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

A new aza-crown macrocyclic fluorescence chemosensor (N_3O_2 donor atoms) for magnesium ions in aqueous ethanol solution

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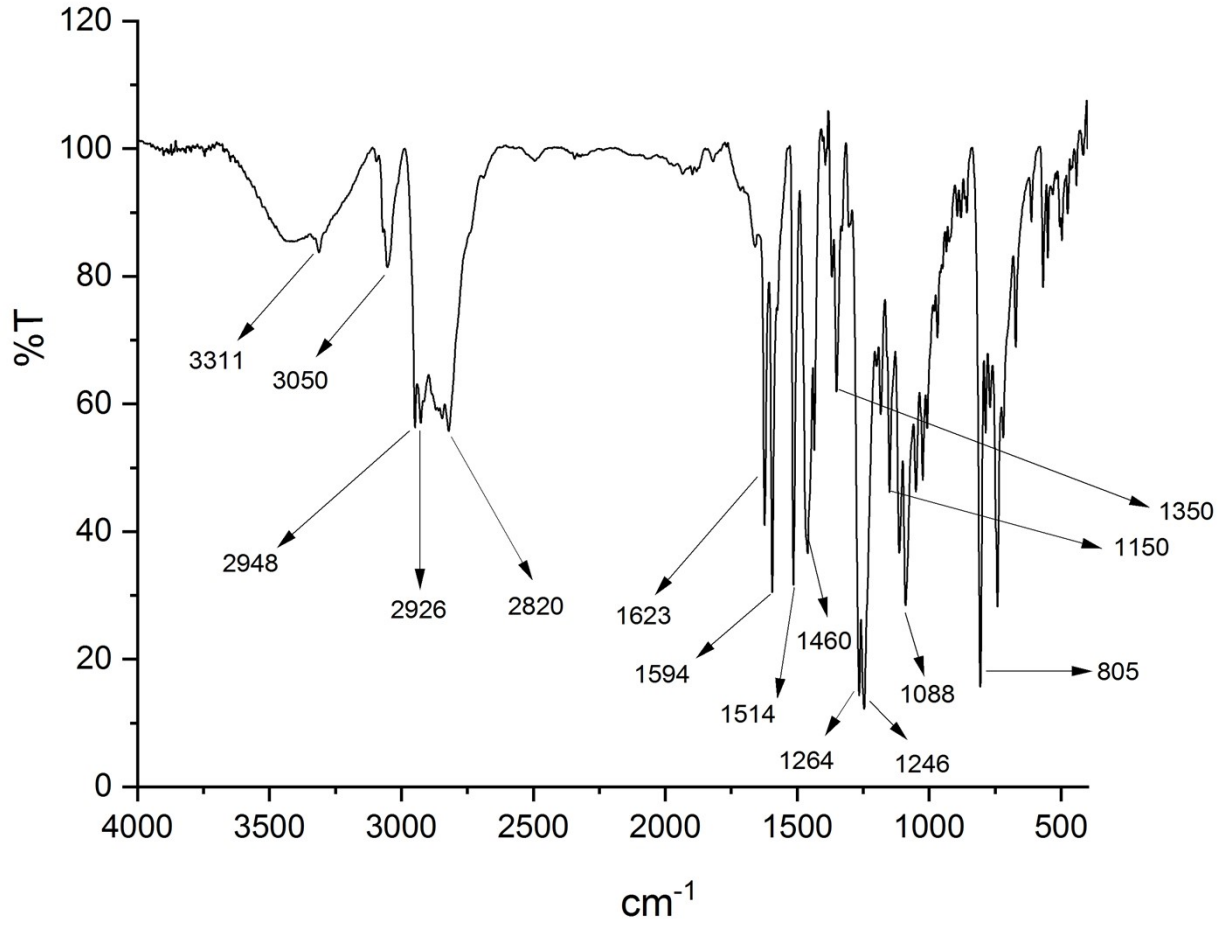

