Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary documents

A highly sensitive reversible fluorescent-colorimetric azino *bis*-Schiff base sensor for rapid detection of Pb^{2+} in aqueous media

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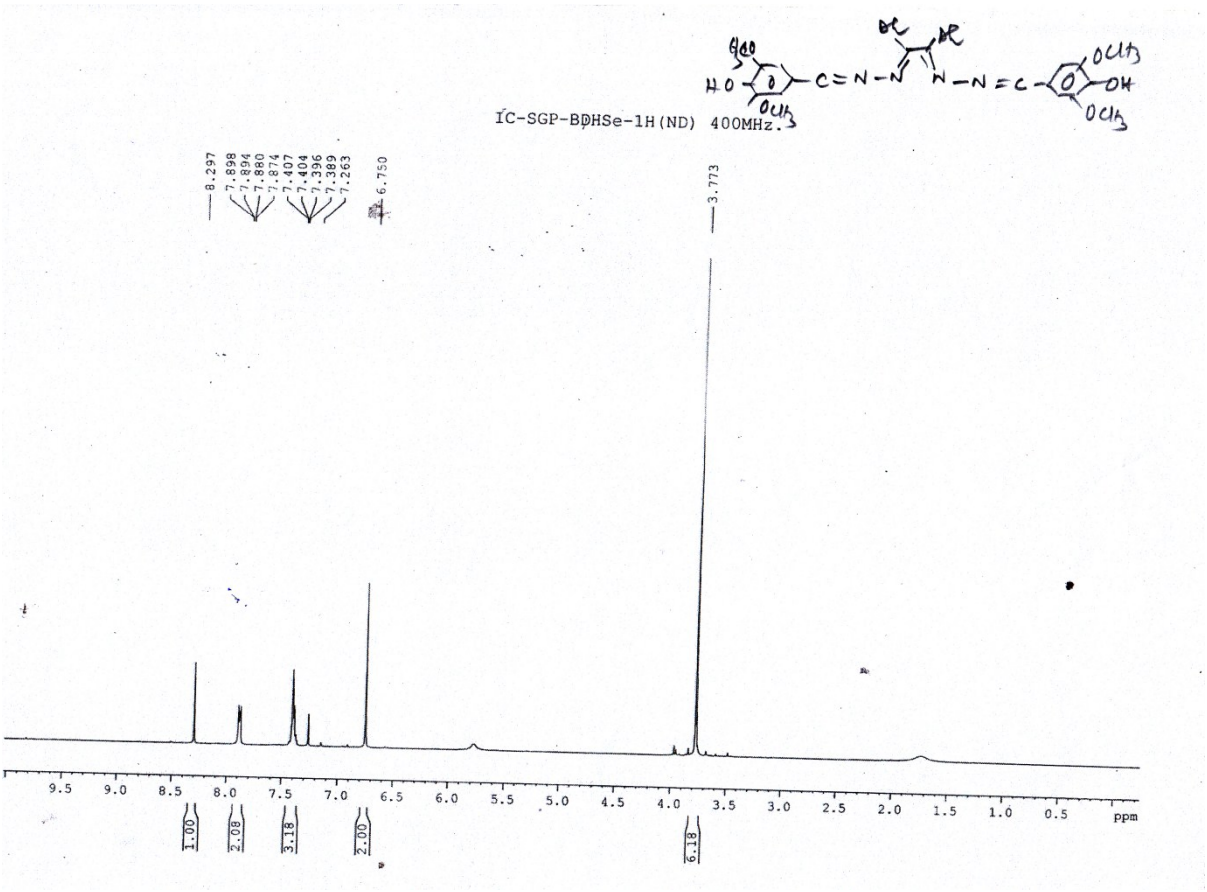


Fig. S1 ^{1}H NMR spectra of **L** in $CDCl_3$.

