Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A highly selective fluorescent chemosensor based on quinoline derivative for zinc ion in pure water

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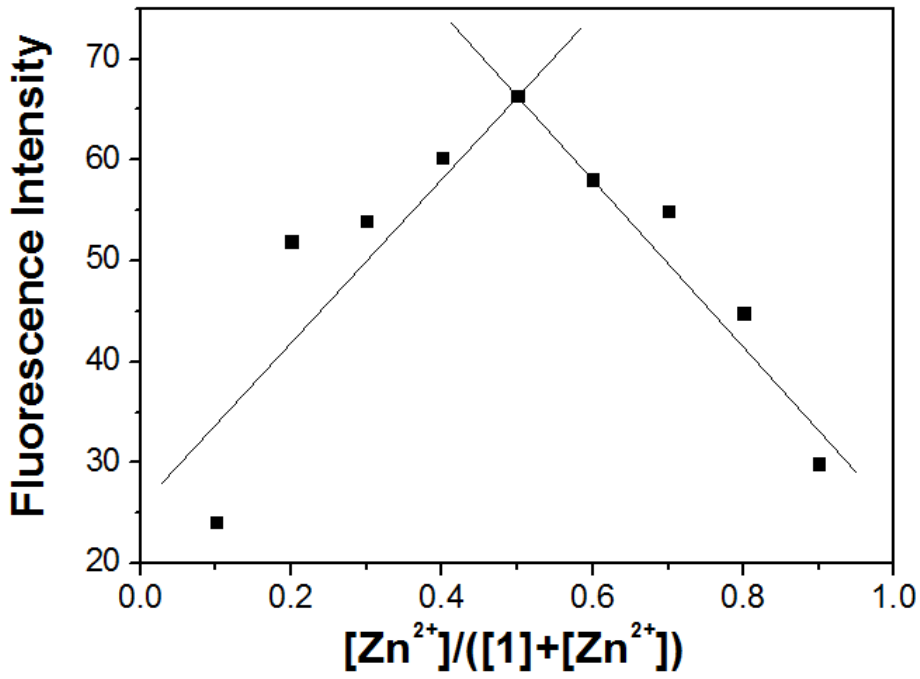
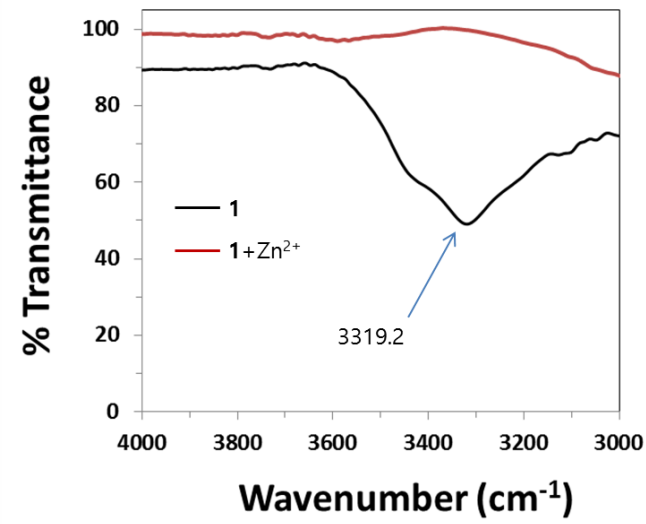


Fig. S1 Job plot of **1** and Zn^{2+} in buffer solution (10 mM bis-tris, pH 7.0). The total concentrations of **1** and Zn^{2+} were 50 μM.

