Electronic Supplementary Material (ESI) for RSC Advances.

A highly selective CHEF-type chemosensor for monitoring Zn^{2+} in aqueous solution and living cells

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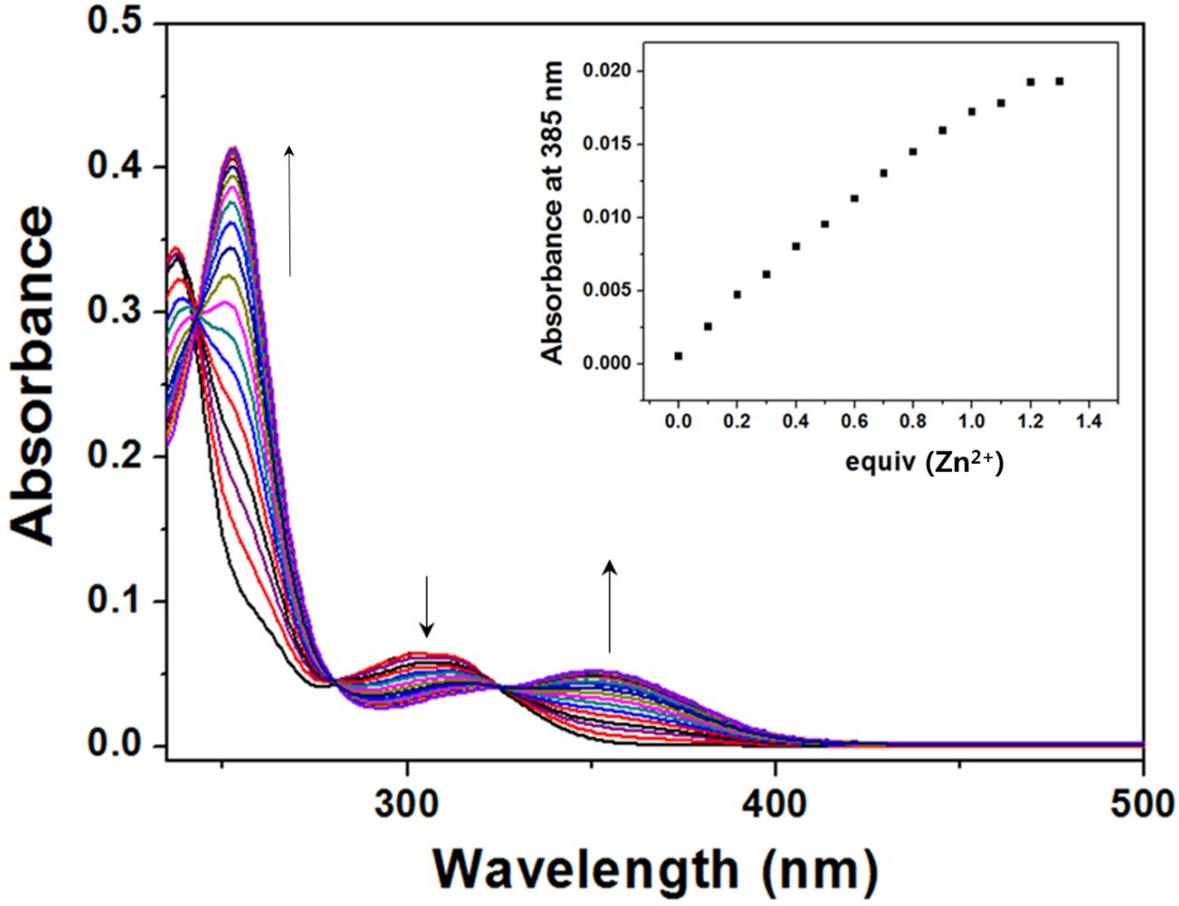


Fig. S1 UV-vis absorption spectra of **1** (10 μM) obtained during the titration with $Zn(NO_3)_2$ (0.1-1.5 equiv) in bis-tris buffer solution at room temperature.

