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Supporting Information

A Novel Peptide-based Fluorescent Chemosensor for Measuring Zinc Ion by Different Excitation Wavelengths and Application in Living Cell Image

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HPLC Chromatogram of L

Sample: L

Column: 4.6*150mm, kromasil C18-5

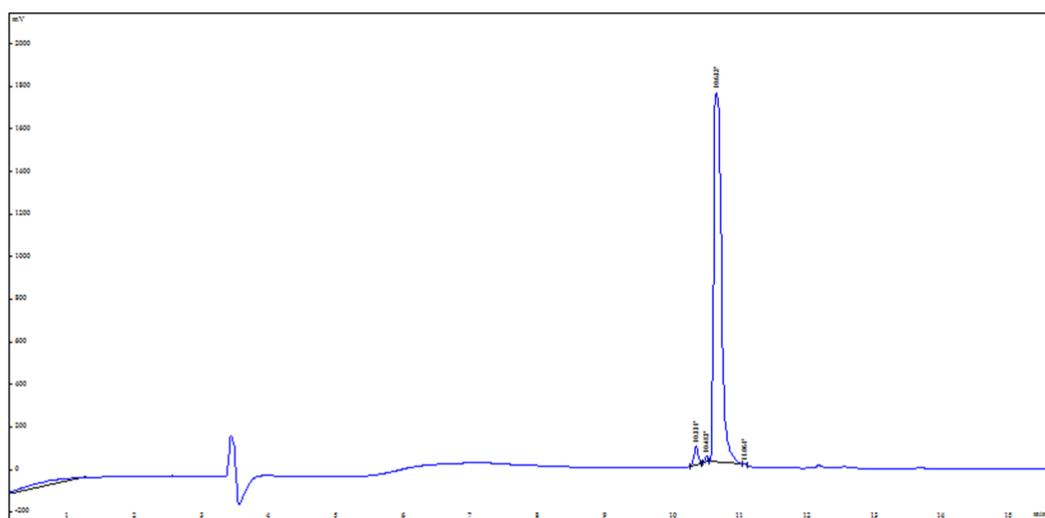
Solvent A: 0.1%Trifluoroacetic acid in 100%Acetonitrile

Solvent B: 0.1%Trifluoroacetic acid in 100% Water

Gradient:	Time	A	B
	0.01min	5%	95%
	25.0min	70%	30%

Flow rate: 1.0 mL min⁻¹

Wavelength: 214 nm

Volume: 10 μ L**Fig. S1** HPLC Chromatogram of L**Table S1.** HPLC Chromatogram data of L

Rank	Time	Name Conc.	Area
1	10.245	0.1522	6838
2	10.441	96.13	4319578
3	12.500	3.725	167377
Total		100	4493793

