Supporting Information

Al^{3+} selective coumarin based reversible chemosensor: application in living cell imaging and as integrated molecular logic gate

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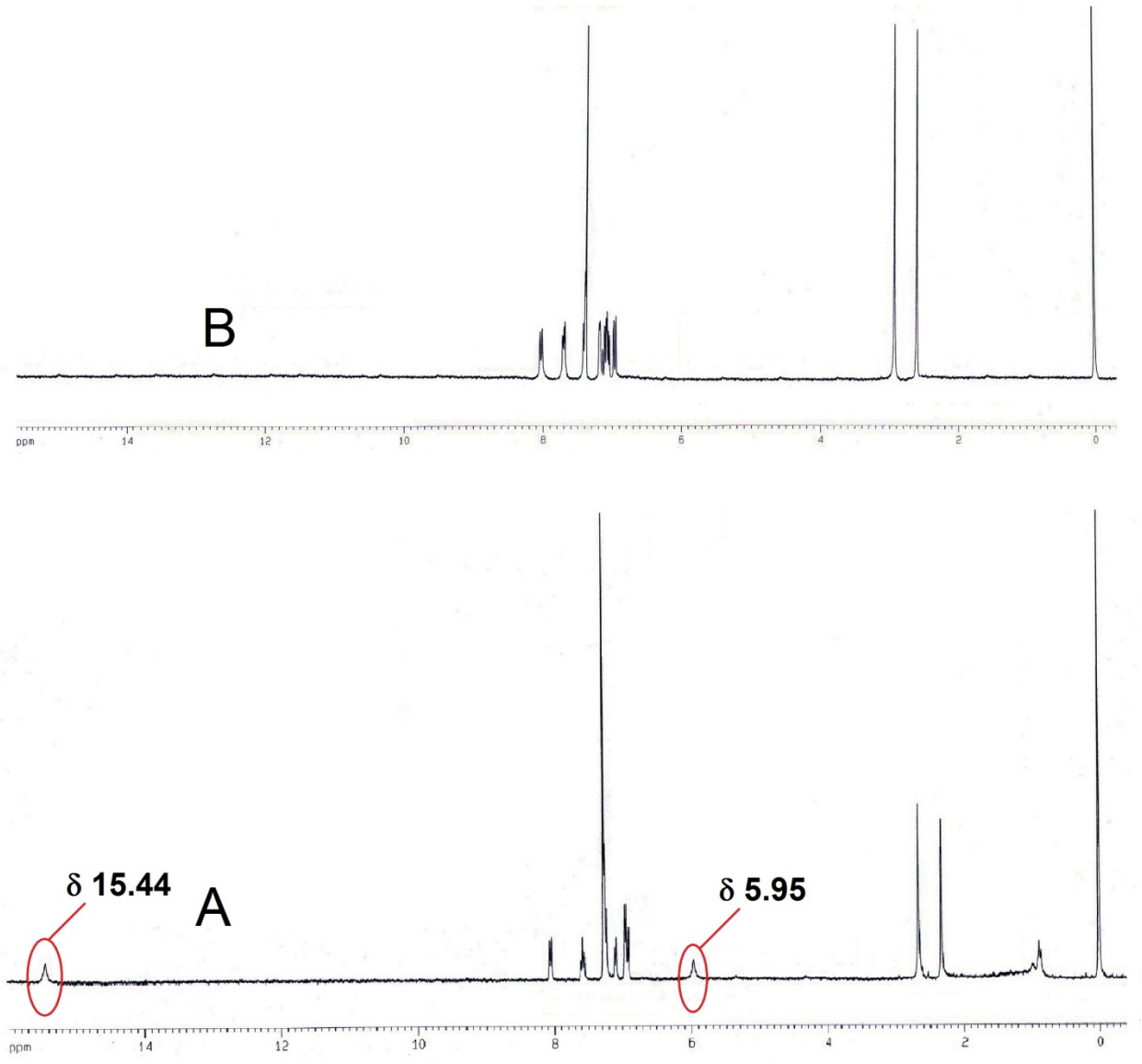

