Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A Single Chemosensor for Bimetal Cu(II) and Zn(II) in Aqueous Medium

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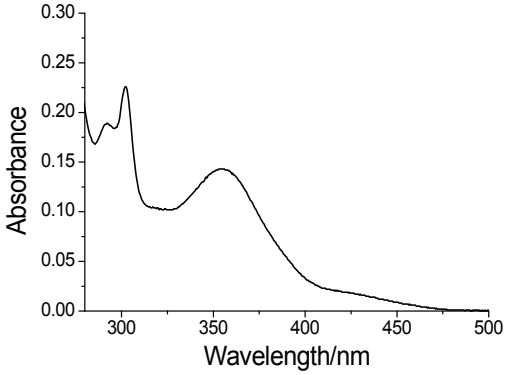


Figure S1 UV-Vis spectrum of HL (10 μM) in DMSO/H_2O (1/1, v/v).

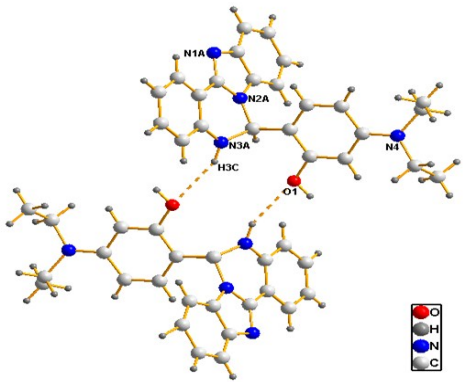


Figure S2 The intermolecular hydrogen bonds in HL.

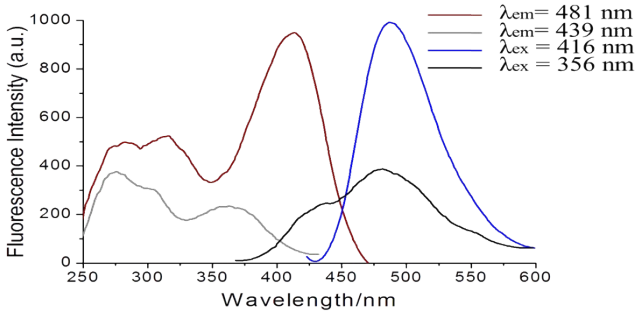
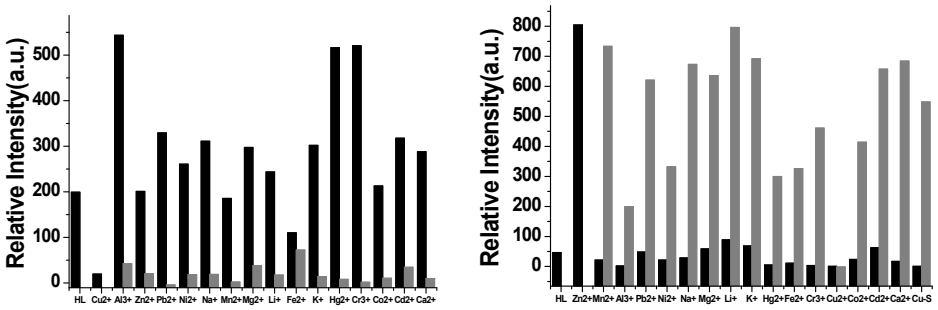


Figure S3 The excitation and fluorescence spectra of HL (10 μM) + 1 equiv. Zn (II) in DMSO/H_2O (v/v, 1:1).



(a) (b)

Figure S4 (a) Relative fluorescence intensity of 10 μM HL with 1 equiv. Cu^{2+} in the presence of 1 equiv. Other metal ions in DMSO/H_2O (1/1, v/v), in the absence (black) and presence (gray) of Cu^{2+}, λ_{ex} = 356 nm; (b) relative fluorescence intensity of HL with 1 equiv. Zn^{2+} in the presence of other metal ions (1 equiv.) in DMSO/H_2O (1/1, v/v), in the absence (black) and presence (gray) of Zn^{2+}, λ_{ex} = 416 nm.