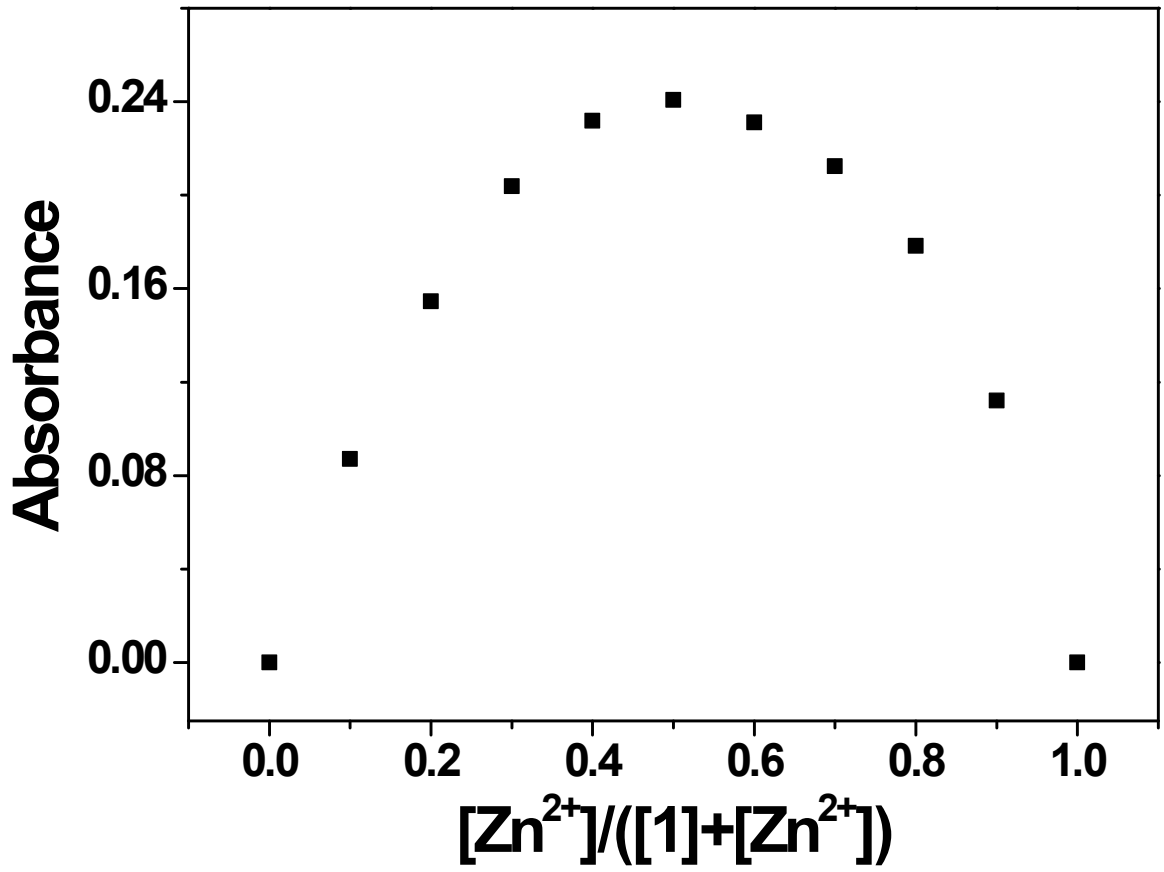


Fig. S2 Job plot for the binding of **1** with Zn^{2+}. Absorbance at 312 nm was plotted as a function of the molar ratio $[Zn^{2+}]/([\mathbf{1}] + [Zn^{2+}])$. The total concentration of zinc ions with receptor **1** was 4.0×10^{-5}M.

