Electronic Supplementary Material (ESI) for New Journal of Chemistry.

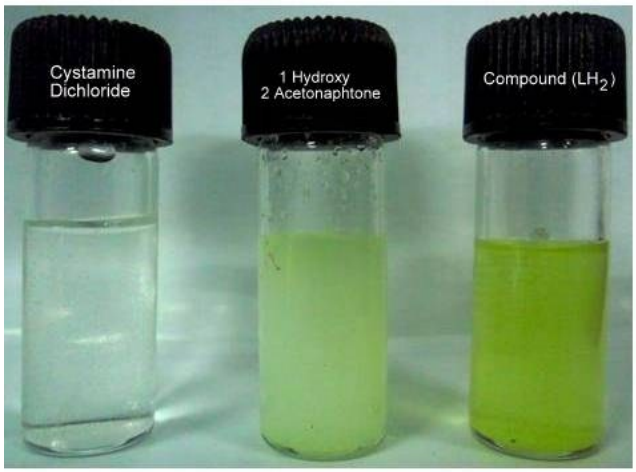
Electronic Supplementary Information (ESI)

Development of Fluorescent Chemosensor towards sensing and separation of Mg^{2+} ions in chlorophyll and Hard Water

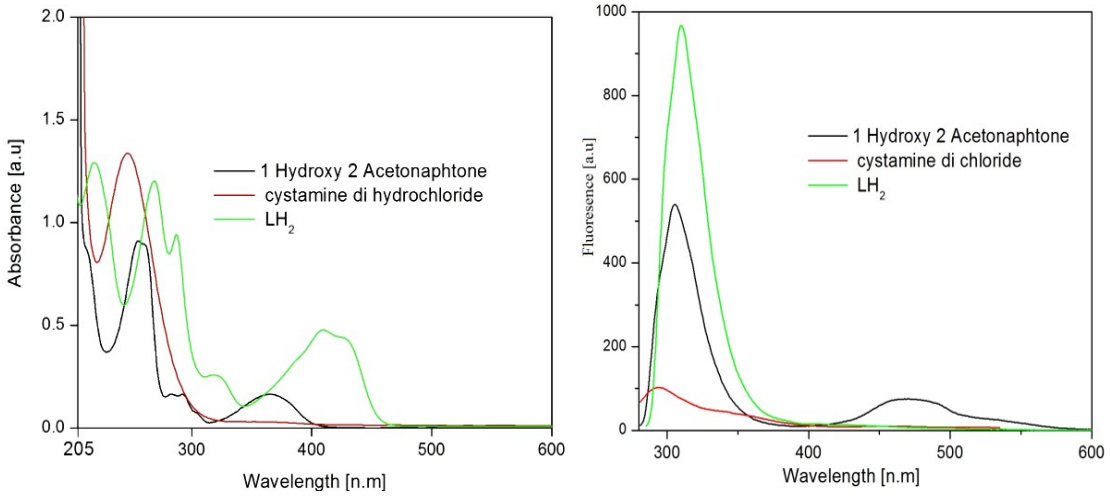
G. Tamil Selvan, [a] V.Chitra, [a] Israel V. M. V. Enoch[a, b] and P. Mosae Selvakumar * [a]

Chemistry Research Lab, Department of Science & Humanities, Karunya Institute of Technology and sciences, Coimbatore, Tamil Nadu, India-641114.