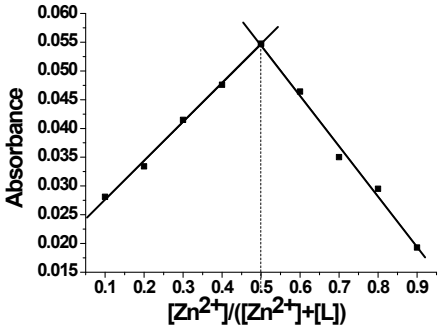
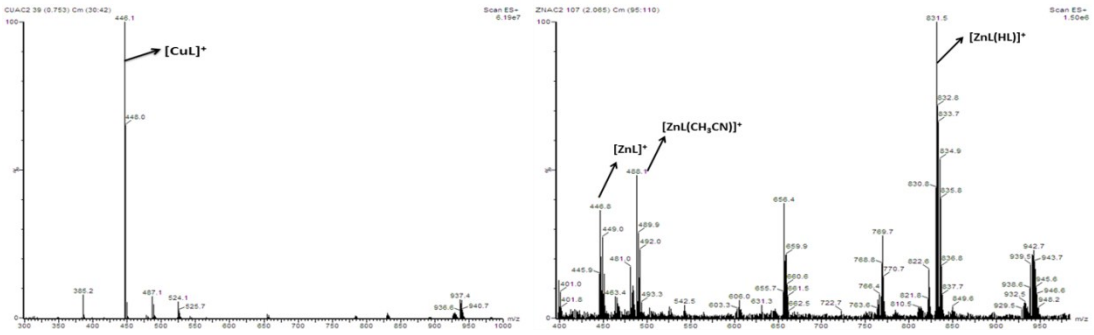


Figure S5 Job plot for the determination of the stoichiometry in the complexation of HL with Zn^{2+} in DMSO/H_2O (v/v, 1/1), absorbance at 416 nm was plotted as a function of the molar ratio $[Zn^{2+}]/([Zn^{2+}]+[HL])$.



(a) (b)

Figure S6 Positive-ion electrospray ionization mass spectra of HL upon addition of $CuCl_2$ (a) and $Zn(Ac)_2$ (b).

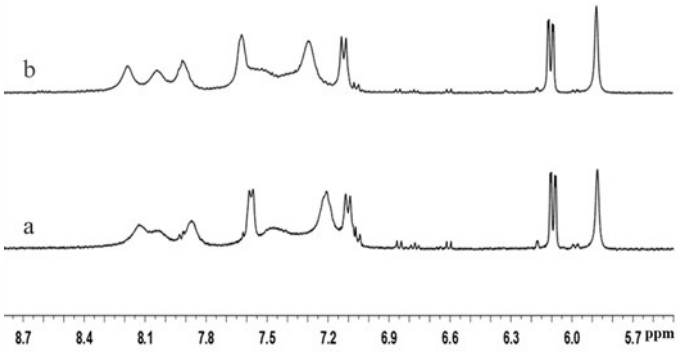
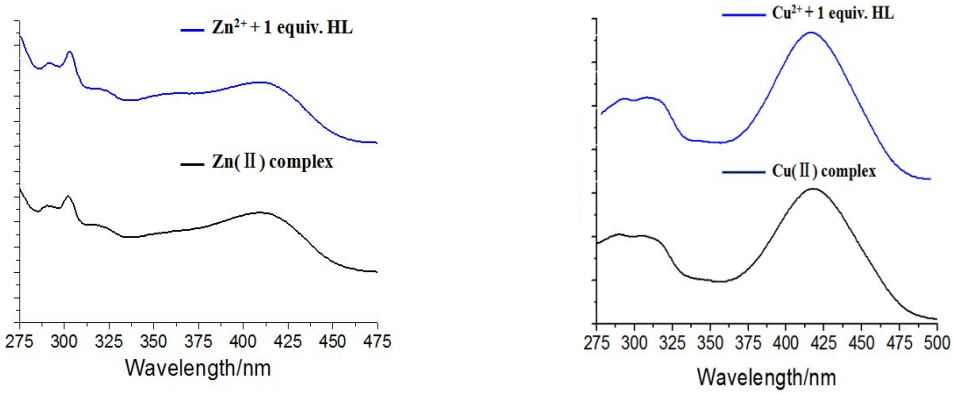
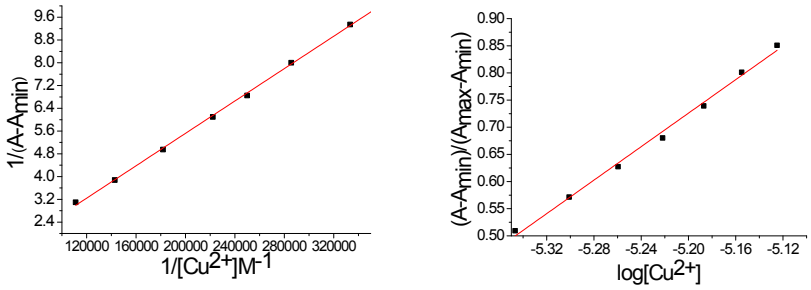


