Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2019

Supporting Information

An easy-to-synthesize multi-photoresponse smart sensor for fast

detecting Zn2+ and quantifying Fe3+ based on the enol/keto binding

mode

Jingzhe Zhang,^a Zheng Zhao,^b Hong Shang,^{c,*} Qingsong Liu,^{a,*} Fei Liu^{a,*}

Content

- 1. The ¹H and ¹³C NMR spectra of EASA-F, Figure S1, Page S3.
- 2. The mass spectroscopy of EASA-F, Figure S2, Page S4.
- Fluorescence Benesi-Hildebrand plot of 1/(F-F_{min}) against 1/[Zn²⁺], Figure S3, Page S5.
- 4. The mass spectroscopy of EASA-F upon addition of Zn^{2+} , Figure S4, Page S6.
- 5. ¹H NMR titration experiments of EASA-F with the Zn^{2+} in CD₃CN, Figure S5, Page S7.
- The electronic absorption and fluorescence emission spectra of EASA-F upon increasing Fe³⁺ amount, Figures S6 and S7, Pages S8 and S9.
- The electronic absorption and fluorescence emission spectra of EASA-F-Zn²⁺/Fe³⁺ upon addition of other tested metal ions, respectively, Figures S8 and S9, Pages S10 and S11.
- The electronic absorption of EASA-F (20 μM) in DMSO/H₂O mixture and in different solvents, Figure S10, Page S12.
- 9. The mass spectroscopy of EASA-F upon addition of Fe³⁺, Figure S11, Page S13.
- 10. The IR spectra for EASA-F upon addition of Zn^{2+}/Fe^{3+} , Figure S12, Page S14.
- 11. The response time of EASA-F to Zn^{2+}/Fe^{3+} , Figures S13 and S14, Pages S15 and S16.



Figure S1 ¹H NMR (A) and ¹³C NMR spectra (B) of EASA-F in DMSO. * indicates the residual solvent signals.



Figure S2 The mass spectroscopy of EASA-F.



Figure S3 Fluorescence Benesi-Hildebrand plot of $1/(F-F_{min})$ against $1/[Zn^{2+}]$. F_{min} and *F* represent the fluorescence emission of EASA-F (10 μ M) in the absence and the presence of Zn²⁺ at 500 nm, respectively.

Based on 1:1 stoichiometry, the Benesi-Hildebrand equation can be used to evaluate the binding strength:

$$\frac{1}{F - F_{\min}} = \frac{1}{K_a \cdot (F_{\max} - F_{\min}) \cdot [Zn^{2+}]} + \frac{1}{F_{\max} - F_{\min}}$$

 F_{max} is the fluorescence intensity obtained with a large excess of Zn²⁺, *K* is the association constant of Zn²⁺ complex of EASA-F. From the Benesi-Hildebrand analysis, the *K* is determined to be 6.7×10^4 .



Figure S4 (A and B) Experimental and (C) simulated isotopic pattern for molecular ion of EASA-F upon addition of Zn^{2+} , respectively.



Figure S5 The ¹H NMR spectra of EASA-F in the absence and the presence of Zn^{2+} (1.0 equiv.) in CD₃CN, respectively.



Figure S6 The fluorescence emission spectra of EASA-F upon increasing Fe^{3+} amount from 0 to 1.5 and from 1.5 to 8 even 10 equiv, respectively.



Figure S7 The absorption spectra of EASA-F upon increasing Fe^{3+} amount from 0 to 1.5 and from 1.5 to 8 equiv, respectively.



Figure S8 The fluorescence emission spectra of EASA-F-Zn²⁺ system in CH₃CN/H₂O (19:1) upon respective addition of other metal ions such as Pb²⁺, Mg²⁺, Co²⁺, Fe³⁺, Hg²⁺, Mn²⁺, Zn²⁺, Ni²⁺, Cd²⁺, Ca²⁺, Ba²⁺, Li⁺, Na⁺, K⁺, Fe²⁺, Al³⁺, or Cr³⁺ (10 equiv), respectively.



Figure S9 The fluorescence emission spectra of EASA-F-Fe³⁺ system in CH₃CN/H₂O (19:1) upon respective addition of other metal ion such as Li⁺, Na⁺, K⁺, Ca²⁺, Ba²⁺, Mg²⁺, Pb²⁺, Co²⁺, Hg²⁺, Mn²⁺, Cu²⁺, Ni²⁺, Cd²⁺, Fe²⁺, Al³⁺, or Cr³⁺ (10 equiv), respectively.



Figure S10 The electronic absorption spectra of EASA-F (20 μ M) in DMSO/H₂O mixture with H₂O fractions (f_w) from 0 to 50% (A) and in different solvent including CH₂Cl₂, THF, CH₃CN, DMSO and MeOH (B), respectively.



Figure S11 The experimental (A and B) and simulated (C) isotopic pattern for molecular ion of EASA-F upon addition of Fe³⁺ (10 equiv.) in CH₃CN/H₂O (19:1), respectively.



Figure S12 The IR spectra for EASA-F upon respective addition of Zn^{2+} (10 eqiuv.)and Fe^{3+} (1and10eqiuv.),respectively.



Figure S13 The fluorescence emission of EASA-F along with the changing time upon addition of 10 equiv. Zn^{2+} in CH₃CN/H₂O (19:1).



Figure S14 The electronic absorption spectra of EASA-F along with the change in time upon addition of Fe^{3+} (10 equiv.) in CH₃CN/H₂O (19:1).