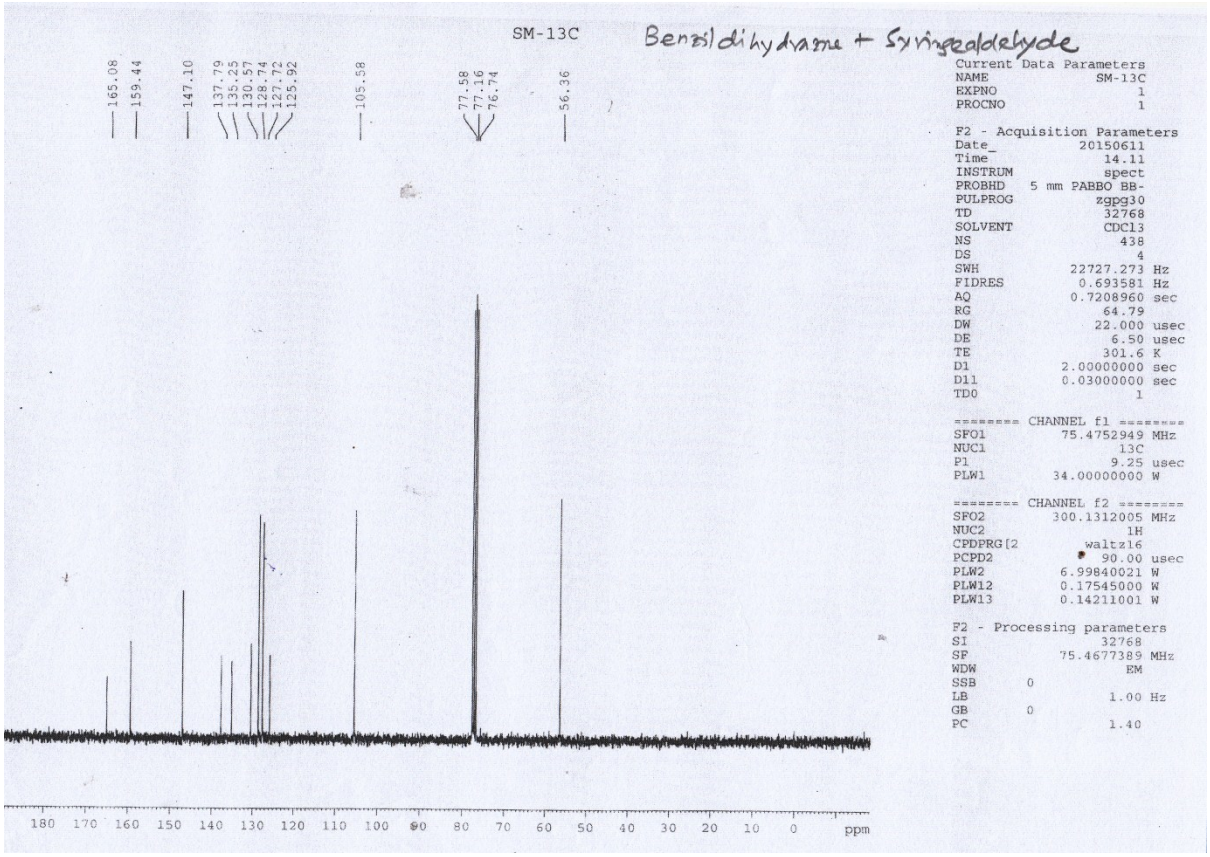


Fig. S2 ^{13}C NMR Spectra of **L** in $CDCl_3$.