MS Analysis data

Sample: L

Expected MS: 922.3043

Buffer: 0.1% TFA in second distilled water

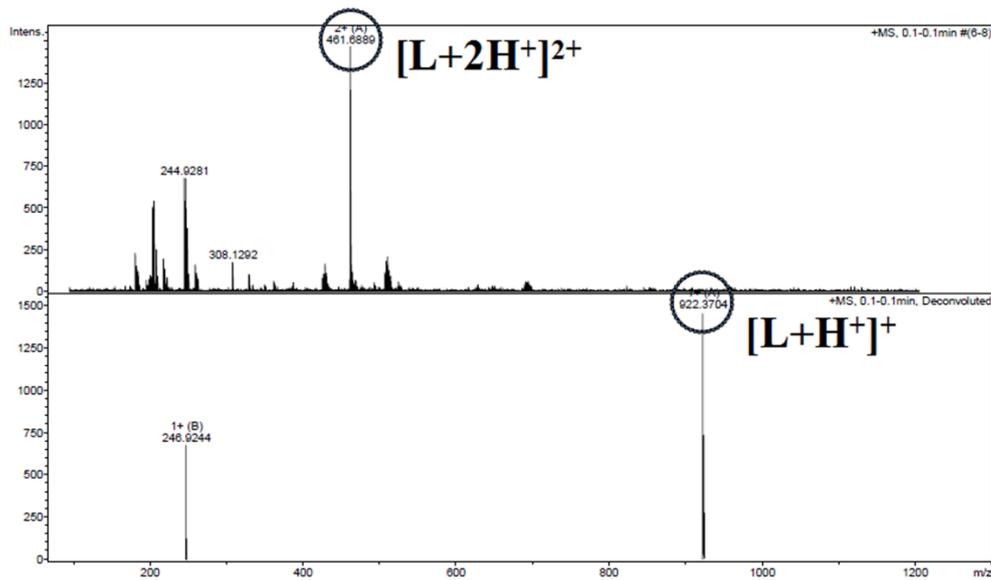


Fig. S2 MS (ESI) Spectrum of L.

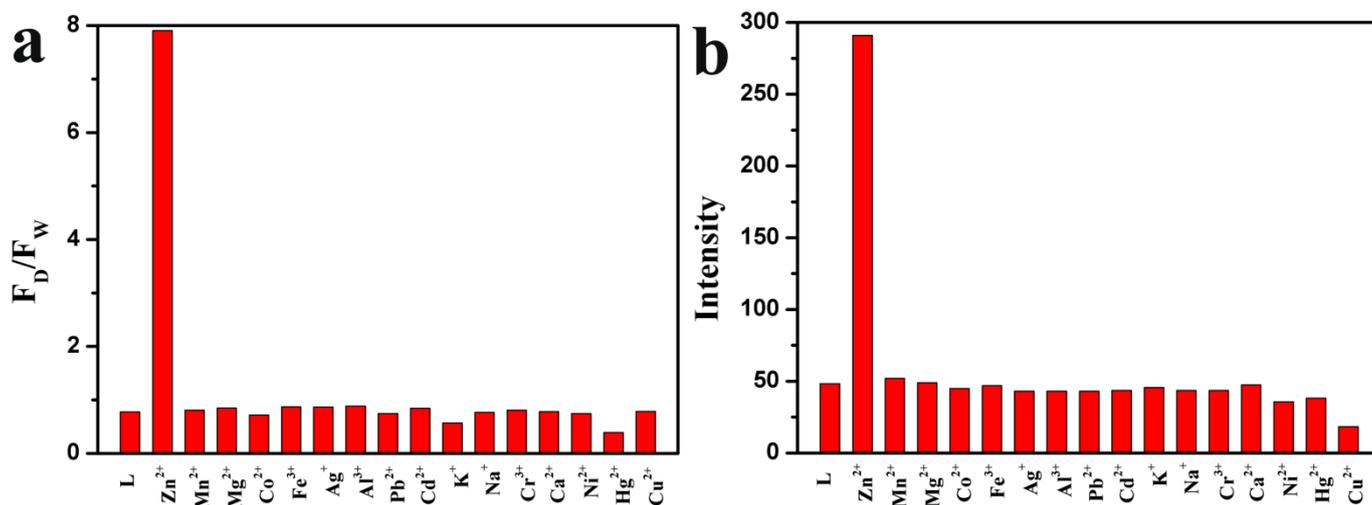
The metal ions selectivity of L

Fig. S3 The metal ion selectivity of L in 10 mM HEPES buffer solution at pH 7.4. The molar ratio of metal:L is 1:2. (a) Excitation wavelength: 290 nm, (b) Excitation wavelength: 330 nm. In the inset of (a), F_D and F_W are the fluorescence emission intensity of dansyl and Tryptophan motifs.