Fig. S1. IR spectrum of L

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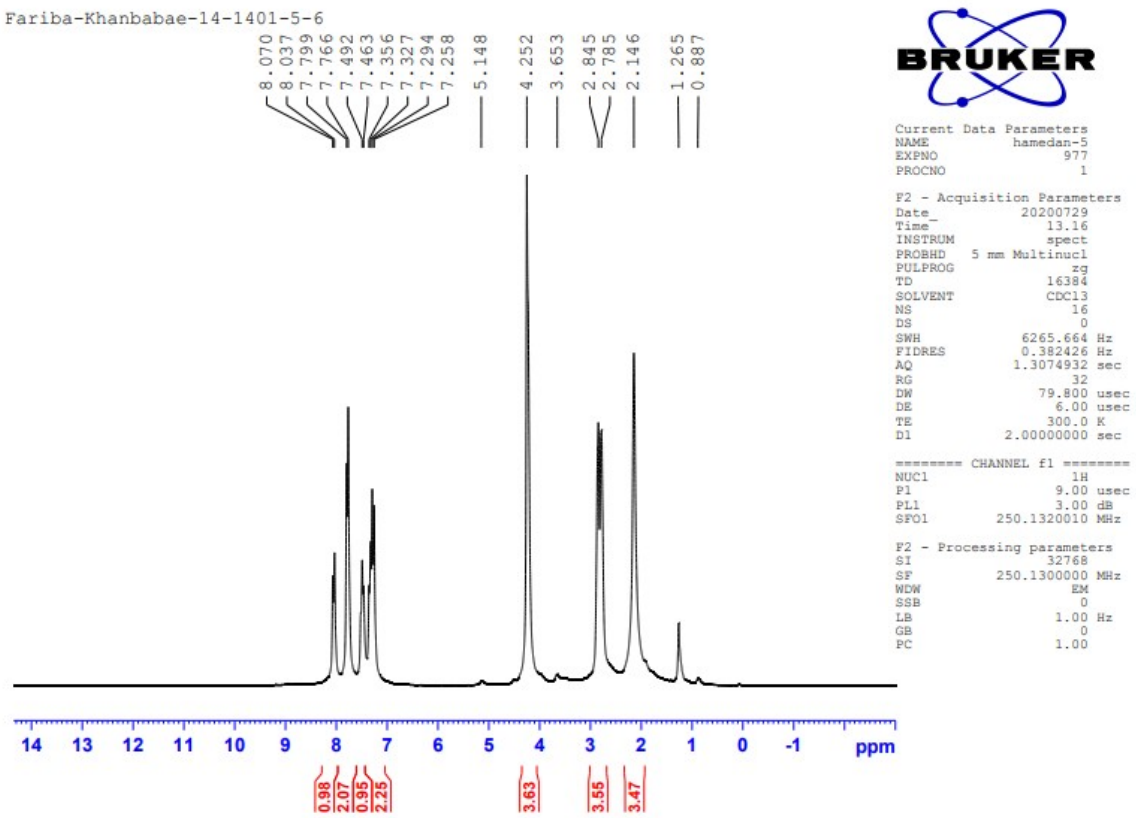

Fig. S2. [1]HNMR spectrum of L in CDCl3.

