Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A highly selective colorimetric chemosensor for cyanide and sulfide in aqueous solution: experimental and theoretical studies

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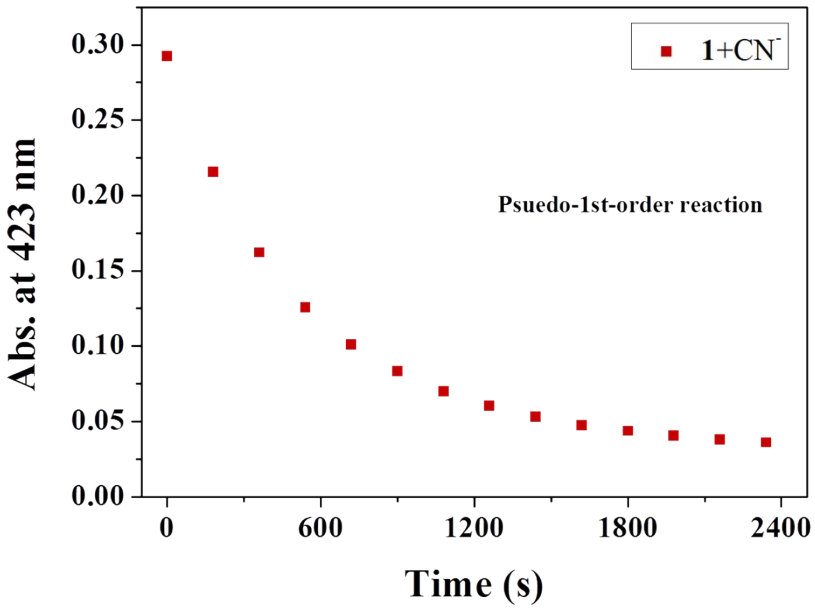
(a)



(b)

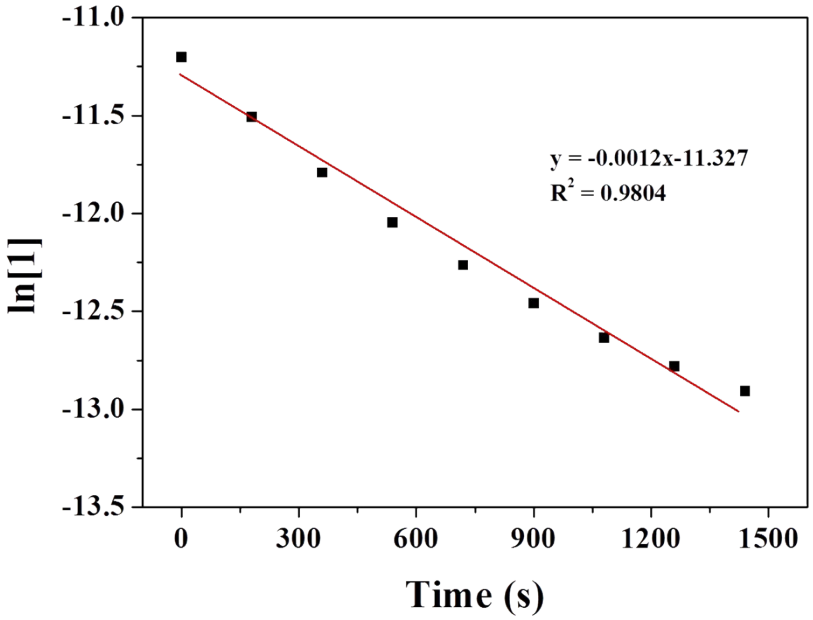


Fig. **S1**. Change of the absorption intensity (423 nm) of **1** (15 μM) with 45 equiv of CN^- under the pseudo-first-order reaction condition. (b) The plot of time vs ln[**1**].