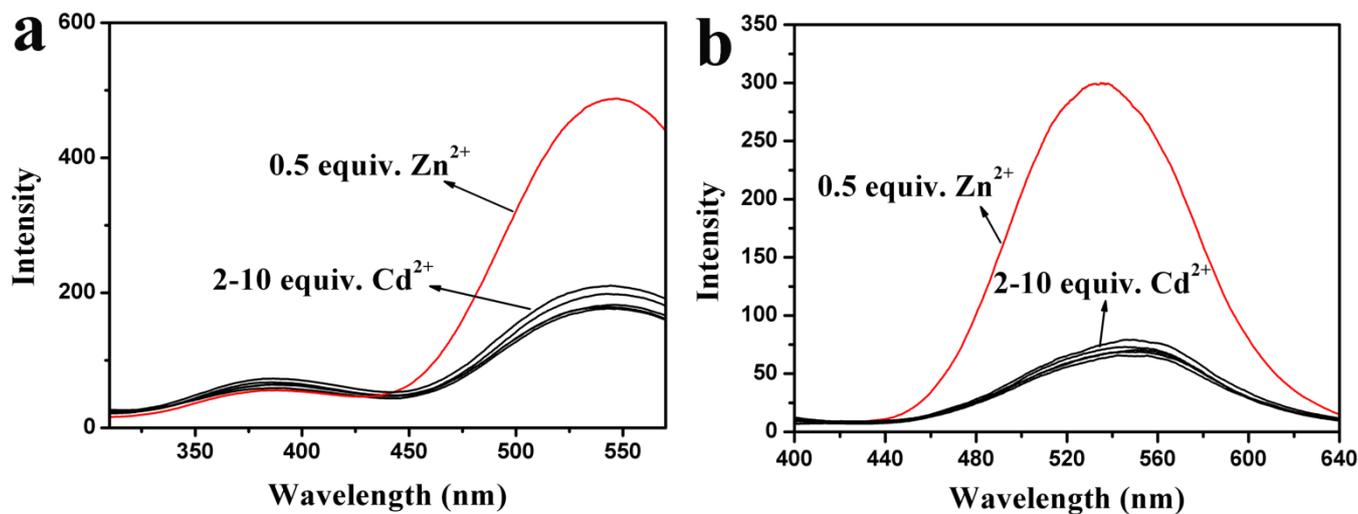
Fluorescence interference test of Cd^{2+} 

Fig. S4 Fluorescence emission spectra of **L** (10 μM) upon addition of Cd^{2+} (2, 4, 6, 8, 10 equiv) in 10 mM HEPES buffer solution at pH 7.4. (a) Excitation wavelength: 290 nm, (b) Excitation wavelength: 330 nm.