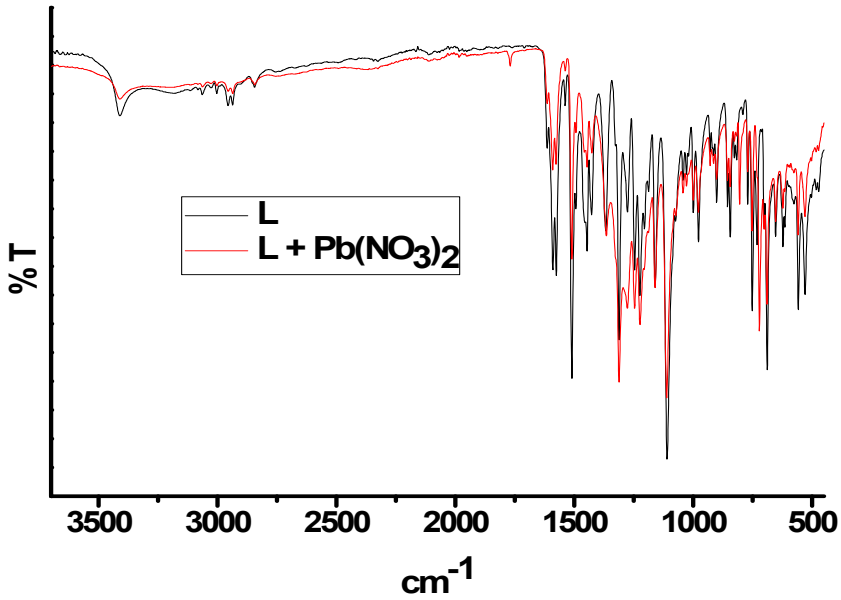


Fig. S3 FTIR spectra of **L.**

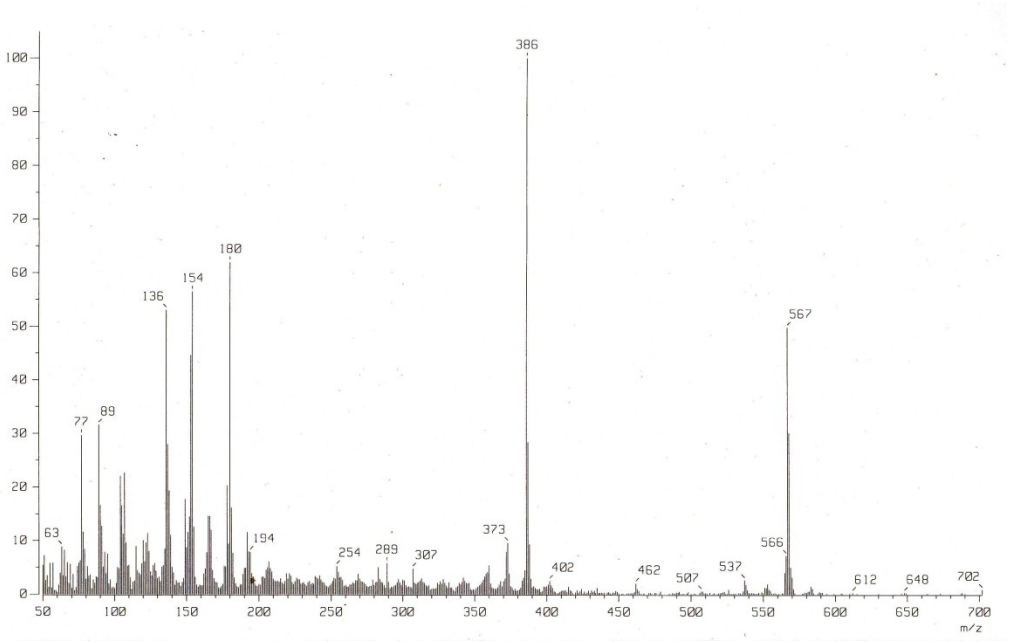


Fig. S4 Mass spectra of **L.**

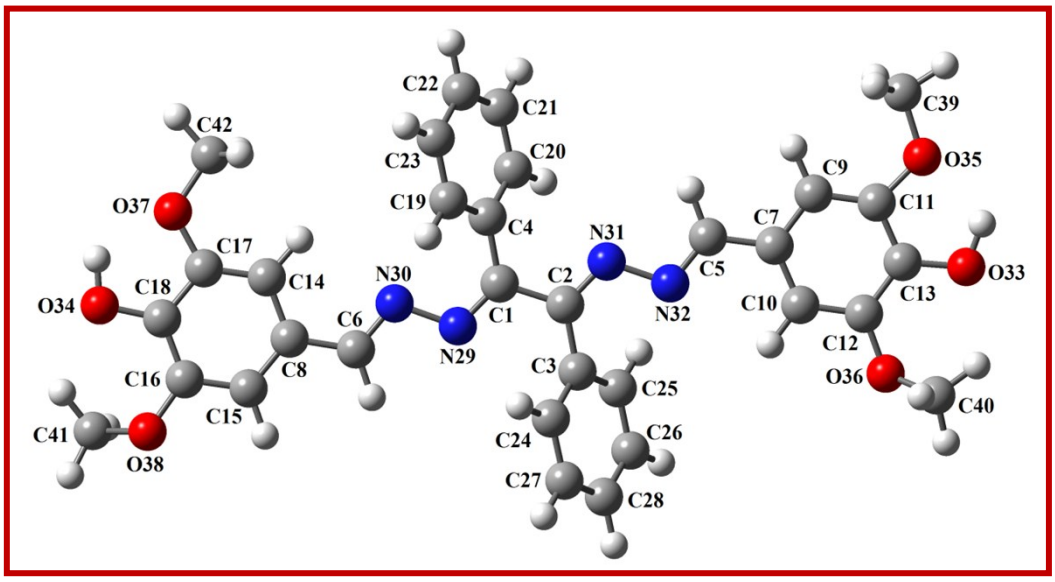


Figure S5. Geometry optimized diagram of the molecule **L.**

