Supporting information

A New Fluorescent Probe for distinguishing Zn^{2+} and Cd^{2+} with High Sensitivity and Selectivity

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1. Characterization data

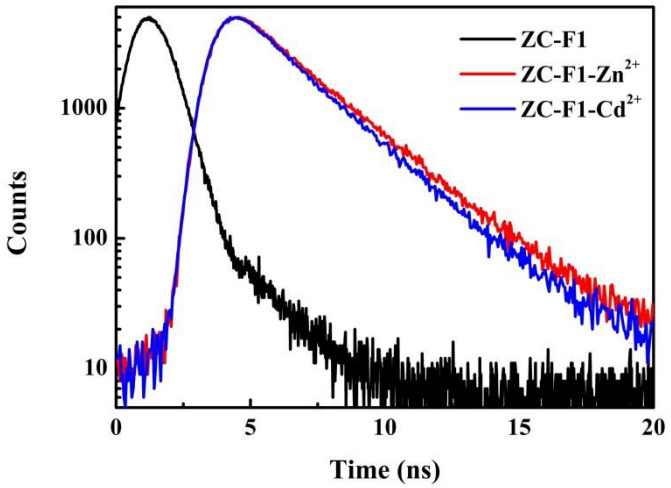

Figure S1. Fluorescence rising and decay curves of probe ZC-F1 (0.45 μM) before and after coordinated with Zn^{2+} and Cd^{2+}.

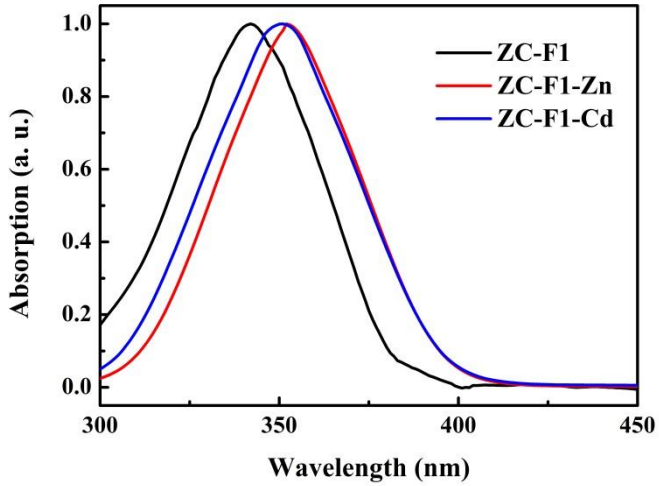

Figure S2. Absorption spectra of ZC-F1 (0.45 μM) before and after coordinated with Zn^{2+} and Cd^{2+} at the concentration of 1 equv.

Table S1. Main photophysical parameters of ZC-F1 and its complexes form.[a]

	ε^{b} [$\times10^{4}$L·mol^{-1}·cm^{-1}]	τ^{c}[ns]	Φ^{d}[%]	$\lambda_{abs}/\lambda_{em}{}^{e}$ [nm]
ZC-F1	0.39	0.19/0.48	28	341/400
ZC-F1-Zn^{2+}	0.43	2.30	58	352/495
ZC-F1-Cd^{2+}	0.45	2.23	56	351/455

a. All the measurements were carried out at the fixed concentration of 0.45 μM in acetonitrile. b. molar extinction coefficient of ZC-F1 and its complexes. c. the fluorescence lifetime. d. quantum yield. e. wavelength of absorption and fluorescence emission peak.

2. Calculation of pKa and competitive experiment.

The pKa of ZC-F1 was calculated by using the Henderson-Hasselbalch equation:

$$-\log\frac{F_{max}-F}{F-F_{min}} = \mathrm{pH} - \mathrm{p}K_a \qquad (1)$$

where F_{max} and F_{min} are the corresponding maximum and minimum fluorescence intensity, F is the fluorescence intensity observed at a fixed wavelength. The pK_a of 3.75 for ZC-F1-Zn^{2+} and 3.62 for ZC-F1-Cd^{2+} indicates ZC-F1 can be used for detection of Zn^{2+} or Cd^{2+} when both of them present.