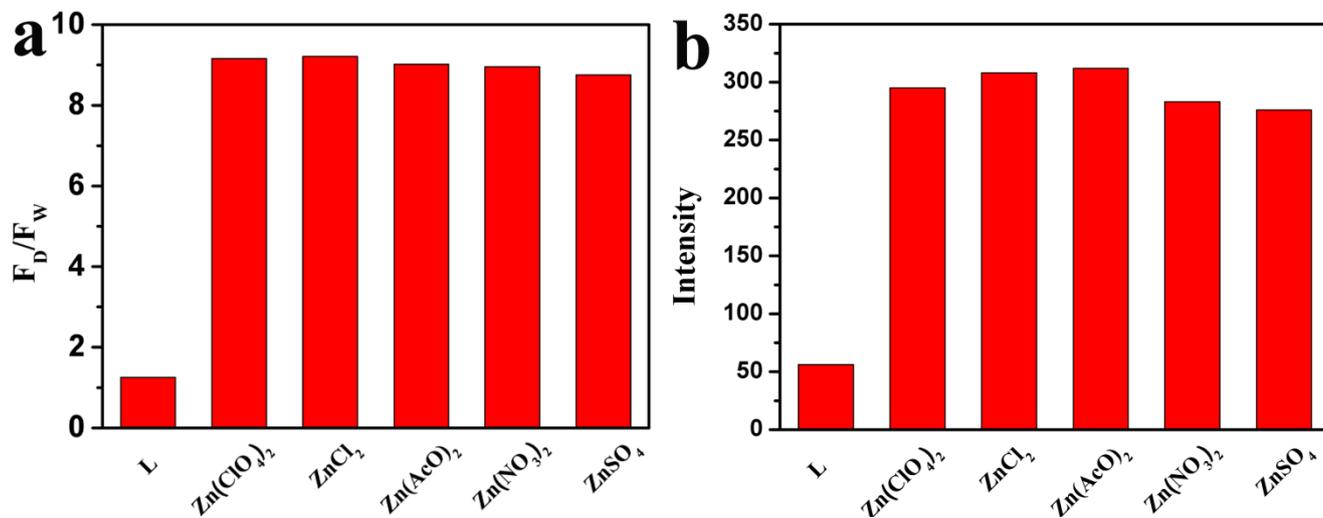
Counter anions test of Zn^{2+} 

Fig. S5 Counter anions test of Zn^{2+} with $\text{Zn}(\text{ClO}_4)_2$, ZnCl_2 , $\text{Zn}(\text{AcO})_2$, $\text{Zn}(\text{NO}_3)_2$, and ZnSO_4 in 10 mM HEPES buffer solution at pH 7.4. (a) Excitation wavelength: 290 nm, (b) Excitation wavelength: 330 nm. In the inset of (a), F_D and F_W are the fluorescence emission intensity of dansyl and Tryptophan motifs.

The pH test for L with Zn²⁺

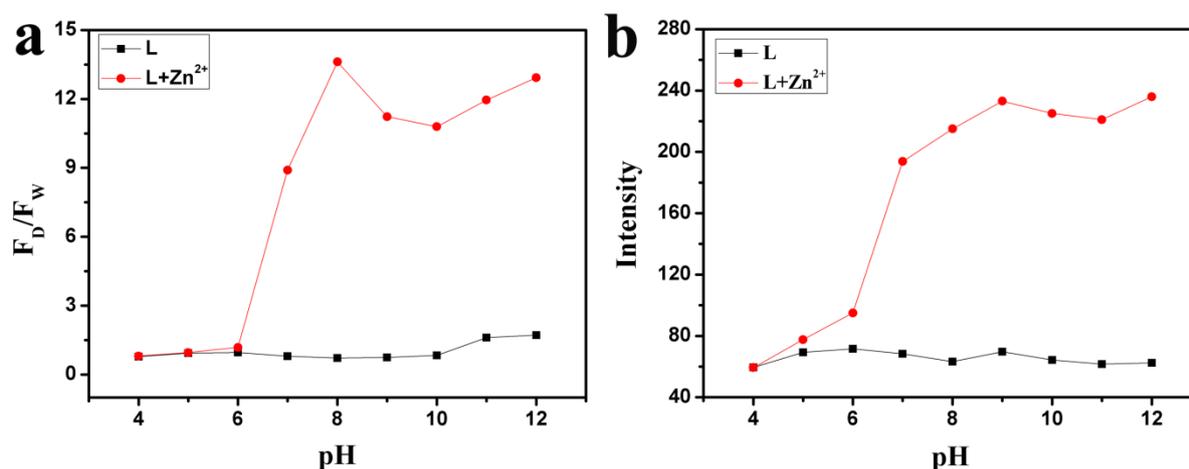


Fig. S6 Influence of pH on the fluorescence intensity of L in the absence and presence of Zn²⁺ ions. (a) Excitation wavelength: 290 nm, (b) Excitation wavelength: 330 nm. In the inset of (a), F_D and F_W are the fluorescence emission intensity of dansyl and Tryptophan motifs.

The binding constant of L-Zn

The association constant for 2:1 complex was calculated based on the titration curve of the probes with metal ions. Association constants was determined by a nonlinear least squares fitting of the data with the following equation according to the reference.^[S1]

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

Where x is $(I - I_0)/(I_{\max} - I_0)$, y is the concentration of metal ions, a is the association constant, and b is the concentration of probe. The binding constant of Zn²⁺ with L is $2.8 \times 10^{11} \text{ M}^{-2}$.

