Figure 6: ^{13}C NMR spectra of **L_2** in $CDCl_3$.

ESI-MS spectra of L_2:



SI Figure 7: ESI-MS spectra of L_2.

FTIR spectra of L_2:



SI Figure 8: FTIR spectra of L_2.

ESI-MS spectra of L_2 in presence of Hg^{2+}:

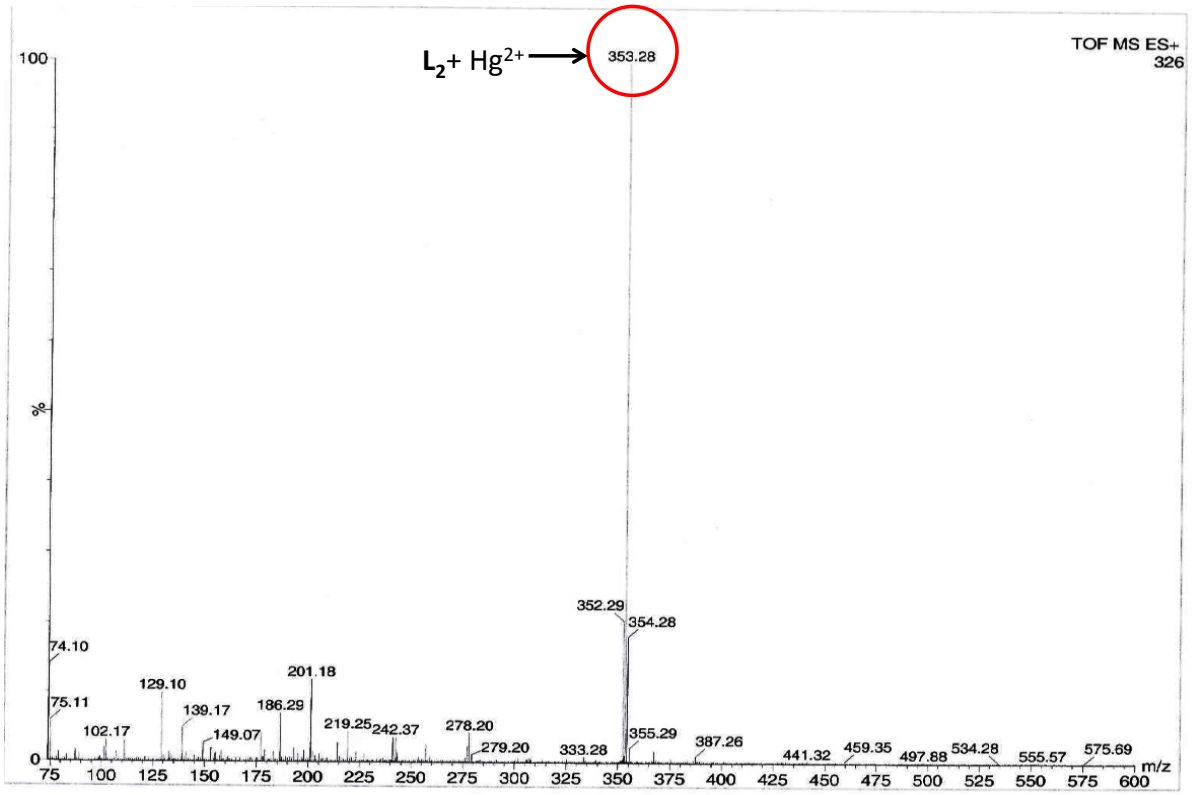


Figure 9: ESI-Ms spectra of L_2 in presence of Hg^{2+} showing the reappearance of L_1 mass peak.

Crystal Data and Refinement Parameters for Compound L_2:

Table S1

Identification code	**Compound1**
Chemical formula	$C_{23}H_{25}BF_2N_2S_2$
Formula weight	442.38
Crystal Colour	orange
Crystal Size (mm)	0.23x0.10 x 0.04
Temperature (K)	150(2)
Crystal System	orthorhombic
Space Group	Pbca
a(Å)	12.572(3)
b(Å)	18.211(5)
c(Å)	19.677(5)
α(°)	90
β(°)	90
γ (°)	90
Z	8
V(Å^3)	4505.1(19)
Density (Mg/m^3)	1.304
Absorption Coefficient(mm^{-1})	0.265
F(000)	1856
Reflections Collected	19526
Independent Reflections	3531
$R_{(int)}$	0.0940
Number of parameters	285
S(Goodness of Fit) on F^2	1.106
Final R1/wR2 (I>2σ(I)	0.0974/ 0.1981
Weighted R1/wR2(all data)	0.1515/ 0.2235
CCDC Number	921458