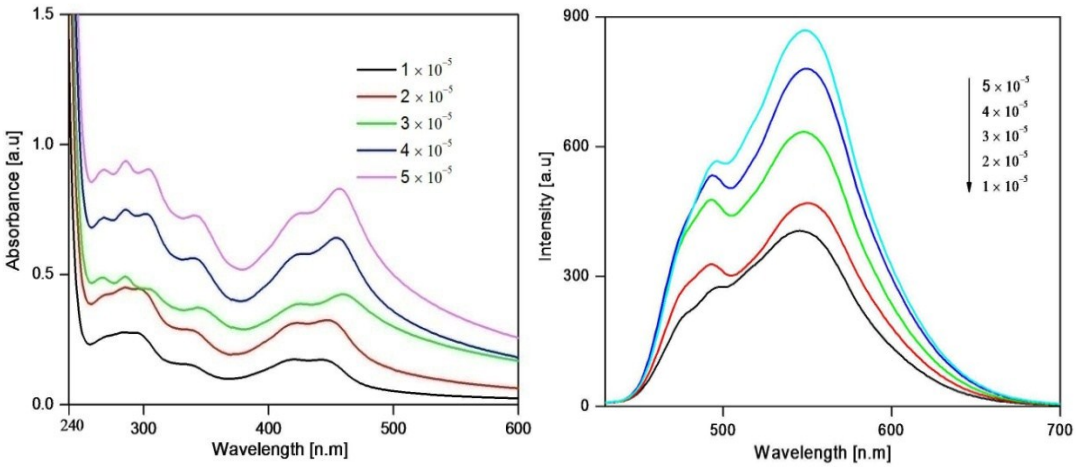
Email:pmosae@gmail.com



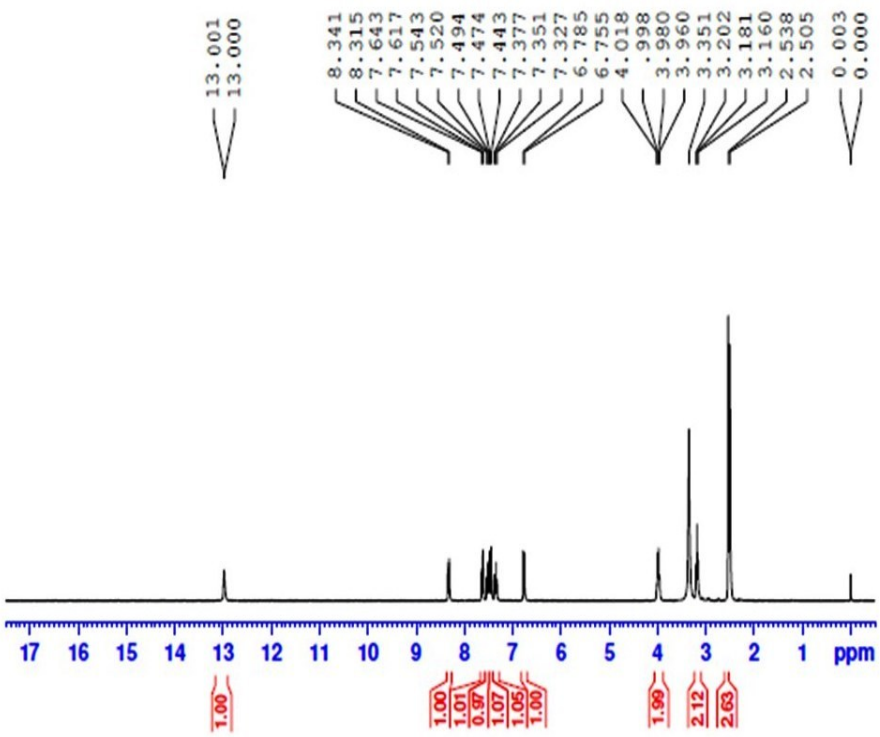
S1. Photographs of starting material and Compound LH_2 preparation



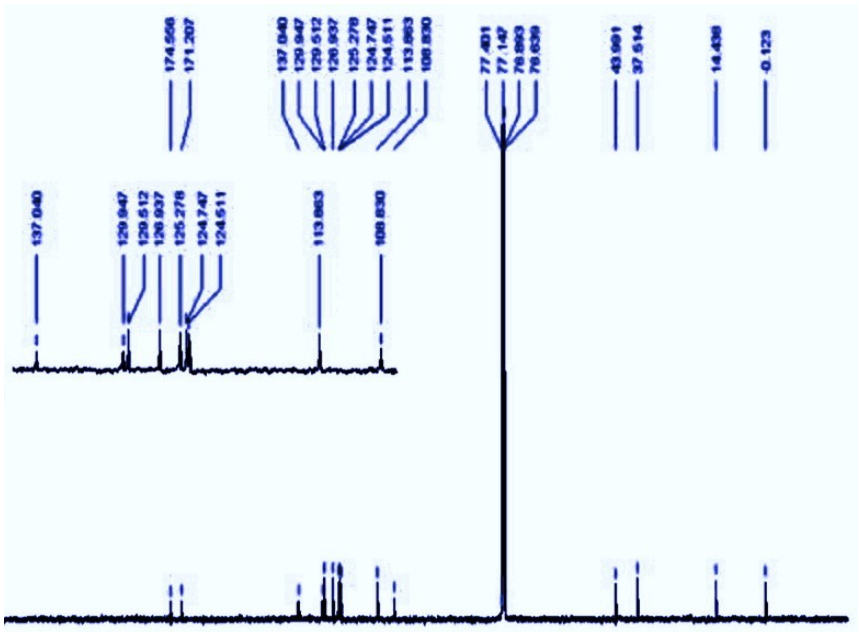
S2. Absorption and Fluorescence spectrum of starting material and Compound LH_2.



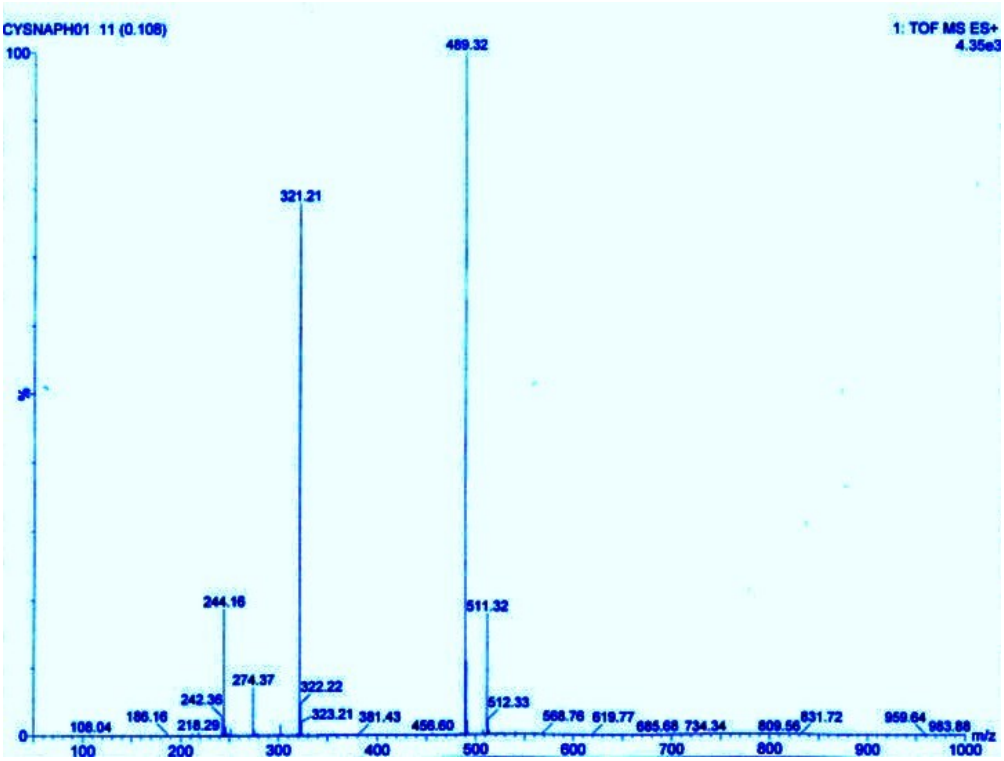
S3. Absorption and Fluorescence spectrum of Receptor in various concentrations.