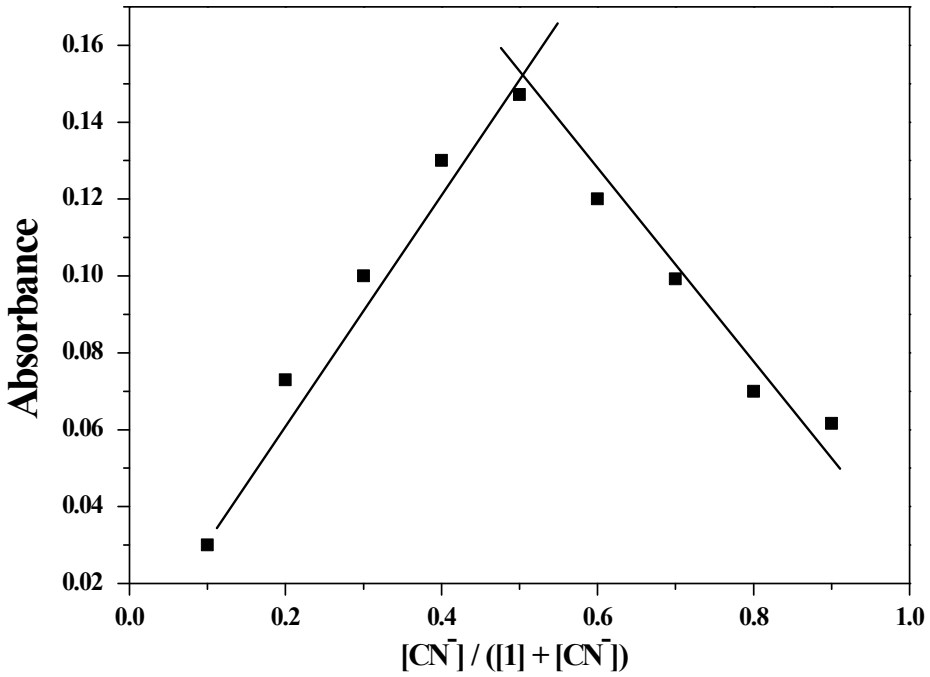


Fig. **S2**. Job plot for the binding of **1** with CN^-. Absorbance at 423 nm was plotted as a function of the molar ratio of $[CN^-]/([\mathbf{1}]+[CN^-])$. The total concentration of CN^- ions with receptor **1** was 1.0×10^{-5} M.

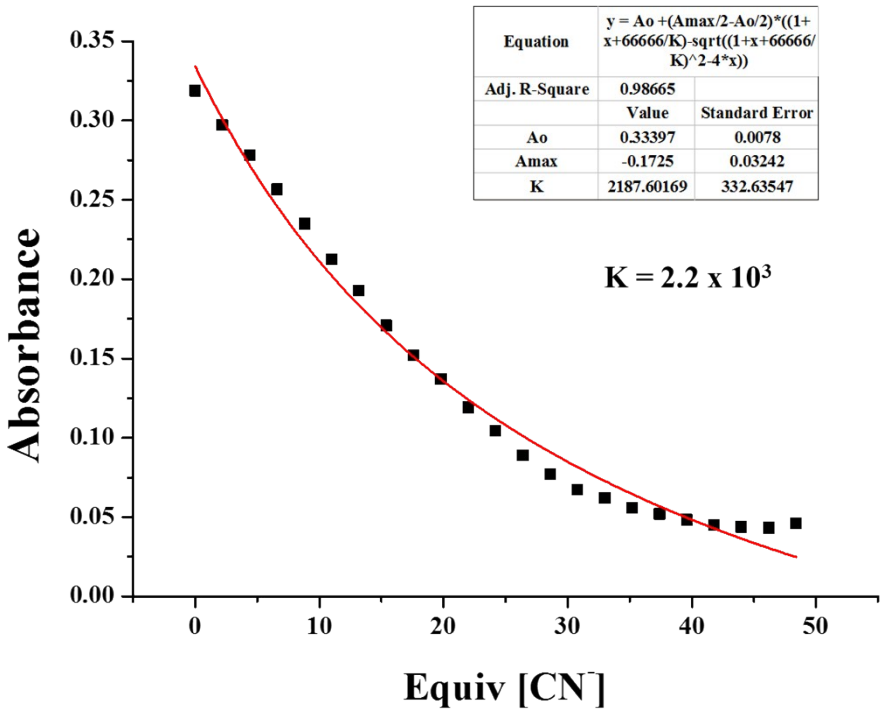


Fig. **S3**. Absorption intensity of **1** (15 μM) at 423 nm after addition of increasing concentration of CN^-. The red line is the non-linear fitting curve between **1** and CN^-. Association constant (K) of **1** with CN^- was calculated by the non-linear least square curve fitting using Origin 8.0.

