Electronic Supplementary Information for

Highly selective colorimetric and reversible fluorometric turn-off sensors based on pyrimidine derivative: mimicking logic gate operation and potential application

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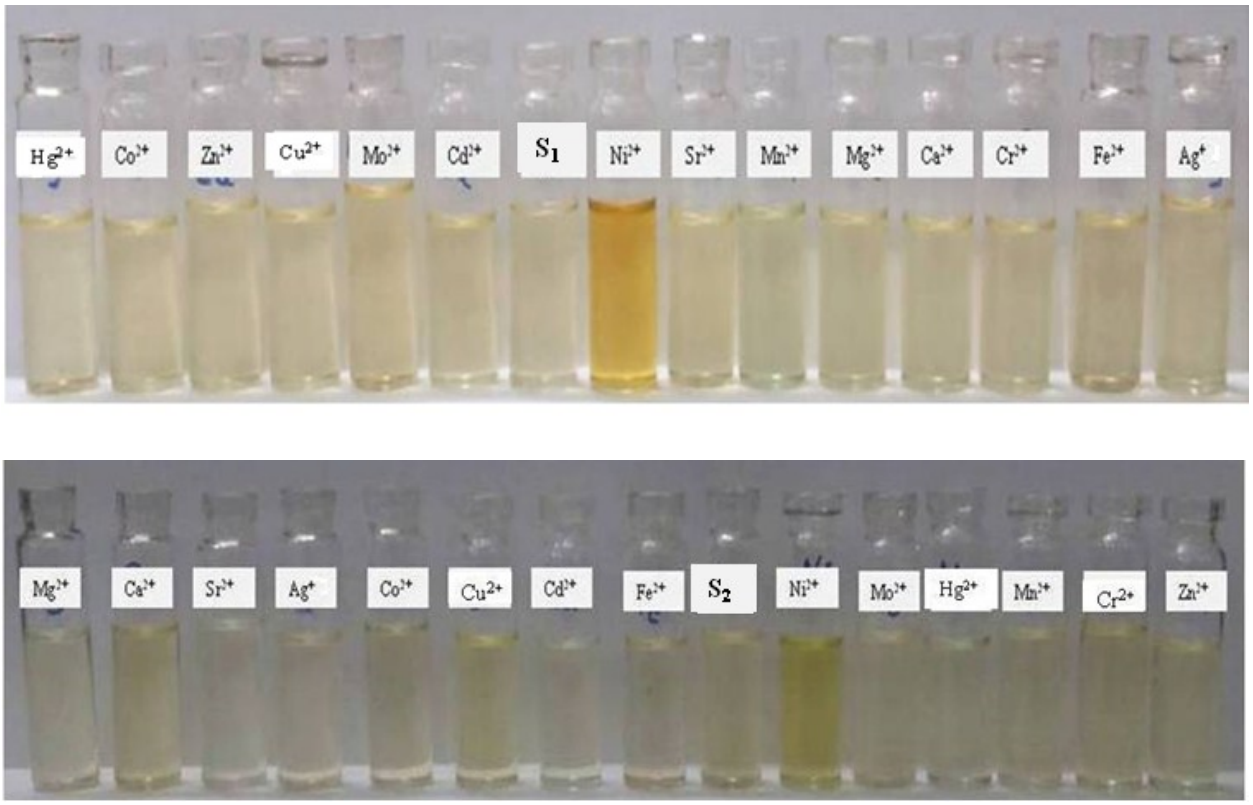
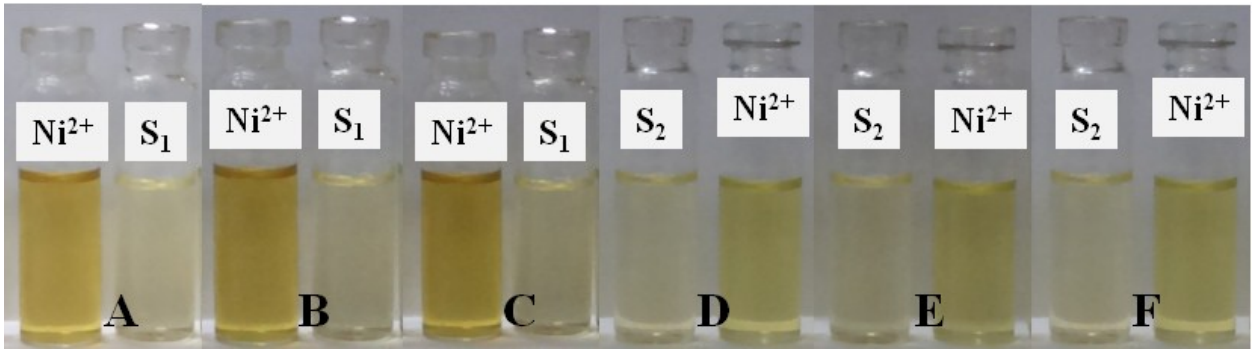
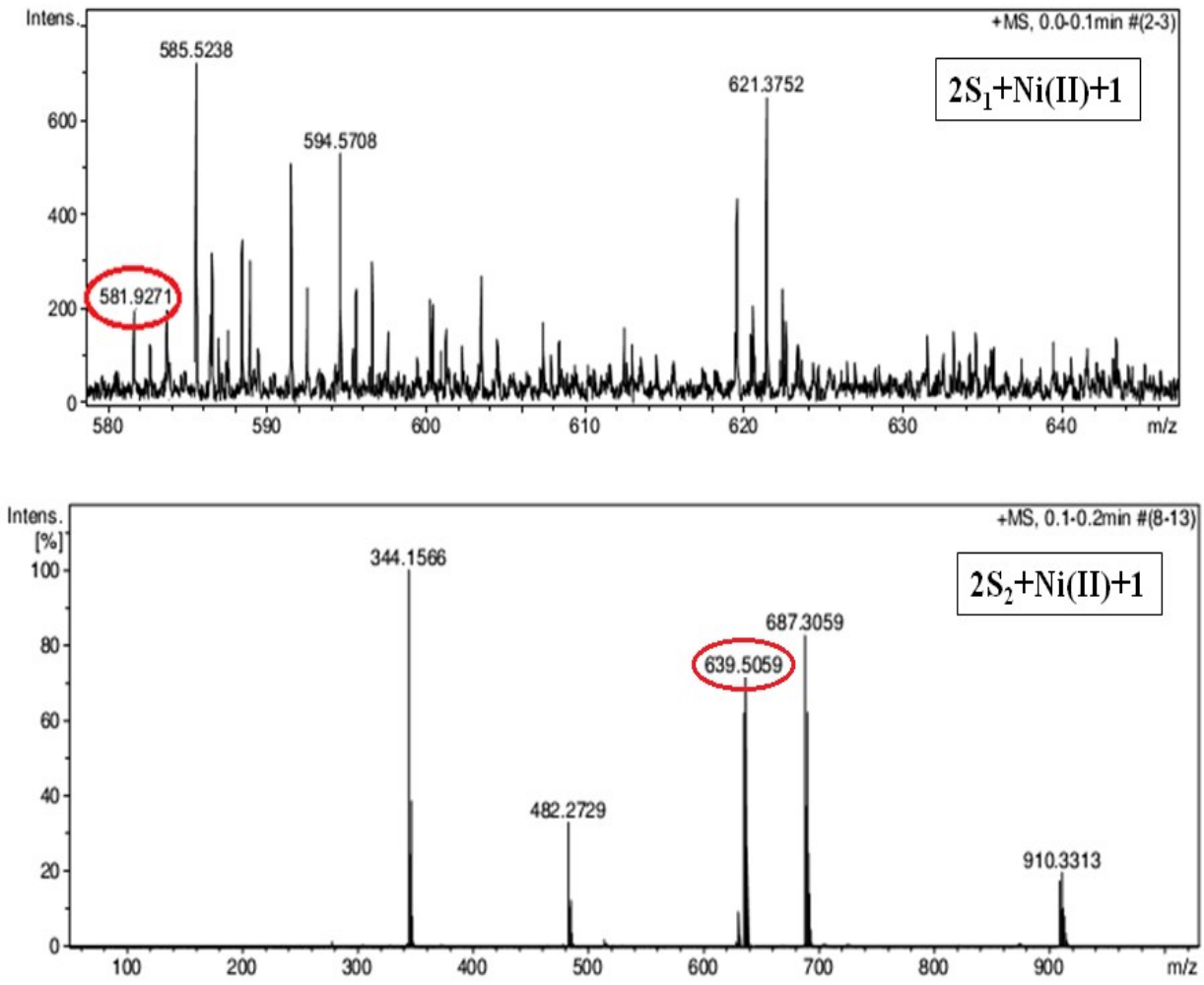