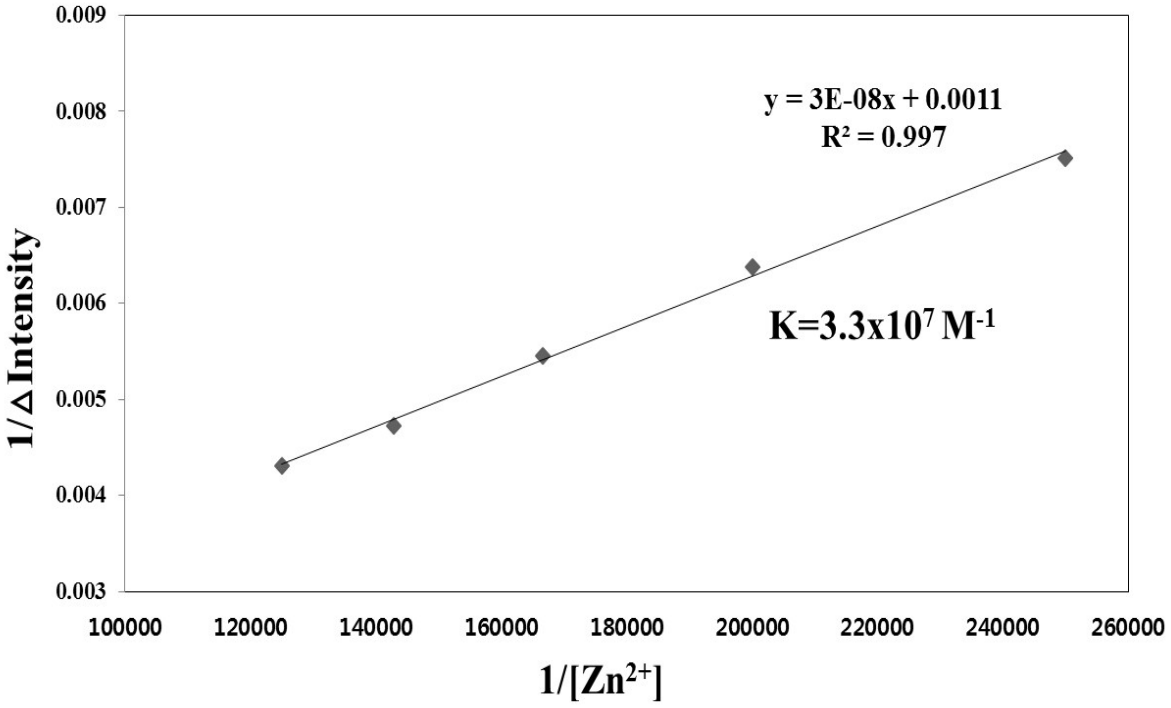


Fig. S3 Benesi-Hildebrand equation plot (fluorescence intensity at 521 nm) of **1**, assuming 1:1 stoichiometry for association between **1** and Zn^{2+}.

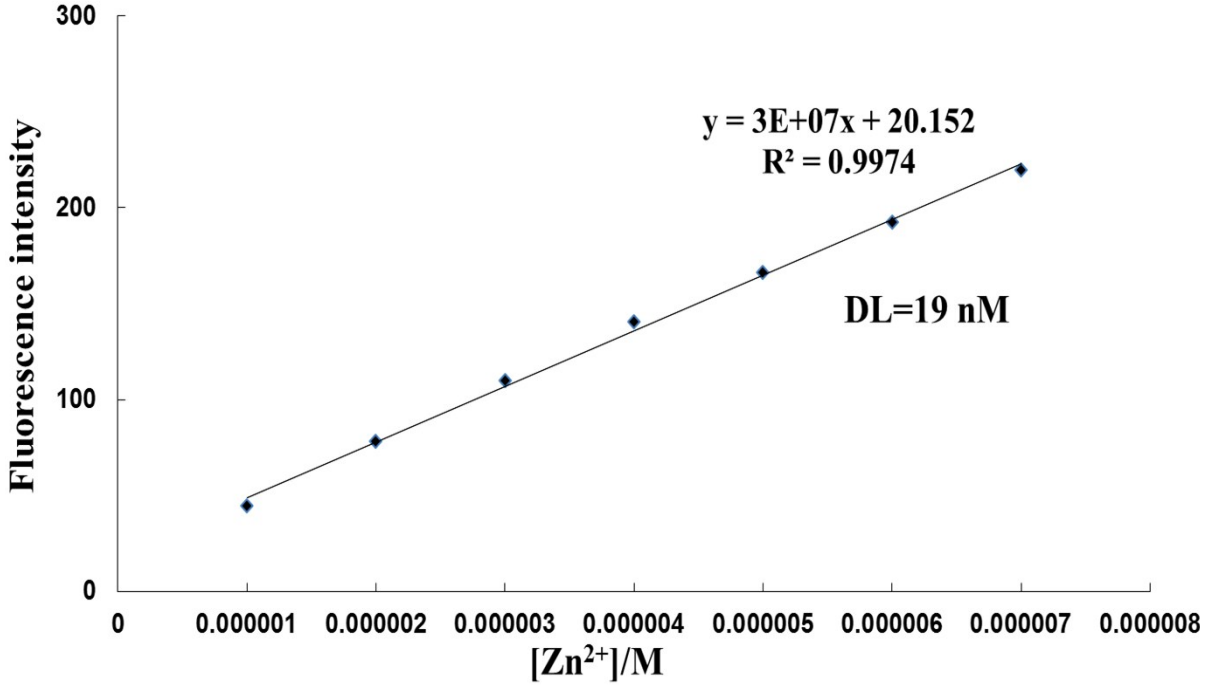


Fig. S4 Determination of the detection limit based on change in the ratio (fluorescence intensity at 521 nm) of **1** (10 μM) with Zn^{2+}.