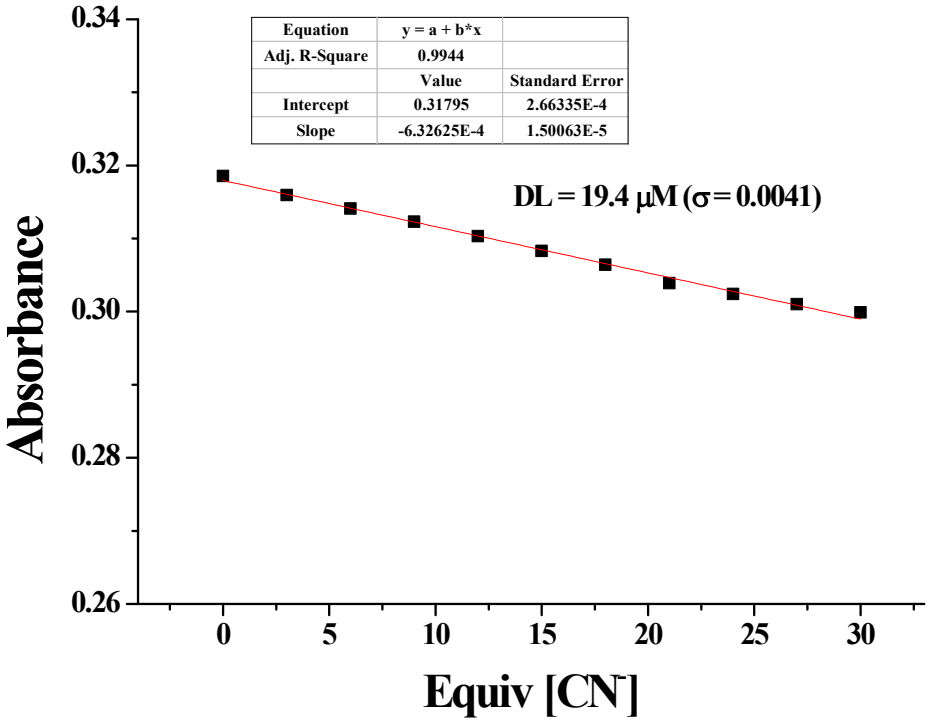


Fig. **S4**. Absorbance (at 423 nm) of **1** as a function of CN^- concentration in bis-tris buffer (10 mM bis-tris, pH = 7.0). [**1**] = 15 µmol/L and [CN^-] = 0-30 µmol/L.

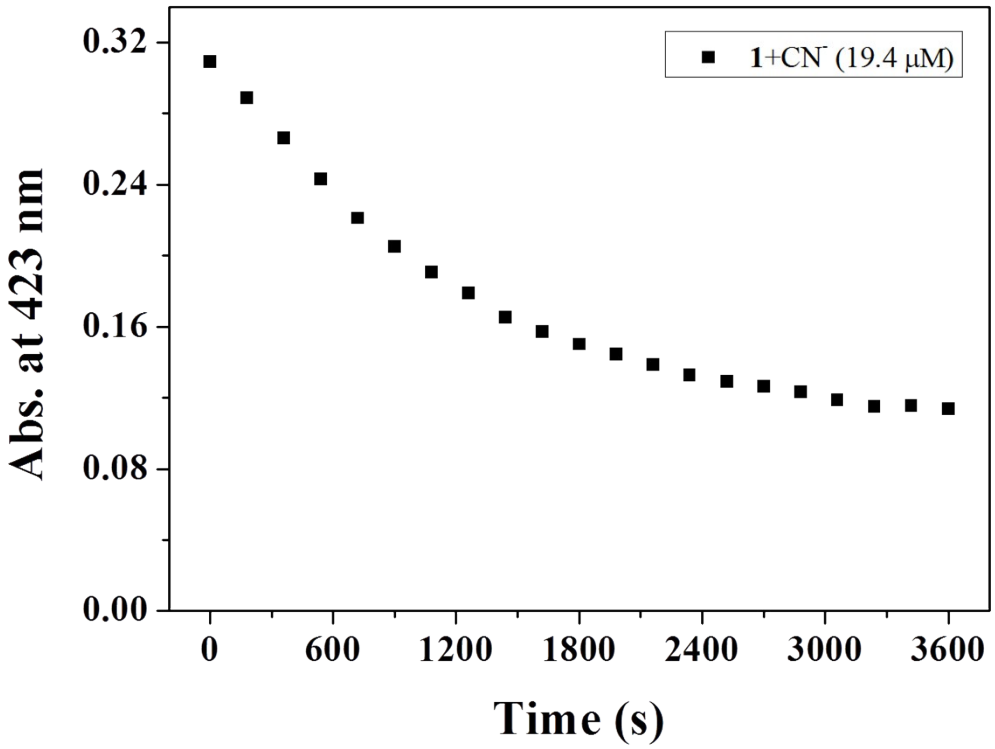
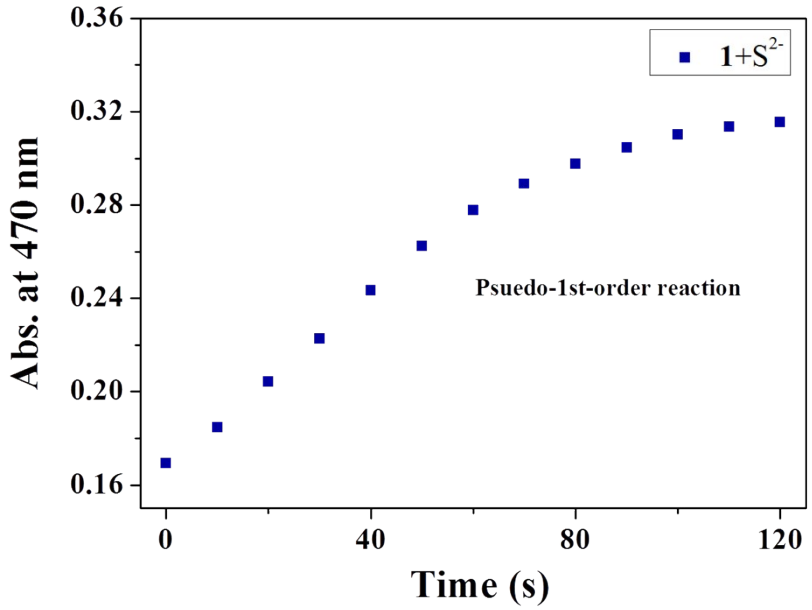


Fig. **S5**. Change of the absorption intensity (423 nm) of **1** (15 μM) with 19.4 μM of CN^- according to time.