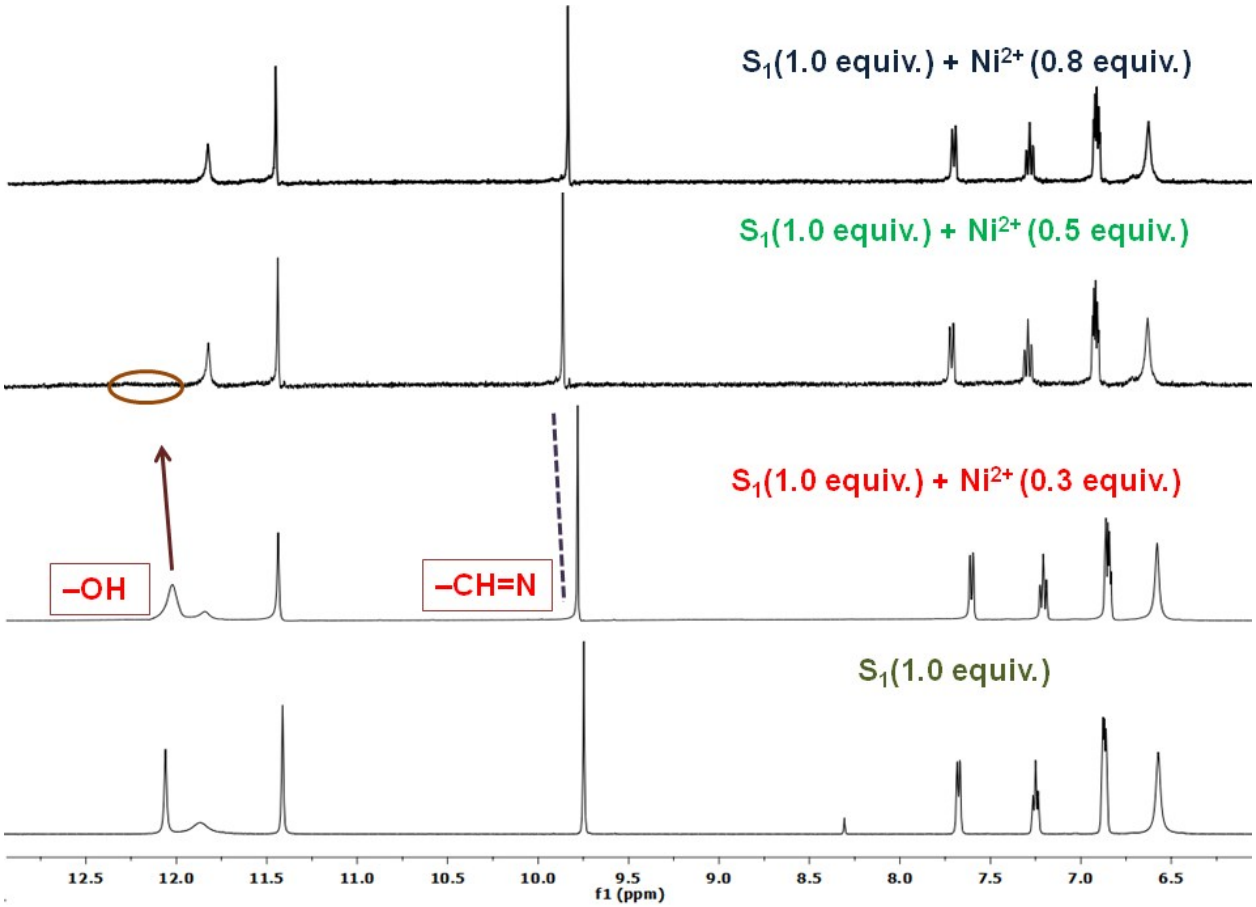
ESI Fig. 1 Visual ion sensing of S_1 and S_2 with various metal ions in DMF.