Figure S7 ^{1}H NMR spectra in DMSO-d_6: (a) HL+1.0 equiv. Zn^{2+}, (b) **2**.



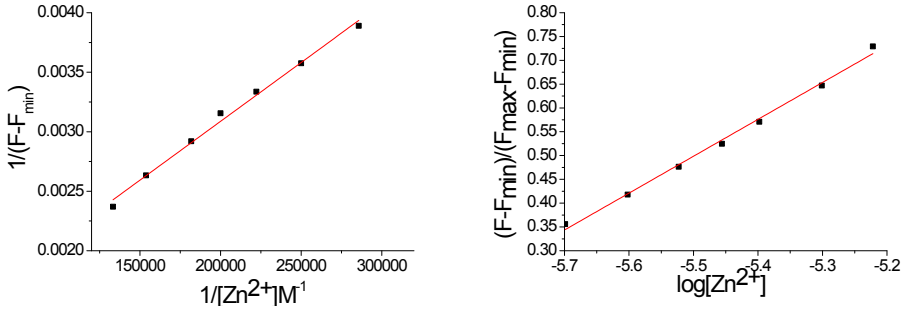
(a) (b)

Figure S8 (a) UV-Vis spectra of Zn (II) complex and HL(10 μM) + 1 equiv. Zn (II), (b) UV-Vis spectra of Cu (II) complex and HL (10 μM) + 1 equiv. Cu (II) (The solvents for a and b were DMSO/H_2O (1/1, v/v)).



(a) (b)

Figure S9 (a) Benesi-Hildebrand plot of HL and Cu^{2+} in DMSO/H_2O (v/v, 1/1), (b) Normalized response of UV absorbances at 418 nm to changing Cu^{2+} concentrations.



(a) (b)

Figure S10 (a) Benesi-Hildebrand plot of HL and $Zinc^{2+}$ in DMSO/H_2O (v/v, 1:1), (b) Normalized response of flouresence signals at 481 nm to changing Zn^{2+} concentrations.

Table S1 Bond Distances (Å) and Angles (deg) for HL.