(a)



(b)

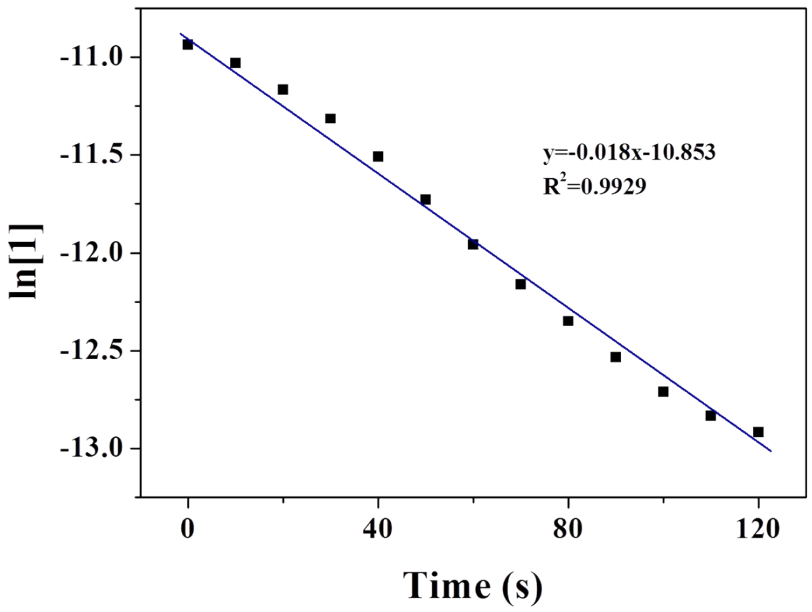


Fig. **S6**. (a) Change of the absorption intensity (470 nm) of **1** (15 μM) with 45 equiv of S^{2-} under the pseudo-first-order reaction condition. (b) The plot of time vs ln[**1**].

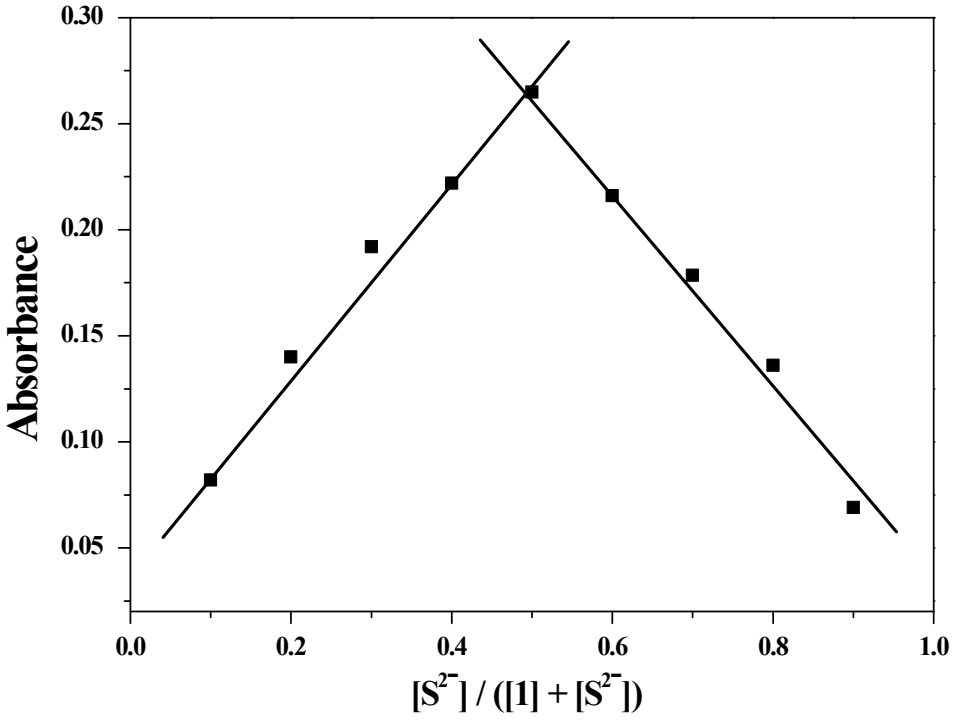


Fig. **S7**. Job plot for the binding of **1** with S^{2-}. Absorbance at 470 nm was plotted as a function of the molar ratio of $[S^{2-}]/([\mathbf{1}]+[S^{2-}])$. The total concentration of S^{2-} ions with receptor **1** was 1.0×10^{-5} M.