ESI Fig. 2 Stability in color of complex S-Ni(II) with definite interval of time (A,D) 0 hour, (B,E) after 24 hours, (C,F) after 36 hours.



ESI Fig. 3 LC-HRMS (ESI+) mass spectra of (2:1) complex of S_1, S_2 with Ni(II) ion.

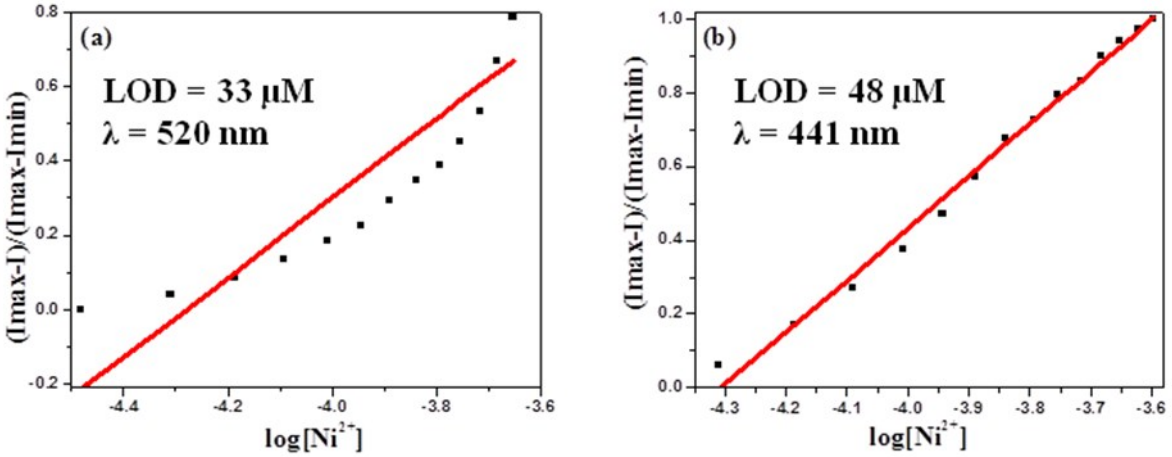


ESI Fig. 4 ^{1}H NMR titration spectra of S_1 in DMSO-d_6 upon addition of different equivalents of Ni(II) ion.

