Electronic Supplemental Information
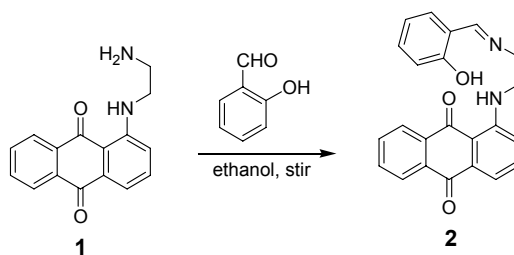
Single Molecular Colorimetric Probe for Simultaneous Estimation of Cu^{2+} and Ni^{2+}

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1. Experimental Section

Scheme-1

1a. Spectral and other data of Schiff base 2, dark red solid; 80%; m.p. 150 - 151 ^{o}C (C$_2$H$_5$OH-CHCl$_3$); FAB mass M$^+$ *m/z* 371 (M$^+$+1); IR υ_{max} (KBr) 1629 (C=O), 1668 (C=O), 3275 (NH/OH) cm^{-1}; ^{1}H NMR (CDCl$_3$): δ 3.72 (q, *J* = 6.0 Hz, 4H, CH$_2$), 3.96 (t, *J* = 6.0 Hz, 2H, CH$_2$), 6.87 (t, *J* = 7.5 Hz, 1H, ArH), 6.97 (d, *J* = 7.8 Hz, 1H, ArH), 7.13 (d, *J* = 8.4 Hz, 1H, ArH), 7.25-7.34 (m, 2H, ArH), 7.53-7.63 (m, 2H, ArH), 7.68 (t, *J* = 7.5 Hz, 1H, ArH), 7.75 (t, *J* = 7.5 Hz, 1H, ArH), 8.24 (t, *J* = 7.5 Hz, 2H, ArH), 8.45 (s, 1H, CH), 9.92 (bs,1H, NH, exchanges with D$_2$O), 12.8 (bs, 1H, OH, exhanges with D$_2$O); ^{13}C NMR (normal / DEPT-135) (CDCl$_3$): δ 43.36 (-ve, CH$_2$), 58.71 (-ve, CH$_2$), 113.36 (absent, ArC), 116.03 (+ve, ArCH), 117.02 (+ve, ArCH), 117.67 (+ve, ArCH), 118.64 (+ve, ArCH), 118.72 (absent, ArC), 126.67 (+ve, ArCH), 126.80 (+ve, ArCH), 131.53 (+ve, ArCH), 132.52 (+ve, ArCH), 132.94 (+ve, ArCH), 132.99 (absent, ArC), 133.92 (+ve, ArCH), 134.70 (absent, ArC), 134.87 (absent, ArC), 135.35 (+ve, ArCH), 151.44 (absent, ArC), 160.92 (absent, ArC), 166.80 (+ve, ArCH), 183.71 (absent, CO), 185.14 (absent, CO); Found C 74.27; H 4.9; N 7.46%. C$_{23}$H$_{18}$N$_2$O$_3$ requires C 74.58, H 4.90; N 7.58%.

1b. Spectral and other data of Schiff base 2 + Ni^{2+} complex. dark green solid; 75%; m.p. 235 ^{o}C (C$_2$H$_5$OH-CHCl$_3$); FAB mass M$^+$ *m/z* 427 (M$^+$+1); IR υ_{max} (KBr) 1629(C=O), 1654(C=O), 3384-3527(b) cm^{-1}; ^{1}H NMR (CDCl$_3$): δ 3.22 (t, *J* = 6.6 Hz, 4H, CH$_2$), 3.51 (t, *J* = 6.6 Hz, 2H, CH$_2$), 6.56 (t, *J* = 7.2 Hz, 1H, ArH), 6.99 (d, *J* = 9.0 Hz, 2H, ArH), 7.07-7.23 (m, 2H, ArH), 7.26 (s, 1H, ArH), 7.53-7.63 (m, 2H, ArH), 7.68 (t, *J* = 7.5 Hz, 1H, ArH), 7.34 (s, 1H, CH), 7.41 (d, *J* = 6.6 Hz, 1H, ArH), 7.63 (t, *J* = 6.9 Hz, 1H, ArH), 7.70 (t, *J* = 6.6 Hz, 1H, ArH), 8.15 (d, *J* = 7.2 Hz, 1H, ArH), 8.29 (d, *J* = 7.8 Hz, 1H, ArH); ^{13}C NMR (normal / DEPT-135) (CDCl$_3$): δ 51.03 (-ve, CH$_2$), 60.12 (-ve, CH$_2$), 113.81 (absent, ArC), 114.77 (+ve, ArCH), 118.51 (+ve, ArCH), 120.54 (+ve, ArCH), 120.64 (absent, ArC), 122.16