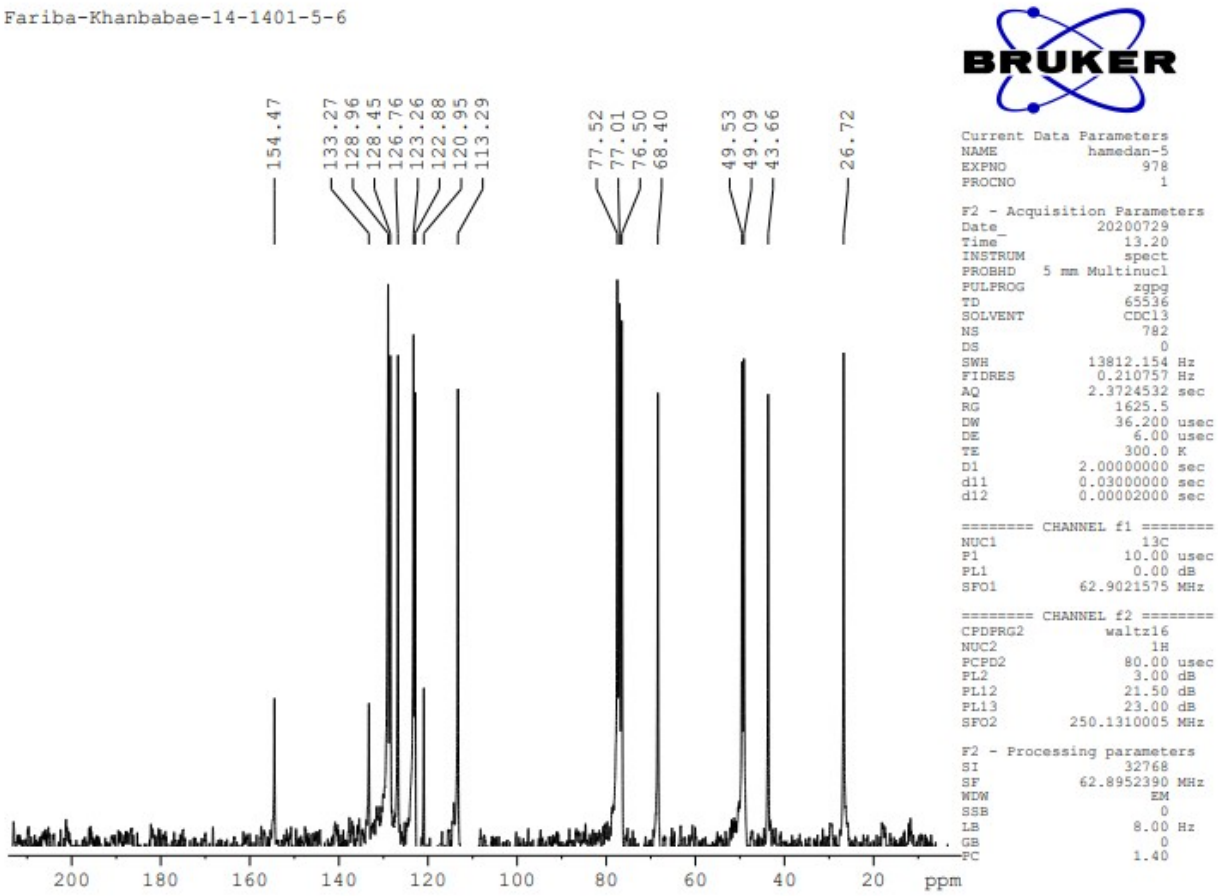

Fig. S3.[13]CNMR spectrum of L in CDCl3.

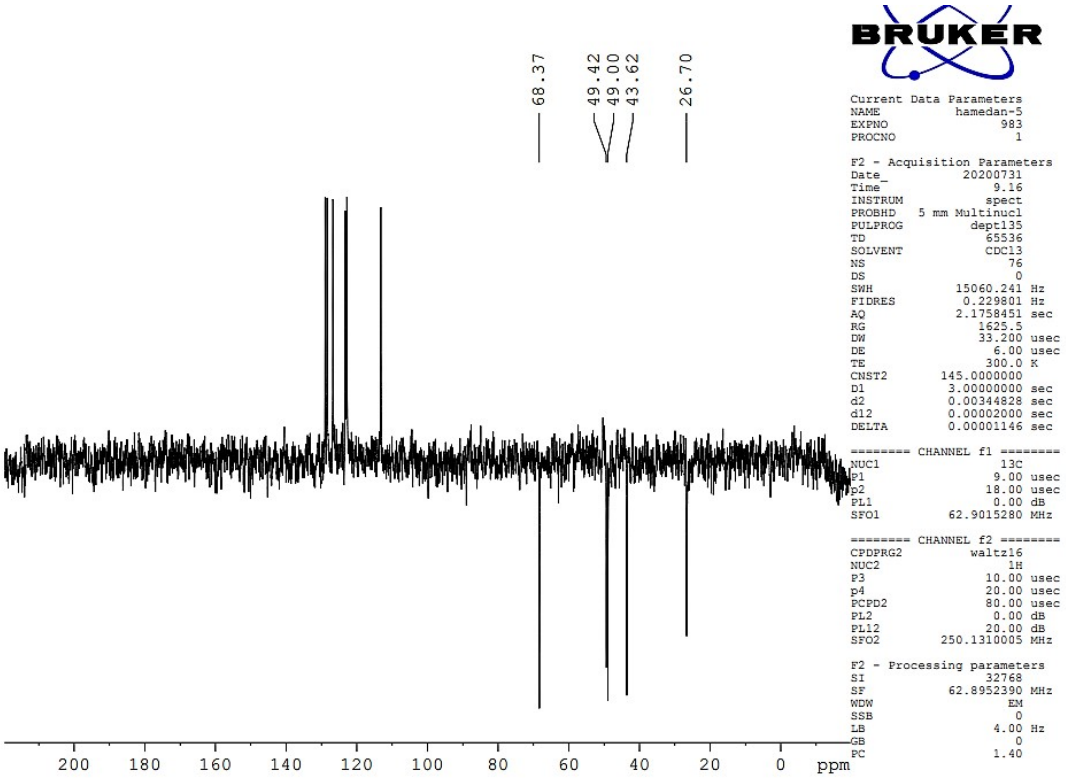

Fig. S4. DEPT spectrum of L in CDCl3.

