

Supporting information

5-(hydroxyimino)quinolin-8-one (**HL**) was prepared as follows: 8-hydroxyquinoline (0.725 g, 5 mmol) was added to a solution of sulphuric acid (0.3 mL, 32 M) in distilled water (20 mL) with vigorous stirring at 15-18°C. A solution of sodium nitrite (0.367 g) in water (10 mL) was added dropwise over 30-40 minute at 18-20°C. The reaction was allowed to proceed under cold condition for 3hs. The reaction mixture was neutralized with solution of 24 % sodium hydroxide to pH 8-9 and then acidified to pH 5-6 by adding glacial acetic acid. At this stage care is taken so that the temperature of the solution does not exceed 25°C. The precipitate was filtered, washed with distilled water (3×50 mL) and recrystallised from 1:1 acetone-DMF solvent mixture. IR (KBr, cm^{-1}): 3436 (w), 3056 (w), 2933 (w), 2814 (w), 2702 (m), 1656 (s), 1601 (w), 1581 (w), 1459 (m), 1388 (w), 1331 (w), 1316 (w), 1131 (m), 1095 (w), 977 (s), 823 (w), 792 (w), 692 (w). $^1\text{H-NMR}$ (DMSO- d_6): 13.4 (s, 1H), 8.87 (t, $J = 0.8$ Hz, 1H), 8.57 (d, $J = 8.4$ Hz, 1H), 8.03 (d, $J = 10.8$ Hz, 1H), 7.74 (q, $J = 4.8$ Hz, 1H), 6.75 (d, $J = 10.4$ Hz, 1H). $^{13}\text{C-NMR}$ (DMSO- d_6): 183.4, 151.6, 145.2, 144.7, 131.9, 131.3, 130.4, 127.4, 126.0.

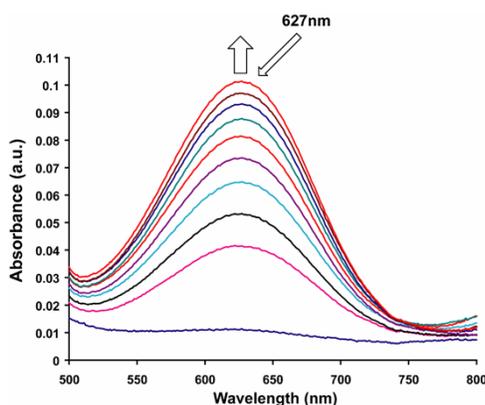


Figure S1: Changes in visible absorption spectra of **HL** (10^{-4} mol/L in DMSO) on several additions of 30 μL of TBAF (10^{-3} mol/L in DMSO) in acidic condition (4.0 pH).

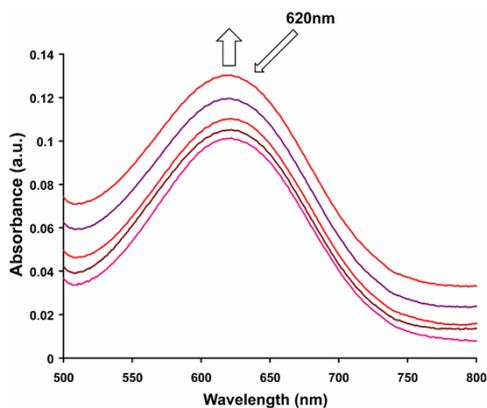


Figure S2: Changes in visible spectra of **HL** (10^{-4} mol/L in DMSO) on several additions of 30 μ L of TBAF (10^{-3} mol/L in DMSO) in neutral condition (7.0 pH).

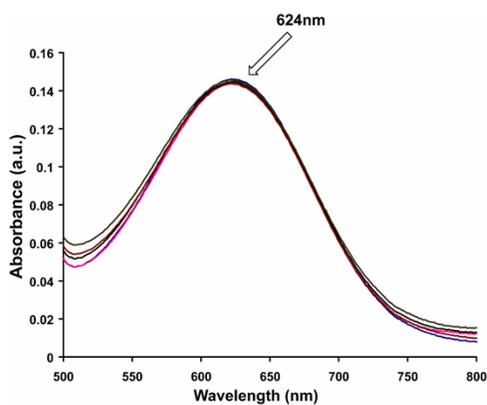


Figure S3: Changes in visible spectra of **HL** (10^{-4} mol/L in DMSO) on several additions of 30 μ L of TBAF (10^{-3} mol/L in DMSO) in basic condition (9.2 pH).

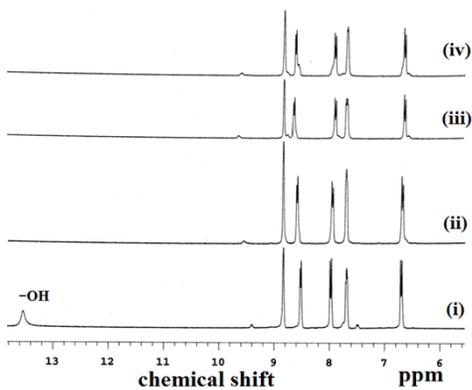


Figure S4: The aromatic region of the ^1H -NMR spectra of **HL** on addition of (ii) 5 μ L (iii) 10 μ L and (iv) 15 μ L triethylamine in DMSO-d_6 .