Change in 1H NMR Spectra of L_2 upon addition of Hg^{2+} ions in CD_3CN medium

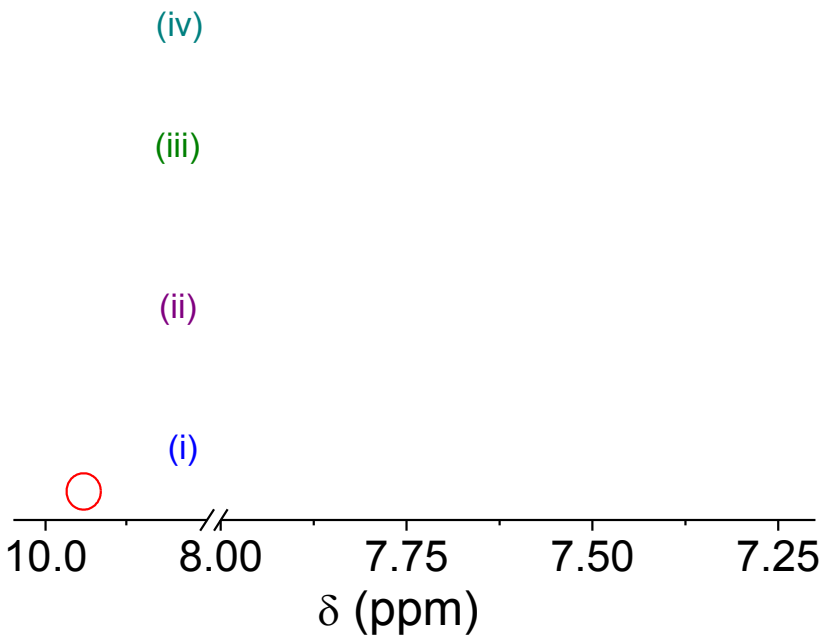


Figure 10: A plot of change in ^1H NMR spectral pattern for the receptor (i) **L_2**; (ii) **L_2** with 0.25 equivalents Hg^{2+}; (iii) **L_2** with 0.5 equivalents Hg^{2+} and (iv) **L_2** with 1 equivalent Hg^{2+} in CD_3CN medium.

2D-ROESY NMR spectra for L_2 in presence of β-CD in DMF-d_7 solvent:

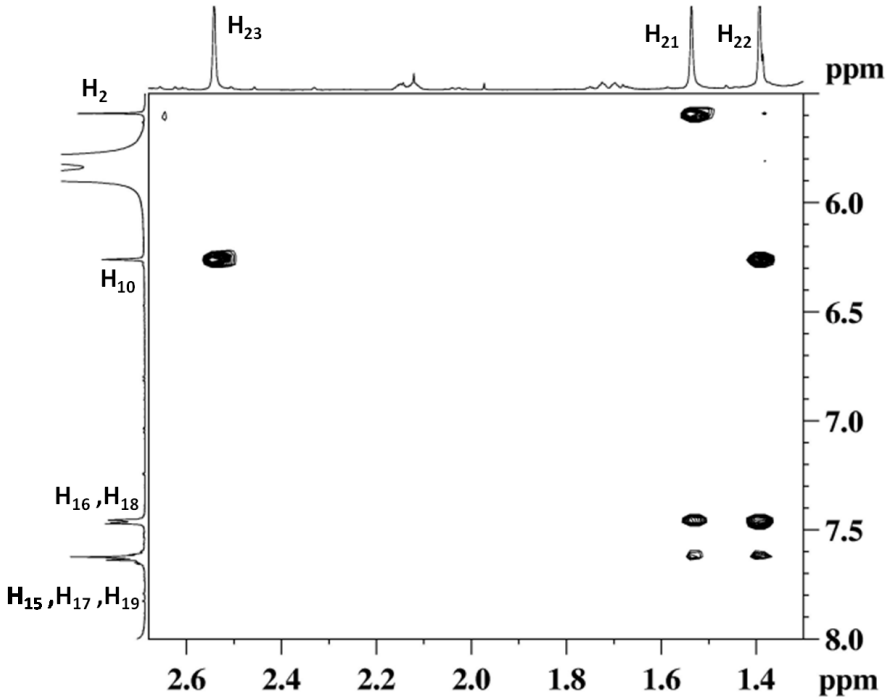


Figure 11: 2D-ROESY NMR showing interaction of Methyl protons (H_{21}, H_{22}) with aromatic protons and nearby protons (H_2 and H_{10}).