O(1)-C(20)	1.368(3)	C(15)-C(14B)	1.512(3)
N(1A)-C(7A)	1.351(9)	C(16)-C(17)	1.369(4)
N(1A)-C(1A)	1.377(6)	C(17)-C(18)	1.407(4)
N(2A)-C(6A)	1.348(6)	C(18)-C(19)	1.397(4)
N(2A)-C(7A)	1.350(11)	C(19)-C(20)	1.382(4)
N(2A)-C(14A)	1.467(5)	C(21)-C(22)	1.426(6)
N(3A)-C(13A)	1.399(5)	C(23)-C(24)	1.459(5)
N(3A)-C(14A)	1.478(5)	N(1B)-C(7B)	1.25(2)
N(4)-C(18)	1.375 (4)	N(1B)-C(1B)	1.429(13)
N(4)-C(21)	1.479(5)	N(2B)-C(6B)	1.372(12)
N(4)-C(23)	1.484(4)	N(2B)-C(7B)	1.39(2)
C(1A)-C(2A)	1.3900	N(2B)-C(14B)	1.429(7)
C(1A)-C(6A)	1.3900	N(3B)-C(13B)	1.398(10)
C(2A)-C(3A)	1.3900	N(3B)-C(14B)	1.477(7)
C(3A)-C(4A)	1.3900	C(1B)-C(2B)	1.3900
C(4A)-C(5A)	1.3900	C(1B)-C(6B)	1.3900
C(5A)-C(6A)	1.3900	C(2B)-C(3B)	1.3900
C(7A)-C(8A)	1.423(8)	C(3B)-C(4B)	1.3900
C(8A)-C(9A)	1.3900	C(4B)-C(5B)	1.3900
C(8A)-C(13A)	1.3900	C(5B)-C(6B)	1.3900
C(9A)-C(10A)	1.3900	C(7B)-C(8B)	1.429(17)
C(10A)-C(11A)	1.3900	C(8B)-C(9B)	1.3900
C(11A)-C(12A)	1.3900	C(8B)-C(13B)	1.3900
C(12A)-C(13A)	1.3900	C(9B)-C(10B)	1.3900
C(14A)-C(15)	1.504(5)	C(10B)-C(11B)	1.3900
C(15)-C(16)	1.386(4)	C(11B)-C(12B)	1.3900
C(15)-C(20)	1.392(3)	C(12B)-C(13B)	1.3900
C(7A)-N(1A)-C(1A)	104.5(6)	C(16)-C(17)-C(18)	120.5(3)
C(6A)-N(2A)-C(7A)	108.1(5)	N(4)-C(18)-C(19)	120.5(3)
C(6A)-N(2A)-C(14A)	127.6(5)	N(4)-C(18)-C(17)	122.7(3)
C(7A)-N(2A)-C(14A)	123.5(5)	C(19)-C(18)-C(17)	116.8(3)
C(13A)-N(3A)-C(14A)	121.2(4)	C(20)-C(19)-C(18)	121.5(3)
C(18)-N(4)-C(21)	122.4(3)	O(1)-C(20)-C(19)	121.0(2)
C(18)-N(4)-C(23)	120.9(3)	O(1)-C(20)-C(15)	117.3(2)
C(21)-N(4)-C(23)	116.4(3)	C(19)-C(20)-C(15)	121.7(2)
N(1A)-C(1A)-C(2A)	130.3(5)	C(22)-C(21)-N(4)	110.7(4)
N(1A)-C(1A)-C(6A)	109.6(5)	C(24)-C(23)-N(4)	112.8(4)
C(2A)-C(1A)-C(6A)	120.0	C(7B)-N(1B)-C(1B)	104.1(12)
C(1A)-C(2A)-C(3A)	120.0	C(6B)-N(2B)-C(7B)	106.7(12)
C(4A)-C(3A)-C(2A)	120.0	C(6B)-N(2B)-C(14B)	122.8(9)
C(3A)-C(4A)-C(5A)	120.0	C(7B)-N(2B)-C(14B)	130.4(12)
C(6A)-C(5A)-C(4A)	120.0	C(13B)-N(3B)-C(14B)	119.9(7)