(+ve, ArCH), 126.42 (+ve, ArCH), 127.62 (+ve, ArCH), 131.06 (+ve, ArCH), 131.37 (absent, ArC), 132.23 (+ve, ArCH), 132.35 (+ve, ArCH), 133.15 (+ve, ArCH), 135.64 (+ve, ArCH), 133.74 (absent, ArC), 133.84 (absent, ArC), 153.78 (absent, ArC), 160.81 (+ve, ArCH), 164.10 (absent, ArC), 170.00 (absent, CO), 182.98 (absent, CO); Found C 63.64; H 4.71; N 6.37 %. $C_{23}H_{16}N_2O_3Ni$ $0.5H_2O$ requires C 63.30, H 4.36; N 6.42%.

2. Photophysical studies – Parameters and Conditions

UV-Vis spectroscopy experiments were carried out on a Shimadzu UV-1601 PC UV-Vis Spectrophotometer by using slit widths of 1.0 nm and matched quartz cells. All metal ion stimulated colour changes have been studied in MeOH-H_2O (4:1) under buffered conditions. 10 mM HEPES Buffer, at pH 7.0 $\pm$ 0.1 was used for these experiments.. However, for the pH dependent studies on receptor – metal complexes, due to poor solubility of the complexes at pH > 9, all respestive evaluations were carried out in DMSO – H_2O (1:1). All absorption scans were saved as ACS II files and further processed in Excel™ to produce all graphs shown. Solutions of **2** were typically 50 µM.
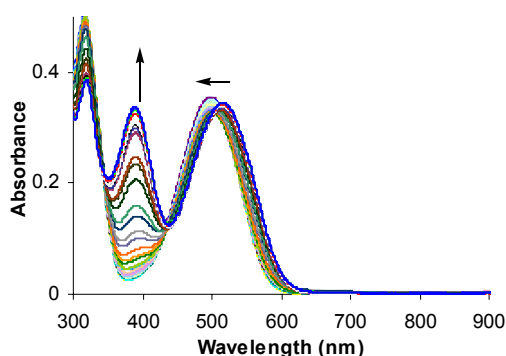
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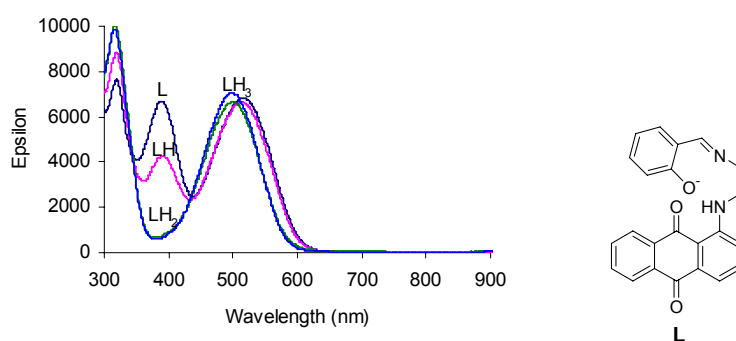**Figure S1: pH titration of 2 in DMSO : H_2O 1:1**

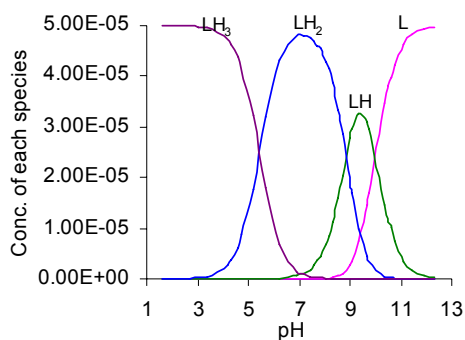**Figure S2. Absorption curves of 2 upon pH titration with acid and base**

Figure S3: Species distribution diagram for a system containing solution of 2 upon pH titration with acid and base
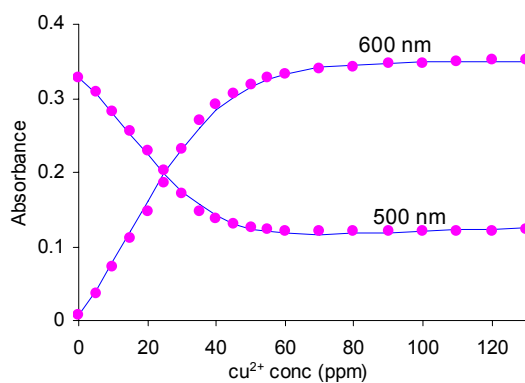