(a)



(b)

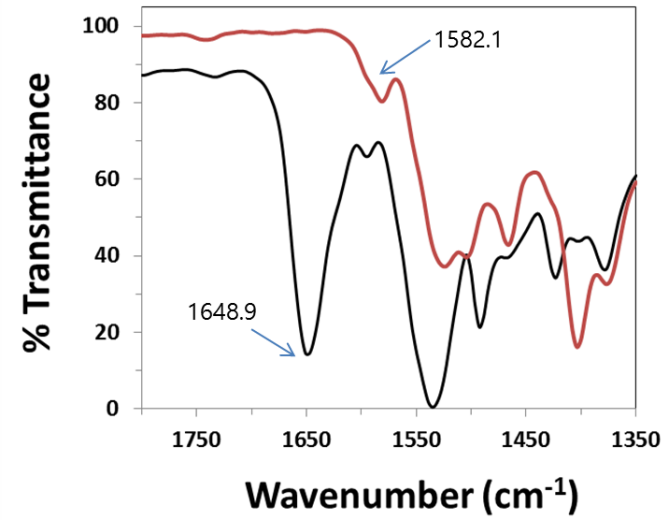


Fig. S2 (a) FT-IR spectra of **1** and **1**-Zn^{2+} complex in the range of wavenumber 4000-3000 cm^{-1}. (b) FT-IR spectra of **1** and **1**-Zn^{2+} complex in the range of wavenumber 1900-1350 cm^{-1}.

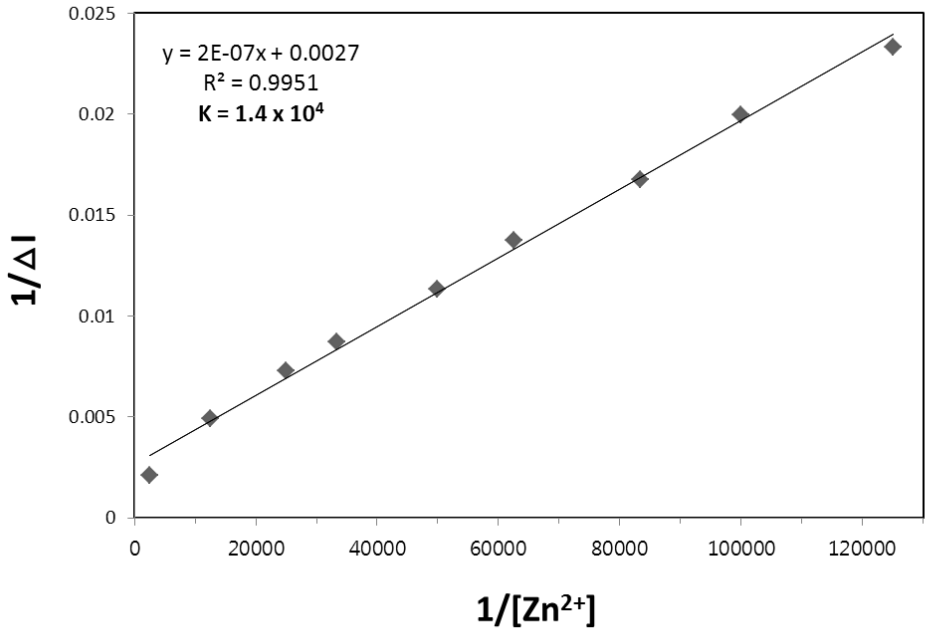


Fig. S3 Benesi-Hildebrand plot of **1** (at 536 nm), assuming 1:1 stoichiometry for association between **1** and Zn^{2+}.

