

## Supporting Information

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

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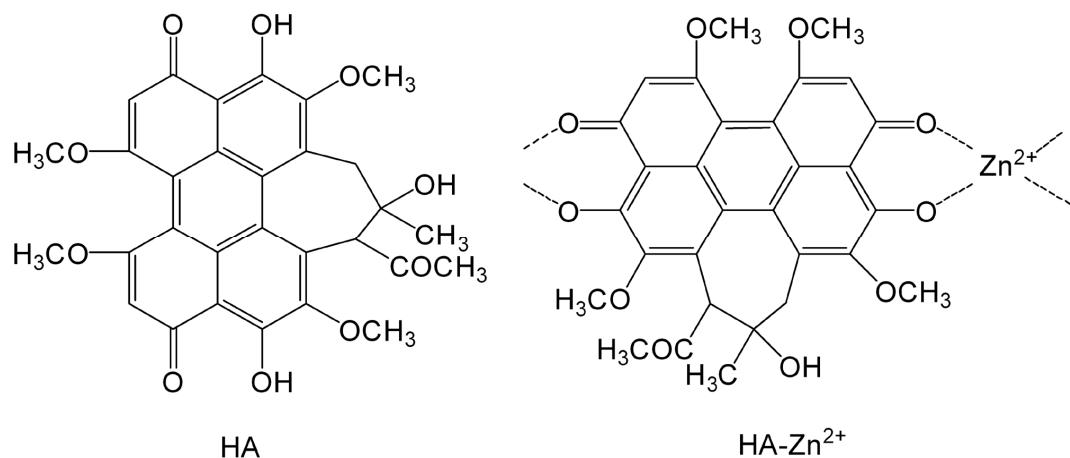


Figure S1 The structures of HA and HA-Zn<sup>2+</sup>.

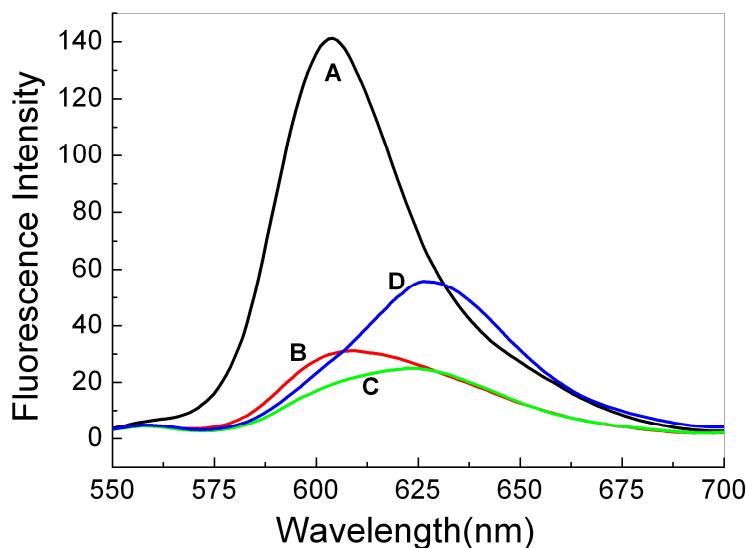


Figure S2 Changes in the fluorescence emission of HA in ethanol solution upon addition of Zn<sup>2+</sup>.

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

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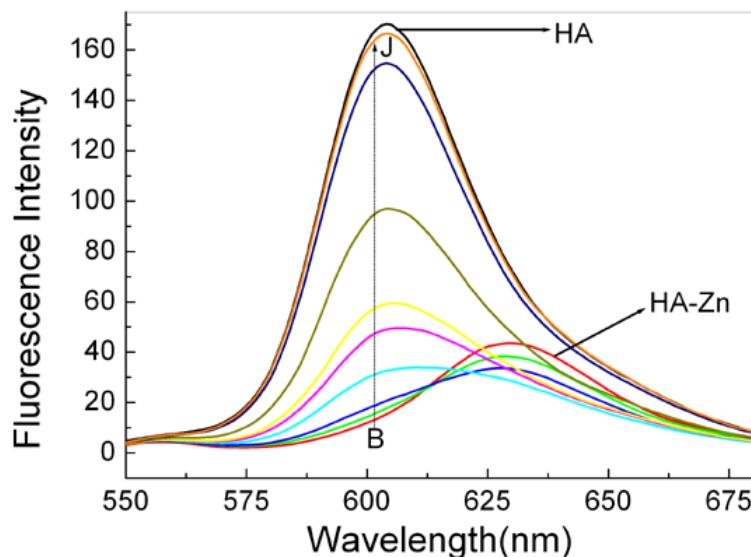


