Supporting Information

A Molecular Logic Gate for Highly Selective Recognition of Pyrophosphate with Hypocrellin A-Zn(II) Complex

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Figure S1 The structures of HA and HA-Zn\textsuperscript{2+}.

Figure S2 Changes in the fluorescence emission of HA in ethanol solution upon addition of Zn\textsuperscript{2+}.

$[\text{HA}] = 5 \text{ mM, } [\text{Zn}^{2+}] = 0, 100, 200, \text{ and } 300 \text{ mM (from A to D).}$

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Figure S3 PPi induced recovery of fluorescence of HA. Curves B-J, HA-Zn$^{2+}$ upon addition of various amounts of PPi; $\lambda_{\text{ex}}$, 466 nm; $c_{\text{HA}}$, 5 $\mu$M; $c_{\text{Zn}^{2+}}$, 350 $\mu$M; Tris-HCl, pH 7.4; $c_{\text{PPi}}$, from curve B to curve J, 0, 3.0×10$^{-5}$ M, 6.0×10$^{-5}$ M, 1.2×10$^{-4}$ M, 1.8×10$^{-4}$ M, 2.4×10$^{-4}$ M, 3.0×10$^{-4}$ M, 3.6×10$^{-4}$ M, 3.96×10$^{-4}$ M.

Figure S4 Changes of the fluorescence emission of HA upon addition of Pb$^{2+}$. $c_{\text{HA}}$, 5 $\mu$M, $c_{\text{Pb}^{2+}}$, 0, 50, 200, 350, and 500 $\mu$M (from A to E), Tris-HCl, pH 7.4.
Figure S5 Changes of the fluorescence emission of HA upon addition of Co$^{2+}$. 

$c_{HA}$, 5 $\mu$M, $c_{Co^{2+}}$, 0, 50, 200, 350, and 500 $\mu$M (from A to E), Tris-HCl, pH 7.4.

Figure S6 Changes of the fluorescence emission of HA upon addition of Cu$^{2+}$. 

$c_{HA}$, 5 $\mu$M, $c_{Cu^{2+}}$, 0, 50, 200, 350, and 500 $\mu$M (from A to E), Tris-HCl, pH 7.4.
Figure S7 Changes of the fluorescence emission of HA upon addition of Tb$^{3+}$.
$c_{HA}$, 5 μM, $c_{Tb^{3+}}$, 0, 50, 200, 350, and 500 μM (from A to E), Tris-HCl, pH 7.4.

Figure S8 Changes of the fluorescence emission of HA upon addition of Cd$^{2+}$.
$c_{HA}$, 5 μM, $c_{Cd^{2+}}$, 0, 50, 200, 350, and 500 μM (from A to E), Tris-HCl, pH 7.4.
Figure S9 Changes of the fluorescence emission of HA upon addition of Zn$^{2+}$.

c_{HA}, 5 \mu M, c_{Zn^{2+}}, 0, 50, 200, 350, and 500 \mu M (from A to E), Tris-HCl, pH 7.4.

Figure S10. pH-dependent fluorescence change curves of HA-Zn$^{2+}$ and HA-Zn$^{2+}$-PPi. (Inset)

Influence of pH on the fluorescence of HA. \(\lambda_{ex}=466\) nm, \(\lambda_{em}=604\) nm, \(c_{HA}, 5 \mu M, c_{Zn^{2+}}, 350 \mu M\),

Tris-HCl, pH 7.2, 7.3, 7.4, 7.6, 8.0, 8.2, 8.6, 9.0.

As shown in Figure S10, the fluorescence intensity of HA-Zn$^{2+}$ and HA-Zn$^{2+}$-PPi was decreased gradually in the range from pH 7.2 to 9.0, while no significant emission changes of HA were observed at pH 7.3-8.0. Since HA-Zn$^{2+}$ had a large fluorescence enhancement (\(F/F_0\)) at pH 7.4 which could sense PPi effectively, the acidity of the medium was adjusted with Tris-HCl buffer solution of pH 7.4.