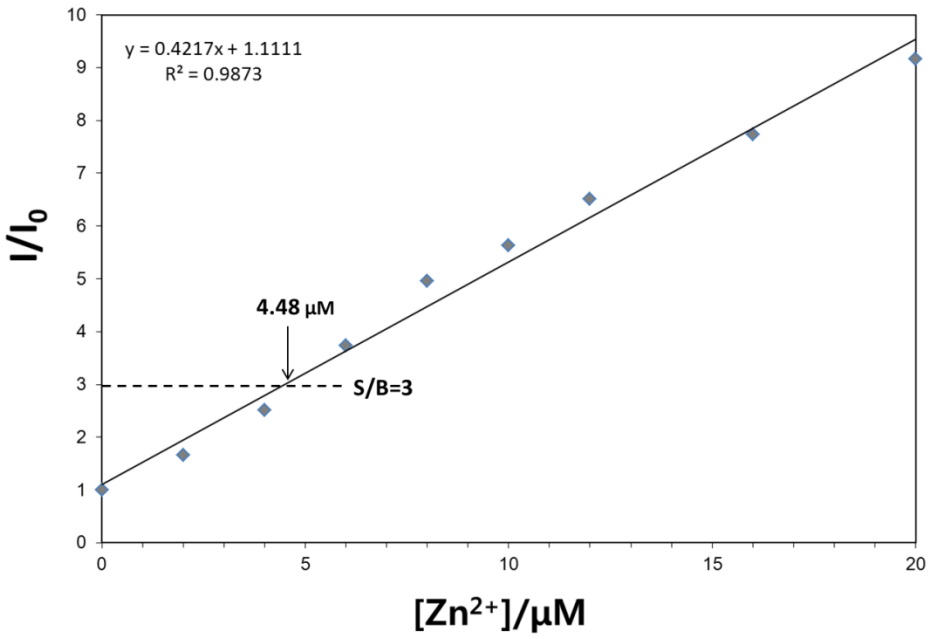


Fig. S4 Change in the ratio of fluorescence intensity (λ_{ex} = 350 nm; λ_{em} = 536 nm) of **1** (20 μM) with Zn^{2+}.

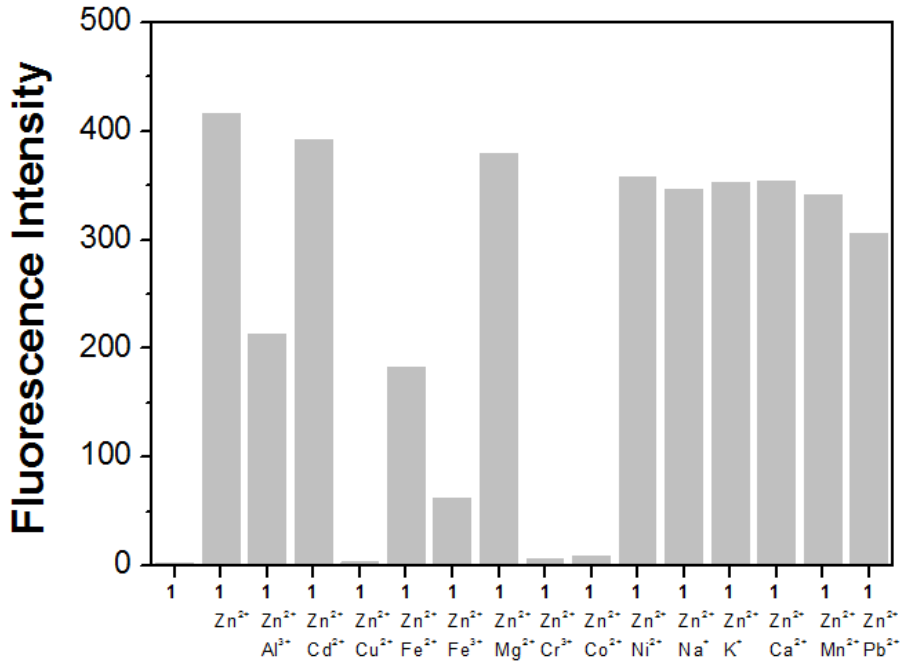


Fig. S5 Competitive selectivity of **1** (20 μM) toward Zn^{2+} (20 equiv) in the presence of other metal ions (20 equiv) in buffer solution (10 mM bis-tris, pH 7.0).