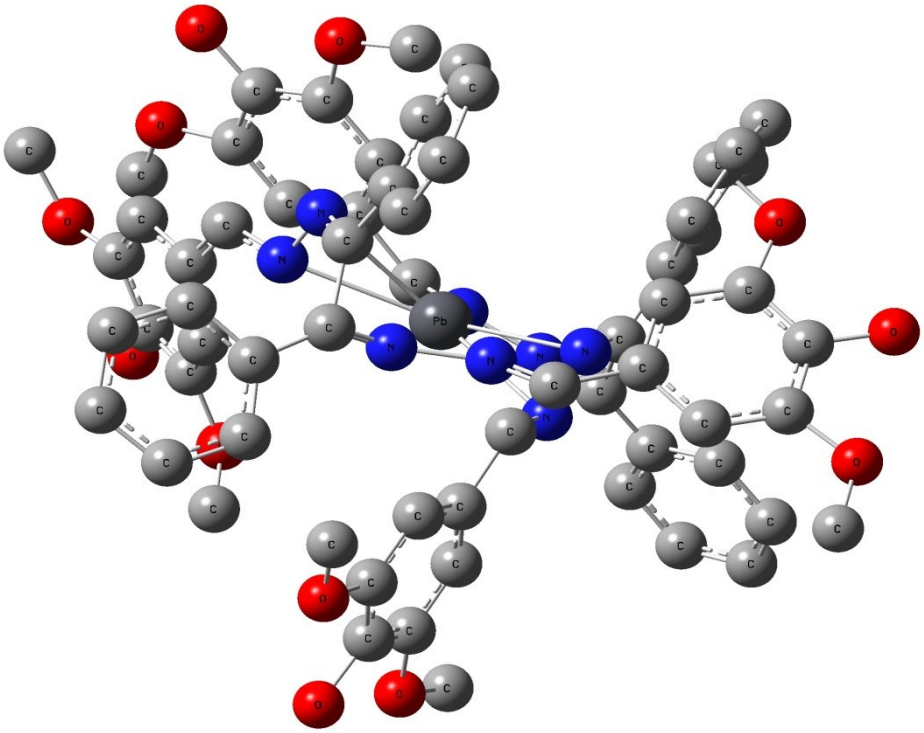


Figure S6. Geometry optimized diagram of the molecule Pb^{2+} complex of **L.**

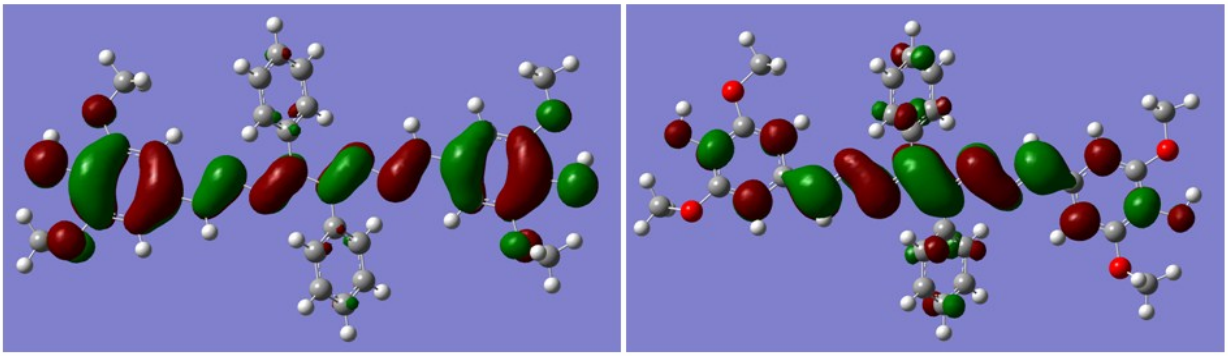
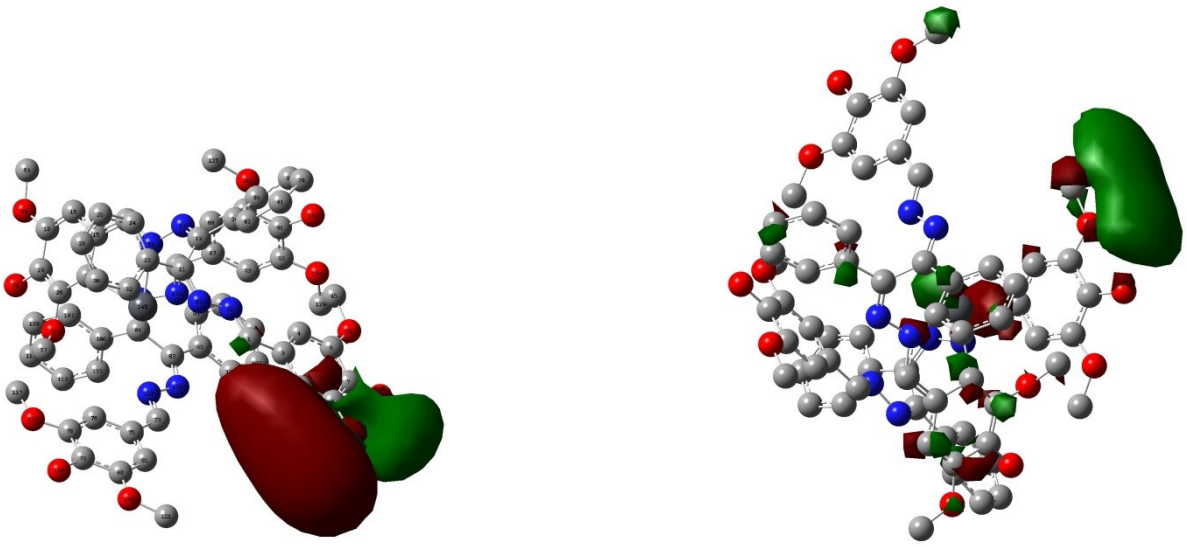


Figure S7. The contour diagrams of HOMO and LUMO of **L.**



(a) (b)