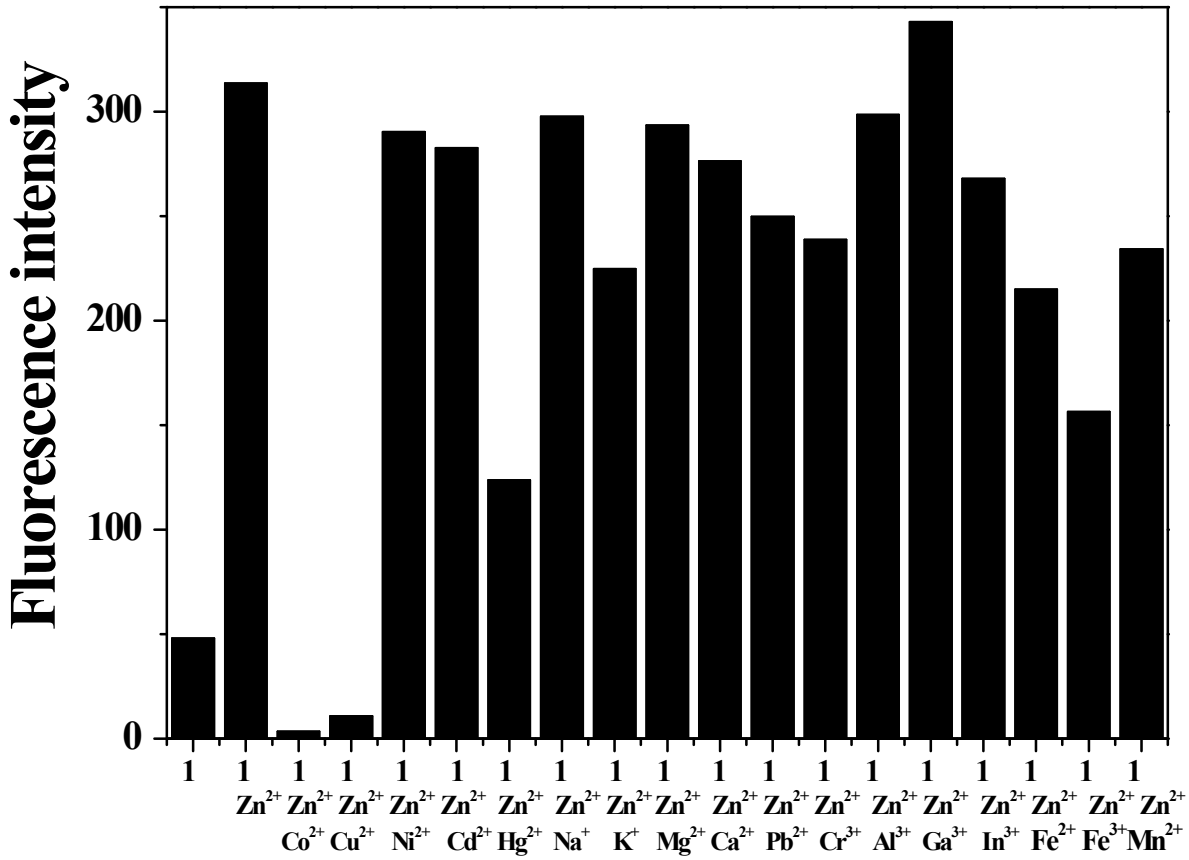


Fig. S5 Competitive selectivity of **1** (10 μM) toward Zn^{2+} (1.5 equiv) in the presence of other metal ions (15 equiv) with an excitation of 355 nm in buffer solution (10 mM bis-tris, pH 7.0).

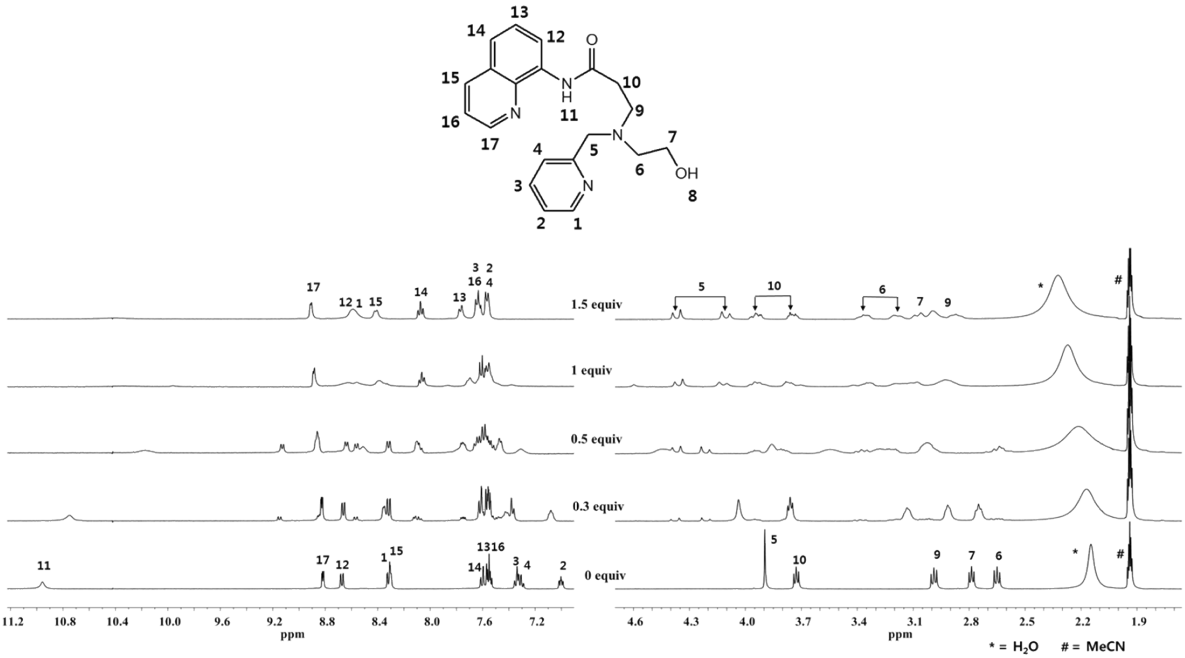
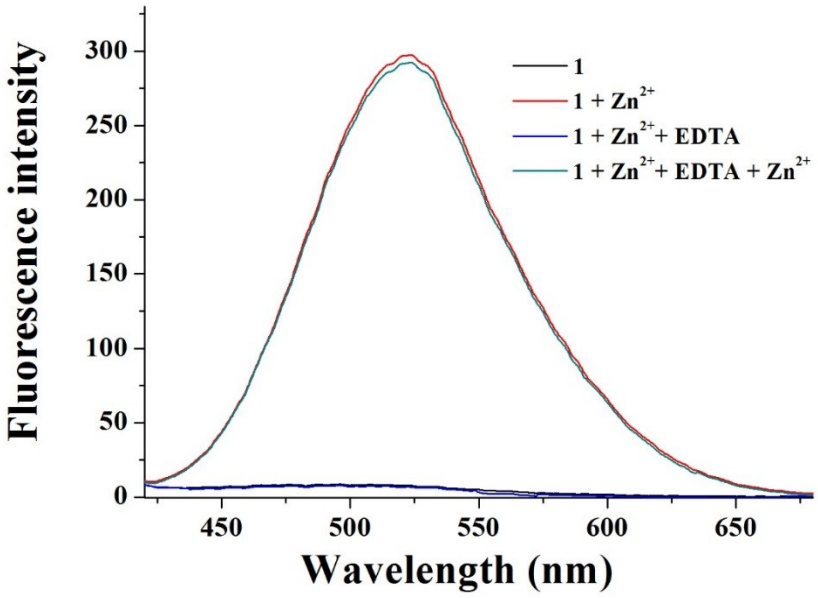