Fig. S1. ^{1}H-NMR spectra of H_2L (A) and H_2L-Al^{3+} (B) in $CDCl_3$

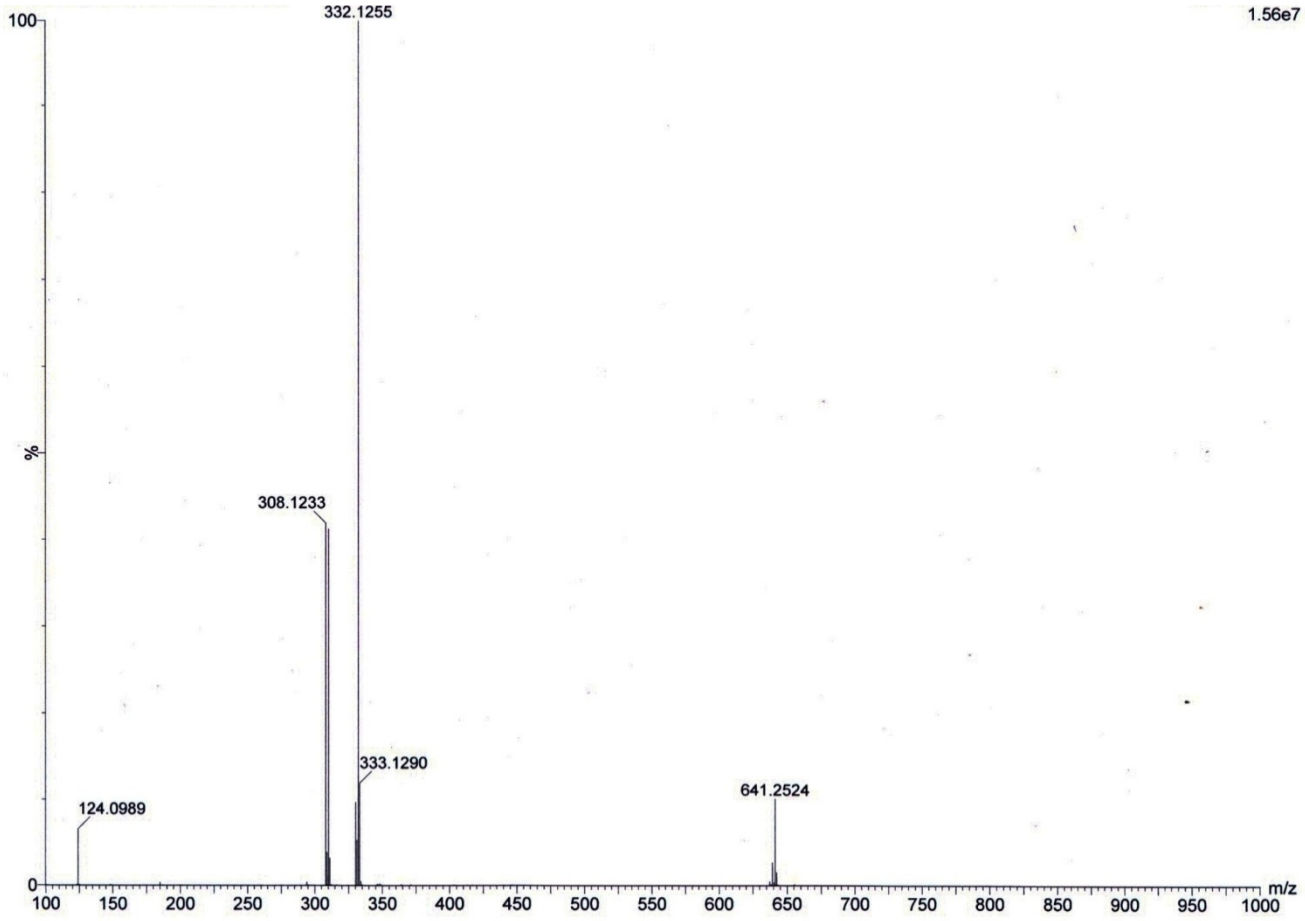

Fig. S2. HRMS spectra of the receptor H_2L

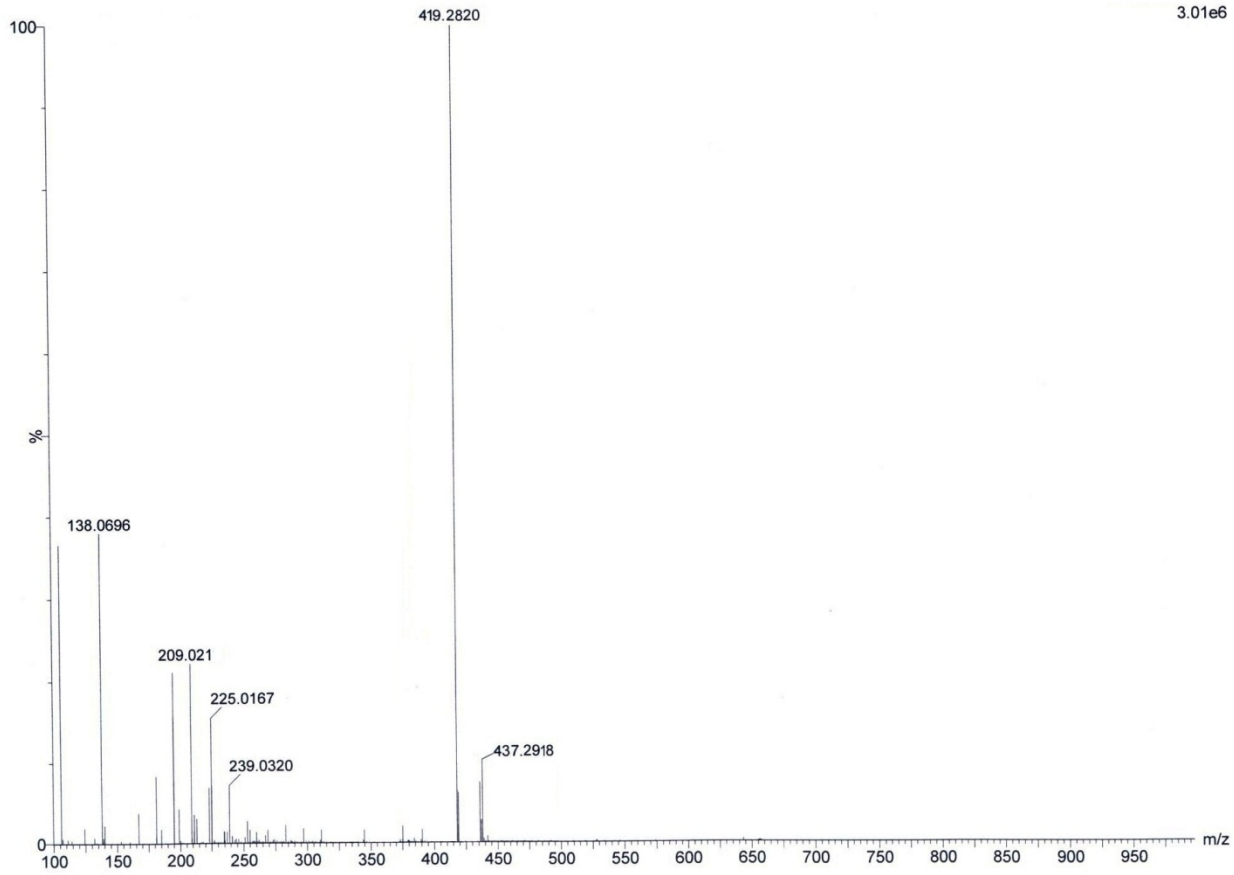