Figure S8. Structure of the (a) HOMO and (b) LUMO of Pb^{2+} complex of **L**. Hydrogen atoms are omitted for the sake of simplicity**.**

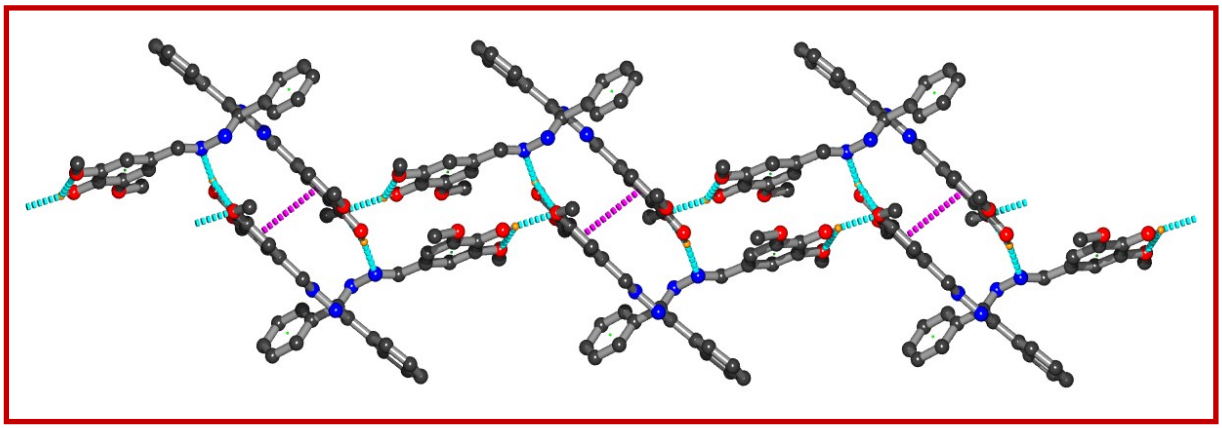


Fig. S9 1D supramolecular chain formation through hydrogen bonding and π···π interactions in **L.**