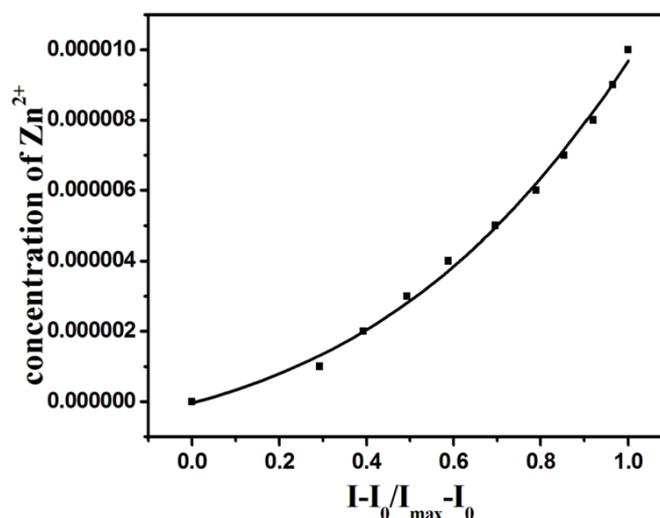


Fig. S7 Fitting of fluorescence titration curve of L with Zn²⁺ in 10 mM HEPES buffer at pH 7.4. Excitation wavelength: 330 nm.

The limit of detection for Zn^{2+}

The limit of detection (LOD) was calculated based on the fluorescence titration. The emission intensity of **L** without Zn^{2+} was measured 10 times and the standard deviation of blank measurements was determined. A good linear relationship between the fluorescence intensity at 545 nm and the Zn^{2+} concentration could be obtained in the 0-1.25 μM concentration range ($R = 0.9985$). The LOD was then calculated with the equation: $LOD = 3\sigma/k$, where σ is the standard deviation of blank measurements, k is the slope between intensity versus sample concentration.^[S2] The LOD of **L** for Zn^{2+} was measured to be 97 nM.

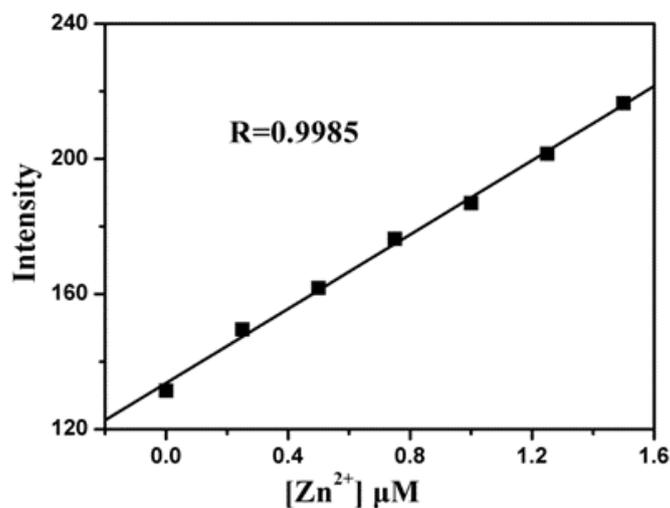


Fig. S8 Fluorescence intensity at 545 nm for **L** (20 μM) as a function of the concentration of Zn^{2+} in 10 mM HEPES buffer at pH 7.4. Excitation wavelength: 330 nm.

The mass spectrum analysis of L-Zn

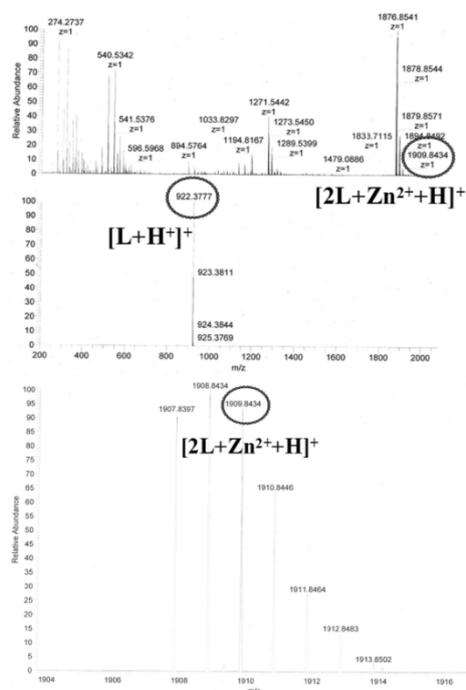


Fig. S9 ESI mass spectrum of **L** (500 μM) in H_2O/CH_3CN (50/50, V/V) including $Zn(ClO_4)_2$ (1 equiv).