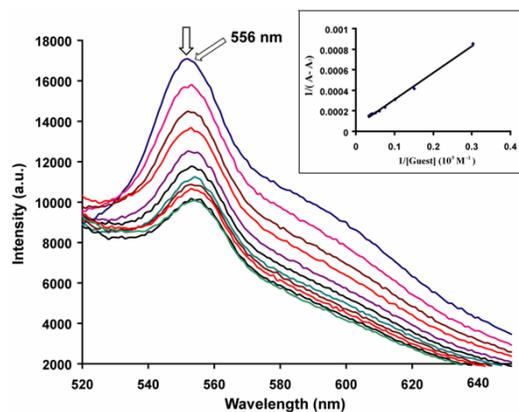


Figure S5: Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L in DMSO) on addition of TBAF in $10 \mu\text{L}$ (10^{-3} mol/L in DMSO) in each aliquot (inset is binding constant plot of **HL** with TBAF).

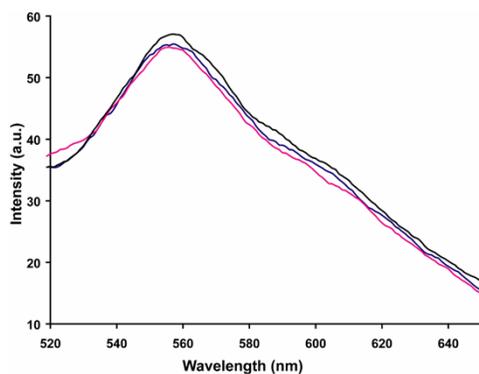


Figure S6: Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L in DMSO) on addition of TBACl in $10 \mu\text{L}$ (10^{-3} mol/L in DMSO) in each aliquot.

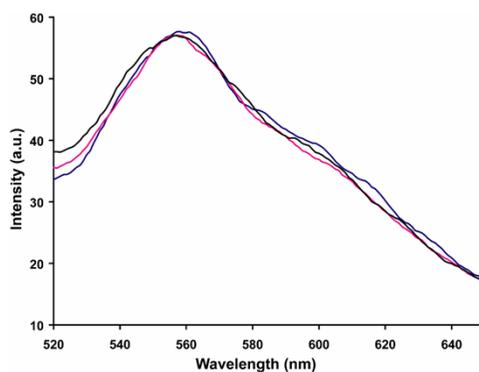


Figure S7: Fluorescence emission of **HL** (10^{-4} mol/L in DMSO) addition of TBABr in $10 \mu\text{L}$ (10^{-3} mol/L in DMSO) in each aliquot ($\lambda_{\text{ex}} = 475 \text{ nm}$).

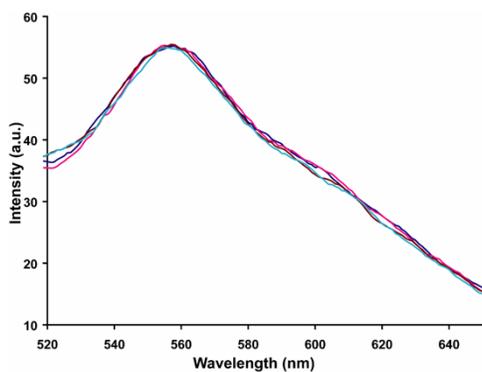


Figure S8: Fluorescence emission of **HL** (10⁻⁴ mol/L in DMSO) addition of TBAI in 10 μL (10⁻³ mol/L in DMSO) in each aliquot ($\lambda_{\text{ex}} = 475$ nm).

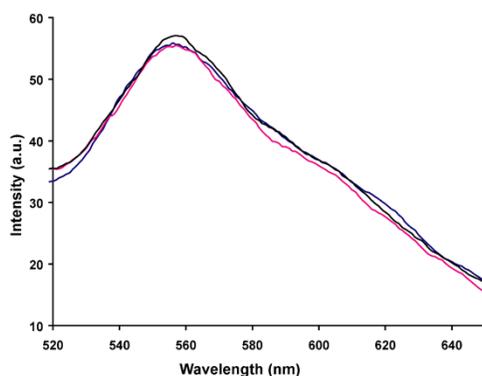


Figure S9: Fluorescence emission of **HL** (10⁻⁴ mol/L in DMSO) on addition of TBANO₃ in 10 μL (10⁻³ mol/L in DMSO) in each aliquot ($\lambda_{\text{ex}} = 475$ nm).

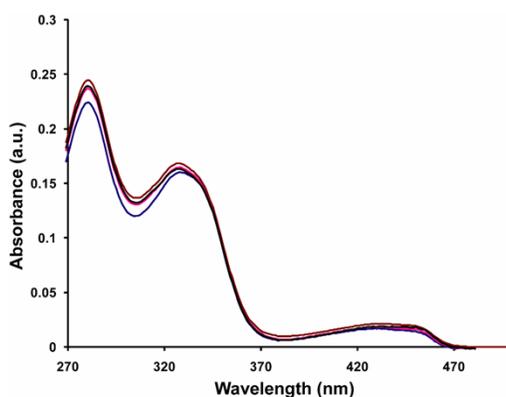


Figure S10: Changes in absorption spectra of **HL** (10⁻⁵ mol/L in methanol) on addition of 10 μL aliquots of Mn²⁺ ions (10⁻⁴ mol/L in methanol).