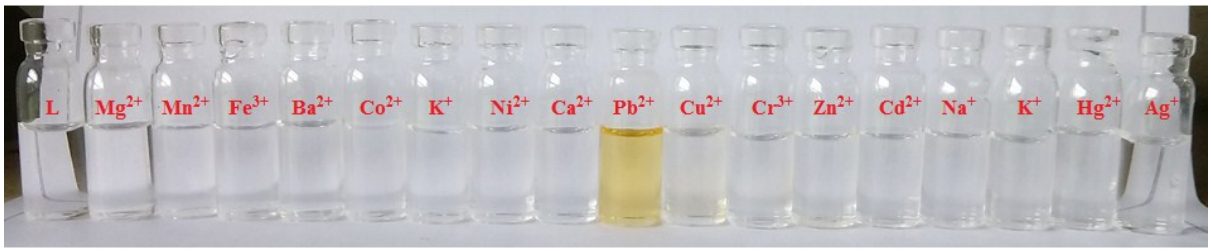


Figure S10. The color changes of **L** (10 μM) upon addition of various cations (10 equiv.) in MeOH-H_2O (1:1, v/v) at room temperature.

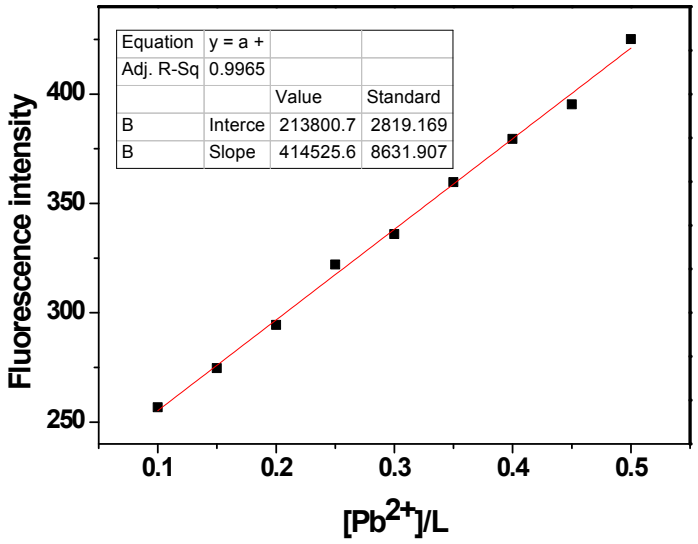


Fig. S11 Detection limit.

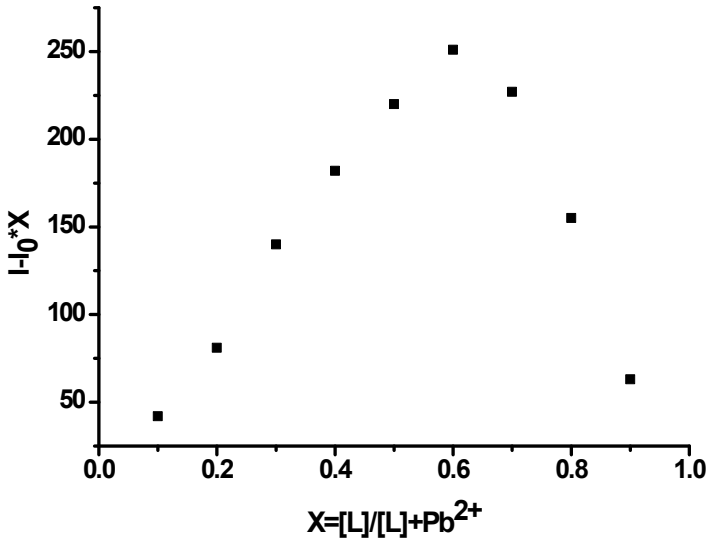


Fig. S12 Job plot for Pb^{2+}.

