Electronic Supplementary Information for Dalton Transactions

A Flexible 1,8-Naphthyridyl Derivative and Its Zn(II) Complexes: Synthesis, Structures, Spectroscopic Properties and Recognition of Cd(II)

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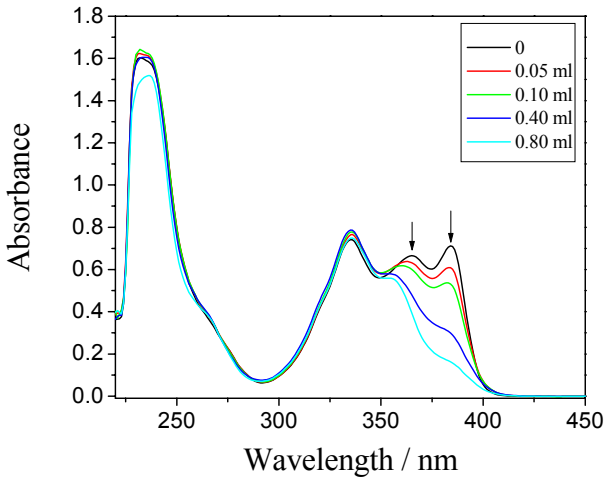

Fig. S1 UV-Vis spectra changes of **1** in CH_2Cl_2 upon addition of CH_3OH.

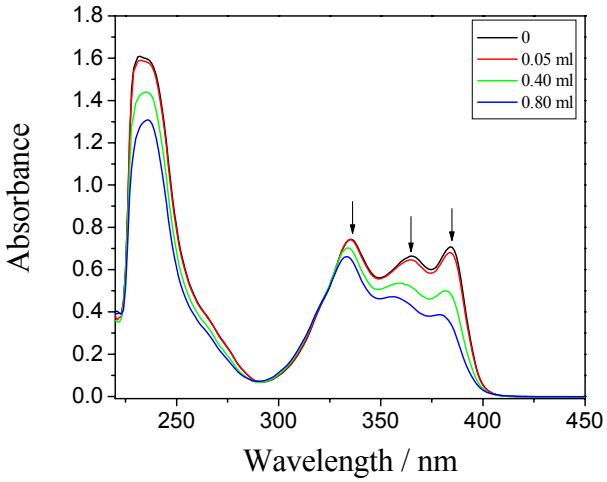

Fig. S2 UV-vis spectra changes of **1** in CH_2Cl_2 upon addition of CH_3CN.

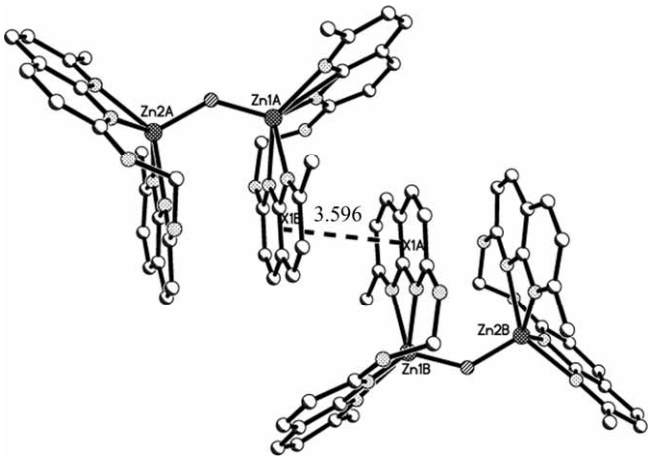

Fig. S3 Crystal packing diagram of **1**.

Calculation of the binding constant of **L**-Cd

$$\frac{I_0}{I-I_0} = \frac{I_0}{[\mathbf{L}]} + \frac{I_0}{[\mathbf{L}]*Ks} * \frac{1}{[Cd]} \qquad (1)^i$$

Ks = Binding constant

I_0 = The fluorescence intensity of **L**

I = The observed fluorescence intensity of **L** in the presence of Cd(II)

Due to the fluorescence intensity of **L**-Cd at 402 nm was four times more than that of **L**, $I-I_0$ can be approximate to I. Plot of 1/I against 1/[Cd] was shown in Fig. S4.