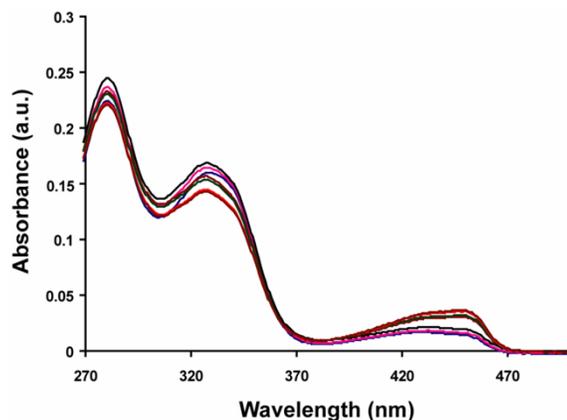


Figure S11: Changes in absorption spectra of **HL** (10^{-5} mol/L in methanol) on addition of Ni^{2+} ions in 10 μL aliquots (10^{-4} mol/L in methanol).

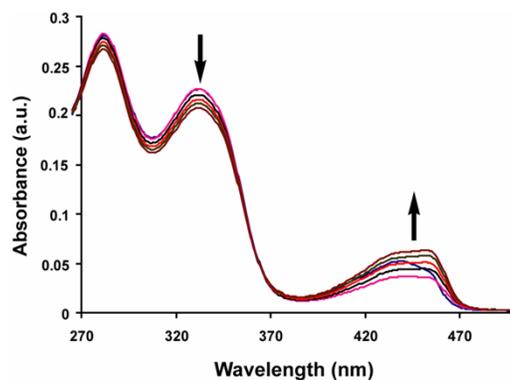


Figure S12: Changes in absorption spectra of **HL** (10^{-5} mol/L in methanol) on addition of 10 μL aliquots of Cu^{2+} ions (10^{-4} mol/L in methanol).

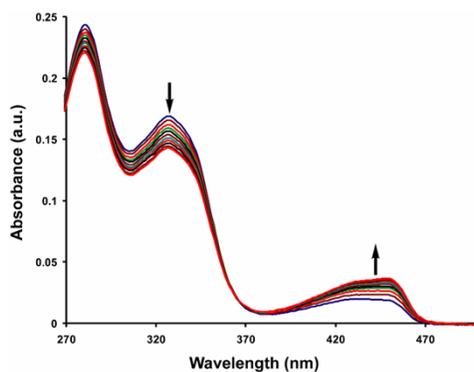


Figure S13: Changes in absorption spectra of **HL** (10^{-5} mol/L in methanol) on addition of 10 μL aliquots of Cd^{2+} ions (10^{-4} mol/L in methanol).

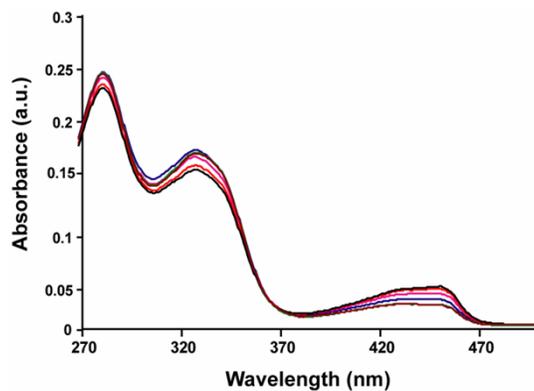


Figure S14: Changes in absorption spectra of **HL** (10^{-5} mol/L in methanol) on addition of 10 μ L aliquots of Al^{3+} ions (10^{-4} mol/L in methanol).

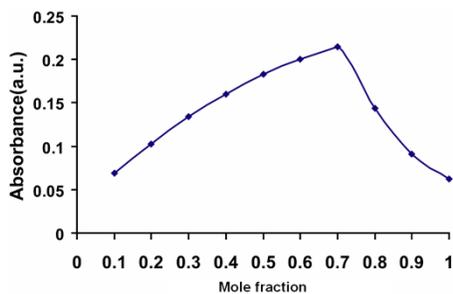


Figure S15: Job's plot for **HL** (10^{-5} mol/L solution in methanol) on addition of Zn^{2+} ions (10^{-4} mol/L solution in methanol).

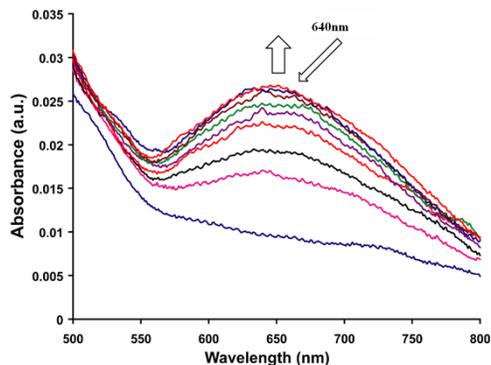


Figure S16: Changes in absorption spectra of **HL** (10^{-4} mol/L in methanol) on addition of 30 μ L aliquots of Zn^{2+} ions (10^{-3} mol/L in methanol) pH = 4.0.