Fig. S3. HRMS spectra of the receptor H_2L-Al^{3+} complex

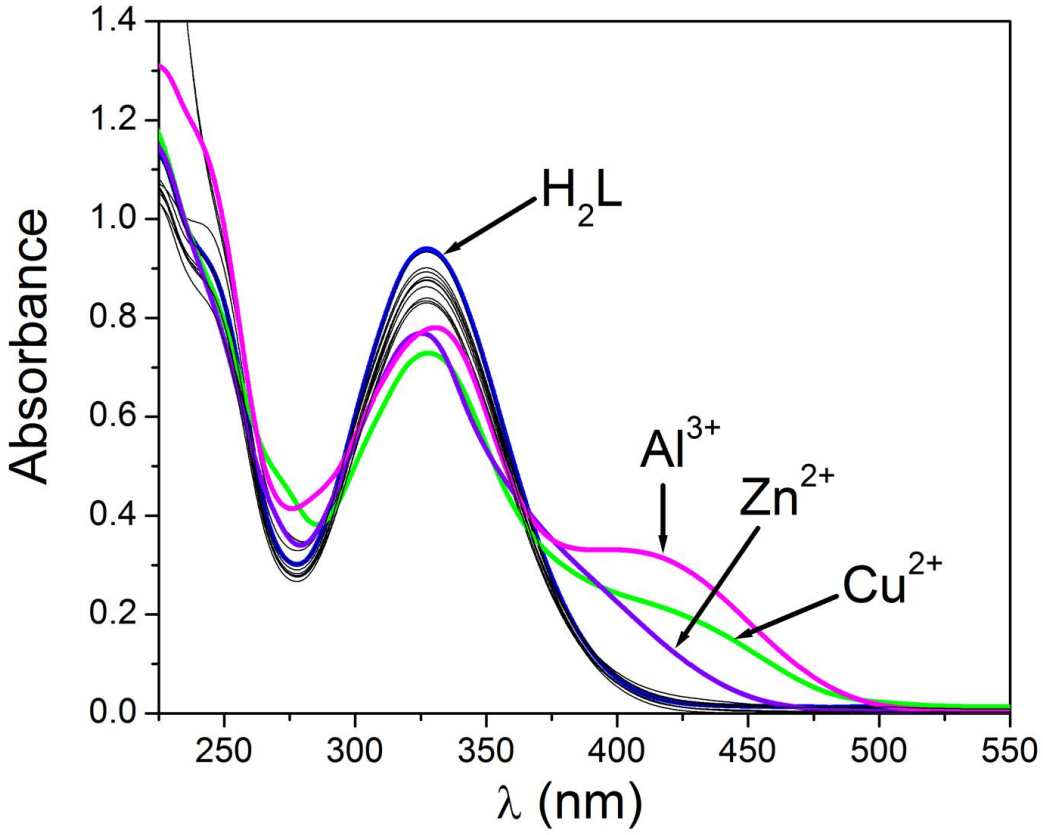

Fig. S4. UV-Vis spectra of chemosensor (HL) (10 μM) upon addition of 2 equivalent of various metal ions i,e, Na^{+}, K^{+}, Ca^{2+}, Mg^{2+}, Mn