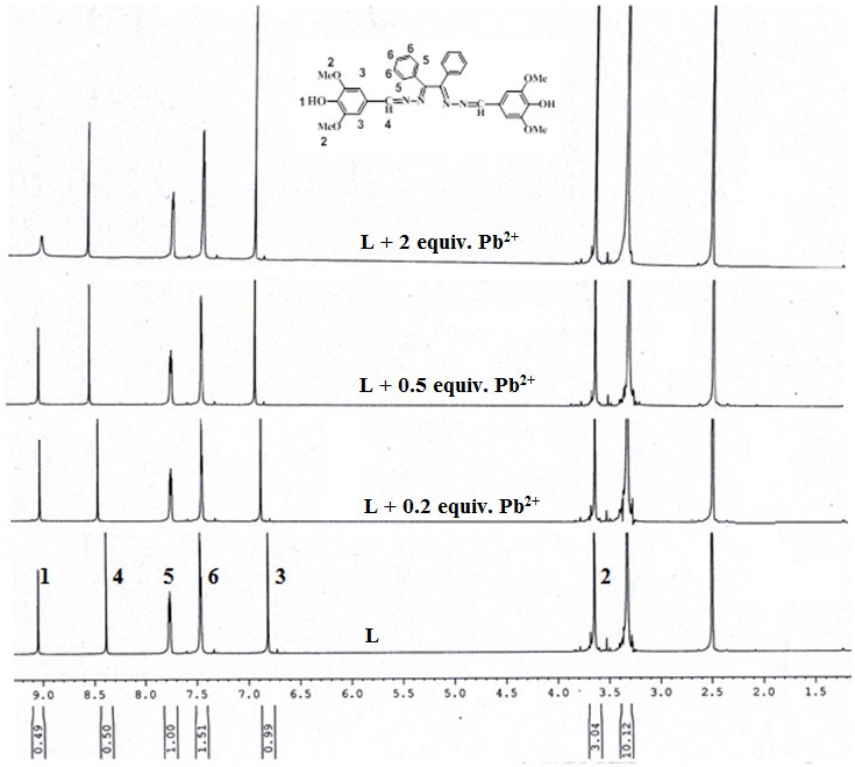


Fig. S13 ^{1}HNMR titration of **L** with Pb^{2+} in d_6-DMSO-D_2O (9/1, v/v).

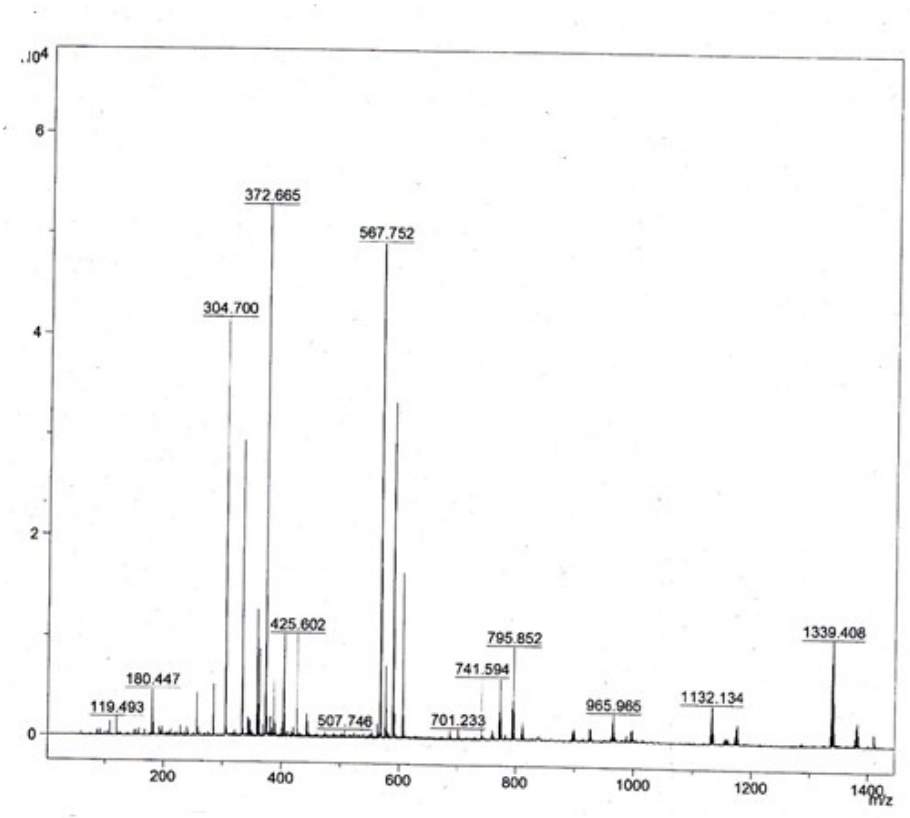


Fig. S14 Mass spectra of **L**+ Pb^{2+}.