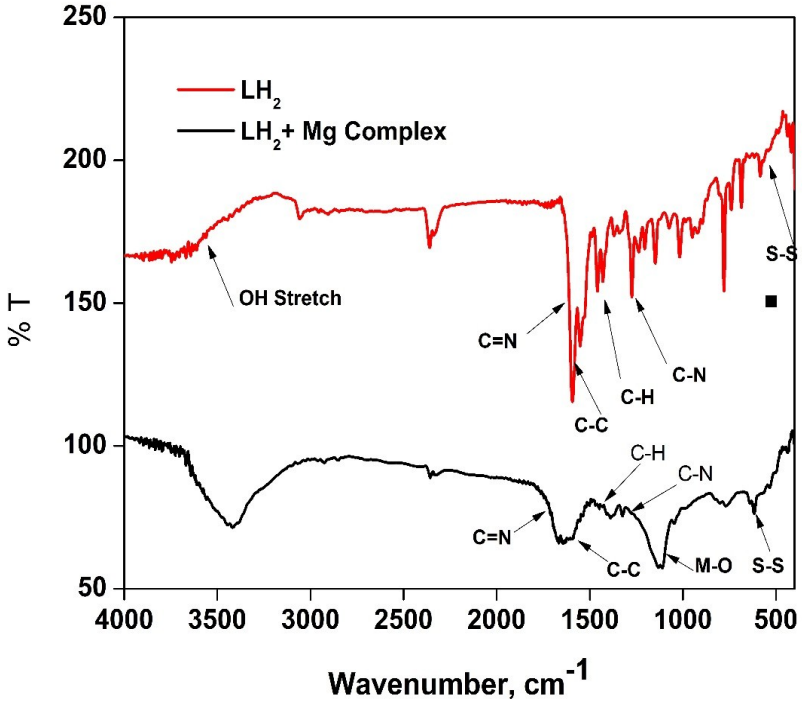
S4.H^1 NMR Spectrum of compound-LH_2



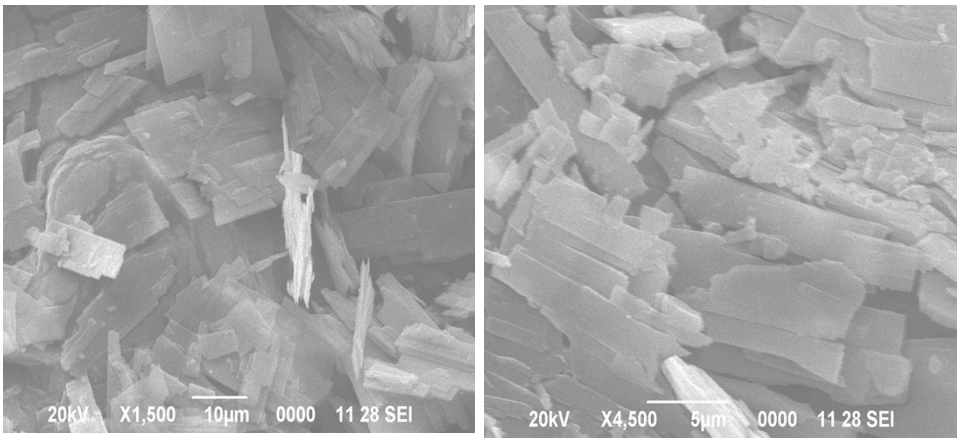
S5.C^{13} NMR Spectrum of compound-LH_2



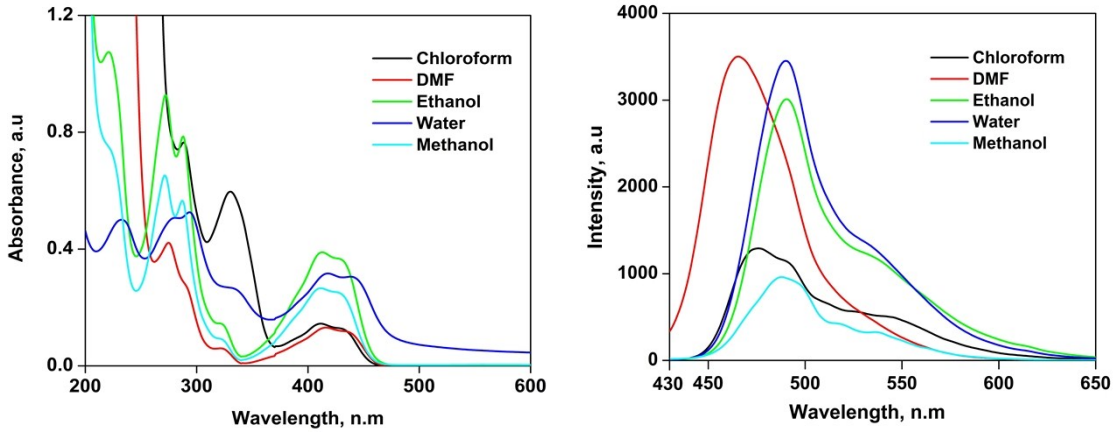
S6.MASS Spectrum of compound-LH_2



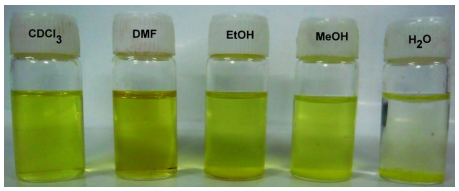
S7. IR spectrum of Compound LH_2 and Mg^{2+} Complex.