^{2+}, Fe^{3+}, Cr^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+} and Hg^{2} (100 μM)

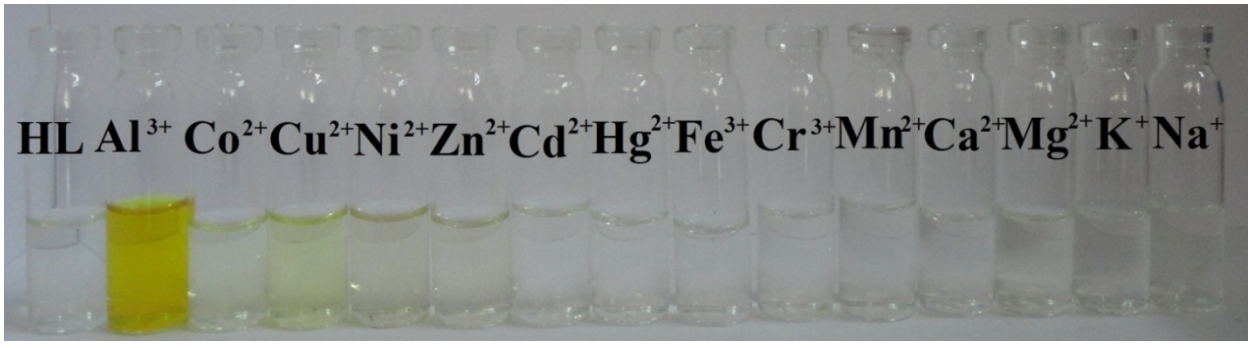

Fig. S5. Visual effect of addition of Al^{3+} to H_2L in comparison to other metals.