Time dependent spectrophotometry study of L_2 in presence of Hg^{2+}:

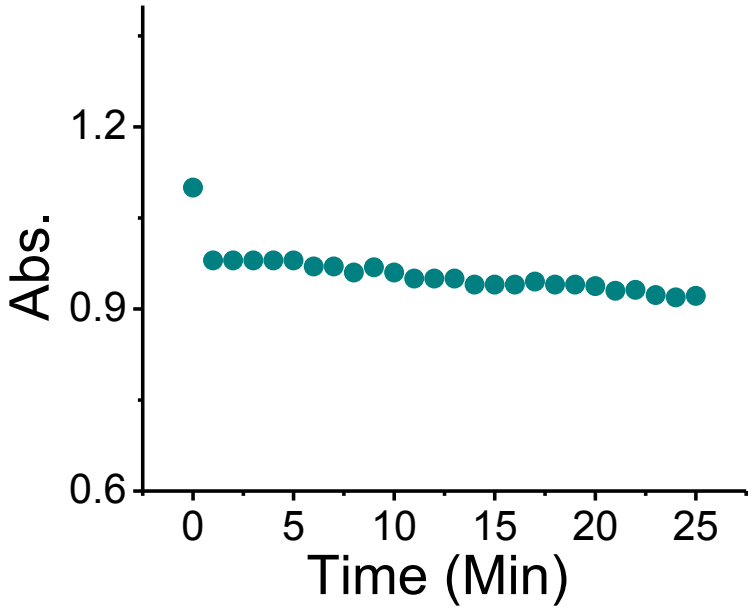


Figure 12: Time dependent absorption spectra of $\mathbf{L_2}$ (1.0×10^{-5} M) in presence of Hg^{2+} (2.8×10^{-5}M) in Acetonitrile/ HEPES buffer medium (3:2, v/v, pH 7.1) over a period of 25 min showing instant conversion of $\mathbf{L_2}$ into $\mathbf{L_1}$.

Hg^{2+} Concentration dependent plot of the absorption titration data of L_2 in Acetonitrile/ HEPES buffer medium in presence of β-CD:

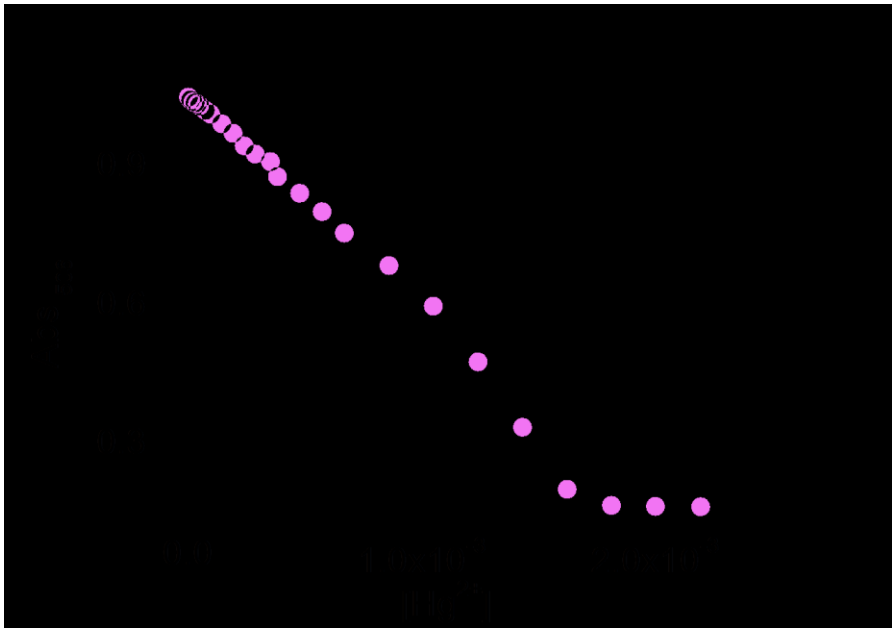


Figure 13: Change in absorption value of **L_2** at 506 nm with changing the [Hg^{2+}].

MTT Assay for the measuring of the Cytotoxicity of Chemodosimeter L_2 to HeLa cells:

Cytotoxicity of **L_2** on HeLa cells was determined by conventional MTT assay (*J. Natl. Cancer Inst.,* **1990,** *8,* 1113-1117). HeLa cells in their exponential growth phase were trypsinised and seeded in 96-well flat-bottom culture plates at a density of 3 x 10^3 cells per well in 100 µl DMEM complete medium (Himedia, India). The cells were allowed to adhere and grow for 24 hr at 37 ºC in CO_2 incubator (New Brunswick Scientific, U.S.A.), and then the medium was replaced with 100 µl fresh incomplete medium containing various concentrations of **L_1** (0 to 5 µM). The assay was performed in quadruplet for each concentration. Cells were then incubated for 6h, after which the culture medium was removed, and 100 µl of 1 mg/ml MTT reagent in PBS was added to each well. Thereafter, it was incubated for 4 hrs; during this period active mitochondria of viable cells reduce MTT to purple formazan. Unreduced MTT were then discarded and DMSO (100 µl) was added into each well to dissolve the formazan precipitate, which was then measured spectrophotometrically using a microplate reader at 570 nm. The cytotoxic effect of each treatment was expressed as percentage of cell viability relative to the untreated control cells. [MTT= (3-(4, 5-Dimethylthiazol-2-yl)-2, 5-diphenyltetrazolium bromide, a yellow tetrazole].