S8. SEM Micrographs of Compound LH_2.



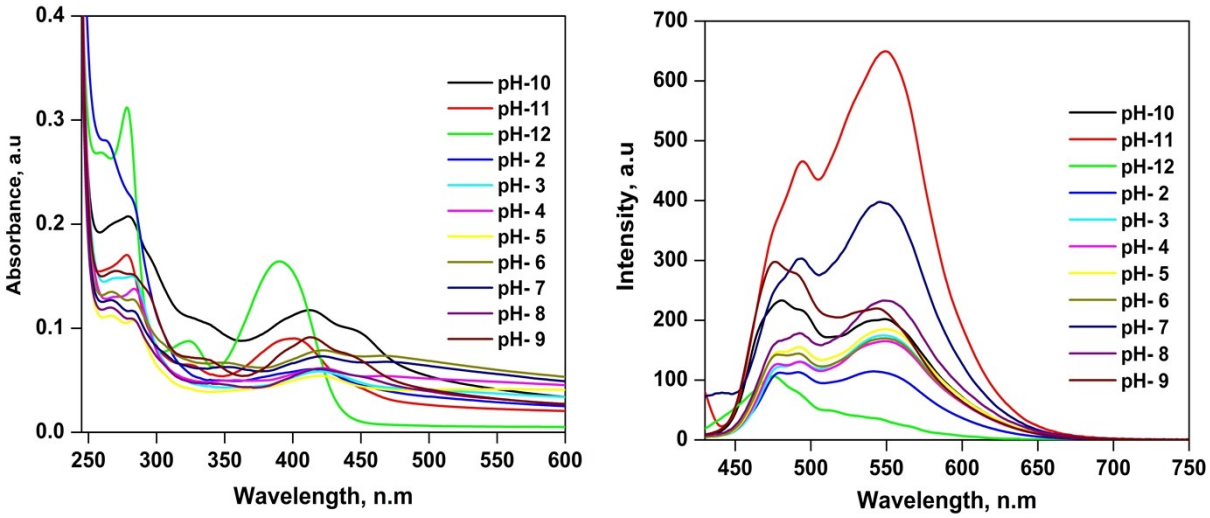
S9. (a) Absorption and (b) Fluorescence spectra of compound LH_2 in various solvents.



Photographs of Various Solvents in Compound LH_2.

Effect of solvents on the absorption and fluorescence spectra of the Compound LH_2 (Solvatochromism)

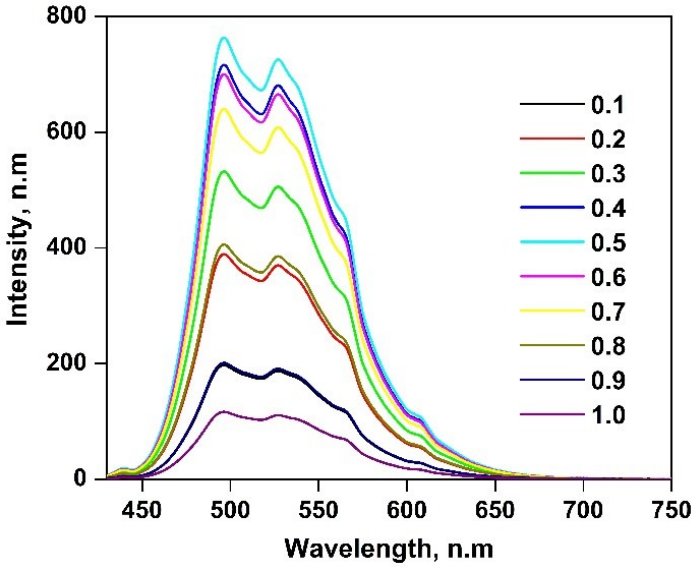
The Compound LH_2 was soluble in common organic solvents. The effect of solvents on the absorption and fluorescence spectra was studied. The properties of Compound LH_2 were studied by UV–visible and fluorescence spectra upon dissolving in different solvents ($CDCl_3$, DMF, EtOH, MeOH, H_2O). The absorption bands of Compound LH_2 were observed around 410 nm. (Fig. S9 (a)). The bathochromic shifts of absorption on shifting polarity (from chloroform and other organic solvents to water) were due to the high polarity of the receptors in the ground state. On excitation at 410 nm, an emission band centered at 480 nm was observed. The broad red shifted band was observed in ethanol and DMF solvents (Fig. S9 (b)). The general observation is that there is an increase in the Stokes shift values with increasing solvent polarity which shows that there is an increase in the dipole moment on excitation. A bathochromic shift was observed in shifting polarity from chloroform and other organic solvents to water.