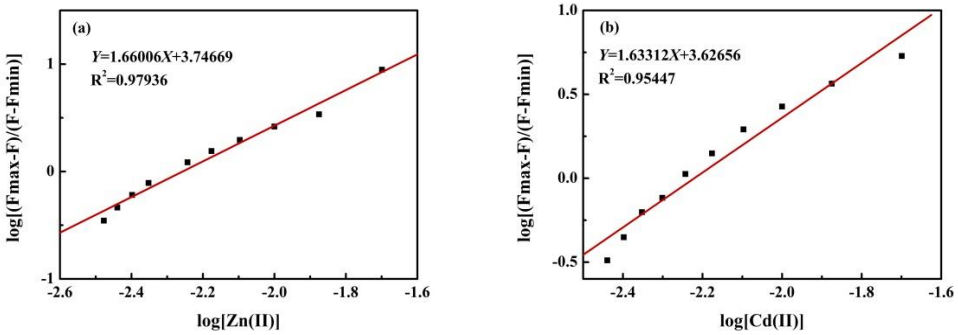

Figure S3. Analysis of fluorescence intensity changes as a function of [Zn^{2+}] (a) / [Cd^{2+}] (b) by using Henderson–Hasselbalch equation.

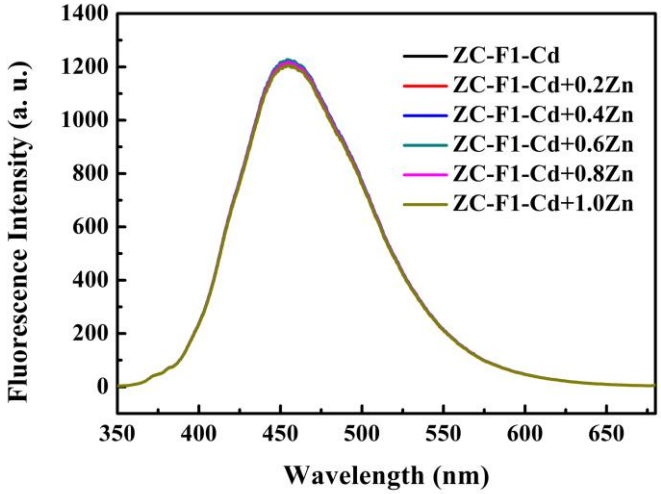

Figure S4. Fluorescence emission spectra (excited at 341 nm) of ZC-F1 (4.5 μM) with Cd^{2+} (1.0 equiv.) upon titration of Zn^{2+} (0.2, 0.4, 0.6, 0.8 and 1.0 equiv.).

3. Job's plot analysis

Job's plot analysis is carried on to determine the stoichiometry of ZC-F1 with Zn^{2+} and Cd^{2+}, during which the summation of $[Zn^{2+}]$ / $[Cd^{2+}]$ and [ZC-F1] is kept as 4.5 μM. The results suggest that both Zn^{2+} and Cd^{2+} complex with ZC-F1 in 1:1 form.

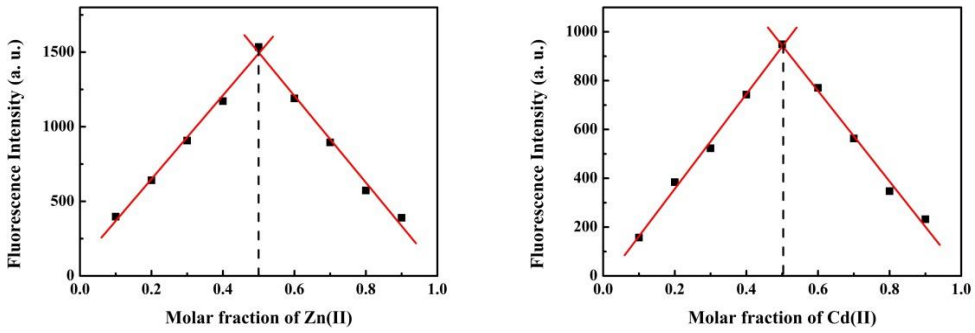

Figure S5. Job plot Analysis of the stoichiometry of ZC-F1 and Zn^{2+} (a)/ Cd^{2+} (b)(excited at 341 nm and monitored at 495 nm for Zn^{2+}, 455nm for Cd^{2+}, respectively)

4. Cartesian coordinates for the optimized structures

Table S2. Standard orientation for ZC-F1

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	12.9326	0.0109	-0.0287
2	6	12.5901	1.2198	-0.6603
3	6	11.2605	1.5753	-0.8469