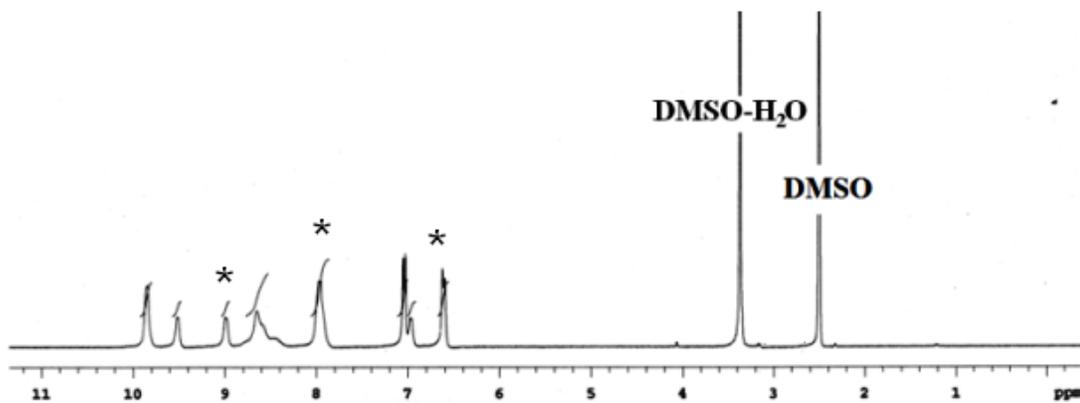


Figure S17: $^1\text{H-NMR}$ (DMSO-d_6) of the zinc complex (peaks marked with asterisk are from dissociated ligand).

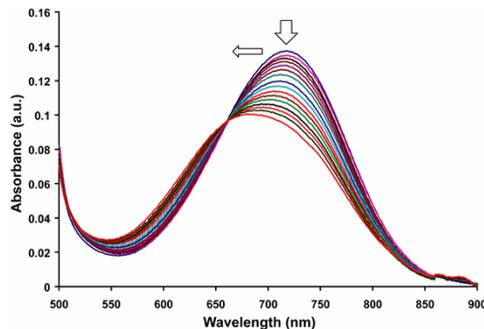


Figure S18: Changes in absorbance spectra of zinc complex (10^{-4} mol/L in DMSO, $\lambda_{\text{max}} = 718$ nm) on addition of TBAF (10^{-3} mole/L in DMSO); absorbance decreases with shift to 676 nm, with an isobestic point at 660 nm ($10 \mu\text{l}$ in each aliquot).

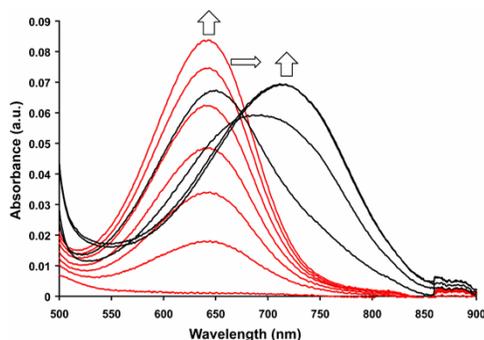


Figure S19: Changes in the visible absorbance of **HL** (10^{-4} mol/L in DMSO) at 640 nm on addition of solution of TBAF (10^{-3} mol/L in DMSO) (red); the black lines show the shifting to 710 nm on addition of ZnCl_2 (10^{-3} mol/L in DMSO) $10\ \mu\text{L}$ in each aliquot.

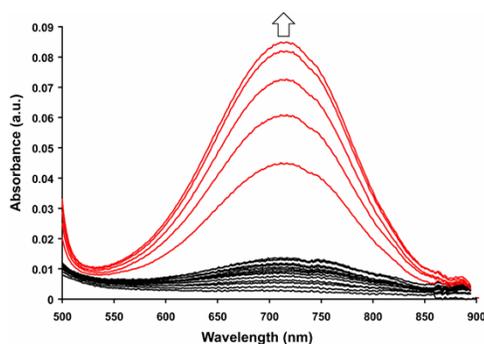


Figure S20: Increase in absorbance of **HL** (10^{-4} mol/L in DMSO) on addition of ZnCl_2 solution at 710 nm (black) redlines shows increase on further addition of TBAF (10^{-3} mol/L in DMSO) solution ($10\ \mu\text{L}$ in each aliquot).

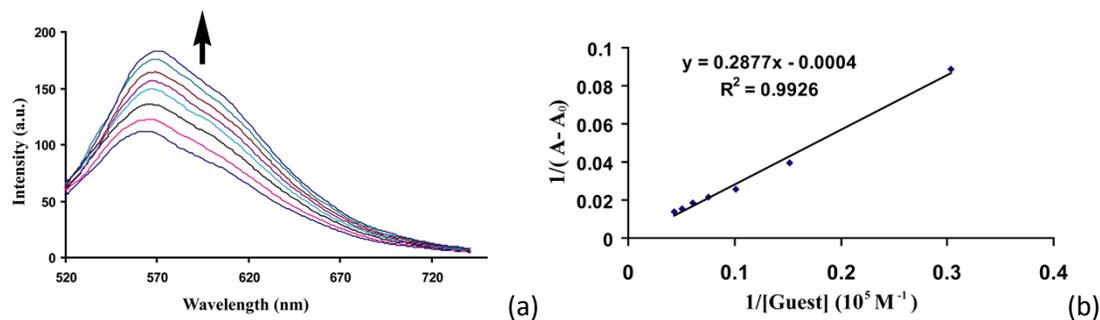


Figure S21: (a) Fluorescence emission at 570 nm ($\lambda_{\text{ex}} = 475$ nm) of **HL** (10^{-4} mol/L in methanol) on addition of Cd^{2+} ions in $10\ \mu\text{L}$ (10^{-3} mol/L in methanol) in each aliquot. (b) Binding constant plot of **HL** with Cd^{2+} ions (binding constant 3.475×10^5 mol.L $^{-1}$).