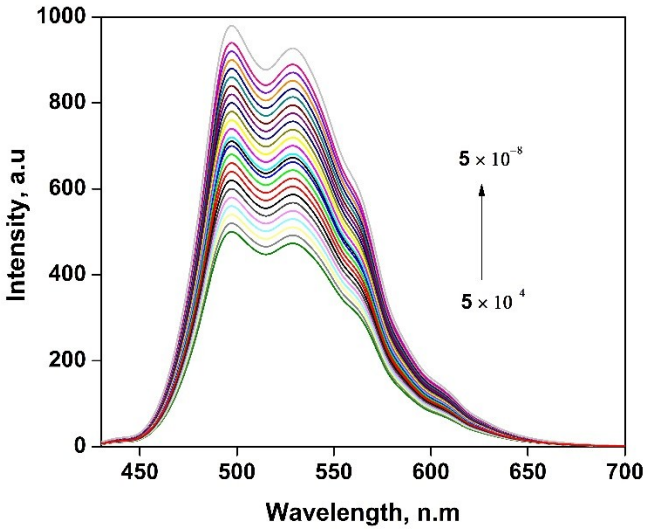
S10. (a) Absorption and (b) Fluorescence Spectra of compound LH_2 at various pH.

Effect of pH with Compound LH_2

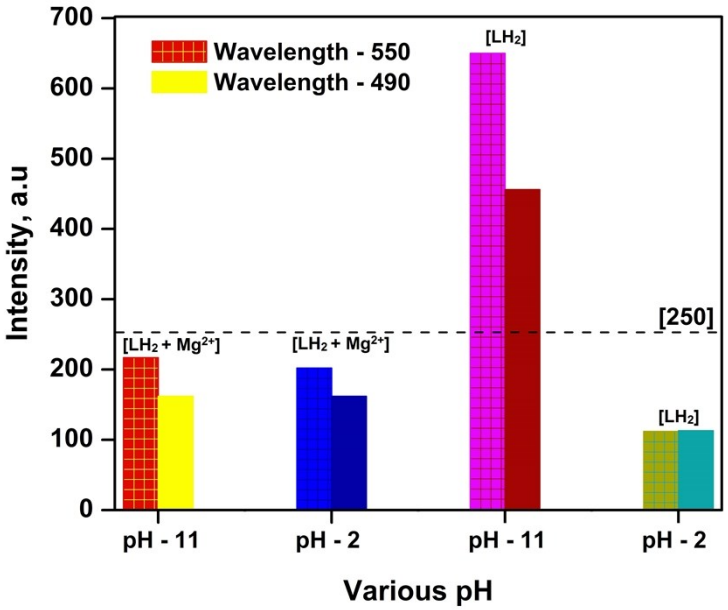
The effect of pH on absorption and fluorescence spectra was studied. The test solution was prepared by adding 9.9 ml in (pH 2-12) to 100 µl of Compound LH_2. The UV–vis absorbance spectra that the absorbance intensity of bands (hyper chromic shift) increased with an increase in pH value from 6.0 to 12.0 but pH value from 2.0 to 5.0 bands hypochromic shifted. The fluorescence intensity was seen to change with the pH value at acidic to basic medium. When the pH increased, the absorption band got enhanced (Fig.S.10. (a)). Similarly, the fluorescence spectrum also showed an enhancement. However, in the acidic range (at lower pH values) a red shift was observed and in the larger pH values, the band was centered at the shorter wavelength (Fig. S.10. (b)).



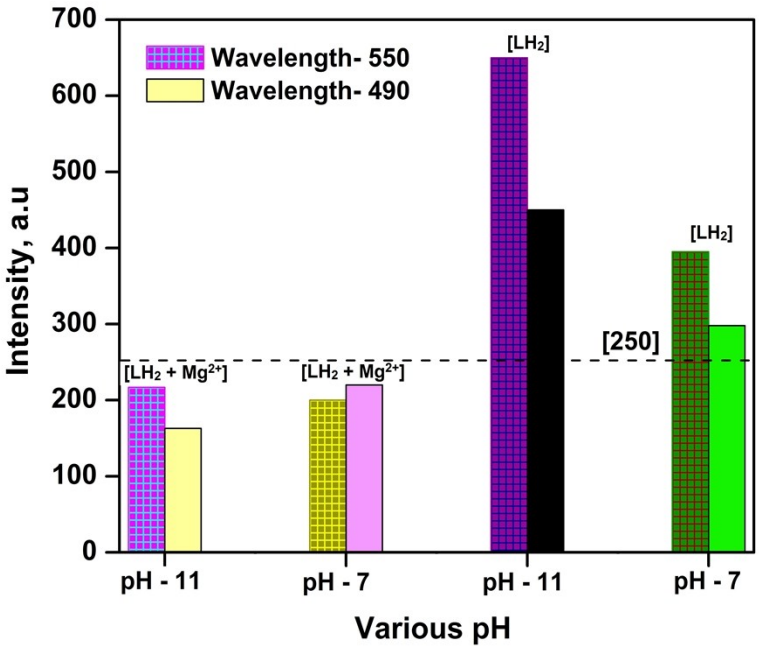
S11. Fluorescence spectra of Mg^{2+} ion for Jobs plot method.



S12. Fluorescence spectra of Mg^{2+}ion for Detection limitation.

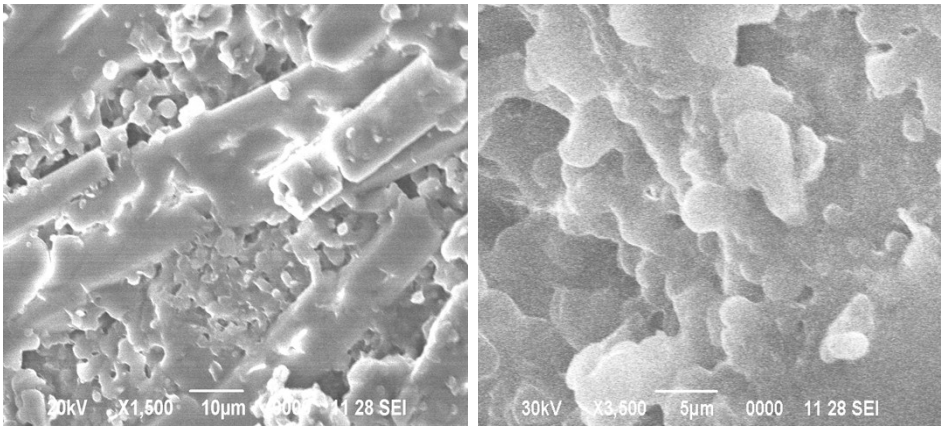


S13. Bar Chart for Fluorescence spectra (λ_{ex} = 410nm) of Compound LH_2 (1×10^{-5}M) in the absence and presence of Mg^{2+} in a mixture of H_2O / DMF (9:1 v/v) at pH 2.0 and pH 11 with 10ml of H_3PO_4 buffer