4	6	10.2541	0.7077	-0.3944
5	6	10.6135	-0.5075	0.2406
6	6	11.9503	-0.8646	0.4279
7	7	8.8978	0.9355	-0.5134
8	6	8.1964	-0.034	-0.0062
9	16	9.1602	-1.373	0.6924
10	6	6.7308	-0.0598	0.0082
11	6	6.0037	-1.1178	0.5797
12	6	4.6159	-1.1107	0.578
13	6	3.9045	-0.0391	0.0007
14	6	4.6363	1.0227	-0.5735
15	6	6.0221	1.0114	-0.5687
16	6	2.483	-0.0291	-0.0013
17	6	1.2658	-0.0209	-0.0014
18	6	-0.1565	-0.0135	0.0012
19	6	-0.8757	1.0213	-0.6304
20	6	-2.2646	1.0246	-0.6224
21	6	-2.9915	0.001	0.0106
22	6	-2.2705	-1.0305	0.6375
23	6	-0.8818	-1.0416	0.6366
24	6	-4.4741	0.0083	0.0196
25	6	-5.2131	-1.1778	-0.0729
26	6	-6.6141	-1.1254	-0.081
27	7	-7.2966	0.0256	-0.009
28	6	-6.6013	1.1668	0.0901
29	6	-5.2003	1.2025	0.1074
30	6	-7.3903	2.4331	0.1925
31	6	-7.4165	-2.3835	-0.1781
32	6	-6.9858	-3.56	0.4548
33	6	-7.759	-4.713	0.3403
34	6	-8.9377	-4.6577	-0.4
35	6	-9.2855	-3.4392	-0.9885
36	7	-8.5559	-2.3265	-0.8877
37	7	-8.5164	2.5073	-0.5362
38	6	-9.2348	3.6295	-0.4635
39	6	-8.8884	4.7291	0.3258
40	6	-7.7237	4.6471	1.0855
41	6	-6.9613	3.4829	1.0195
42	1	13.9793	-0.2465	0.1064
43	1	13.3775	1.8833	-1.0064
44	1	10.9804	2.5047	-1.3325
45	1	12.22	-1.7966	0.915
46	1	6.5243	-1.9572	1.0328
47	1	4.0661	-1.9337	1.023

48	1	4.0997	1.8533	-1.0212
49	1	6.584	1.8275	-1.0093
50	1	-0.3312	1.8143	-1.1333
51	1	-2.7964	1.8182	-1.139
52	1	-2.8072	-1.82	1.1554
53	1	-0.3419	-1.8407	1.1348
54	1	-4.7041	-2.1282	-0.1943
55	1	-4.681	2.1518	0.1853
56	1	-6.0755	-3.5636	1.0463
57	1	-7.4499	-5.6334	0.8286
58	1	-9.5751	-5.529	-0.5178
59	1	-10.1995	-3.3543	-1.5749
60	1	-10.1381	3.6536	-1.0718
61	1	-9.5164	5.6148	0.344
62	1	-7.4168	5.4697	1.7261
63	1	-6.0622	3.3779	1.6189

Table S3. Standard orientation for ZC-F1-Cd

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-14.3286	0.2778	-0.1678
2	6	-14.0519	-0.9738	-0.7494
3	6	-12.7445	-1.4263	-0.882
4	6	-11.6938	-0.6131	-0.4249
5	6	-11.9877	0.6446	0.1596
6	6	-13.3019	1.1001	0.2928
7	7	-10.3513	-0.934	-0.4941
8	6	-9.6012	0.0061	0.0046
9	16	-10.4926	1.4246	0.6288
10	6	-8.1365	-0.0589	0.0597
11	6	-7.3646	0.9691	0.6297
12	6	-5.9793	0.8847	0.6605
13	6	-5.3169	-0.2368	0.1182
14	6	-6.092	-1.2715	-0.4497
15	6	-7.4759	-1.1817	-0.4769
16	6	-3.8965	-0.3084	0.1378
17	6	-2.6794	-0.3408	0.1522
18	6	-1.2568	-0.3267	0.1678
19	6	-0.5064	-1.3548	-0.4399
20	6	0.8827	-1.3077	-0.4415
21	6	1.5709	-0.2354	0.1548
22	6	0.8198	0.7816	0.773