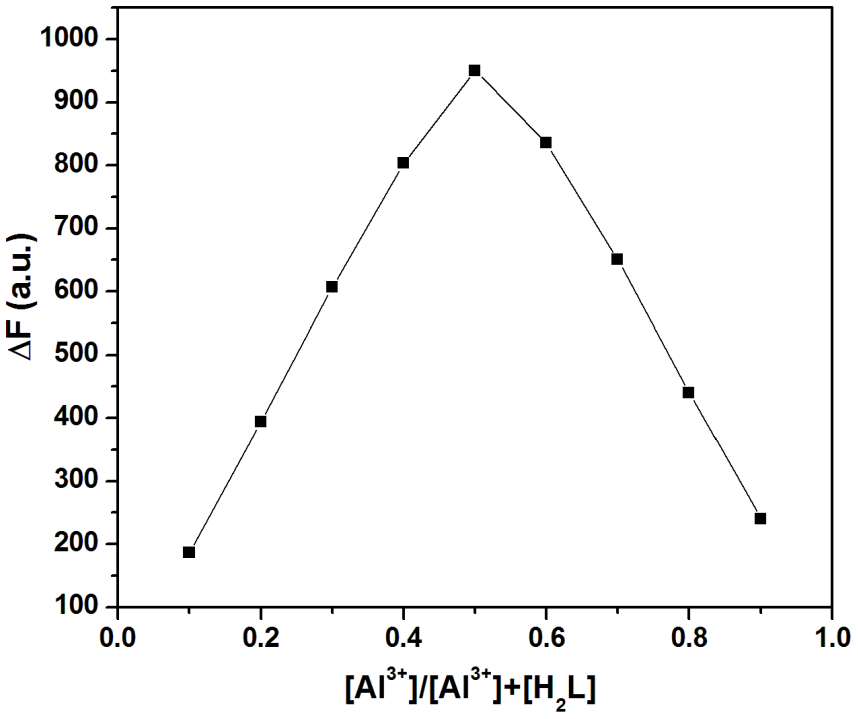

Fig. S6. Job's plot diagram of the receptor (H_2L) for Al^{3+} (where ΔF indicates the change of emission intensity at 398 nm)

Determination of detection limit:

The detection limit was calculated based on the fluorescence titration. To determine the S/N ratio, the emission intensity of H_2L without any analyte was measured by 10 times and the standard deviation of blank measurements was found to be 1.370320319×10^{-4}.

The limit of detection (LOD) of H_2L for Al^{3+} was determined from the following equation: LOD = K × σ Where K = 3 in this case and σ = $(Sb_1)/(S)$; Sb_1 is the standard deviation of the blank solution; S is the slope of the calibration curve.

From the graph we get slope = 104.52, and Sb_1 value is 1.370320319×10^{-4} (**Fig. S8**). Thus using the formula we get the LOD = 0.393 μM.

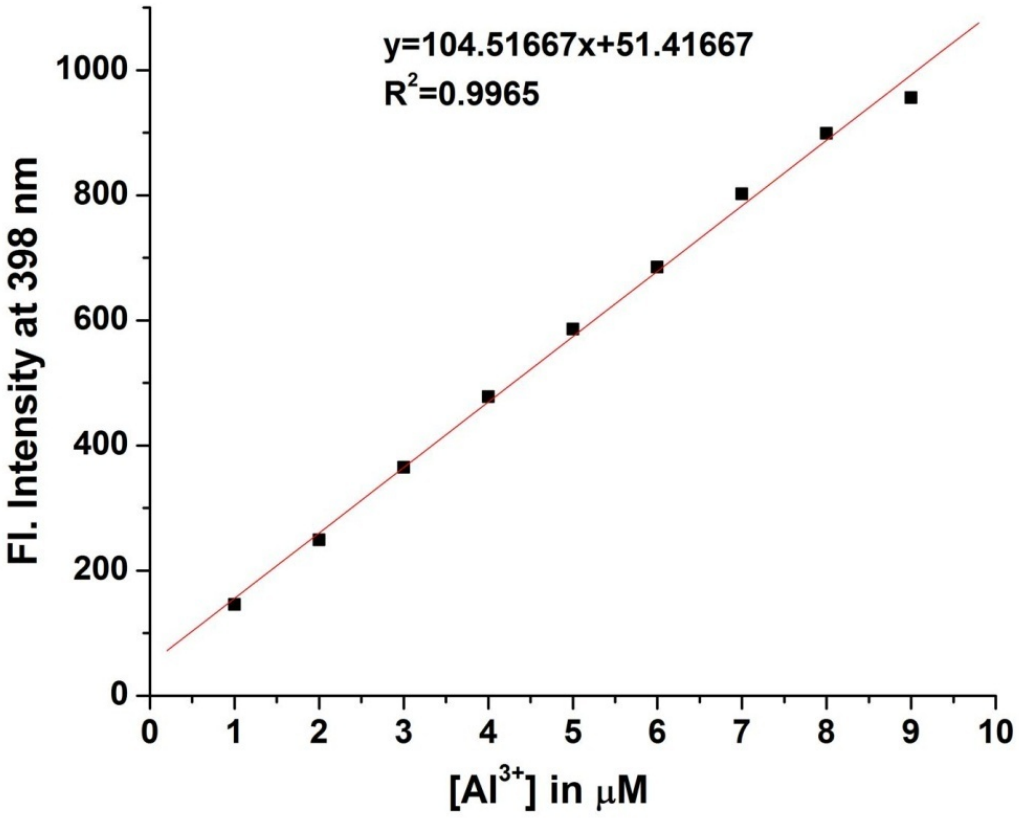

Fig. S7. Linear response curve of H_2L at 398 nm depending on the Al^{3+} concentration.