Figure S4: Cu(II) nitrate Titration of 2 (50 μM), CH$_3$OH :H$_2$O 4:1, pH 7.0 $\pm$ 0.1, [10mM HEPES] points refer to experimental values and line to curve fit
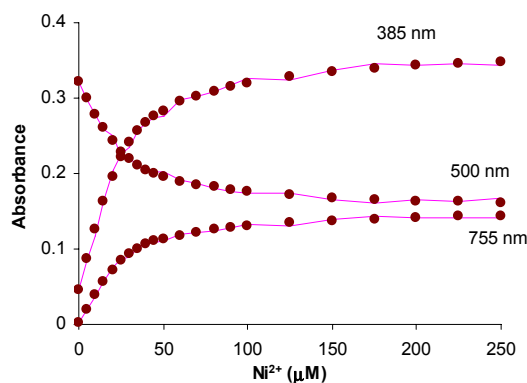

Figure S5: Ni(II) nitrate Titration of 2 (50 μM), CH$_3$OH :H$_2$O 4:1, pH 7.0 $\pm$ 0.1, [10mM HEPES] points refer to experimental values and line to curve fit
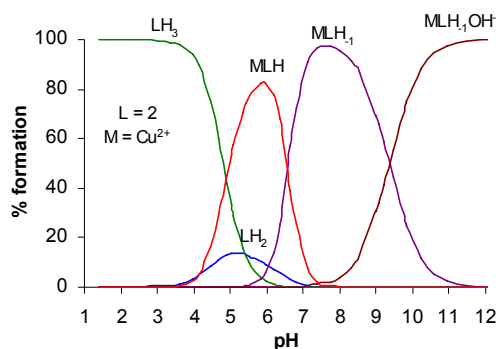
Figure S6: Species distribution diagram for a system containing 2 and Cu^{2+} (1 : 1) at variable pH.
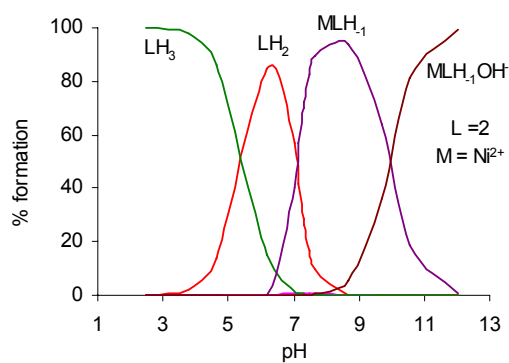

Figure S7: Species distribution diagram for a system containing 2 and Ni^{2+} (1 : 1) at variable pH.
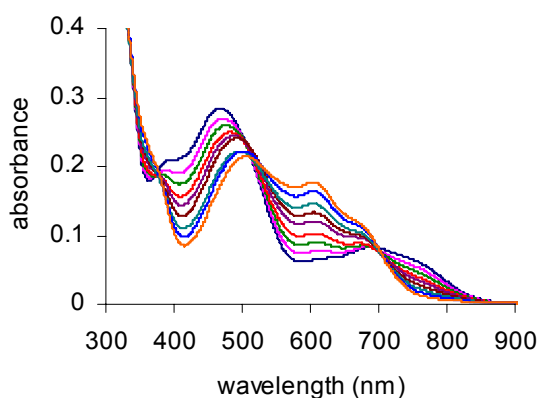

Figure S8: UV-Vis spectra of 50 μM of receptor 2 in the presence of 25 μM of Cu^{2+} and 25 μM of Ni^{2+}.

Table 1: Optical properties and binding characteristics of Schiff base **2** with Ni^{2+} and Cu^{2+} and effect of pH on logβ values

	Receptor **2**	**2**-Cu^{2+} complex	**2**-Ni^{2+} complex	
λ_{max} (nm)	500	600	385	750
ε value	6500	6900	6300	2300
logβ values at constant pH 7.0				
log β_{ML}	---	5.22	5.33	
log β_{ML2}	---	--	10.47	
log β_{M2L3}	---	18.47		
Logβ values from **2** – metal complex Vs.pH titration				
log β_{MLH-1}	---	5.86	2.14	
log $\beta_{MLH-1(OH-1)}$	---	-3.49	-7.79	
log β_{MLH}	---	18.98		