23	6	-0.5675	0.739	0.7842
24	6	3.0492	-0.1581	0.1176
25	6	3.6937	1.0836	0.011
26	6	5.0877	1.1413	-0.0258
27	7	5.8209	0.0198	0.0284
28	6	5.2428	-1.1859	0.1281
29	6	3.8509	-1.3084	0.1777
30	6	6.1661	-2.3638	0.1874
31	6	5.8395	2.4304	-0.1338
32	6	5.1948	3.6726	-0.1283
33	6	5.9497	4.8393	-0.2343
34	6	7.3352	4.7469	-0.3413
35	6	7.9096	3.478	-0.3347
36	7	7.1846	2.3551	-0.2337
37	7	7.4911	-2.1244	0.0514
38	6	8.3581	-3.1457	0.0941
39	6	7.9584	-4.4674	0.2781
40	6	6.5983	-4.7268	0.4246
41	6	5.6942	-3.6671	0.3788
42	48	8.1694	0.1612	-0.1923
43	1	-15.3582	0.6107	-0.0755
44	1	-14.8727	-1.593	-1.0992
45	1	-12.5195	-2.3896	-1.3291
46	1	-13.5203	2.0646	0.7403
47	1	-7.844	1.8465	1.0543
48	1	-5.3964	1.6867	1.1014
49	1	-5.5956	-2.1405	-0.8695
50	1	-8.0673	-1.9771	-0.9164
51	1	-1.0219	-2.1793	-0.9215
52	1	1.4356	-2.0955	-0.9438
53	1	1.3246	1.6035	1.2709
54	1	-1.1315	1.529	1.2691
55	1	3.1	1.9833	-0.0744
56	1	3.3815	-2.2779	0.2775
57	1	4.1186	3.7415	-0.0382
58	1	5.4562	5.8058	-0.2313
59	1	7.9609	5.6281	-0.426
60	1	8.9845	3.3495	-0.4132
61	1	9.4066	-2.8918	-0.0222
62	1	8.6969	-5.2606	0.3067
63	1	6.2388	-5.7397	0.5745
64	1	4.6367	-3.8643	0.4976

Table S4. Standard orientation for ZC-F1-Zn

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-13.805	0.4289	-0.3536
2	6	-13.3883	1.6315	0.2477
3	6	-12.0454	1.8669	0.5173
4	6	-11.1015	0.8825	0.1796
5	6	-11.5355	-0.3234	-0.4262
6	6	-12.8857	-0.5607	-0.6969
7	7	-9.7391	0.9828	0.3871
8	6	-9.1055	-0.0771	-0.0261
9	32	-10.1477	-1.3463	-0.7316
10	6	-7.6498	-0.2406	0.0605
11	6	-6.9919	-1.3838	-0.4272
12	6	-5.6097	-1.4984	-0.3479
13	6	-4.8383	-0.467	0.2263
14	6	-5.5007	0.6762	0.7265
15	6	-6.88	0.7856	0.6429
16	6	-3.4198	-0.5525	0.2853
17	6	-2.203	-0.5804	0.3243
18	6	-0.7814	-0.5398	0.352
19	6	-0.1206	0.5368	0.9812
20	6	1.2638	0.6249	0.9572
21	6	2.0412	-0.3572	0.3145
22	6	1.3829	-1.4484	-0.282
23	6	-0.004	-1.5398	-0.2685
24	6	3.5117	-0.2128	0.2336
25	6	4.3673	-1.3307	0.2451
26	6	5.7452	-1.1365	0.1349
27	7	6.2443	0.0996	0.0255
28	6	5.4689	1.1892	0.0126
29	6	4.0856	1.0668	0.1159
30	6	6.211	2.4737	-0.14
31	6	6.7783	-2.2158	0.1211
32	6	6.4709	-3.5671	0.2828
33	6	7.4996	-4.5094	0.257
34	6	8.8123	-4.0832	0.071
35	6	9.0492	-2.7188	-0.0831
36	7	8.0627	-1.8111	-0.0588
37	7	7.5536	2.3666	-0.2949
38	6	8.2978	3.4723	-0.442
39	6	7.7427	4.7501	-0.4424
40	6	6.3645	4.8721	-0.2818

41	6	5.589	3.7227	-0.1284
42	30	8.3013	0.3305	-0.2581
43	1	-14.86	0.2673	-0.5549
44	1	-14.1276	2.3847	0.5035
45	1	-11.7123	2.7907	0.9803
46	1	-13.212	-1.4859	-1.1612
47	1	-7.5582	-2.1927	-0.8798
48	1	-5.1157	-2.3837	-0.7347
49	1	-4.9181	1.4757	1.1729
50	1	-7.3833	1.6678	1.0219
51	1	-0.7052	1.3028	1.4798
52	1	1.7461	1.4574	1.4595
53	1	1.955	-2.2116	-0.8003
54	1	-0.497	-2.3741	-0.7567
55	1	3.9517	-2.3245	0.3505
56	1	3.4472	1.939	0.0684
57	1	5.4472	-3.8879	0.4309
58	1	7.2721	-5.5629	0.3826
59	1	9.6393	-4.7832	0.0455
60	1	10.0527	-2.3335	-0.2296
61	1	9.3651	3.32	-0.5624
62	1	8.3798	5.6183	-0.5648
63	1	5.8924	5.849	-0.2744
64	1	4.5171	3.8059	0.0007