Figure S3 PPi induced recovery of fluorescence of HA. Curves B-J, HA-Zn<sup>2+</sup> upon addition of various amounts of PPi;  $\lambda_{\text{ex}}$ , 466 nm;  $c_{\text{HA}}$ , 5  $\mu\text{M}$ ;  $c_{\text{Zn}^{2+}}$ , 350  $\mu\text{M}$ ; Tris-HCl, pH 7.4;  $c_{\text{PPi}}$ , from curve B to curve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

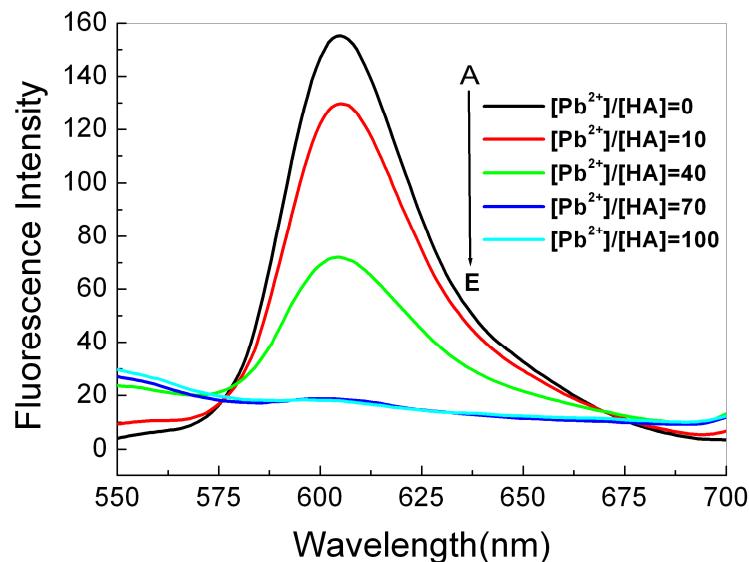


Figure S4 Changes of the fluorescence emission of HA upon addition of  $\text{Pb}^{2+}$ .  
 $c_{\text{HA}}$ , 5  $\mu\text{M}$ ,  $c_{\text{Pb}^{2+}}$ , 0, 50, 200, 350, and 500  $\mu\text{M}$  (from A to E), Tris-HCl, pH 7.4.

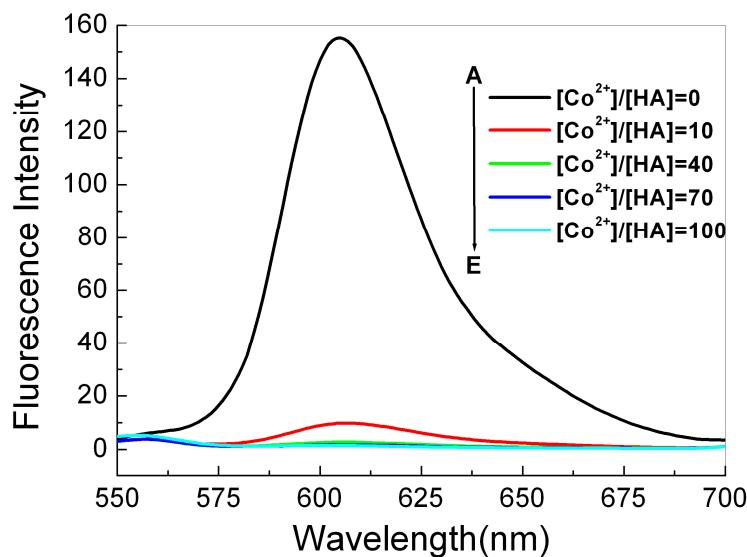


Figure S5 Changes of the fluorescence emission of HA upon addition of  $\text{Co}^{2+}$ .