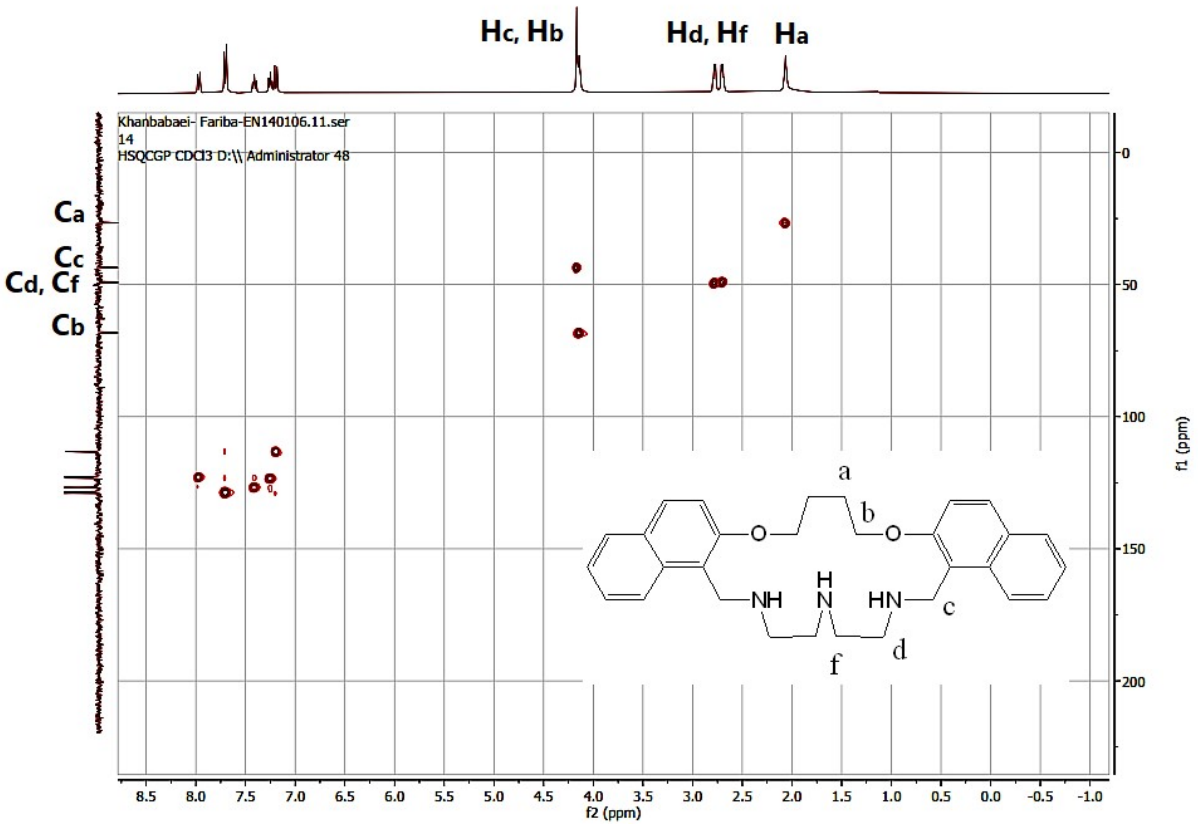

Fig. S5. HSQCGP spectrum of L in CDCl3 along with numbering scheme of the proton and carbon assignments for L.