Determination of binding constant from Fluorescence titration data:

Binding constant was calculated according equation. The binding constant β was calculated following the equation stated below.

$$\text{Log } (F-F_{min})/(F_{max}-F) = n\log [M^{n+}] + B$$

Here F_{min}, F and F_{max} indicate the emission intensity in absence of, at intermediate and at infinite concentration of metal ion respectively. $B = \log\beta$, where β is the total binding constant and n is the number of Al^{3+} bind per ligand. From the plot n = 1.17 indicating 1:1 stoichiometry for the formed HL-Al^{3+} complex (**Fig. S8**). From the intercept β is found to be 1.48×10^6.

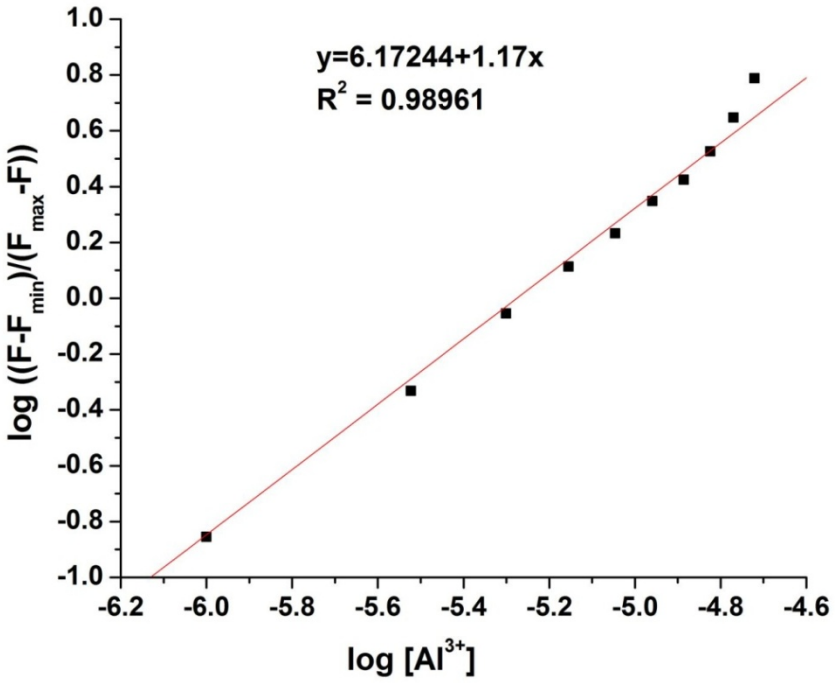

Fig. S8. Determination of binding constant of H_2L for Al^{3+} from fluorescent titration data

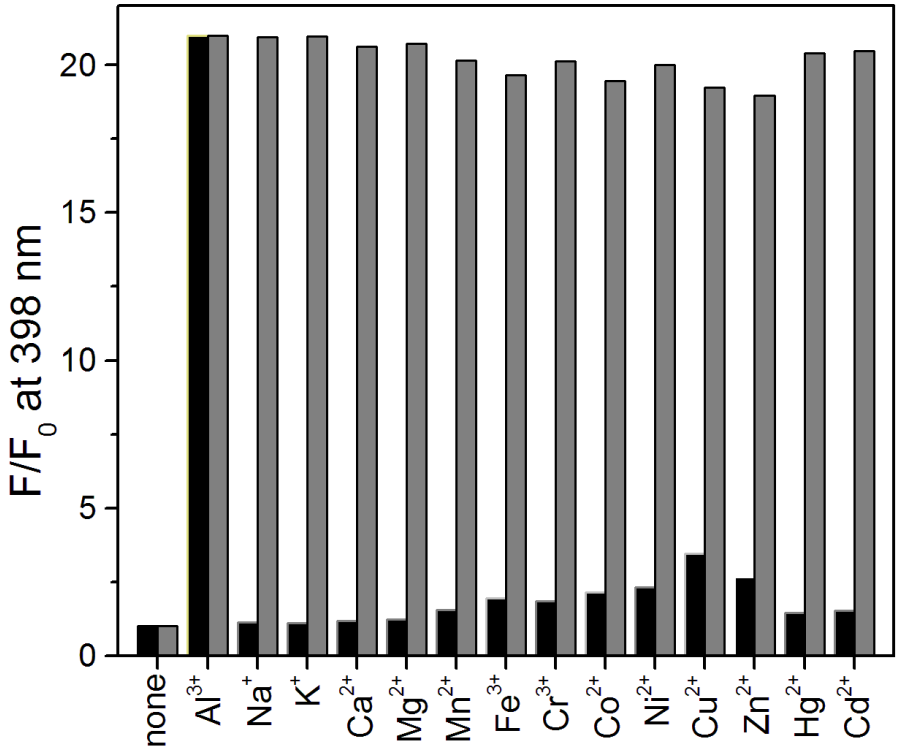

Fig. S9. Change in emission intensity of chemosensor (H_2L) upon addition of 1 equivalent of Al^{3+} along with 2 equivalents of other metal ions to the receptor H_2L