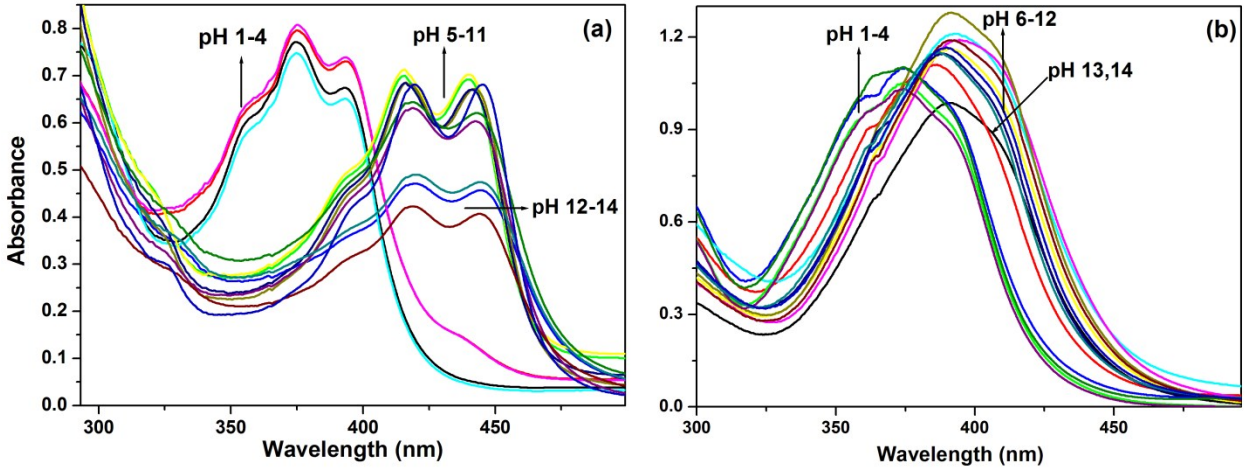
Determination of detection limit

Fluorescence intensity of S_1 and S_2 at each concentration of Ni(II) added, normalized between the maximum fluorescence intensity, found at zero equiv of Ni(II), and the minimum fluorescence intensity, found at [Ni(II)] = 5×10^{-6} M.

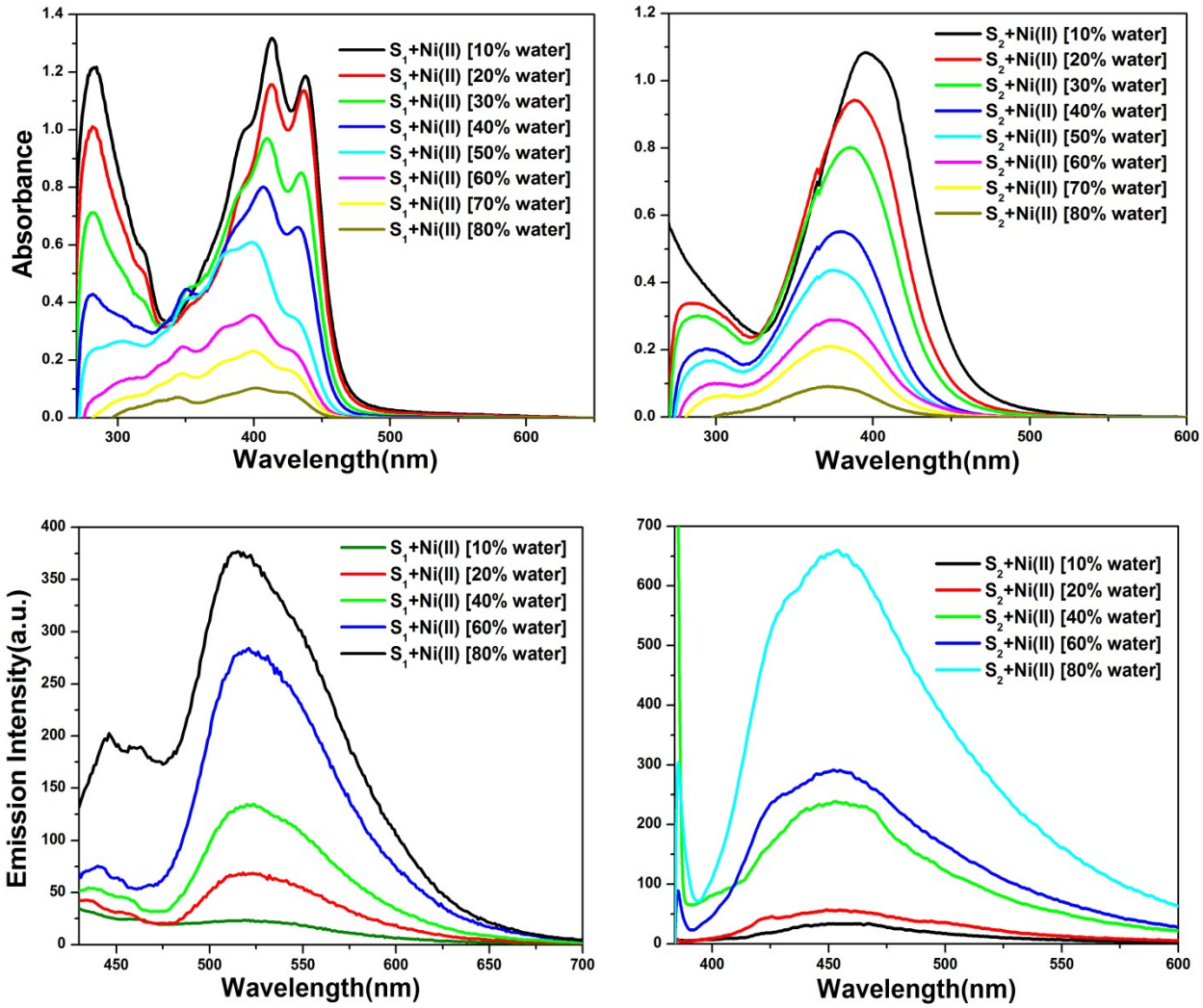
The limit of detection (LOD) values have been calculated by using the intercept of a plotted graph between $(I - I_{min})/(I_{max} - I_{min})$ and log[Ni(II)].