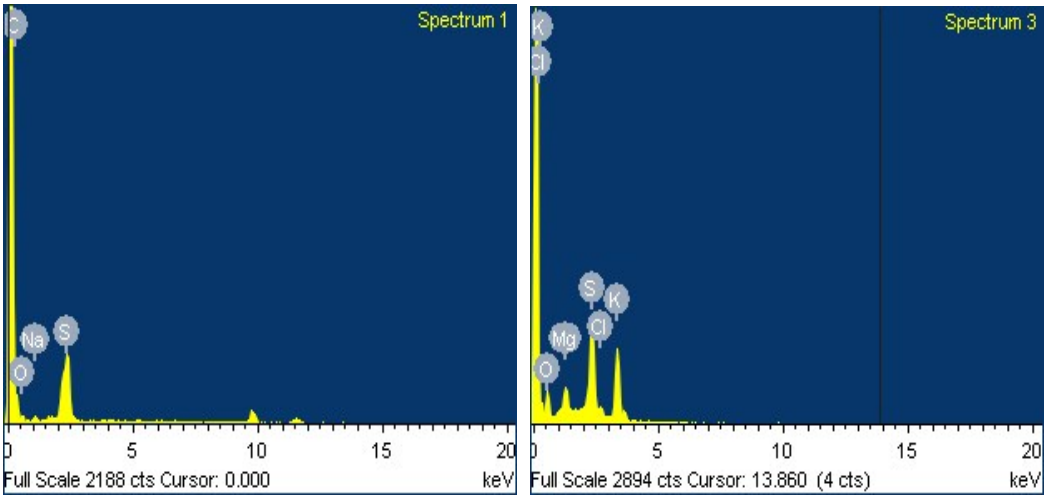


S14. Bar Chart for Fluorescence spectra (λ_{ex} = 410 nm) of Compound LH_2 (1×10^{-5} M) in the absence and the presence of Mg^{2+} (solvent: H_2O/ DMF, 9:1 v/v) at pH 7.0 and pH 11.

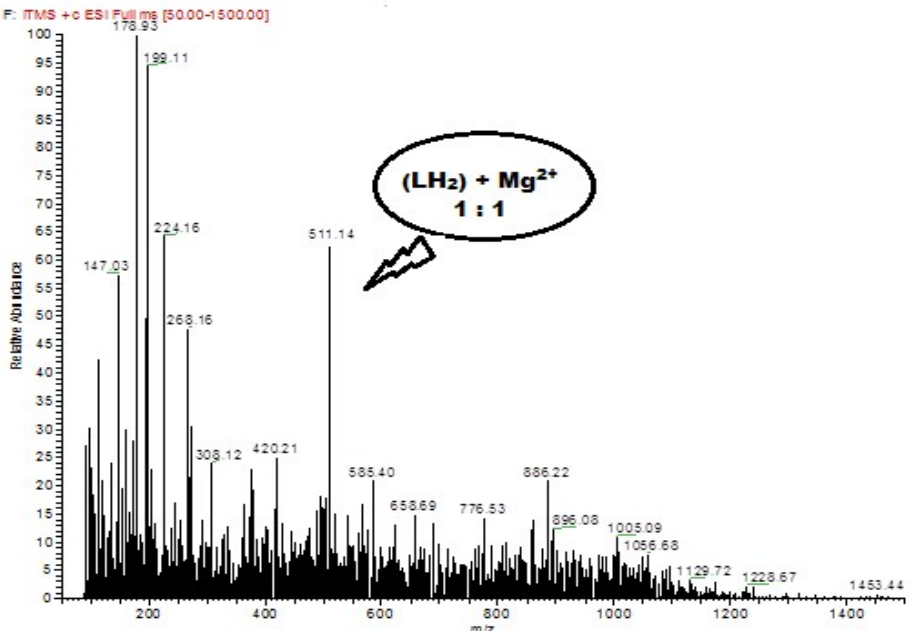
S15. Photographs of starting material, Compound LH_2 and Mg^{2+} Complex Preparation.