Fig. S6 ^{1}H NMR titration of **1** with $Zn(NO_3)_2$ in CD_3CN.

(a)



(b)

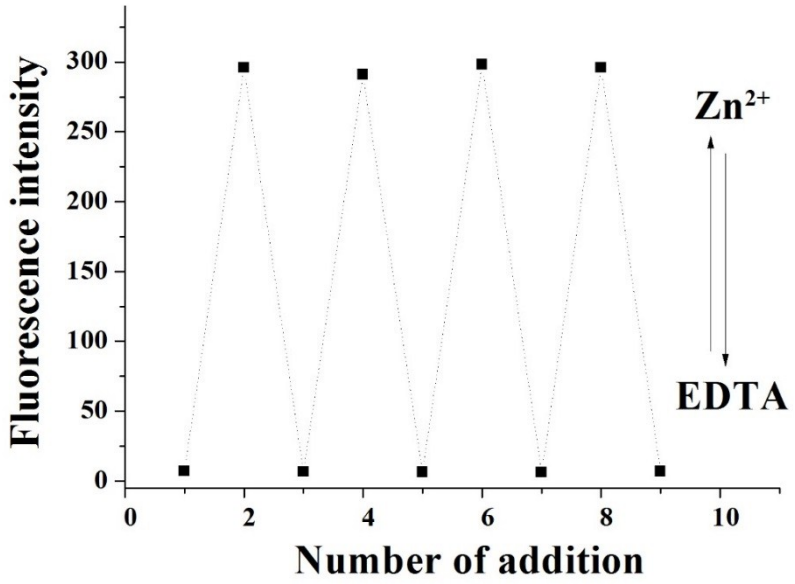


Fig. S7 (a) Fluorescence spectral changes of **1** (10 μM) after the sequential addition of Zn^{2+} and EDTA in buffer solution (10 mM bis-tris, pH 7.0). (b) Reversible changes in fluorescence

intensity of **1** (10 μM) at 521 nm after the sequential addition of Zn^{2+} and EDTA.

