Electronic Supplementary Information

A Highly Selective Fluorescence Turn–On Chemosensor for Zn$^{2+}$, its Application in Live Cell Imaging, and a Colorimetric Sensor for Co$^{2+}$: Experimental and TD-DFT Calculations

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Synthesis of carboxamide ligand, Hbpq

A mixture of triphenylphosphite (TPP) (5 mmol, 1.55 g), tetrabutylammonium bromide (TBAB) (5 mmol, 1.61 g), pyridine-2-carboxilic acid (5 mmol, 0.62 g), and 8-aminoquinoline (5 mmol, 0.72 g) in a 25-mL round bottom flask was placed in an oil bath. The reaction mixture was heated until a homogeneous solution was formed, and the solution was stirred for 30 min at 120°C. The final viscous solution was cooled to room temperature and then treated with 10 mL of cold ethanol. The product was precipitated out and filtered off and washed with cold ethanol.

Yield 84%. Anal. Caled. for C₁₅H₁₁N₃O: C, 72.28; H, 4.45; N, 16.86. Found: C, 72.18; H, 4.27; N, 16.76%. FT–IR (KBr, cm⁻¹) $ν_{max}$: 3295 (s, N-H), 1681 (s, C=O), 1529 (m, C=C), 1487 (m, C–N). UV–Vis: [CH₃CN; $λ_{max}$ (nm) (ε, L mol⁻¹ cm⁻¹)]: 328 (12240), 276 (7510), 241 (23950). ¹H NMR (δ, CDCl₃, 500 MHz): 7.45-7.63 (m, 4H, Hₐ,b,d,e,i) 7.91 (td, H₇), 8.18 (dd, H₉), 8.35 (bd, H₈), 8.78 (bd, H₇), 8.96 (dd, H₉), 9.01 (dd, H₈), 12.27 (s, NH).
Scheme S1. One pot synthesis of N-(8-quinolyl)pyridine-2-carboxamide ligand, Hbpq.

Fig. S1-1. UV-vis spectrum of Hbpq in acetonitrile, solution at room temperature.

Fig. S1-2. FT-IR spectrum of Hbpq (KBr pellet).
Determination of association constant for Zn$^{2+}$ complex

An association constant (2:1) was calculated according to the titration curve for complex formation between the chemosensors and the metal ions, using the following nonlinear least squares fitting equation:

$$y = \frac{x}{2 \times a \times b \times (1 - x)^2} + \frac{x \times b}{2}$$

Where $a$ is the association constant, $b$ is the concentration of chemosensor, $x$ is $A_x - A_0 / A_{\text{max}} - A_0$ and $y$ is the concentration of metal ions [1].

Fig. S2. The Benesi-Hildebrand plot of Hbpq with Zn$^{2+}$ based on the absorption titration.
**Fig. S3.** The linear fitting of the fluorescence intensity of Hbpq toward the concentrations of Zn$^{2+}$.

**Fig. S4.** The relative fluorescence intensity of Hbpq and [Zn(bpq)$_2$] in the presence of interfering anions.
Fig. S5. Job's plot of the [Co(bpq)$_2$] complex in acetonitrile solution, with the monitoring wavelength set at 401 nm.

**Determination of association constant for Co$^{2+}$ complex**

An association constant (2:1) was calculated according to the titration curve for complex formation between the chemosensors and the metal ions, using the following nonlinear least squares fitting equation:

$$y = \frac{x}{2 \times a \times b \times (1-x)^2} + \frac{x \times b}{2}$$

Where $a$ is the association constant, $b$ is the concentration of chemosensor, $x$ is $A_x - A_0 / A_{\text{max}} - A_0$ and $y$ is the concentration of metal ions [1].

Fig. S6. The Benesi-Hildebrand plot of Hbpq with Co$^{2+}$ based on the absorption titration.
Fig. S7. The linear fitting of the absorption intensity of Hbpq toward the concentrations of Co$^{2+}$.

Reference


Fig. S8. FT-IR spectrum of [Zn(Hbpq)$_2$] as KBr pellet.
Fig. S9. UV-vis spectrum of [Zn(bpq)$_2$] in acetonitrile, solution at room temperature.

Fig. S10. $^1$H-NMR spectrum of [Zn(Hbpq)$_2$] in CDCl$_3$ solution at room temperature.
Fig. S11. FT-IR spectrum of [Co(Hbpq)$_2$] as KBr pellet.

![FT-IR spectrum of [Co(Hbpq)$_2$]](image)

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Fig. S12. UV-vis spectrum of [Co(bpq)$_2$] in acetonitrile, solution at room temperature.

![UV-vis spectrum of [Co(bpq)$_2$]](image)