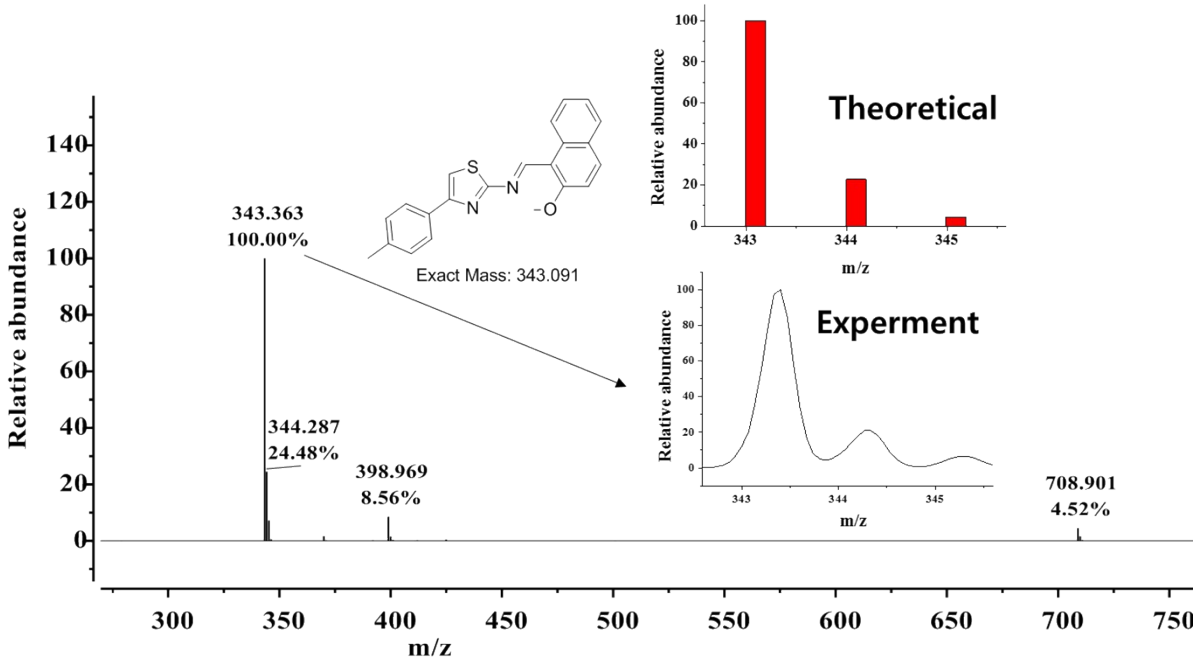


Fig. **S8**. Negative-ion electrospray ionization mass spectrum of **1** (15 μM) upon addition of $Na_2S·9H_2O$ (45 equiv).

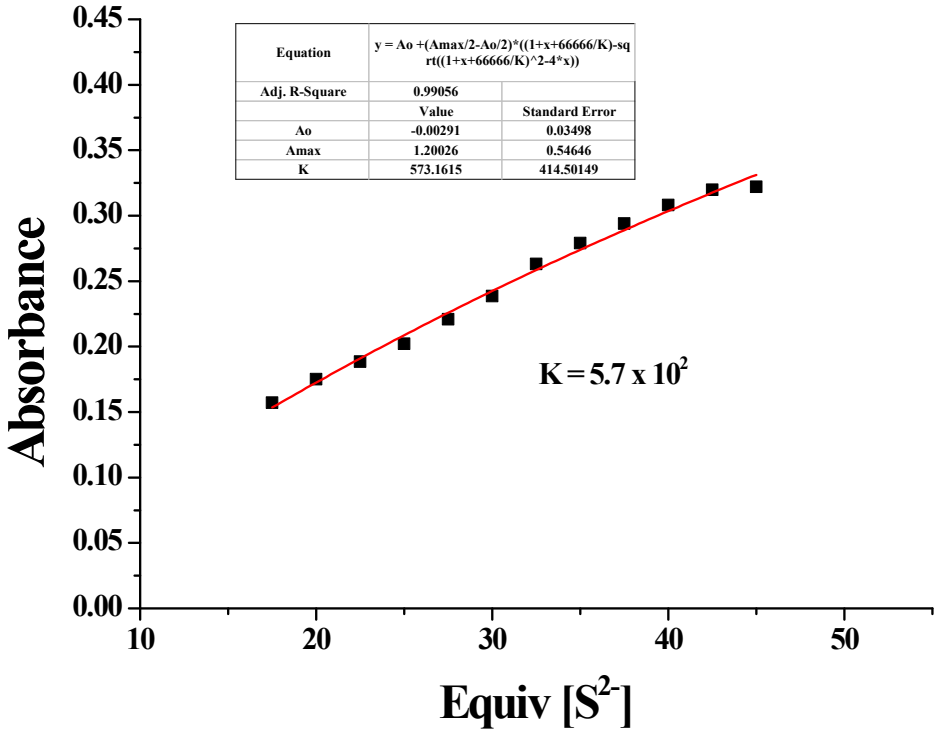


Fig. **S9**. Benesi-Hildebrand plot (λ_{abs} = 470 nm) of **1** (15 μM), assuming a 1:1 stoichiometry for association between **1** and S^{2-}.