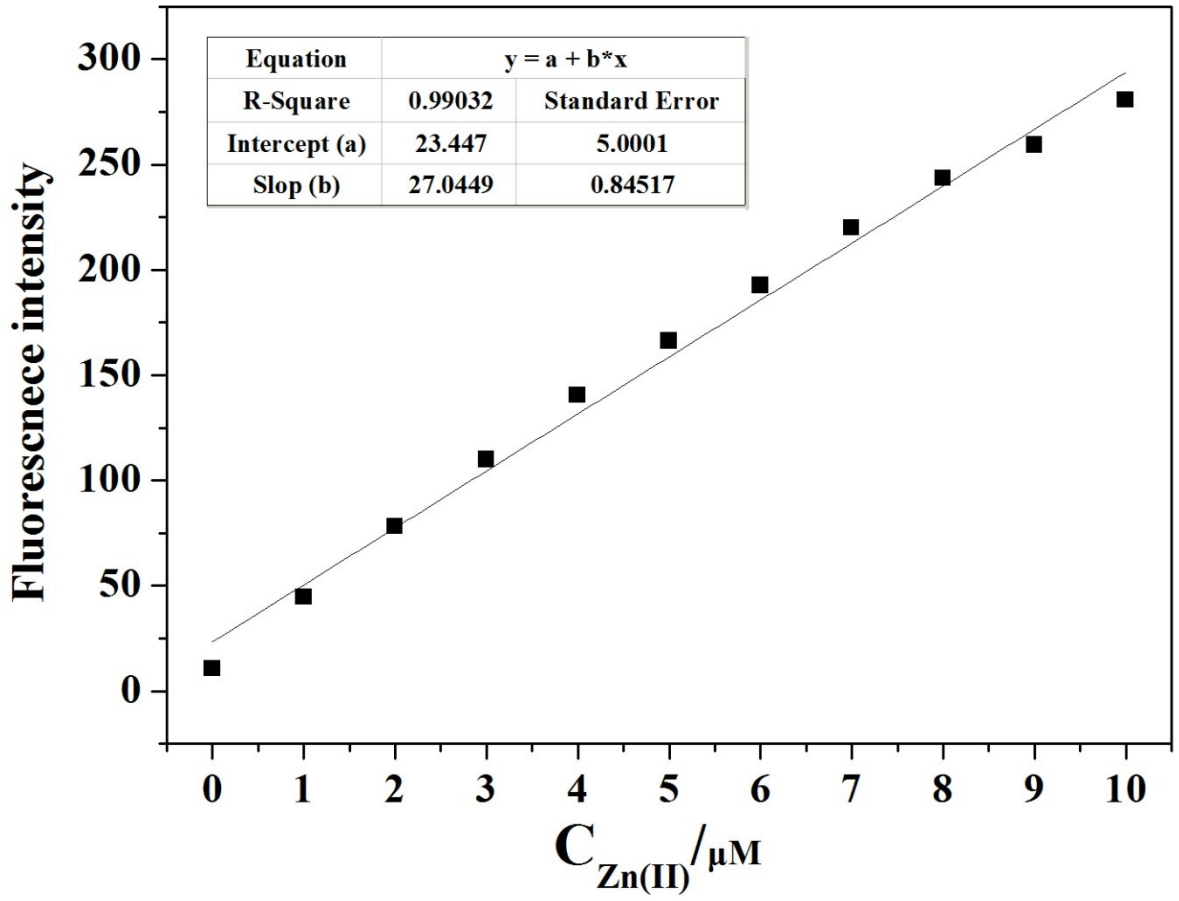
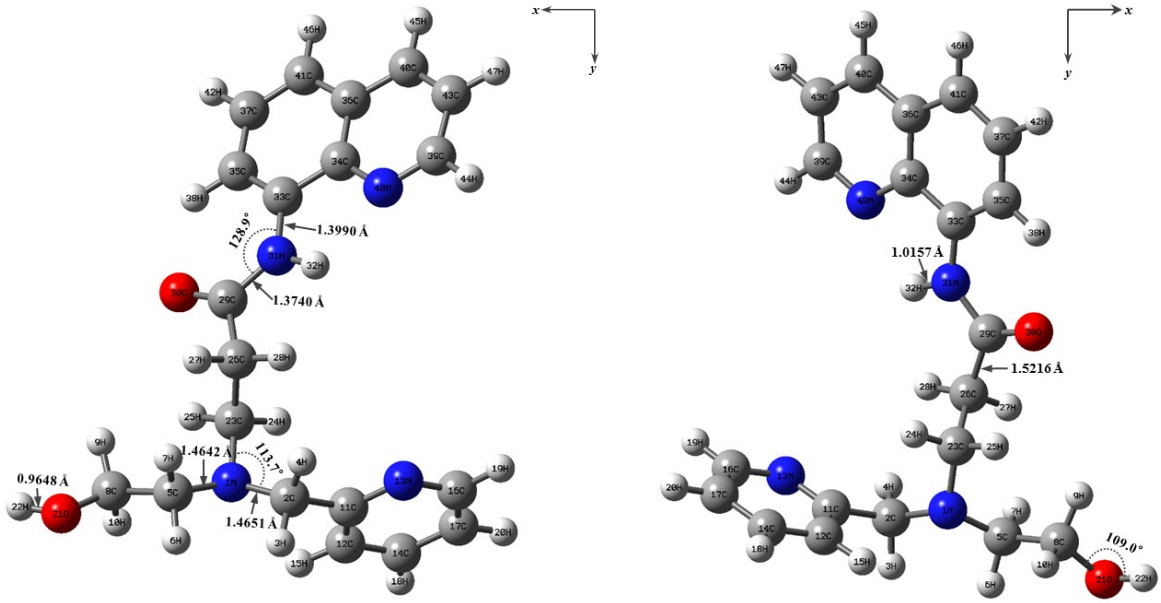


Fig. S8 Fluorescence intensity (at 521 nm) of **1** as a function of Zn(II) concentration ([**1**] = 20 μmol/L and [Zn(II)] = 1.00-10.00 μmol/L). Conditions: all samples were conducted in buffer-MeOH solution (999:1, 10 mM bis-tris, pH 7.0). λ_{ex} and λ_{em} were 355 and 521 nm, respectively.