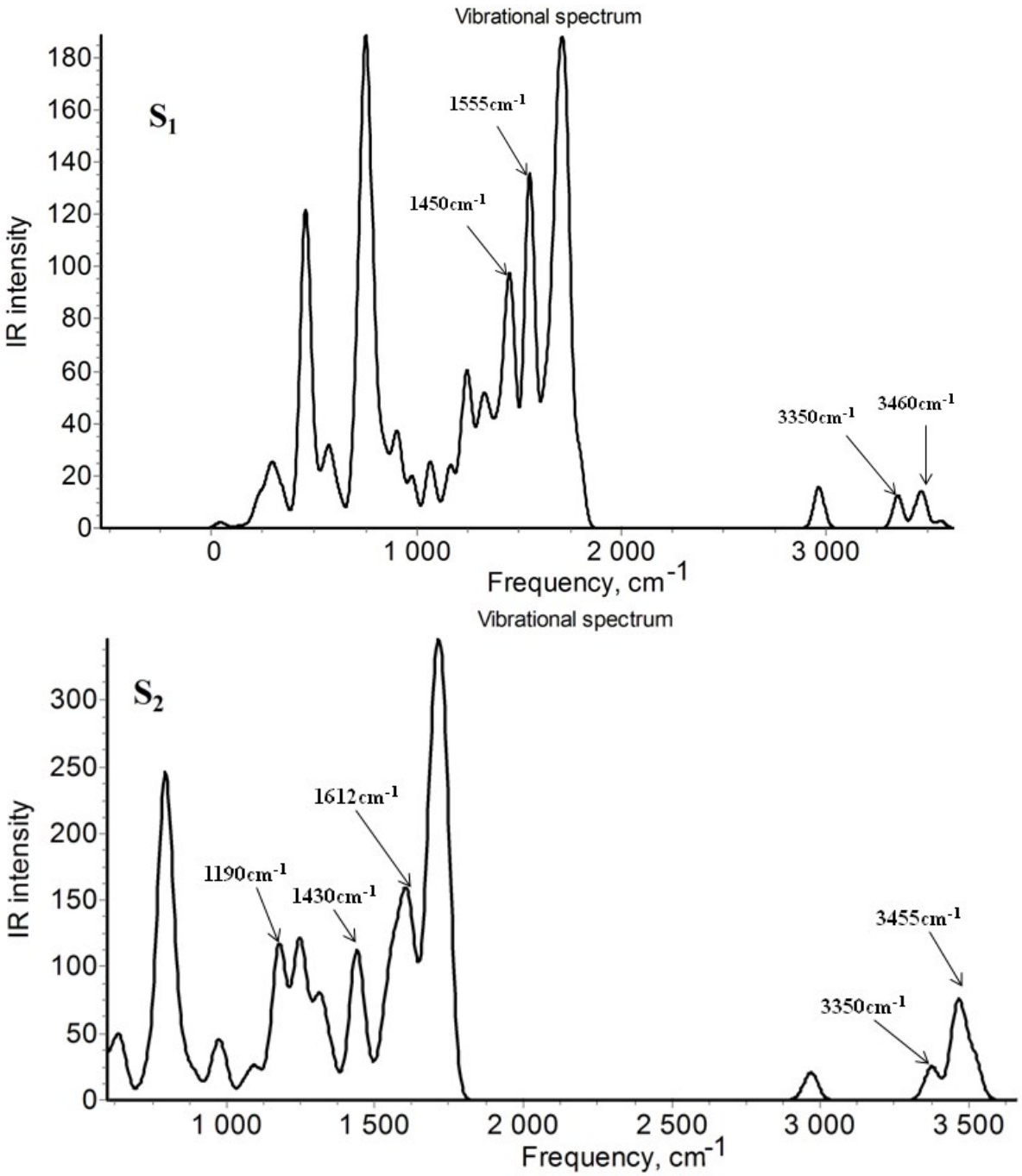
ESI Fig. 5 The limit of detection (LOD) calculated by fluorescence emission linear fitting.