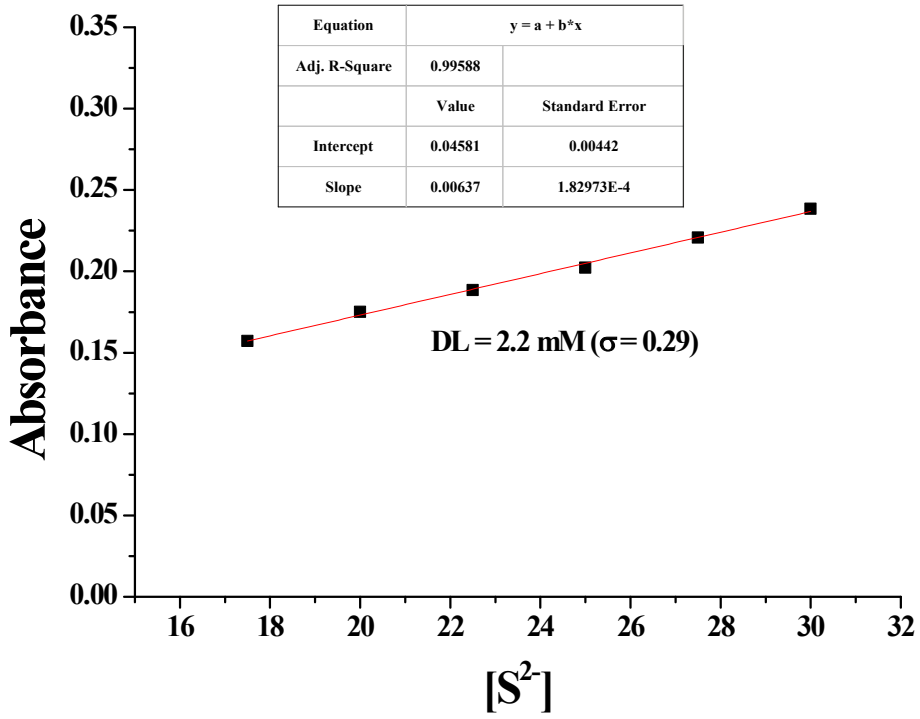
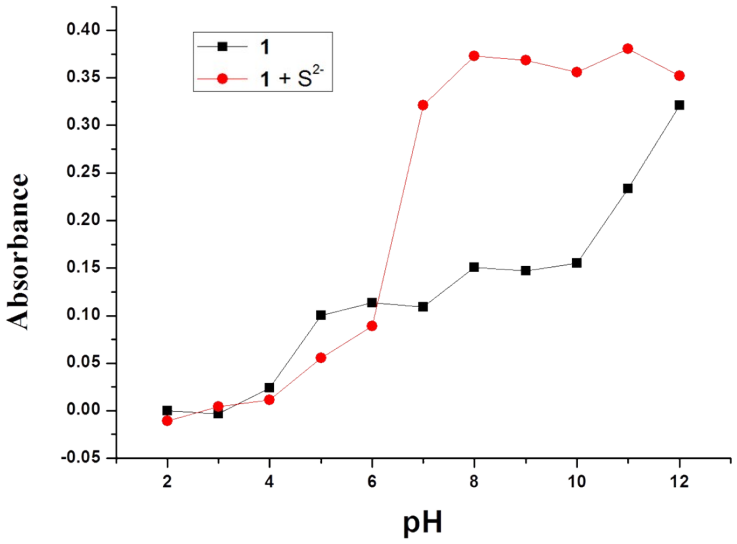


Fig. **S10**. Absorbance (at 470 nm) of **1** as a function of S^{2-} concentration in bis-tris buffer (10 mM bis-tris, pH = 7.0). [**1**] = 15 µmol/L and [S^{2-}] = 18-30 µmol/L.

(a)



(b)