(a)



(b)

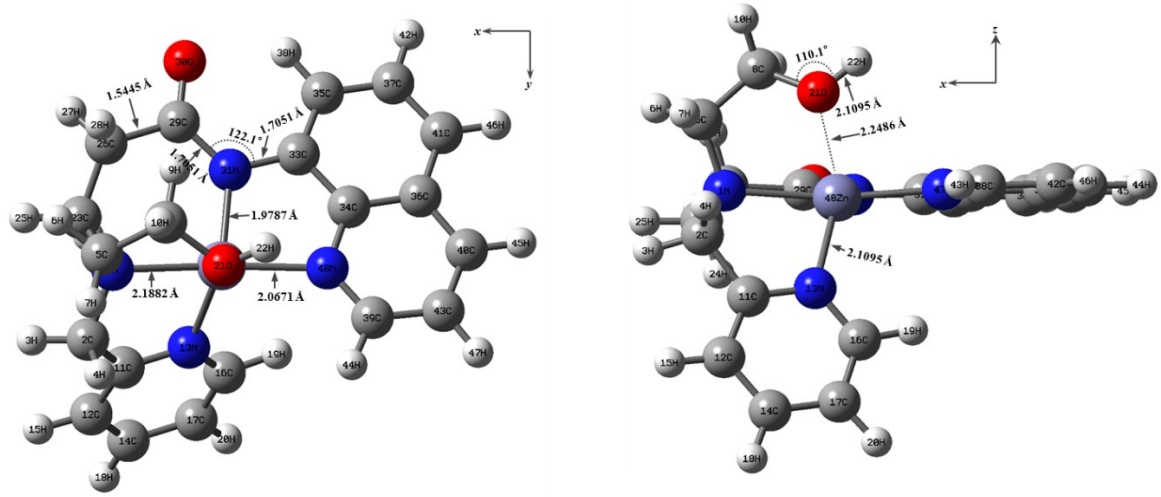
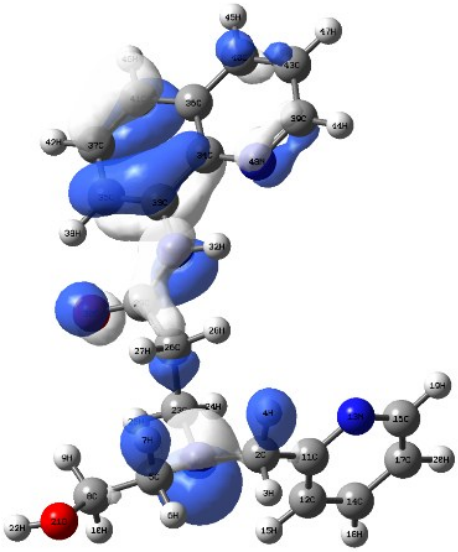
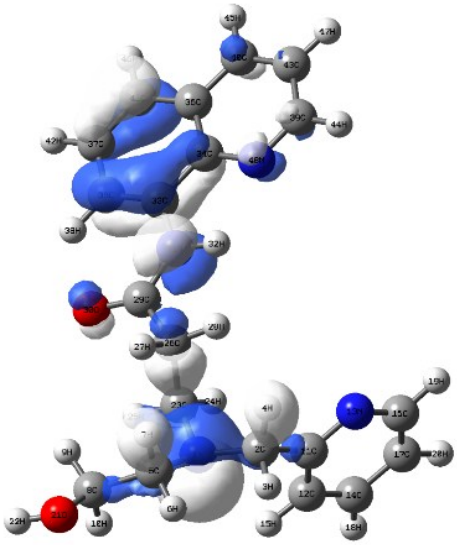
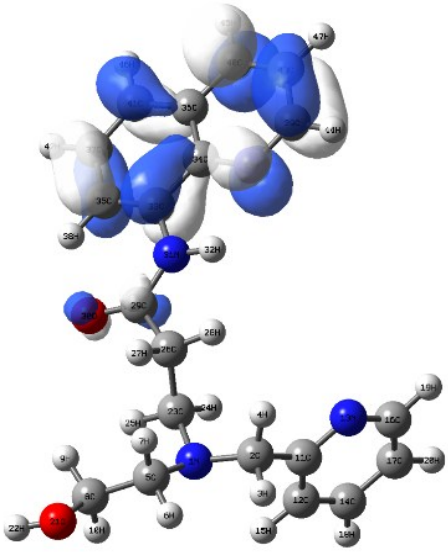
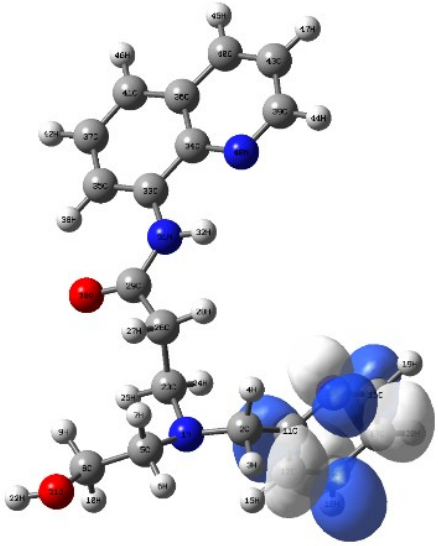