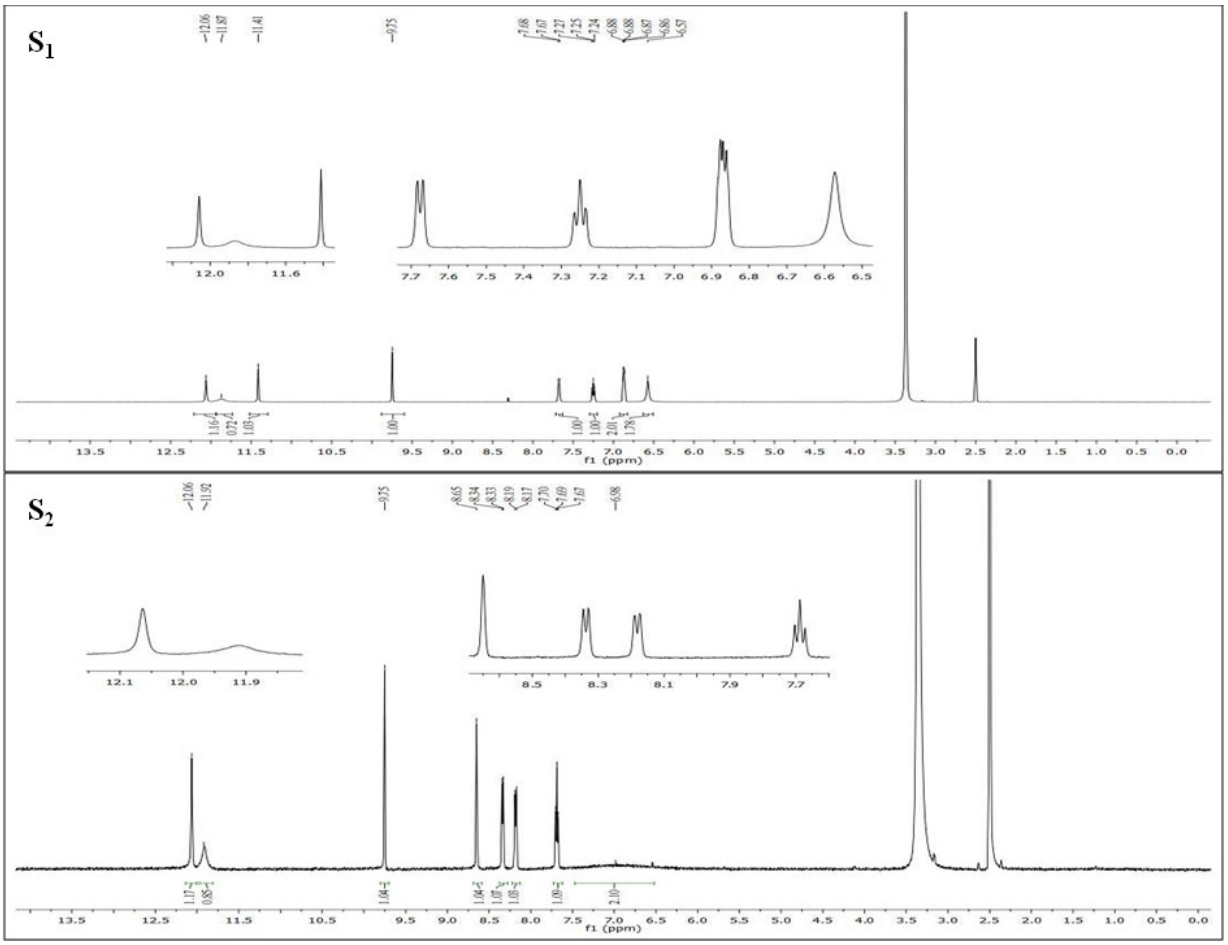
ESI Fig. 6 Effect of pH on absorption study of S_1 (a) and S_2 (b) in DMF.