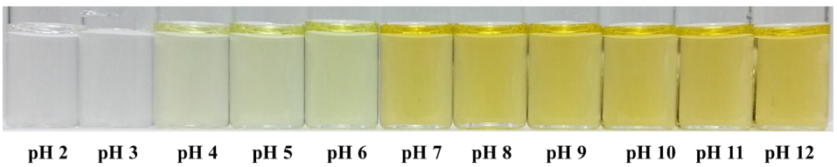
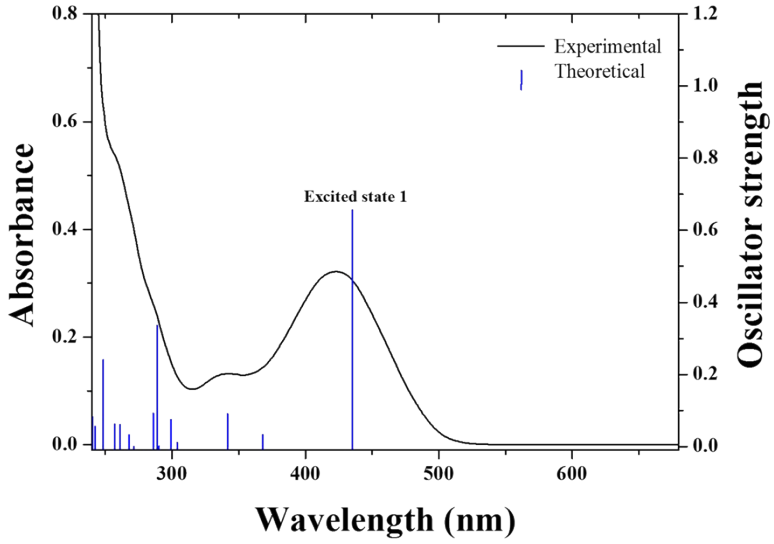


Fig. **S11**. (a) Absorbance (at 470 nm) of **1** (15 μM) with S^{2-} (45 equiv) at different pH (2-12). (b) The color of **1** (15 μM) with S^{2-} (45 equiv) at different pH (2-12).

(a)



(b)

Excited State 1	Wavelength	Percent (%)	Oscillator strength
H → L	435.33 nm	99 %	0.6561

(c)

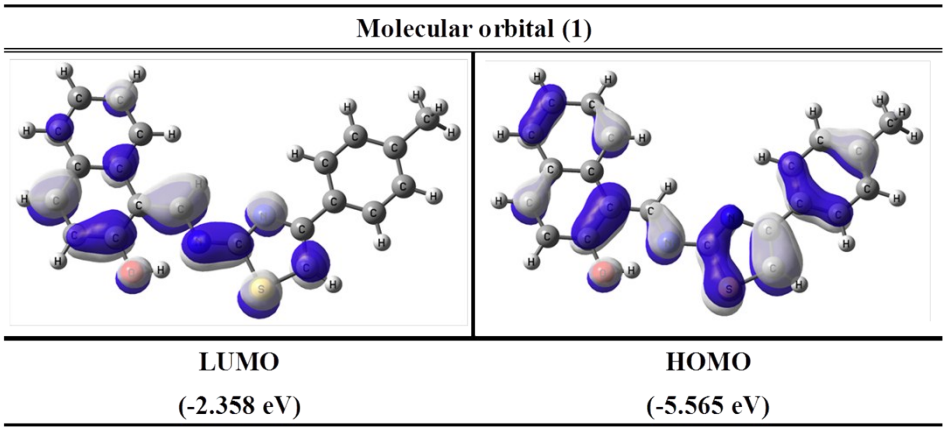
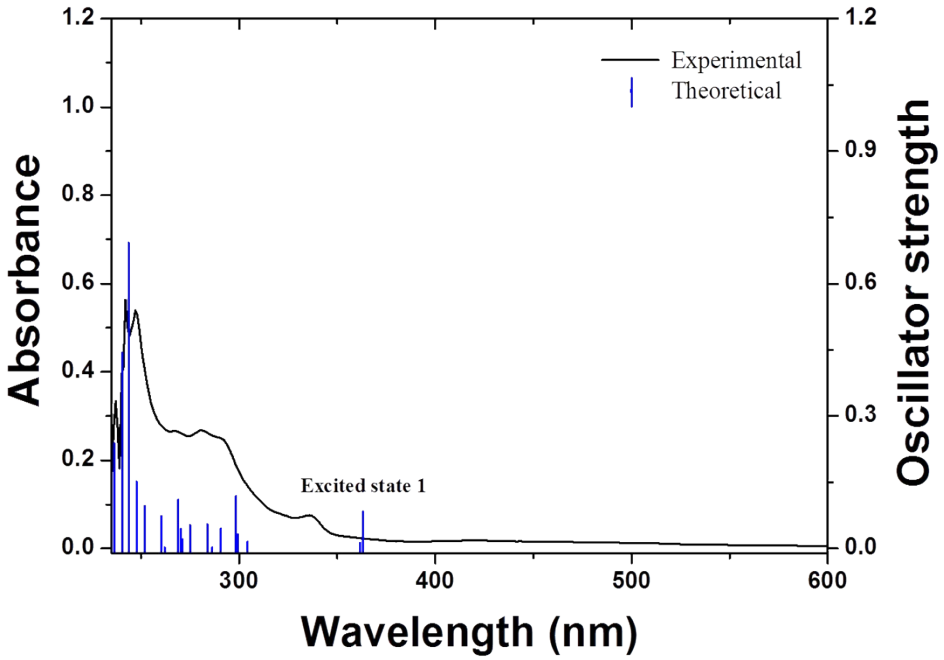


Fig. **S12**. (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**. (b) The major electronic transition energies and molecular orbital contributions for **1** (H = HOMO and L = LUMO). (c) Isosurface (0.030 electron bohr^{-3}) of molecular orbitals participating in the major singlet excited state of **1**.