Fig. S9 Energy-minimized structures for (a) **1** and (b) **1**-Zn^{2+} complex. The major bond length and angle are indicated.

(a)

Molecular orbital (1)	
	
HOMO -1 (-6.1432 eV)	**HOMO (-5.9694 eV)**
	
LUMO (-1.9430 eV)	**LUMO + 1 (-0.9878 eV)**

(b)

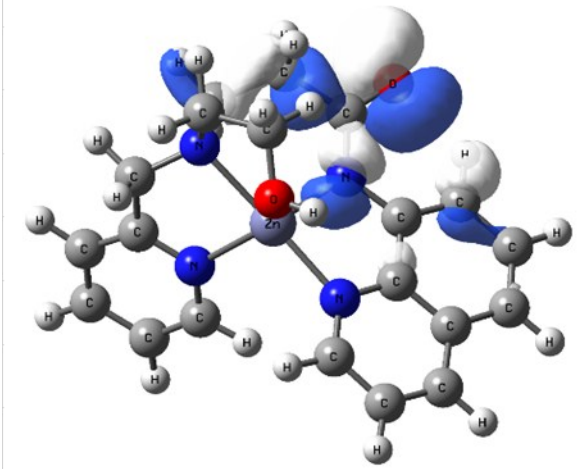
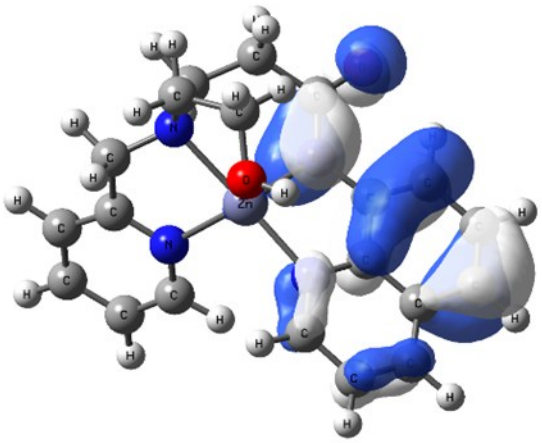
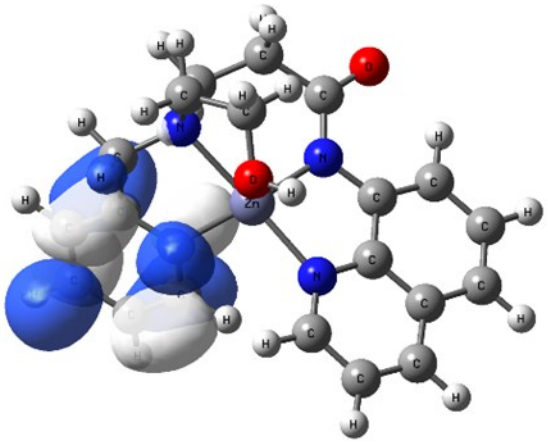
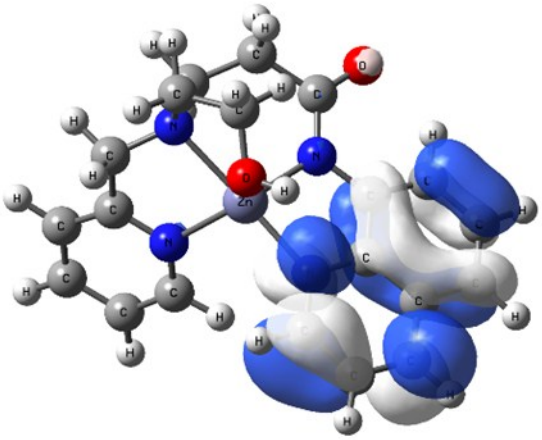
Molecular orbital (1 -Zn^{2+})	
	
HOMO -1 (-9.0573 eV)	**HOMO (-8.3183 eV)**
	
LUMO (-5.0137 eV)	**LUMO + 1 (-4.8047 eV)**

Fig. S10 The major molecular orbital contours for (a) **1** and (b) **1**-Zn^{2+} complex (Isosurface = 0.030 electron $bohr^{-3}$).