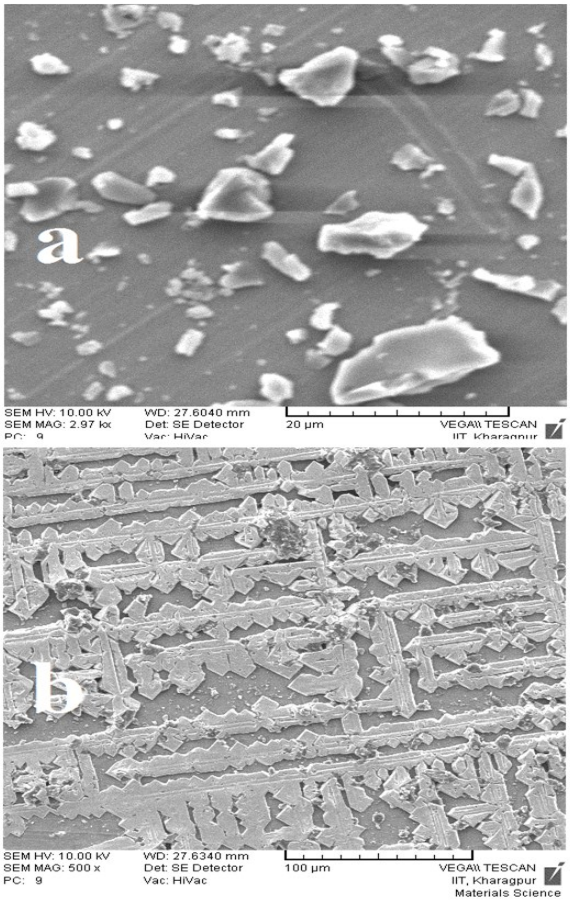


Fig. S15 FTIR spectra of **L** and **L+ $Pb(NO_3)_2$.**

Table S1 Crystallographic data and structure refinement parameters for receptor **L**

Formula	$C_{32}H_{30}N_4O_6$
Formula Weight	566.60
Crystal System	Monoclinic
Space group	P21/c (No. 14)
a [Å]	11.840(5)
b [Å]	10.520(5)
c [Å]	23.100(5)
β [°]	96.951(5)
V [$Å^3$]	2856.1(19)
Z	4
D(calc) [g/cm^3]	1.318
μ(MoKα) [/mm]	0.092
F(000)	1192

Crystal Size [mm]	0.14 x 0.16 x 0.20
Temperature (K)	293
Radiation [Å]	MoKα, 0.71073
Θ Min-Max [°]	2.1; 28.8
Dataset	-15: 15 ; -14: 14 ; -30: 30
Total Data	92134
Uniq. Data	7313
R(int)	0.168
Observed data [I > 2.0 sigma(I)]	3856
N_{ref}	7313
N_{par}	380
R	0.0964
wR_2	0.2885
S	1.09

Table S2 Hydrogen bond dimensions of the molecule **L**

D-H···A	D-H/(Å)	H···A/(Å)	D···A/(Å)	<D-H···A/(°)	Symmetry
O2-H1O2···O3	0.91	2.34	2.682(3)	102	.
O2-H1O2···N4	0.91	1.99	2.877(4)	165	-x, -y, -z
O5-H1O5···O3	0.86	2.07	2.849(3)	151	1+x, -1+y, z
O5-H1O5···O4	0.86	2.25	2.642(4)	108	.
C1-H1···O6	0.93	2.55	3.355(5)	146	1-x, -y, -z
C16-H16···O2	0.93	2.59	3.363(4)	142	-x, -y, -z
C32-H32A···N2	0.96	2.57	3.462(5)	155	1-x, -y, -z
C32-H32B···O1	0.96	2.48	3.196(5)	131	1+x, y, z

Table S3 All π···interactions of the molecule **L.**

π···π interactions			
Cgi···Cgj	Distance between ring Centroids/(Å)	Dihedral Angle between Planes I and J/(°)	Symmetry
Cg1···Cg1	3.744(3)	0	-x, -y, -z
Cg2···Cg2	3.595(3)	0	1-x, -1-y, -z
C-H···π interactions			
C-H···Cgi	H···Cg/(Å)	<X-H···Cg/(°)	Symmetry
C10-H10···Cg3	2.94	167	1-x, -1/2+y, 1/2-z
C31-H31C···Cg4	2.75	134	1-x, -1/2+y, 1/2-z

***Cg1: C2-> C3-> C4-> C5-> C6-> C7->; Cg2: C11-> C12-> C13-> C14-> C15-> C16->; Cg3: C17-> C18-> C19-> C20-> C21-> C22->; Cg4: C23-> C24-> C25-> C26-> C27-> C28->**