N(2A)-C(6A)-C(5A)	133.6(5)	C(2B)-C(1B)-C(6B)	120.0
N(2A)-C(6A)-C(1A)	106.3(5)	C(2B)-C(1B)-N(1B)	130.0(12)
C(5A)-C(6A)-C(1A)	120.0	C(6B)-C(1B)-N(1B)	109.9(12)
N(2A)-C(7A)-N(1A)	111.4(7)	C(1B)-C(2B)-C(3B)	120.0
N(2A)-C(7A)-C(8A)	120.4(7)	C(4B)-C(3B)-C(2B)	120.0
N(1A)-C(7A)-C(8A)	128.2(8)	C(3B)-C(4B)-C(5B)	120.0
C(9A)-C(8A)-C(13A)	120.0	C(6B)-C(5B)-C(4B)	120.0
C(9A)-C(8A)-C(7A)	121.9(7)	N(2B)-C(6B)-C(5B)	135.5(12)
C(13A)-C(8A)-C(7A)	118.0(7)	N(2B)-C(6B)-C(1B)	104.5(12)
C(8A)-C(9A)-C(10A)	120.0	C(5B)-C(6B)-C(1B)	120.0
C(9A)-C(10A)-C(11A)	120.0	N(1B)-C(7B)-N(2B)	114.6(15)
C(10A)-C(11A)-C(12A)	120.0	N(1B)-C(7B)-C(8B)	130.6(18)
C(13A)-C(12A)-C(11A)	120.0	N(2B)-C(7B)-C(8B)	114.5(18)
C(12A)-C(13A)-C(8A)	120.0	C(9B)-C(8B)-C(13B)	120.0
C(12A)-C(13A)-N(3A)	121.8(6)	C(9B)-C(8B)-C(7B)	120.8(14)
C(8A)-C(13A)-N(3A)	118.1(6)	C(13B)-C(8B)-C(7B)	119.1(14)
N(2A)-C(14A)-N(3A)	105.5(3)	C(10B)-C(9B)-C(8B)	120.0
N(2A)-C(14A)-C(15)	113.8(3)	C(9B)-C(10B)-C(11B)	120.0
N(3A)-C(14A)-C(15)	113.6(3)	C(12B)-C(11B)-C(10B)	120.0
C(16)-C(15)-C(20)	116.3(2)	C(11B)-C(12B)-C(13B)	120.0
C(16)-C(15)-C(14A)	124.9(2)	C(12B)-C(13B)-C(8B)	120.0
C(20)-C(15)-C(14A)	118.3(2)	C(12B)-C(13B)-N(3B)	118.8(11)
C(16)-C(15)-C(14B)	125.4(2)	C(8B)-C(13B)-N(3B)	121.2(11)
C(20)-C(15)-C(14B)	118.3(2)	N(2B)-C(14B)-N(3B)	106.0(5)
C(14A)-C(15)-C(14B)	0.53(16)	N(2B)-C(14B)-C(15)	111.2(3)
C(17)-C(16)-C(15)	123.2(3)	N(3B)-C(14B)-C(15)	107.0(3)

Table S2 Selected Bond Distances (Å) and Angles (deg) for 1.

Cu(1)-Cl(1)	2.2752(13)	Cu(1)-N(2A)	1.984(3)
Cu(1)-O(1)	1.927(3)	Cu(1)-N(3A)	1.962(3)
O(1)-Cu(1)-N(3A)	93.44(14)	O(1)-Cu(1)-Cl(1)	90.94(10)
O(1)-Cu(1)-N(2A)	141.91(14)	N(3A)-Cu(1)-Cl(1)	164.35(11)
N(3A)-Cu(1)-N(2A)	88.33(13)	N(2A)-Cu(1)-Cl(1)	97.43(10)

Table S3 Selected Bond Distances (Å) and Angles (deg) for 2

O(4)-Zn(1)	1.915(11)	O(1)-Zn(2)	1.956(11)
O(5)-Zn(1)	2.295(12)	O(2)-Zn(2)	2.336(10)
O(6)-Zn(1)	2.031(11)	O(3)-Zn(2)	2.009(12)
N(2B)-Zn(1)	1.920(12)	N(2A)-Zn(2)	2.065(10)
N(3B)-Zn(1)	2.028(12)	N(3A)-Zn(2)	2.065(12)
O(4)-Zn(1)-N(2B)	127.8(5)	O(1)-Zn(2)-O(3)	110.6(5)
O(4)-Zn(1)-N(3B)	94.2(5)	O(1)-Zn(2)-N(2A)	128.6(5)
N(2B)-Zn(1)-N(3B)	90.5(4)	O(3)-Zn(2)-N(2A)	115.5(5)
O(4)-Zn(1)-O(6)	116.5(5)	O(1)-Zn(2)-N(3A)	95.2(5)
N(2B)-Zn(1)-O(6)	111.5(5)	O(3)-Zn(2)-N(3A)	109.6(5)
N(3B)-Zn(1)-O(6)	107.0(5)	N(2A)-Zn(2)-N(3A)	89.8(5)
O(4)-Zn(1)-O(5)	88.6(4)	O(1)-Zn(2)-O(2)	88.7(4)
N(2B)-Zn(1)-O(5)	95.9(5)	O(3)-Zn(2)-O(2)	57.0(5)
N(3B)-Zn(1)-O(5)	169.4(5)	N(2A)-Zn(2)-O(2)	97.9(4)
O(6)-Zn(1)-O(5)	62.8(5)	N(3A)-Zn(2)-O(2)	166.5(5)