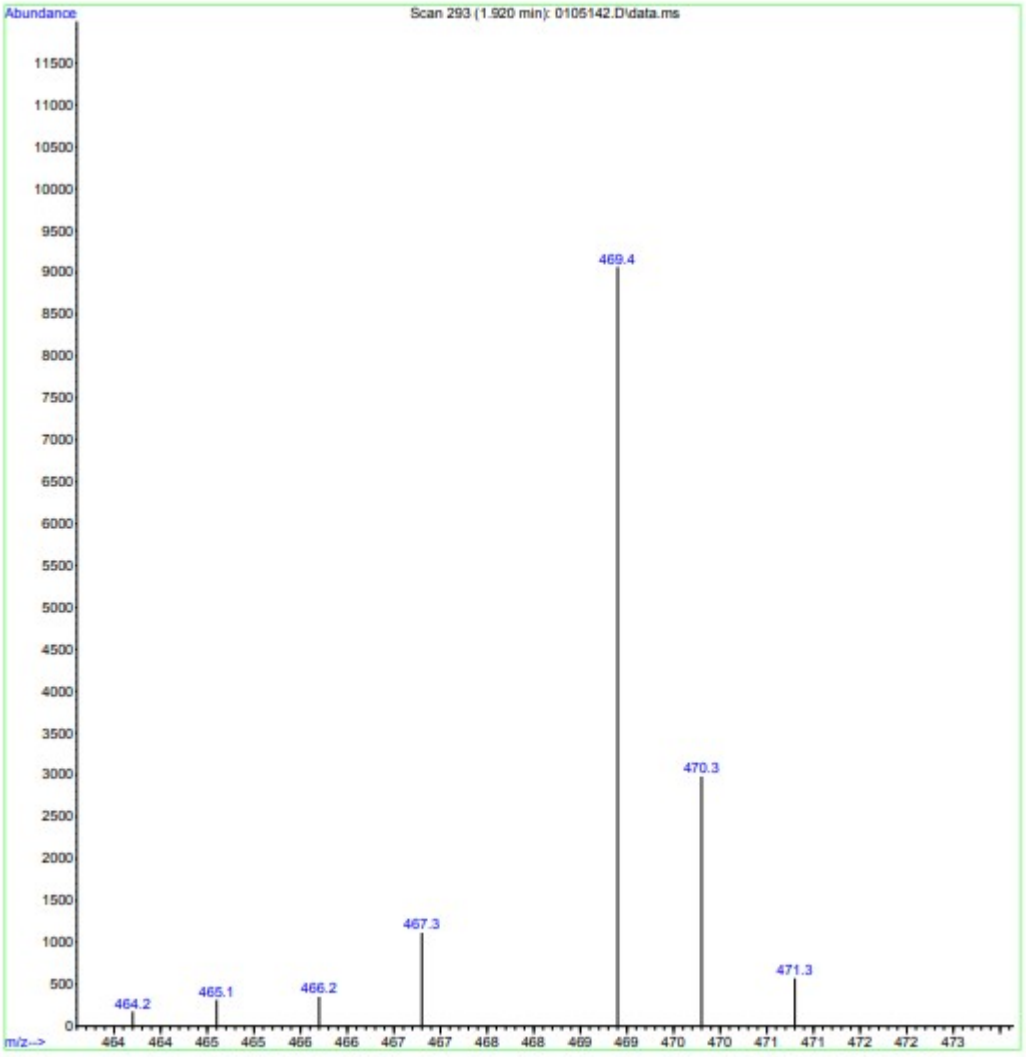

Fig. S6. Mass spectrum of L

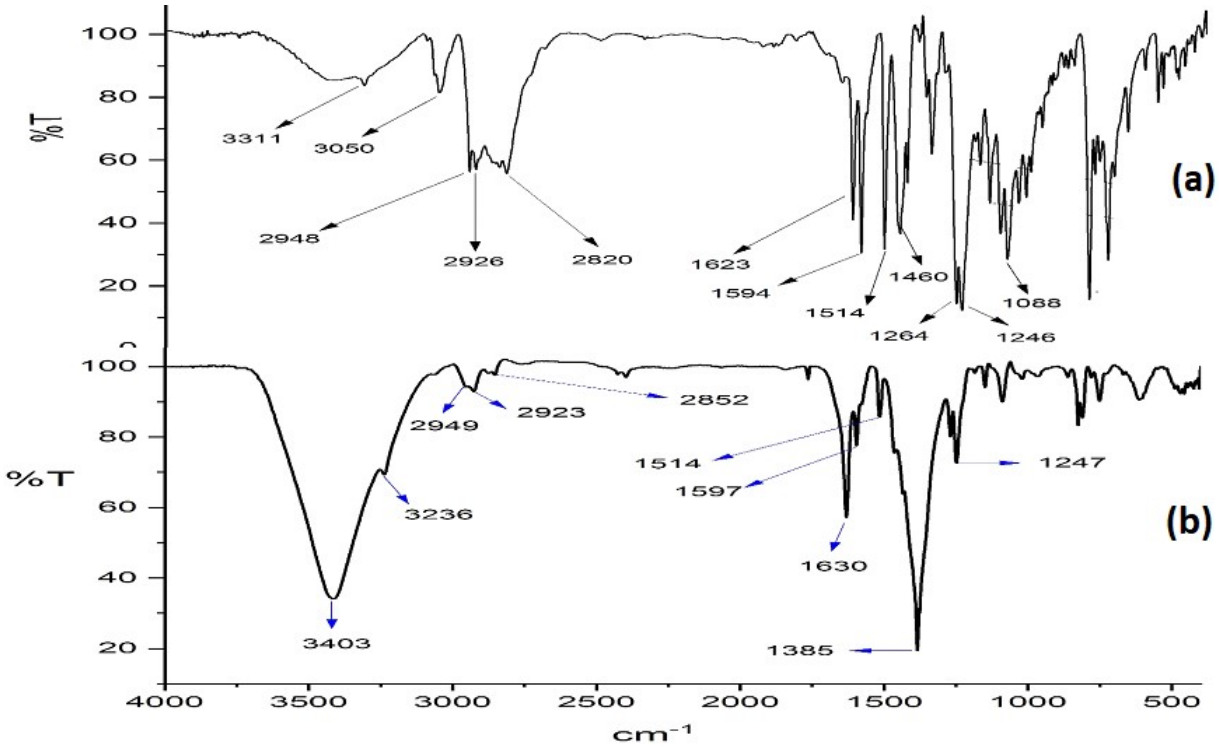

Fig. S7. IR spectra of L (a) L and (b) $[MgL]^{2+}$

Table S1. Selected bond lengths (Å) and angles (°) for $[MgL]^{2+}$ and L.

	$[MgL]^{2+}$		L
Bond length	(Å)	Distance	(Å)
Mg-O(1)	2.079	O(1)-N(1)	3.43
Mg-O(2)	2.110	O(1)-N(2)	5.16
Mg-N(1)	2.113	O(1)-N(3)	7.13
Mg-N(2)	2.200	O(2)-N(1)	5.76
Mg-N(3)	2.174	O(2)-N(2)	4.59
Bond angle	(°)	O(2)-N(3)	3.71
O(1)-Mg-O(2)	85.39	O(1)-O(2)	5.83