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

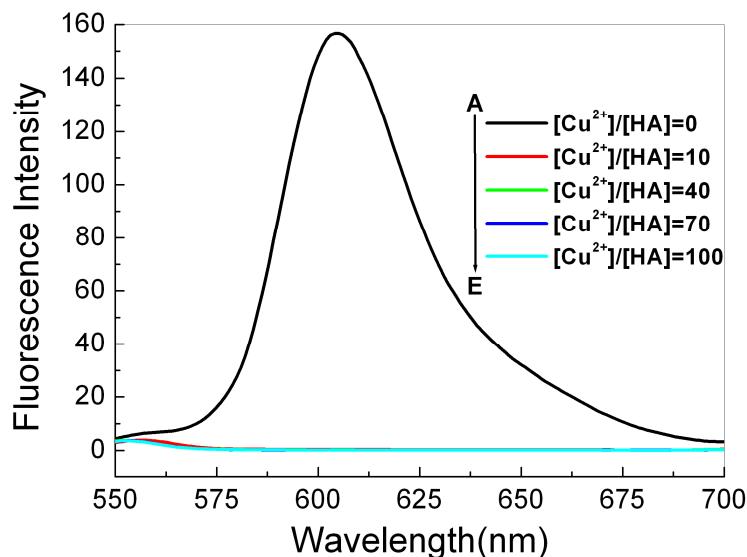


Figure S6 Changes of the fluorescence emission of HA upon addition of  $\text{Cu}^{2+}$ .

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

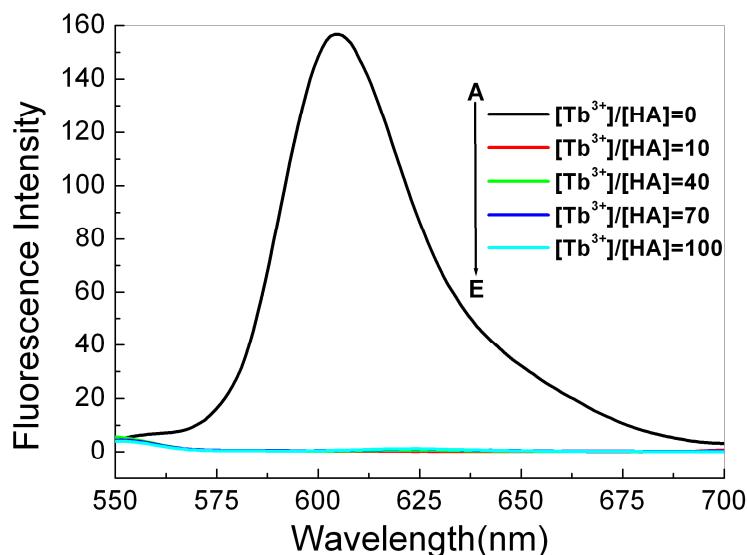


Figure S7 Changes of the fluorescence emission of HA upon addition of  $\text{Tb}^{3+}$ .

$c_{\text{HA}}$ , 5  $\mu\text{M}$ ,  $c_{\text{Tb}^{3+}}$ , 0, 50, 200, 350, and 500  $\mu\text{M}$  (from A to E), Tris-HCl, pH 7.4.