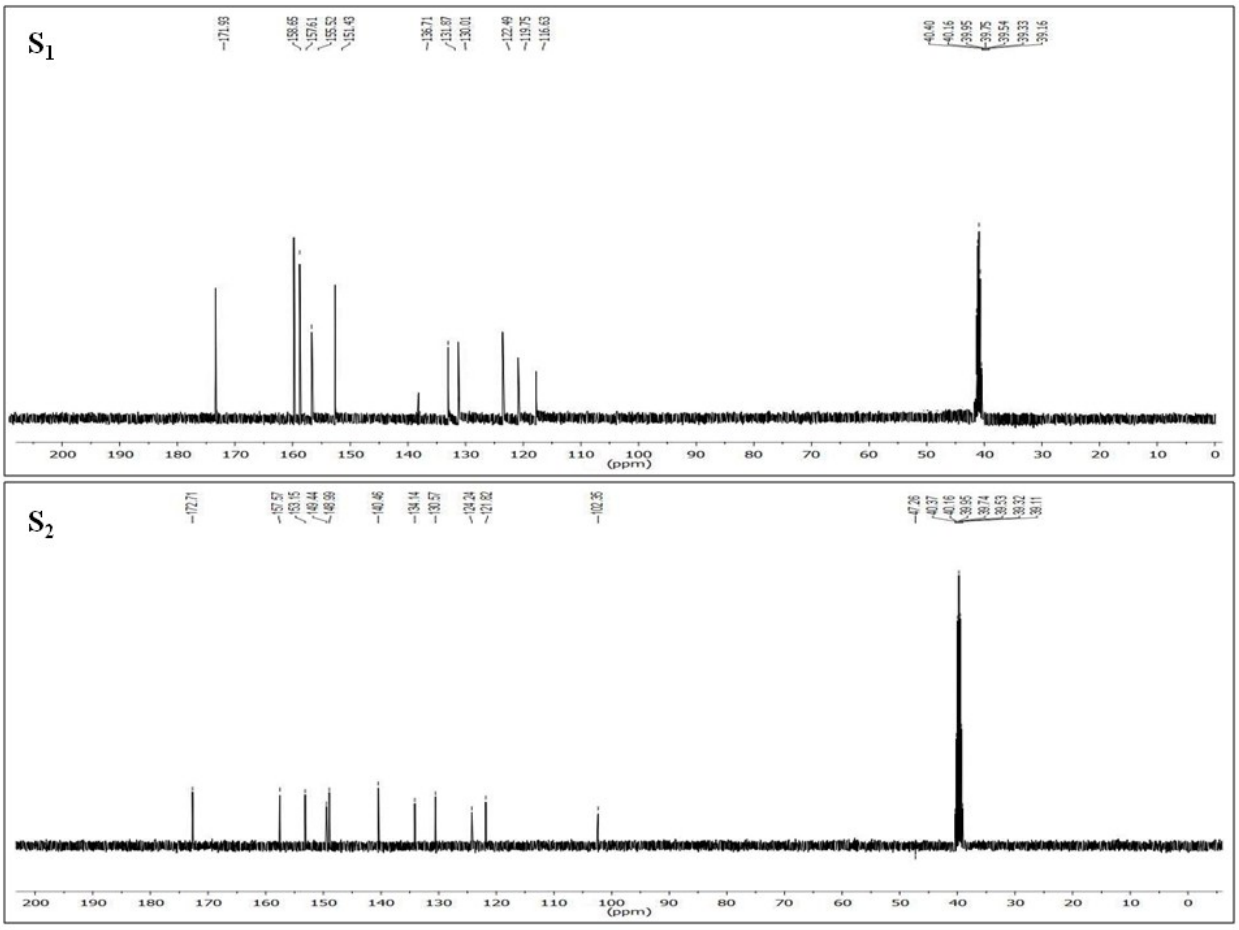
ESI Fig. 7 Effect of water content on absorption study and emission intensity of S_1 and S_2 in DMF.



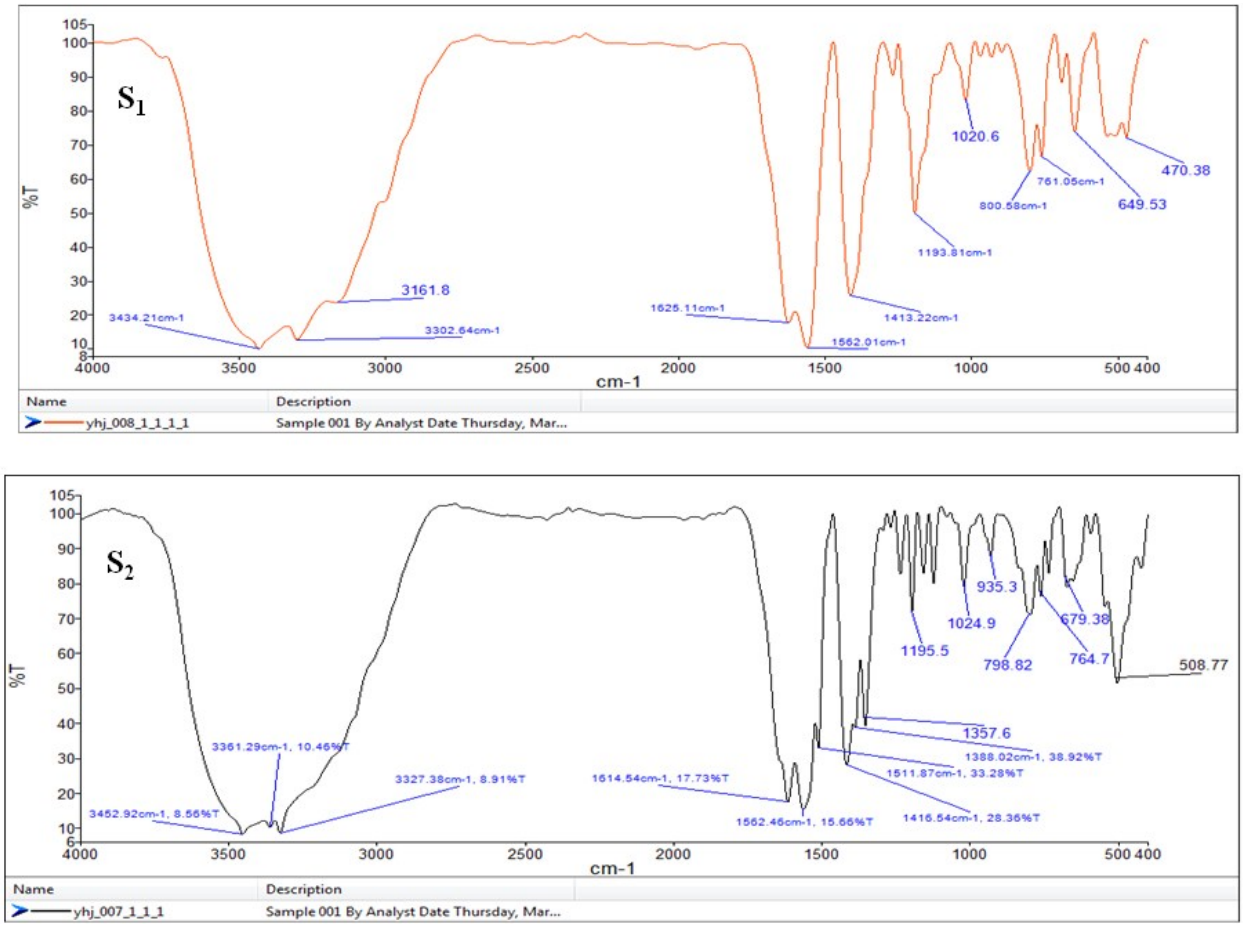
ESI Fig. 8 Optimised IR frequencies of receptors S_1 and S_2.