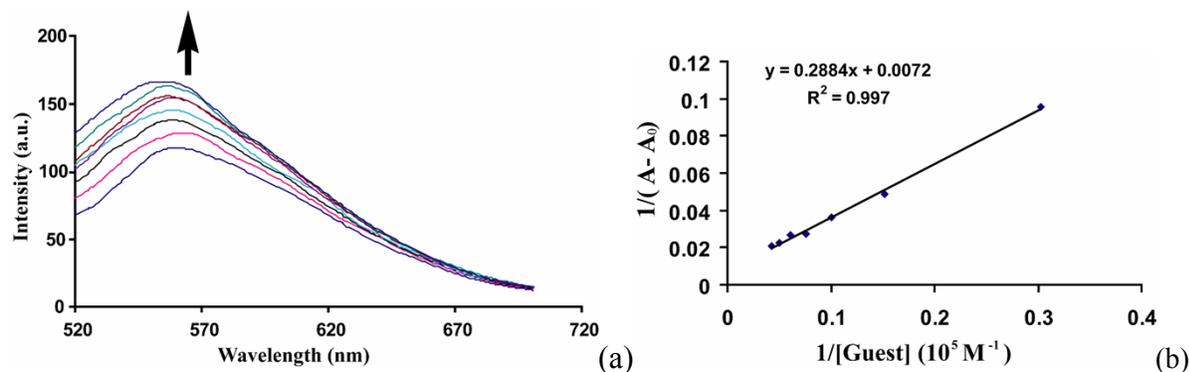


Figure S22: (a) Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L methanol solution) on addition of Al^{3+} ions in $10 \mu\text{L}$ (10^{-3} mol/L in methanol) in each aliquot. (b) Binding constant plot ($M = \text{mol/L}$) of **HL** with Al^{3+} ions (binding constant $3.46 \times 10^5 \text{ mol.L}^{-1}$).

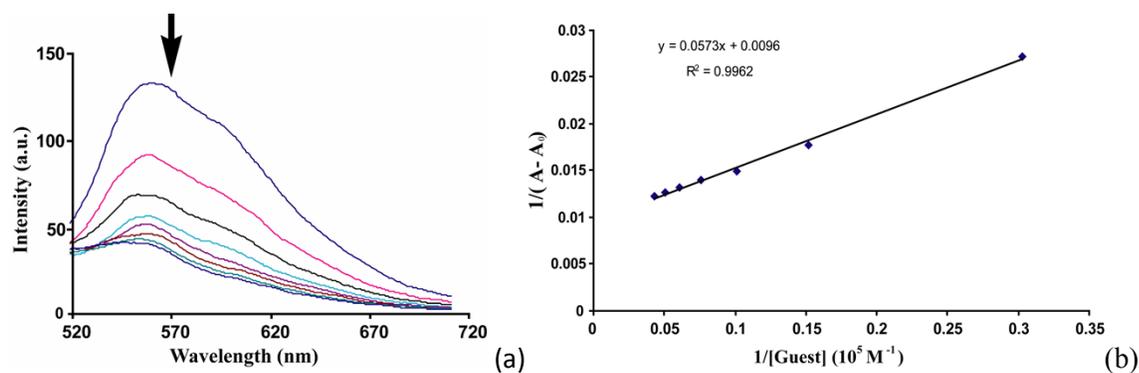


Figure S23: (a) Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L in methanol) on addition of Cu^{2+} ions in $10 \mu\text{L}$ (10^{-3} mol/L in methanol) in each aliquot. (b) Binding constant plot ($M = \text{mol/L}$) for **HL** with Cu^{2+} ions (binding constant $17.45 \times 10^5 \text{ mol.L}^{-1}$).

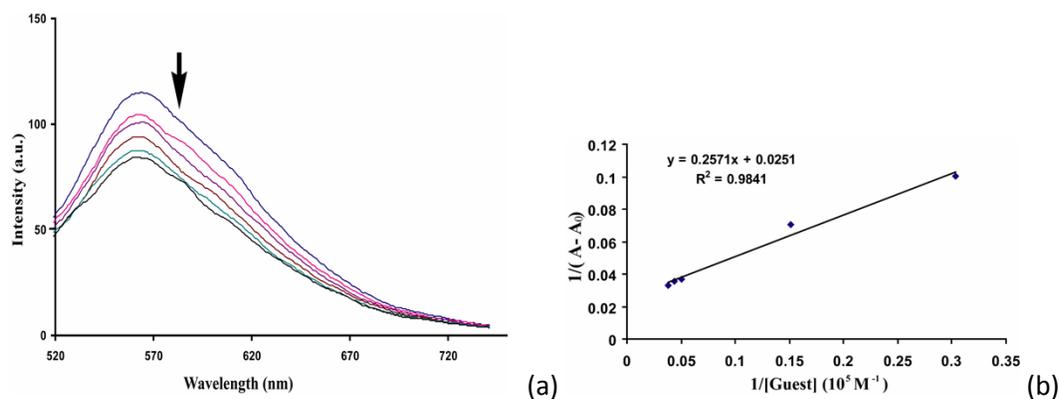


Figure S24: (a) Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L in methanol) on addition of Mn^{2+} in $10 \mu\text{L}$ (10^{-3} mol/L in methanol) in each aliquot. (b) Binding constant determination plot ($M = \text{mol/L}$) for **HL** with Mn^{2+} ions (binding constant $3.89 \times 10^5 \text{ mol}^{-1}\text{L}$).