Recognition of Hg^{2+} ions in presence of other metal ions by L_2:

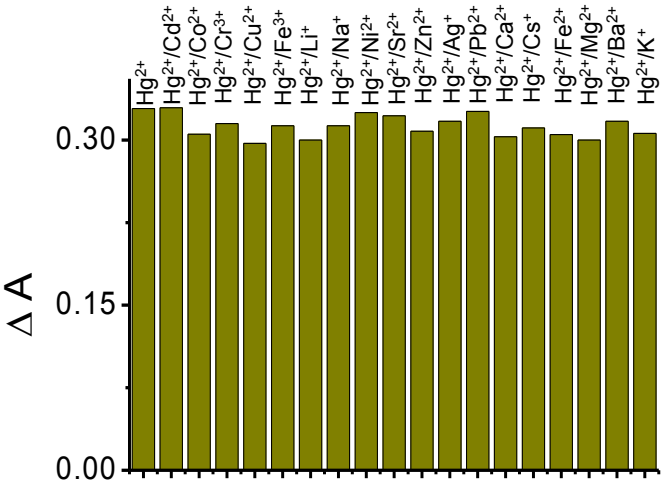


Figure 14: Recognition of Hg^{2+} ion (1.0×10^{-4} M) in presence of different metal (M^{n+} = 1.0×10^{-4} M) ions as their perchlorate salts by **L_2** (1.1×10^{-5} M) in acetonitrile/HEPES (3:2, v/v) buffer medium (ΔA is the change in absorbances at λ_{abs} 490 nm).

Recognition of Hg^{2+} ions in presence of other anions by L_2:

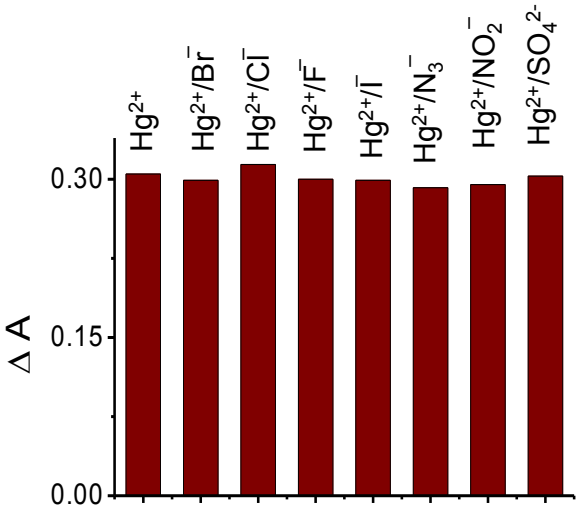


Figure 15: Recognition of Hg^{2+} ion (1.0×10^{-4} M) in presence of different anions (X^{n-} = 1.0×10^{-4} M) as their sodium salt by **L_2** (1.1×10^{-5} M) in acetonitrile/ HEPES (3:2, v/v) buffer medium (ΔA is the change in absorbances at λ_{abs} 490 nm).

^{1}H NMR spectra of L_2 in presence and absence of Hg^{2+} ions related to disappearance of $-CH_2$ protons of dithiane group:

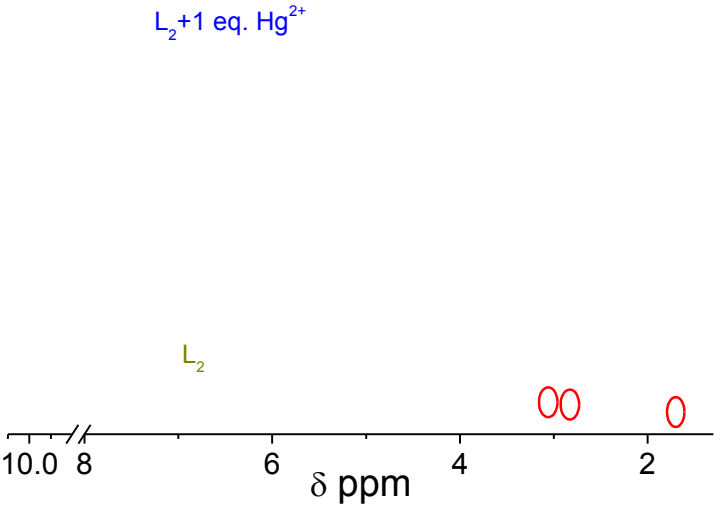


Figure 16: ^{1}H NMR spectra of **L_2** in presence and absence of Hg^{2+} ions showing disappearance of $-CH_2$ protons of dithiane group in CD_3CN medium (Red circles for indicating the $-CH_2$ protons of dithiane moiety).