O(1)-Mg-N(1)	91.30	N(1)-N(2)	3.30
N(1)-Mg-N(2)	81.59	N(1)-N(3)	5.19
N(2)-Mg-N(3)	80.75	N(2)-N(3)	2.91
N(3)-Mg-O(2)	76.49		

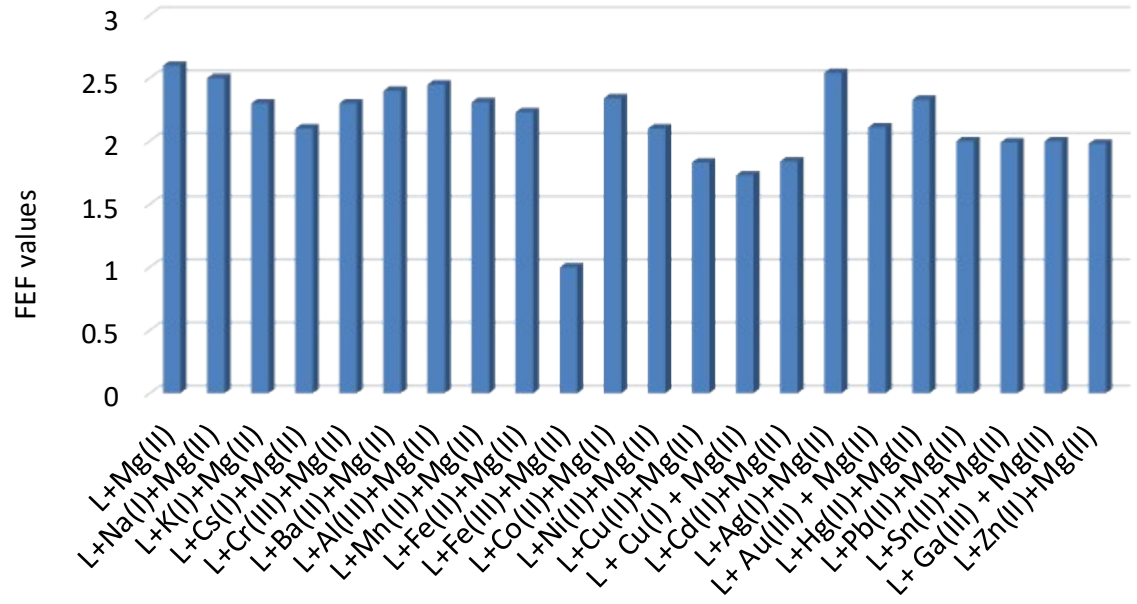

Fig. S8. The FEF value of (L + Mg^{2+}) in the presence of various metal ions in EtOH–H_2O solution (9:1, v/v) at room temperature.

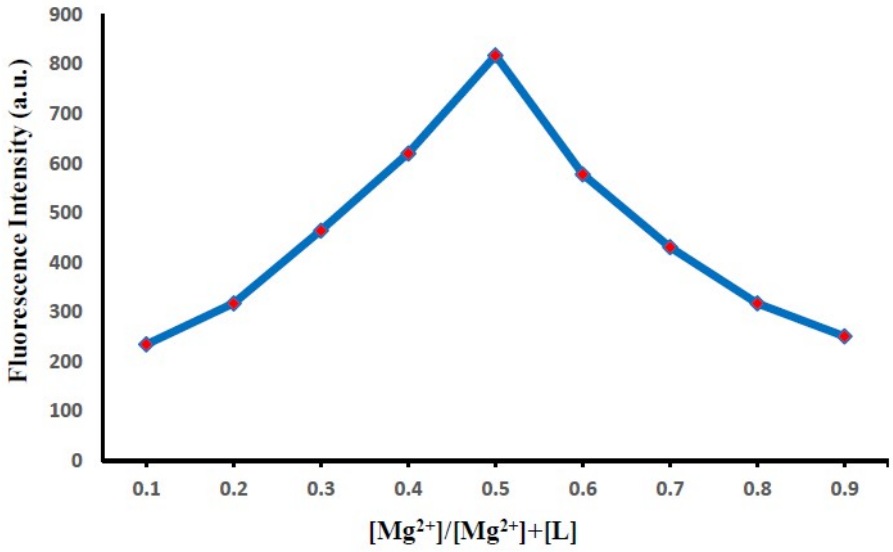

Fig. S9. Job's plot analysis of L and Mg^{2+}.

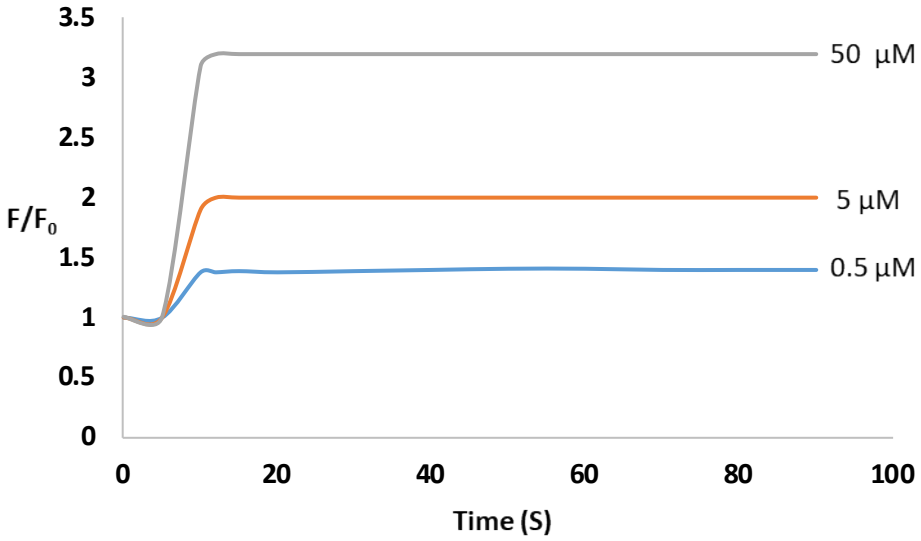

Fig. S10. Kinetics of the fluorescence enhancement of L (10 µM) in the presence of different concentrations of Mg^{2+}. Fluorescence intensity was recorded at 360 nm.