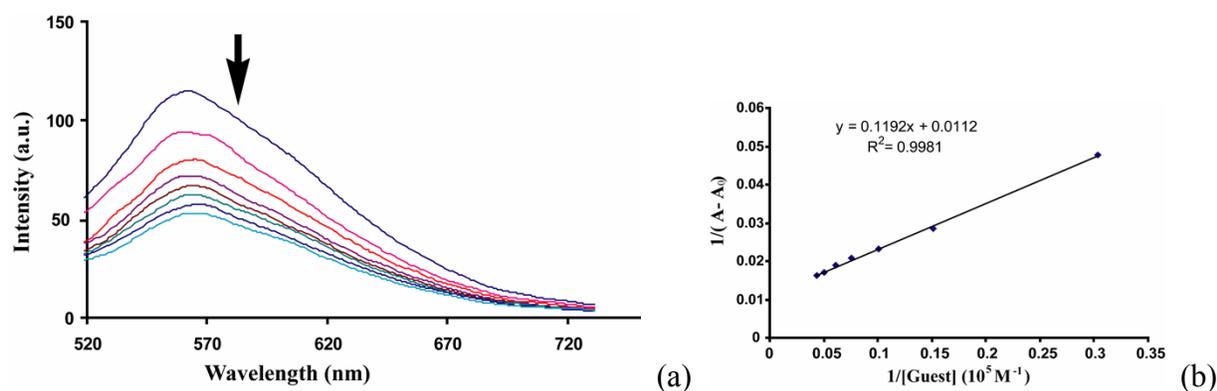


Figure S25: (a) Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L in methanol) on addition of Fe^{3+} ions in $10 \mu\text{L}$ (10^{-3} mol/L in methanol) in each aliquot. (b) Binding constant determination plot for **HL** ($M = \text{mol/L}$) with Fe^{3+} ions (binding constant $8.39 \times 10^5 \text{ mol}^{-1}\text{L}$).

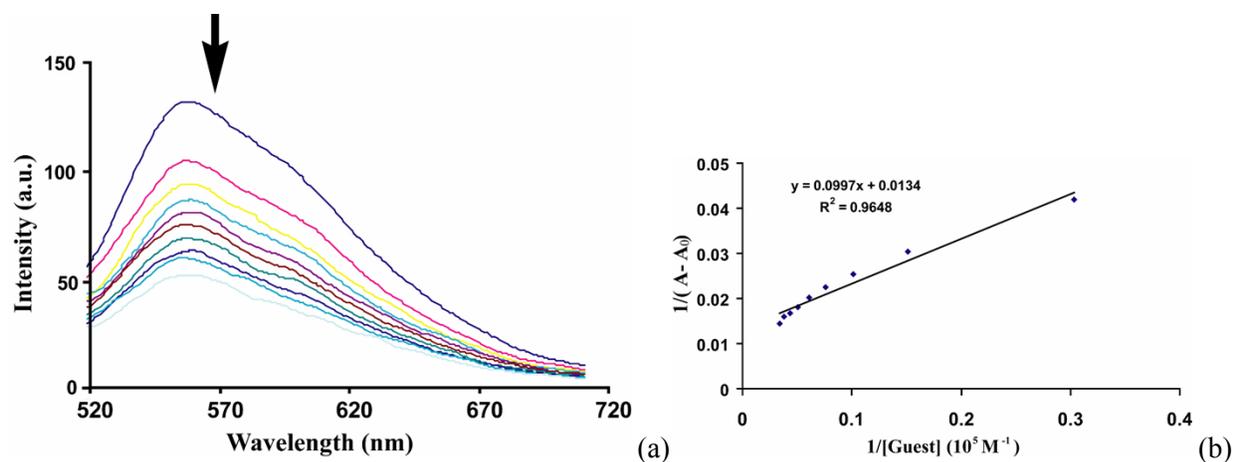


Figure S26: (a) Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L in methanol) on addition of Co^{2+} ions in $10 \mu\text{L}$ (10^{-3} mol/L in methanol) in each aliquot. (b) Binding constant determination plot ($M = \text{mol/L}$) for **HL** with Co^{2+} ions (binding constant $10.03 \times 10^5 \text{ mol.L}^{-1}$).