(a)



(b)

Excited State 1	Wavelength	Percent (%)	Oscillator strength
H → L+1	363.19 nm	82 %	0.0837
H → L		14 %	

(c)

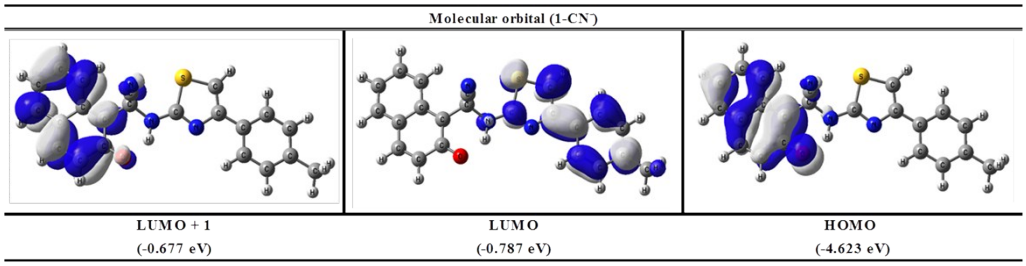
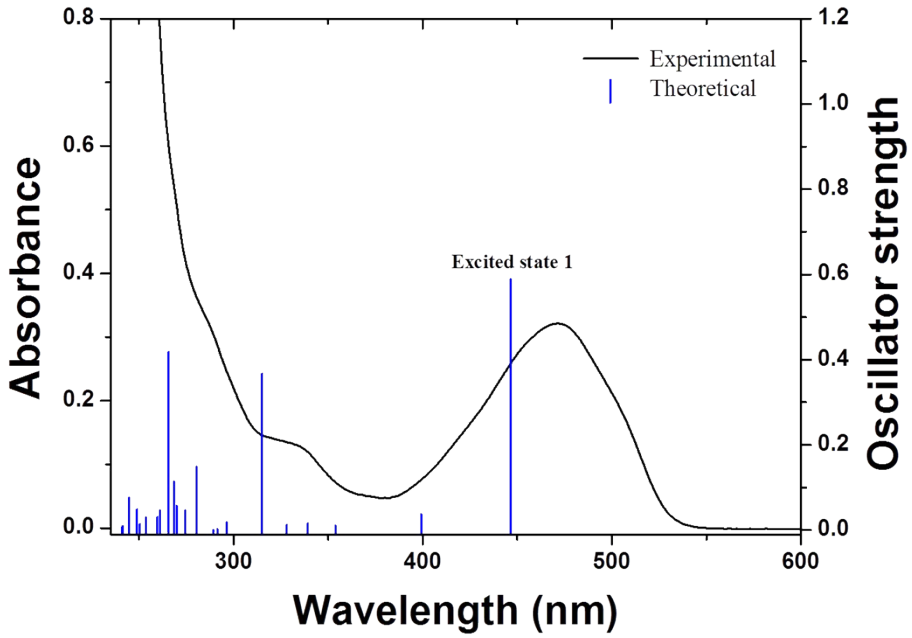


Fig. **S13**. (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**. (b) The major electronic transition energies and molecular orbital contributions for **1** (H = HOMO and L = LUMO). (c) Isosurface (0.030 electron bohr^{-3}) of molecular orbitals participating in the major singlet excited states of **1**-CN^{-}.

(a)



(b)

Excited State 1	Wavelength	Percent (%)	Oscillator strength
H → L	446.40 nm	96 %	0.5891
H-2 → L		2 %	

(c)

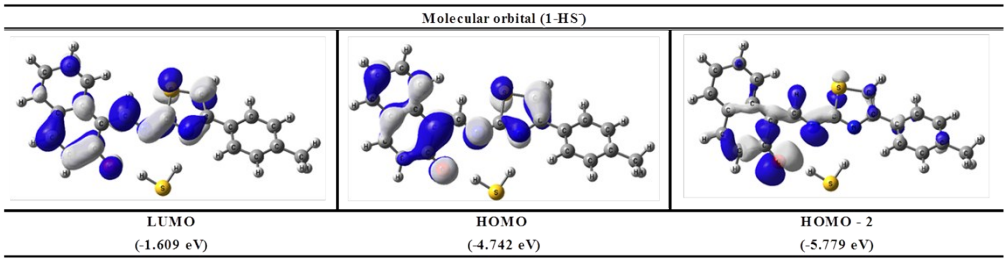


Fig. **S14**. (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**. (b) The major electronic transition energies and molecular orbital contributions for **1** (H = HOMO and L = LUMO). (c) Isosurface (0.030 electron bohr^{-3}) of molecular orbitals participating in the major singlet excited states of **1**-CN^{-}.