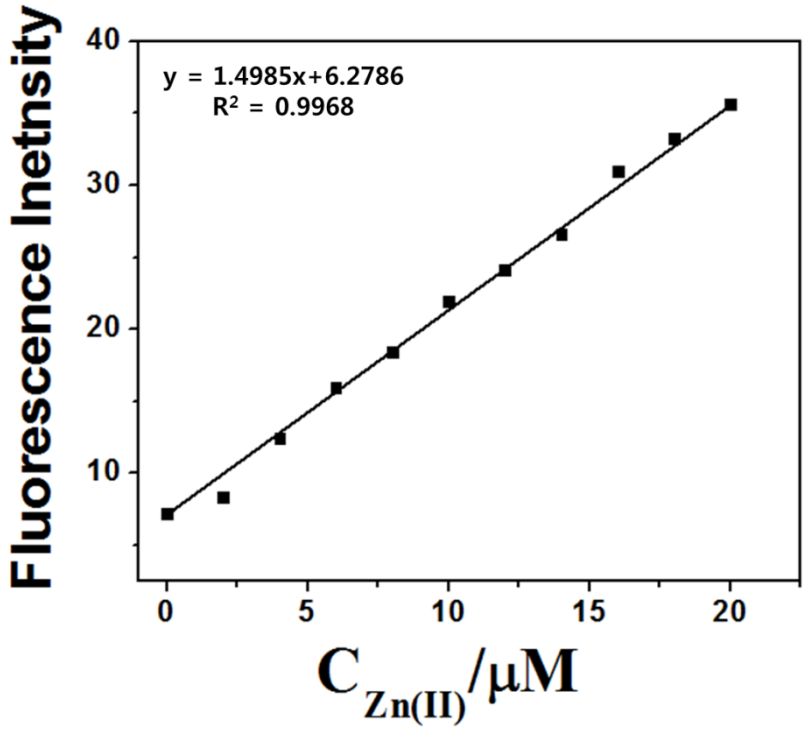
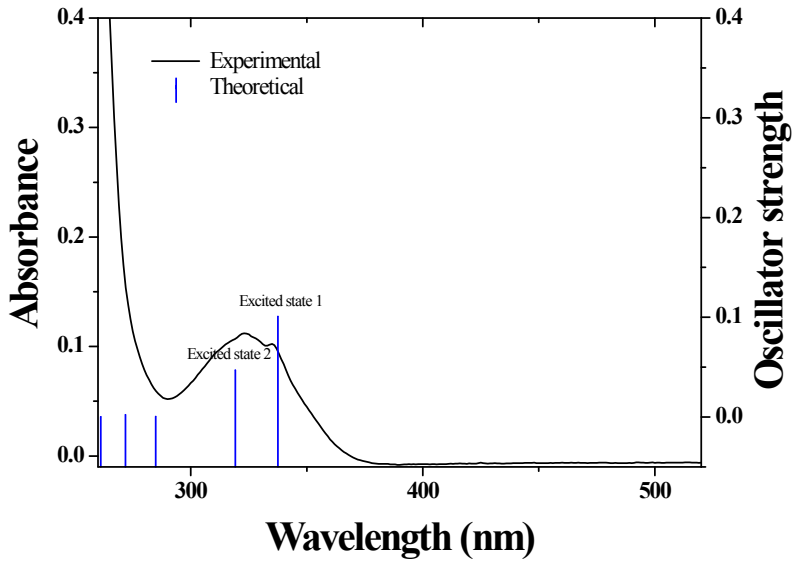


Fig. S6 Fluorescence intensity (at 536 nm) of **1** as a function of Zn^{2+} concentration ([**1**] = 20 μmol/L and [Zn^{2+}] = 0.0-20.0 μmol/L).

(a)



(b)

Excited State 1	Wavelength	Percent (%)	Oscillator strength
H → L	337.51 nm	99 %	0.1009
Excited State 2	**Wavelength**	**Percent (%)**	**Oscillator strength**
H-1 → L	319.24 nm	96 %	0.047
H → L		2 %	

(c)