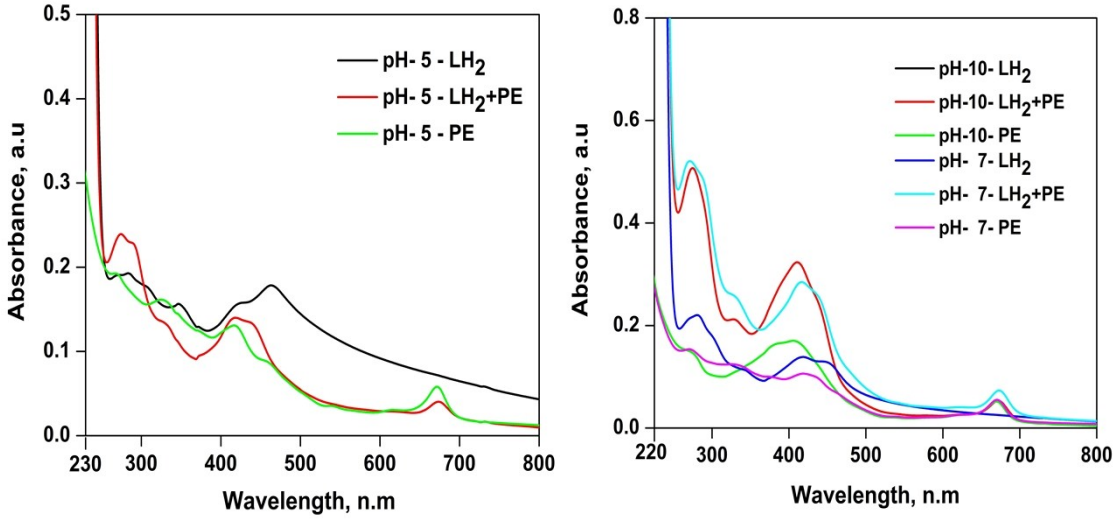
S16.SEM Micrographs of Mg^{2+} complex for compound LH_2.



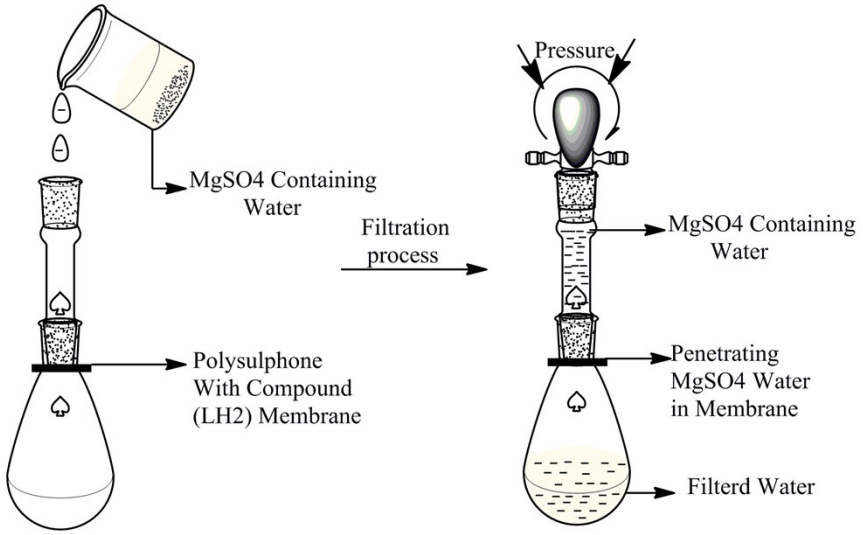
S17. EDX Spectrum of Compound LH_2 with Mg^{2+} complex.



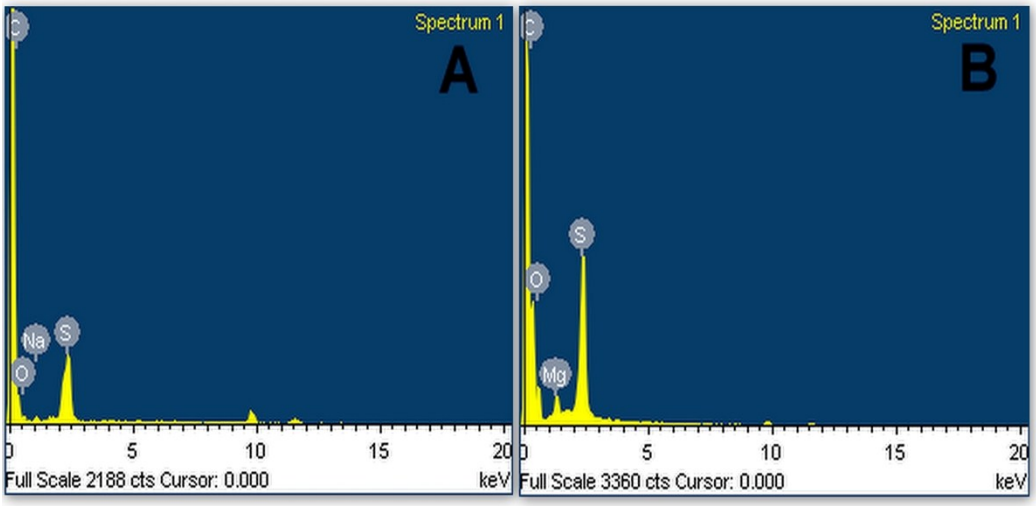
S18. Mass spectrum of Mg^{2+} Complex



S19. Absorption Spectra of Compound LH_2 with plant extraction in (pH-5, 7, 10) condition.

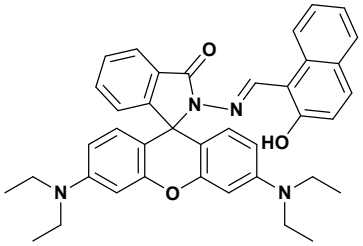
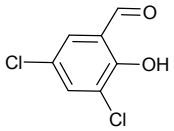
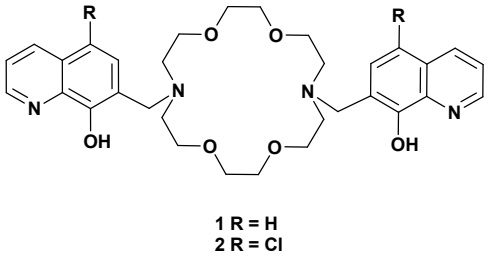
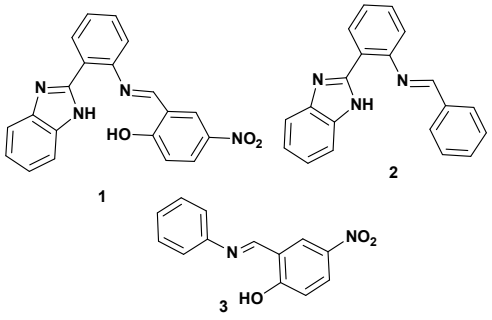