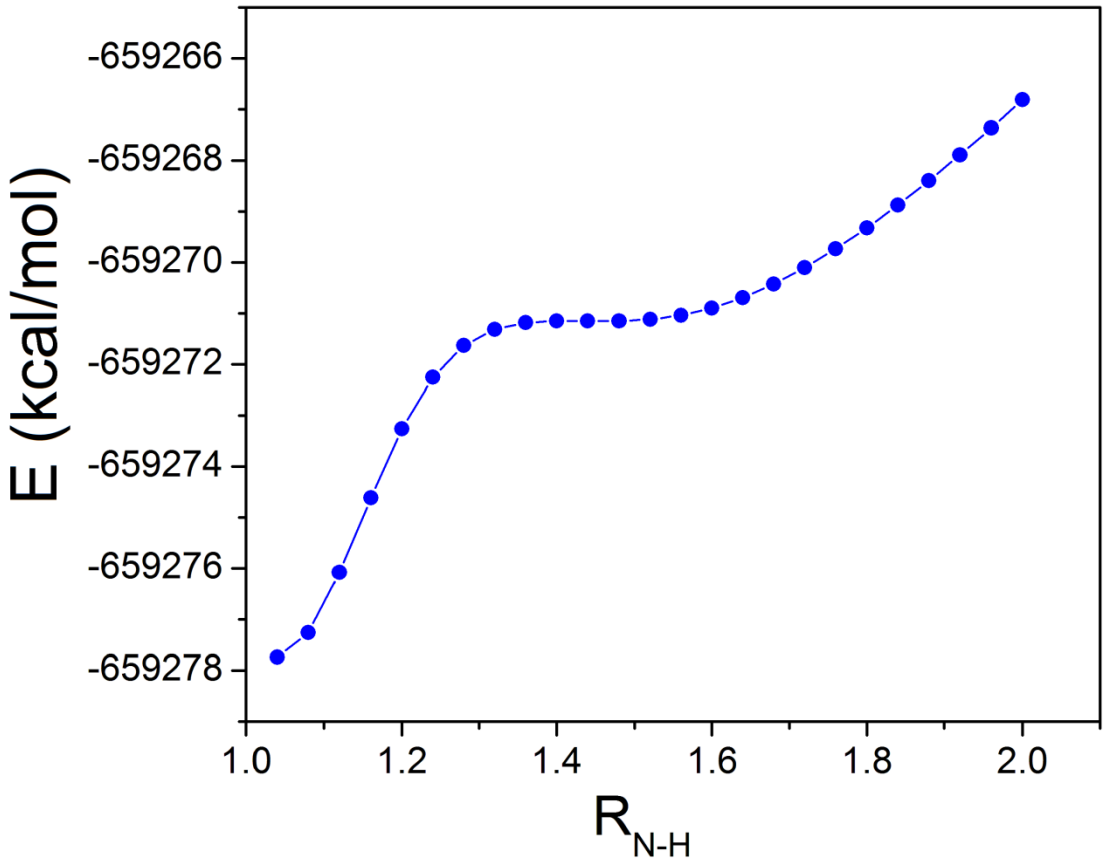

Fig. S10. Potential energy scan in singlet ground (S_0) state of H_2L by DFT/B3LYP/6-311G(d) method

