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Supporting Information

A Peptide-based Fluorescent Chemosensor for Measuring Cadmium Ions in Aqueous Solutions and Live Cells

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HPLC Chromatogram of H_2L

Sample: **H_2L**

Column: 4.6*150 mm, 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
	0.01 min	5%	95%
	25.0 min	70%	30%

Flow rate: 1.0 ml/min

Wavelength: 214 nm

Volume: 10 μL

Figure S1. HPLC Chromatogram of **H_2L**.

Table S1. HPLC Chromatogram data of **H_2L**

Rank	Time	Name Conc.	Area
1	10.331	2.611	370547
2	10.493	0.687	97491
3	10.632	96.59	13707005
4	11.061	0.1133	16082
Total		100	14191125

MS Analysis data

Sample: **H_2L**

Expected MS: 817.2514

Buffer: 10% CH_3CN in double distilled water

Figure S2. MS (ESI) spectrum of **H_2L**.

Counter anions test of Cd^{2+}

Figure S3. Counter anions test of Cd^{2+} with $Cd(ClO_4)_2$, $CdCl_2$, $Cd(NO_3)_2$, and $CdSO_4$ in 10mM HEPES buffer solution at pH 7.4. Excitation wavelength: 330 nm.

The pH test for H_2L with Cd^{2+}

Figure S4. The pH influence on the fluorescence intensity of **H_2L** in the absence and presence of Cd^{2+} ion. Excitation wavelength: 330 nm.

The binding constant of L-Cd

The association constant for 2:1 complex was calculated based on the titration curve of the probes with metal ions. Association constants were determined by a nonlinear least squares fitting of the data with the following equation as referenced elsewhere.

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

Where ***x*** is I-I_o/I_{max}-I_o, ***y*** is the concentration of metal ions, ***a*** is the association constant, and ***b*** is the concentration of chemosensor.[S1]

Figure S5. Fitting of fluorescence titration curve of $\mathbf{H_2L}$ with Cd^{2+} in 10 mM HEPES buffer at pH 7.4. The binding constant of **L-Cd** is 3.26×10^{10} M^{-2}.

The detection limit for Cd^{2+}

The detection limit was calculated based on the fluorescence titration. The emission intensity of **H_2L** without Cd^{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 Cd^{2+} concentration could be obtained in the 0-1.25 μM concentration range (R = 0.9987). The detection limit was then calculated with the equation: detection limit = $3\sigma/k$, where σ is the standard deviation of blank measurements, k is the slope between intensity versus sample concentration.[S2] The detection limits of Cd^{2+} was measured to be 52 nM.

Figure S6. Fluorescence intensity at 545 nm for **H_2L** (20 μM) in aqueous solution (10 mM HEPES buffer, pH 7.4) as a function of the concentration of Cd^{2+} (λ_{ex} = 330 nm). The lowest detection limits of Cd^{2+} is 52 nM.

Fluorescence decay profile of H_2L, L-Cd

Figure S7. Fluorescence decay curve of **H_2L** (a), **L-Cd** (b). The lifetime of **H_2L** is 9.76 ns and contains two lifetime components: 3.36 ns (40.19%) and 14.06 ns (59.81%) (330 nm excitation, decay time at 545 nm emission). The average lifetime **L-Cd** is 12.67 ns and contains two lifetime components: 4.41 ns (17.97%) and 14.48 ns (82.03%) (330 nm excitation, decay time at 545 nm emission). The average lifetime was calculated according to $\langle \tau \rangle = \frac{\Sigma A_i \tau_i^2}{\Sigma A_i \tau_i}$.

The mass spectrum analysis of L-Cd

Figure S8. ESI mass spectrum of **H_2L** (500 μM) in H_2O/CH_3CN (80/20, V/V, pH 7.4) including $Cd(ClO_4)_2$ (1 equiv).

The ^{1}H NMR spectra analysis of L-Cd

Figure S9. ^{1}H NMR spectra of **H_2L** in the absence (a) and presence (b) of $Cd(ClO_4)_2$ (10 equiv) in D_2O/CD_3CN (80: 20, v/v, pH 7.4).

The optimized configurations for the ligand H_2L and complex L-Cd

Figure S10. The optimized configurations for the ligand **H_2L** (a) and complex **L-Cd** (b).

Table S2. Comparison of chemosensors for Cd^{2+} assays in the literatures

Cd^{2+} Chemosensor	**Detection condition**	**Detection limit**	**Detection method**	**Reference**
BODIPY derivative	Aqueous solution	77 nM	Turn-on	Inorg. Chem., 2015, **54**, 3929-3936
Ratiometric electrochemical	PBS buffer	10 nM	Ratiometric	Anal. Chem., 2014, **86**, 10668-10673
Double 1,3,4-oxadiazole derivatives	Aqueous solution	20 nM	Turn-on	Chem. Commun., 2014, **50**, 2498-2501
Two benzoxazole-derived	Aqueous solution	133 nM	Turn-on	Chem. Commun., 2014, **50**, 7514-7516
Norbornene derived 8-hydroxyquinoline	Aqueous solution	1.6 nM	Turn-on	ACS. Appl. Mater. Interfaces., 2013, **5**,7379-7383
Phenanthroxazole platform	Buffer solution	1.3 μM	Ratiometric	RSC. Adv., 2013, **3**, 21409-21412
Quinoline-based Two-photon	PBS buffer	2.72 nM	Turn-on	Dalton Trans., 2012, **41**, 6189-6194
Click functionalized poly (*p*-phenylene ethynylene)s	THF/Water	0.3 μM	Ratiometric	Chem. Commun., 2011, **47**, 11014-11016
Tricabolyanine derivative	Tris-HCl buffer	2.3 μM	Turn-on	Org. Lett., 2011, **13**, 264-267
Quinoline with DPA	Buffer solution	2.38 μM	Ratiometric	Org. Lett., 2009, **11**, 3454-3457
Peptide	HEPES buffer	52 nM	Turn-on	This work

Reference

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[S2] L. Wang, W. Qin, X. Tang, W. Dou, W. Liu, Q. Teng, X. Yao, *Org. Bio. Chem.*, 2010, **8**, 3751-3757.