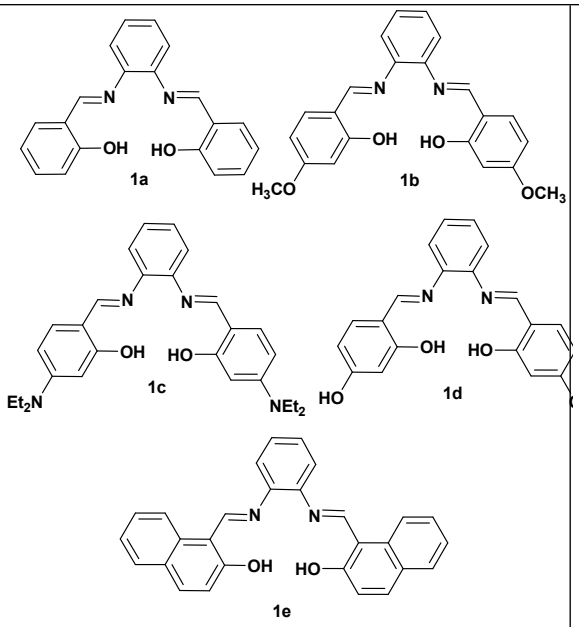
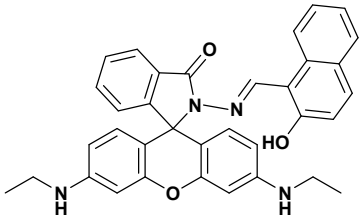
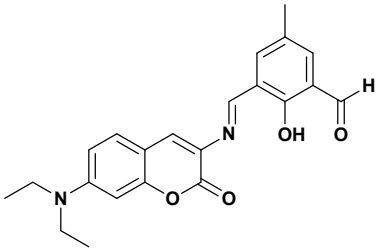
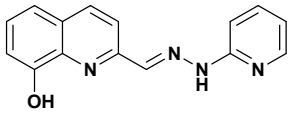
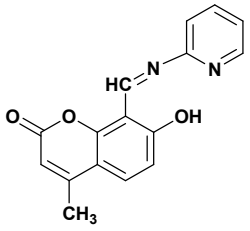
S20. Schematic representation of water filtration process using compound LH_2 incorporated membrane.

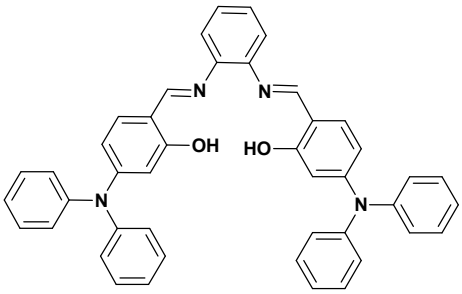
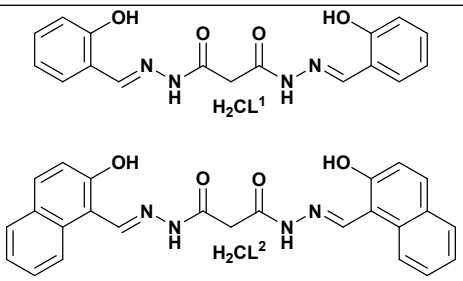
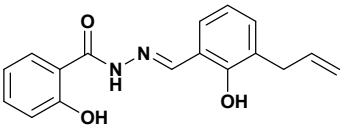
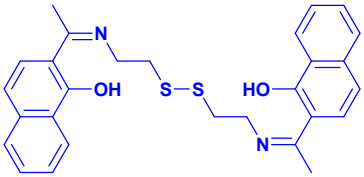


S21. EDX spectrum of (A) before filtration process of membrane spectrum. (B) After filtration process of membrane spectrum.

S22. Comparison with other Mg^{2+} fluorescent chemosensors.

S.No	Chemosensor	Binding constant	Detection limit	Application(s)	Literature
1		1.0×10^5 L mol^{-1}	80 nmol L^{-1}	Fluorescence imaging in Hela cells	29
2		Weak binding constant	2.89×10^{-7} mol/L	Real-time detection in drinking water samples	30
3	 1 R = H 2 R = Cl	44 and 73 µM	-	HC11 mouse mammary cells	31
4	 1 2 3	1.6 (±0.1)10^4 M^2	79.4 - 340 mM	Straining microbial cells (yeast) without breakage	32

5.		-	10^{-7} M	Detection in pond, tap and groundwater samples	33
6.		1.16 x 10^5	1.44 x 10^{-6} M	-	34
7.		2.39 x 10^4 M^{-1}	-	-	35
8.		1.91 x 10^7 M^{-1}	19.1 ppb	Lake, tap and groundwater samples	36
9.		2.17 x 10^4 M^{-1}	-	-	37

10.		-	10^{-6} M	River, pond and groundwater	38
11.		5.31 ± 0.18	-	-	**39**
12.		1.02 x 10^{7} M^{-1}	4.88 x 10^{-8} mol/L	Serum and tap water samples	40
13.		**5667.9703 M^{-1}**	**10^{-8} mol/L**	**Polysulphone membrane to filter Mg^{2+} ions from hard water**	**Present work**