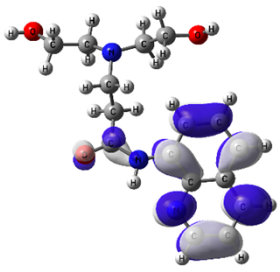
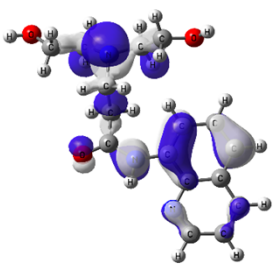
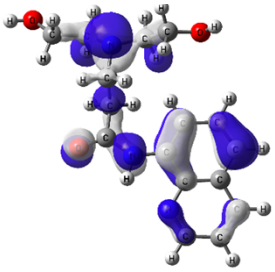
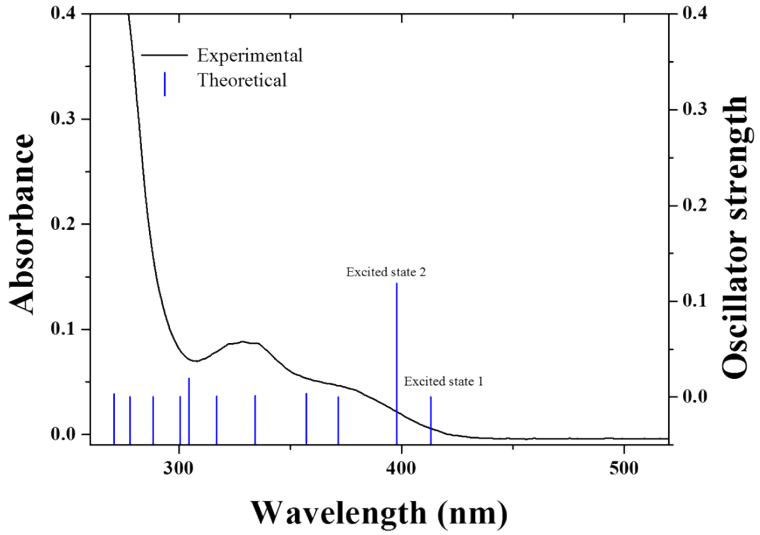
Molecular orbital (1)		
		
LUMO	**HOMO**	**HOMO - 1**
(-1.646 eV)	**(-5.829 eV)**	**(-5.999 eV)**

Fig. S7 (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**. (b) The major electronic transition energies and molecular orbital contributions for **1** (H = HOMO and L = LUMO). (c) Isosurface (0.030 electron bohr^{-3}) of molecular orbitals participating in the major singlet excited states of **1**.

(a)



(b)

Excited State 1	Wavelength	Percent (%)	Oscillator strength
H → L	412.99 nm	99 %	0.0004
Excited State 2	**Wavelength**	**Percent (%)**	**Oscillator strength**
H-1 → L	397.83 nm	98 %	0.1188

(c)

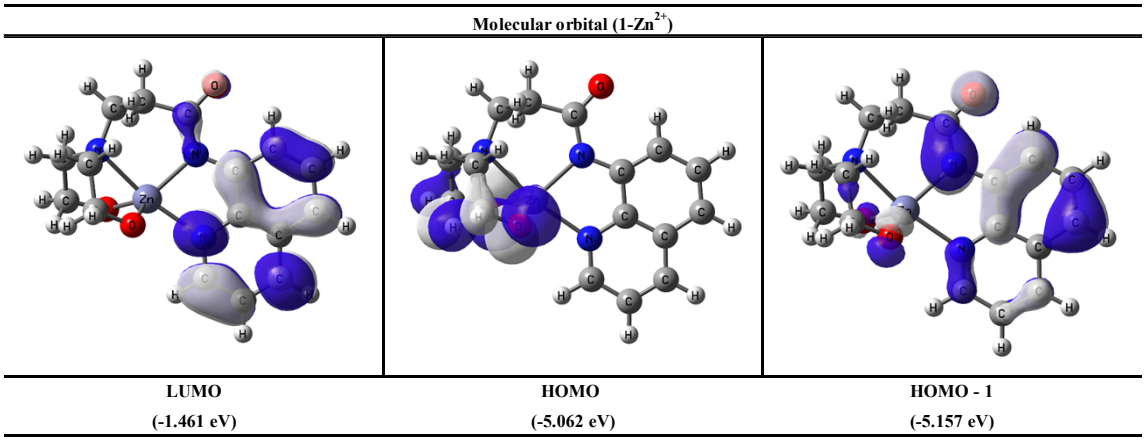


Fig. S8 (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**-Zn^{2+}. (b) The major electronic transition energies and molecular orbital contributions for **1**-Zn^{2+} (H = HOMO and L = LUMO). (c) Isosurface (0.030 electron $bohr^{-3}$) of molecular orbitals participating in the major singlet excited states of **1**-Zn^{2+}.