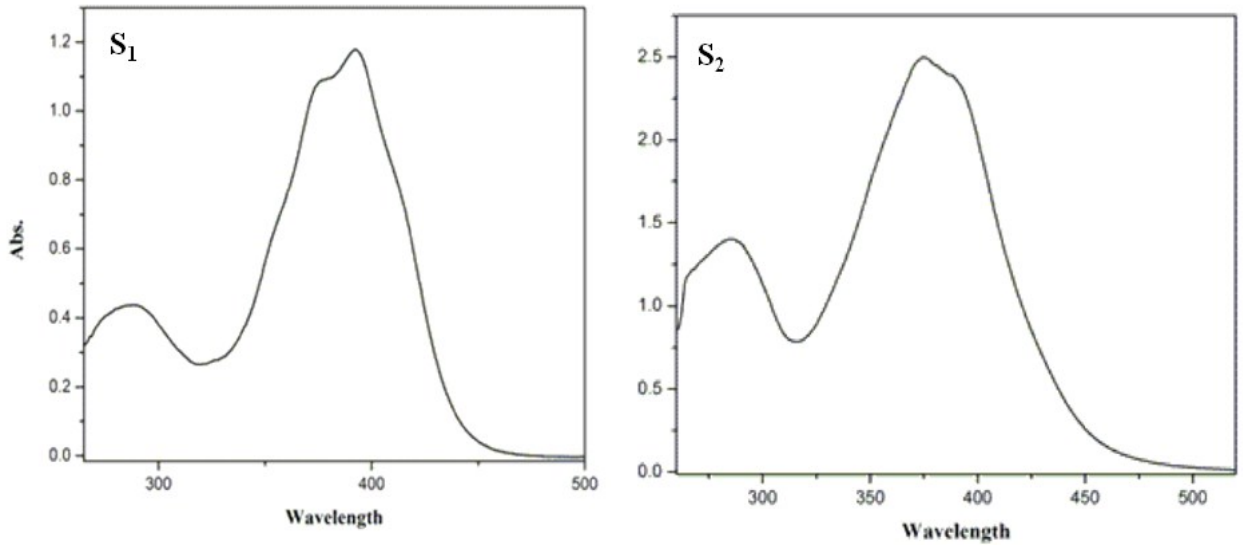
ESI Fig. 9 ^{1}H NMR spectra of receptors S_1 and S_2 in DMSO-d_6 at room temperature.



ESI Fig. 10 ^{13}C NMR spectra of receptors S_1 and S_2 in DMSO-d_6 at room temperature.



ESI Fig. 11 FT-IR spectra of receptor S_1 and S_2.



ESI Fig. 12 UV-Vis spectra of receptor S_1 and S_2.

ESI Table 1 Determination of nickel ion concentration in waste water samples with the receptor S_1.

Sample	Addition of nickel ion	Uv-Vis study[a]	AAS study[a]	Recovery of Receptor S_1(%)
River Ganga (Roorkee)	4.00×10^{-5}	3.75×10^{-5}	3.60×10^{-5}	93.75%
River Ganga (Haridwar)	4.00×10^{-5}	3.88×10^{-5}	3.72×10^{-5}	97.0%
Tap Water (Roorkee)	4.00×10^{-5}	3.91×10^{-5}	3.65×10^{-5}	97.75%

[a]Standard deviation calculation for five measurements