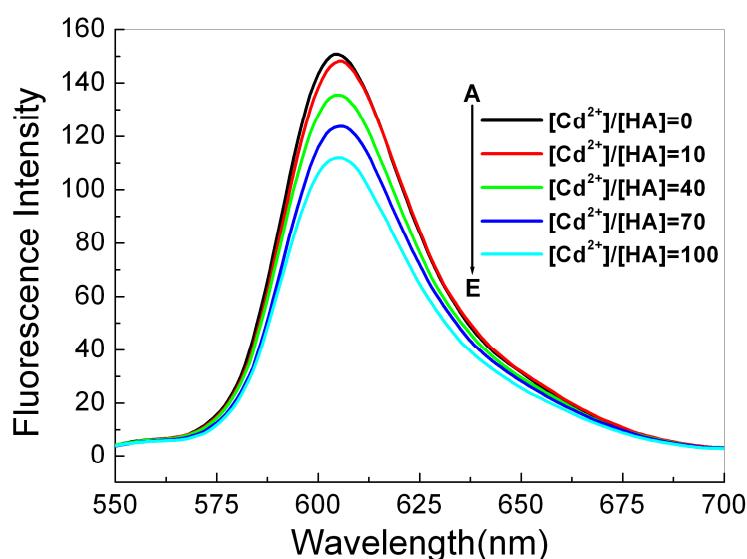


Figure S8 Changes of the fluorescence emission of HA upon addition of  $\text{Cd}^{2+}$ .

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

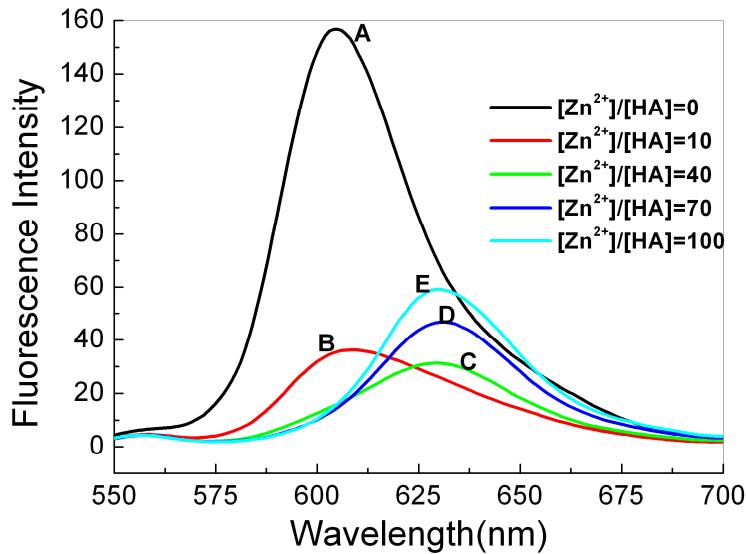


Figure S9 Changes of the fluorescence emission of HA upon addition of  $Zn^{2+}$ .

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

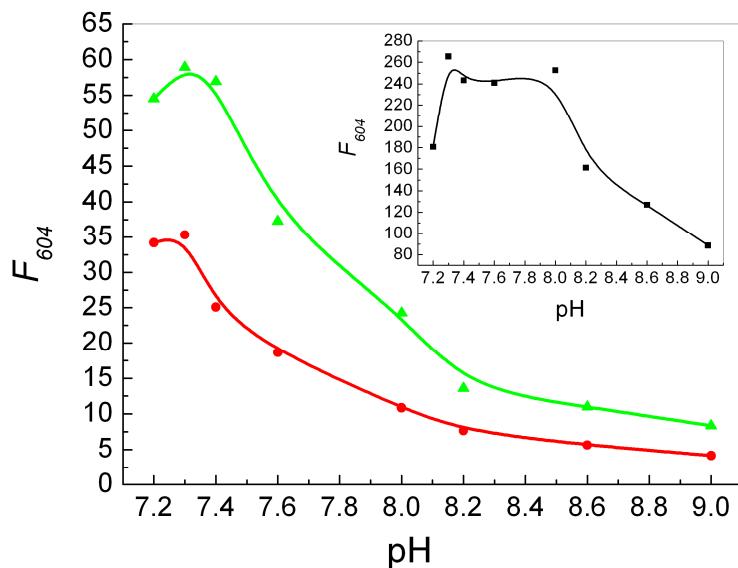


Figure S10. pH-dependent fluorescence change curves of HA- $Zn^{2+}$  and HA- $Zn^{2+}$ -PPi. (Inset)

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