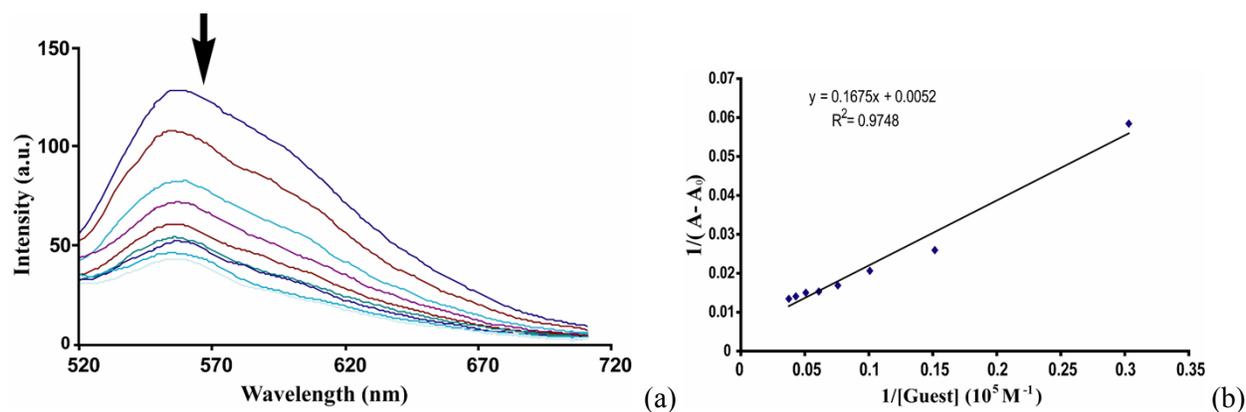


Figure S27: (a) Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L methanol) on addition of Ni^{2+} ions in $10 \mu\text{L}$ (10^{-3} mol/L methanol) in each aliquot. (b) Binding constant plot ($M = \text{mol/L}$) of **HL** with Ni^{2+} ions (binding constant $5.97 \times 10^5 \text{ mol.L}^{-1}$).

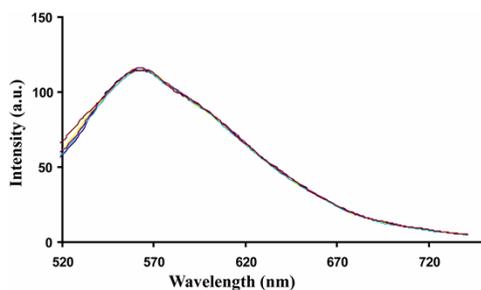


Figure S28: Fluorescence emission ($\lambda_{\text{ex}} = 475 \text{ nm}$) of **HL** (10^{-4} mol/L in methanol) on addition of Hg^{2+} ions in $10 \mu\text{L}$ aliquots (10^{-3} mol/L in methanol).

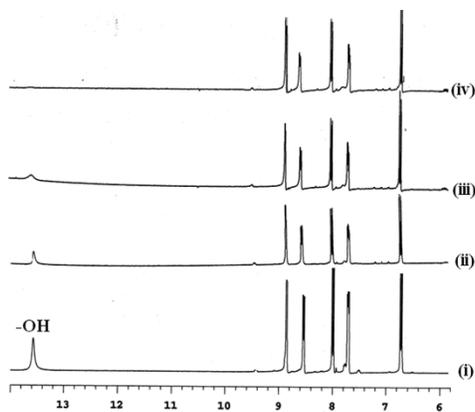


Figure S29: $^1\text{H-NMR}$ titration of **HL** with Zn^{2+} ions (i) **HL**, (ii) **HL** with 0.33 mole equivalent with Zn^{2+} ions, (iii) **HL** with 0.66 mole equivalent with Zn^{2+} ions and (iv) **HL** with 0.99 mole equivalent with Zn^{2+} ions. Peak for $-\text{OH}$ gradually disappears upon addition of Zn^{2+} ions.

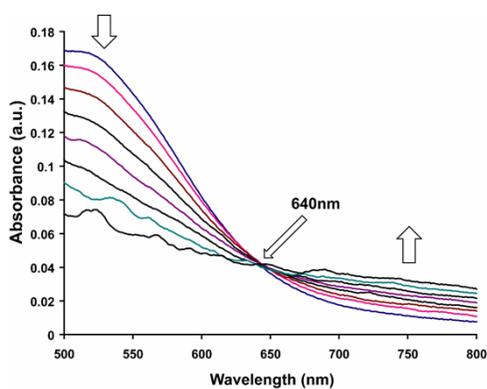


Figure S30: Changes in absorption spectra of 5-(hydroxyimino)quinolin-8-one (10^{-4} mol/L in methanol) on addition of $30\ \mu\text{L}$ of Zn^{2+} ions (10^{-3} mol/L in methanol) at $\text{pH} = 7.0$.

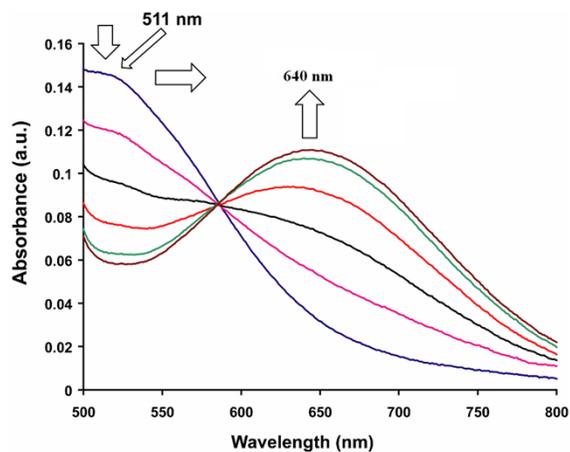


Figure S31: Changes in absorption spectra of 5-(hydroxyimino)quinolin-8-one (10^{-4} mol/L in methanol) on addition of 30 μL of Zn^{2+} -ions (10^{-3} mol/L in methanol) in basic condition (9.2 pH).