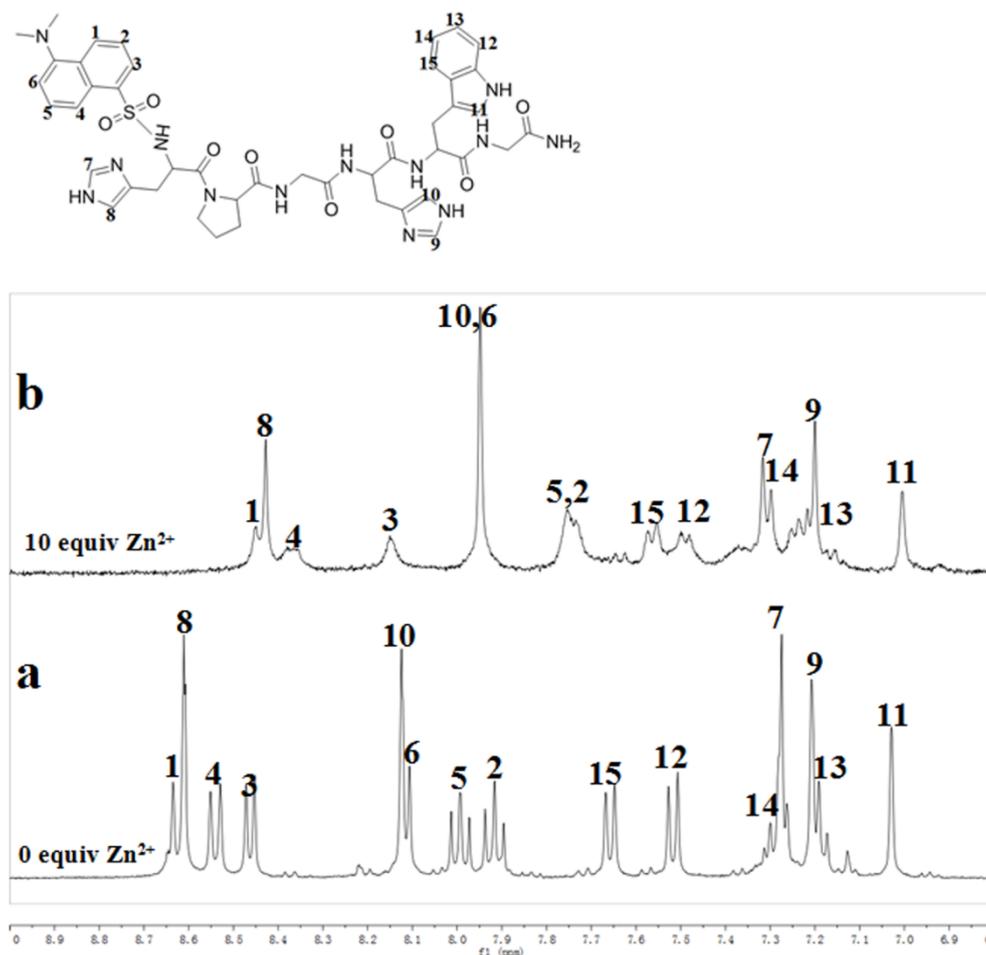
The ^1H NMR spectra analysis of L-Zn

Fig. S10 Partial ^1H NMR spectra of L in the absence (a) and presence (b) of $\text{Zn}(\text{ClO}_4)_2$ (10 equiv) in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ (80: 20, v/v).

References

- [S1] L. N. Neupane, J. Y. Park, J. H. Park and K. H. Lee, *Org. Lett.*, 2013, **15**, 254-257.
[S2] L. Wang, W. Qin, X. Tang, W. Dou, W. Liu, Q. Teng, X. Yao, *Org. Bio. Chem.*, 2010, **8**, 3751-3757.