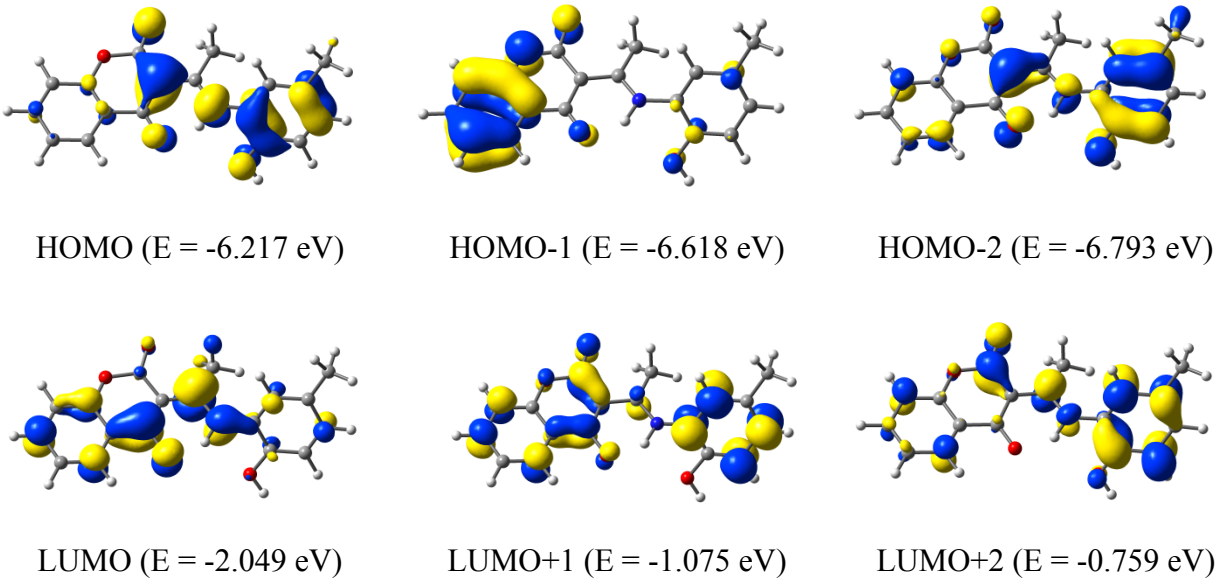

Fig. S11. Contour plots of selected molecular orbitals of chemosensor (H_2L)

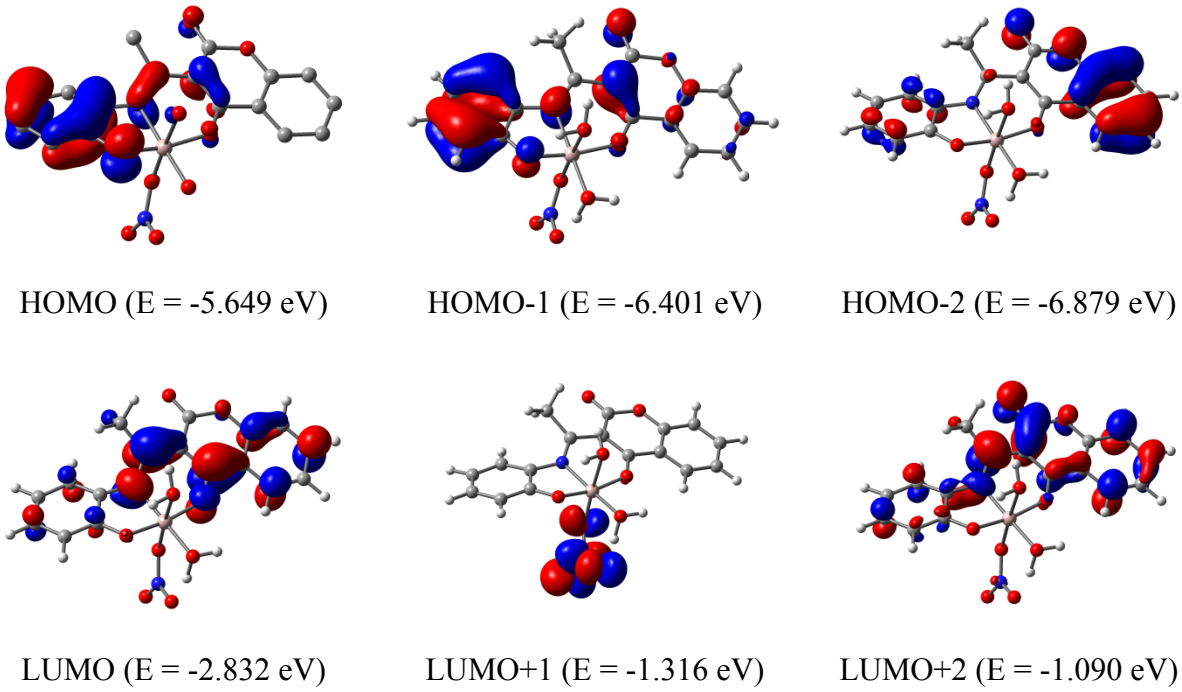

Fig. S12. Contour plots of selected molecular orbitals of H_2L-Al^{3+}