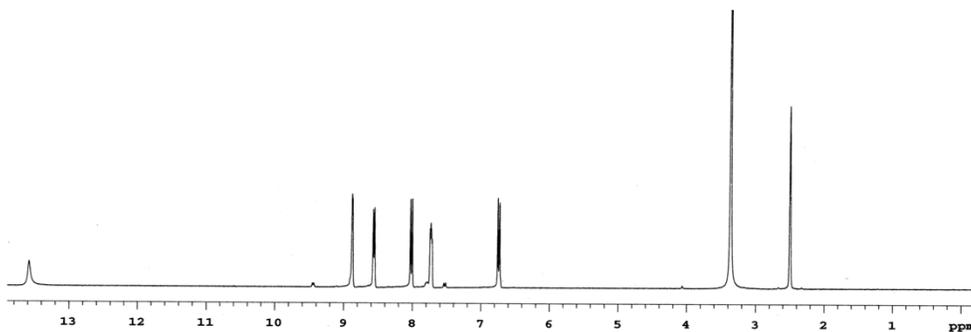


Figure S32: ¹H-NMR spectra (DMSO-d₆) of **HL**

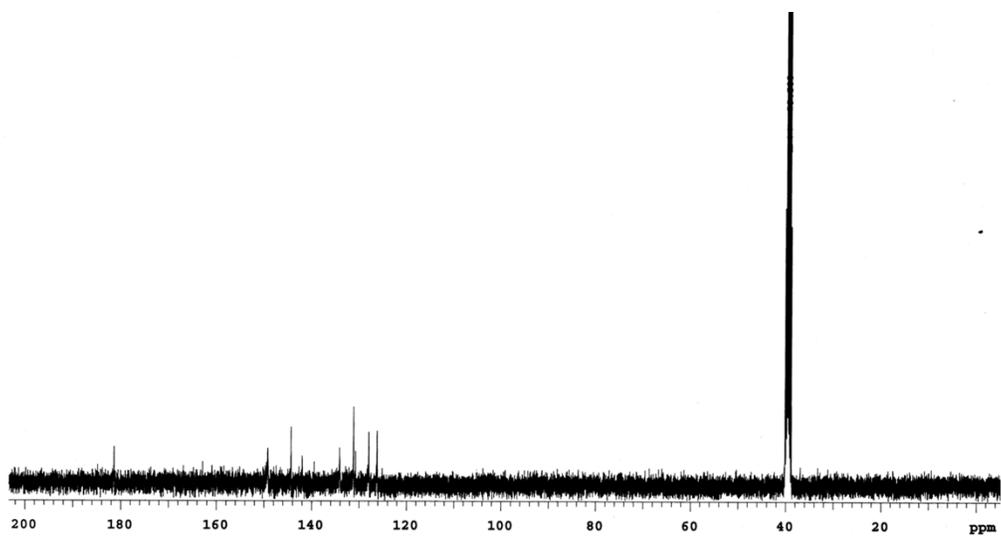


Figure S33: $^{13}\text{C}\{^1\text{H}\}$ -NMR spectra (DMSO- d_6) of HL

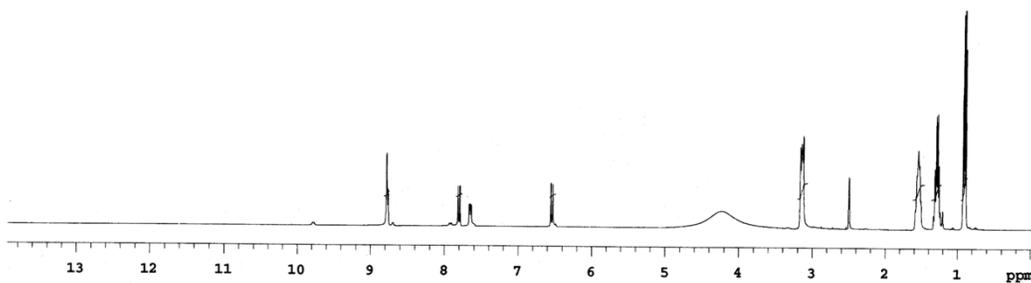


Figure S34: ^1H -NMR spectra (DMSO- d_6) of supramolecular adduct of HL and TBAF.

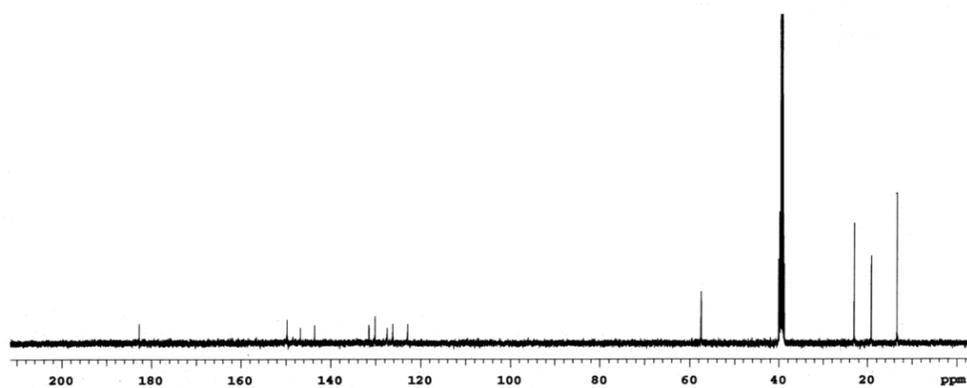


Figure S35: $^{13}\text{C}\{^1\text{H}\}$ -NMR spectra (DMSO- d_6) of supramolecular adduct of HL and TBAF.