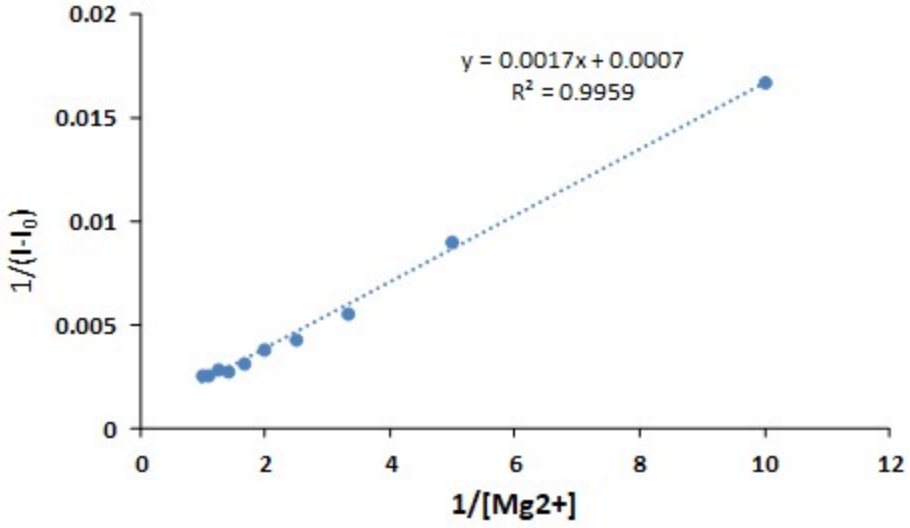

Fig. S11. Benesi-Hildebrand plot of L (10 μM) with Mg^{2+} in EtOH/H_2O (9:1, v/v) solution.

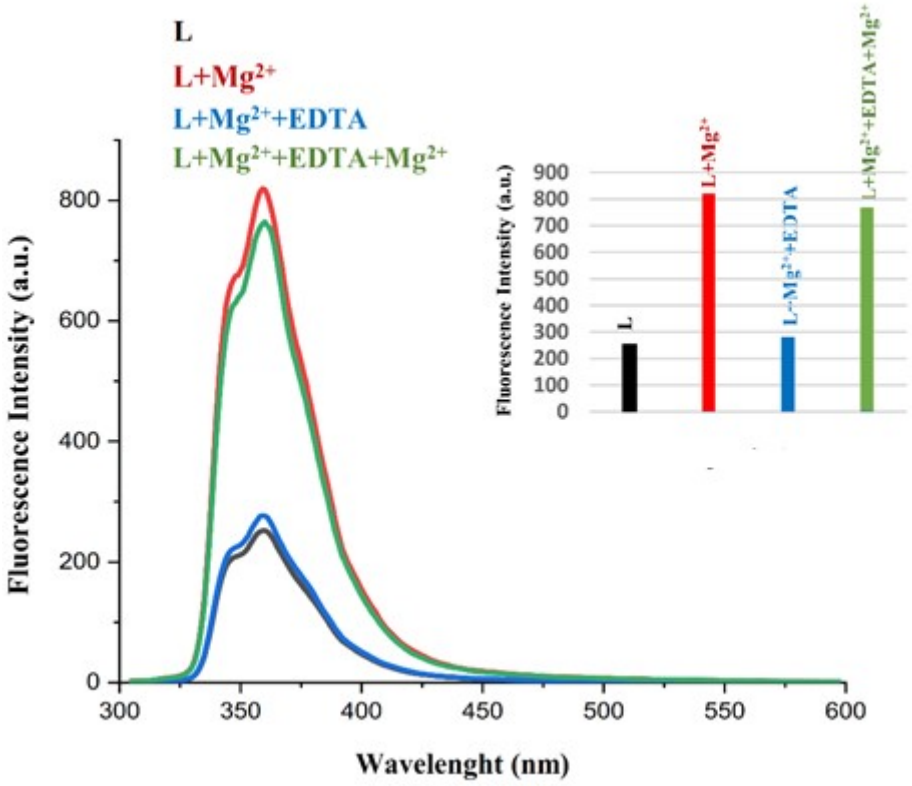

Fig. S12. Chemical reversibility behavior of the binding of L and $[MgL]^{2+}$ ions. Fluorescence intensity was recorded at 360 nm.