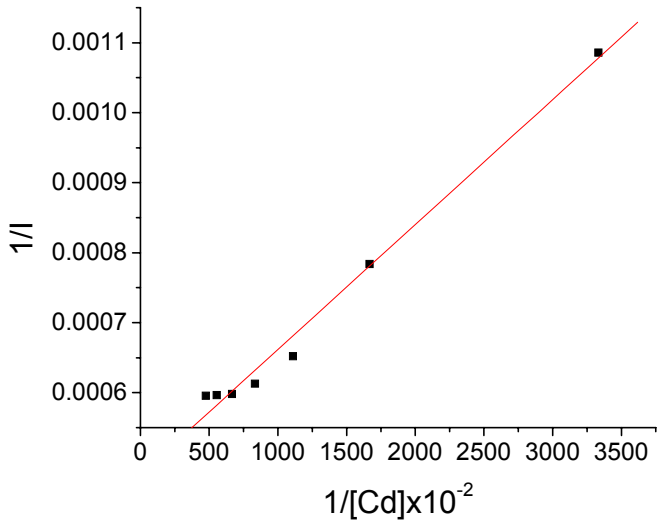

Fig. S4 Fitting analysis of **L**-Cd at different Cd(II) concentrations. Emission was recorded at 402 nm.

Linear Regression for Data1_B:

Y = A + B * X

Parameter	Value	Error
A	4.83087E-4	1.3307E-5
B	1.7856E-9	8.59022E-11

R	SD	N	P
0.99426	2.12622E-5	7	<0.0001

Ks = A/B = (4.83087/1.7856) × 10^5 = 2.71×10^5

$\Delta Ks = |\Delta A/A - \Delta B/B| \times Ks = 5.60\times10^3$

K = Ks + Δ Ks = (2.71 ± 0.056) × 10^5

Calculation of the binding constant of **L**-Zn (**1**)

$$\frac{A_0}{A_0-A} = \frac{A_0}{[L]} + \frac{A_0}{[L]*Ks} * \frac{1}{[Zn]} \qquad (2)^{ii}$$

Ks = Binding constant;

A_0 = The observed absorbance at the absence of cation;

A = The observed absorbance in the presence of cation.

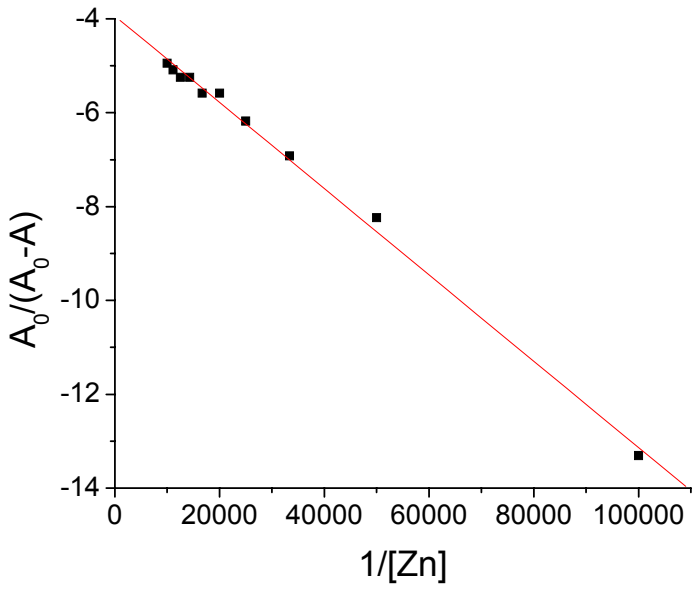

Fig. S5 Fitting analysis of **L**-Zn (**1**) at different Zn(II) concentrations. Absorptions were recorded at 332 nm.

Linear Regression for Data6_B:

Y = A + B * X

Parameter	Value	Error
A	-3.93859	0.07987
B	-9.19632E-5	2.02894E-6

R	SD	N	P
-0.99806	0.16877	10	<0.0001

$Ks = A/B = (-3.93859/-9.19632) \times 10^5 = 4.28\times10^4$

$\Delta Ks = |\Delta A/A - \Delta B/B| \times Ks = 80$

$K = Ks + \Delta Ks = (4.28 \pm 0.008) \times 10^4$

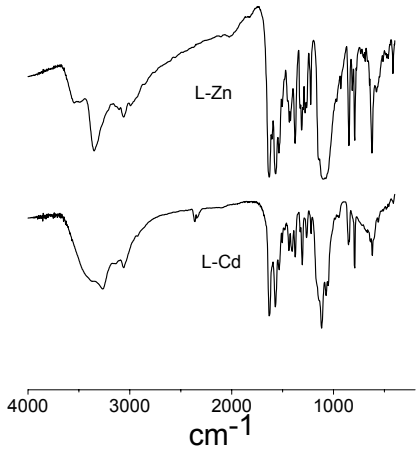

Fig. S6 Comparison of IR spectra of **L**-Cd and **L**-Zn (**1**).
Top: **L**-Zn (**1**); Bottom: **L**-Cd.

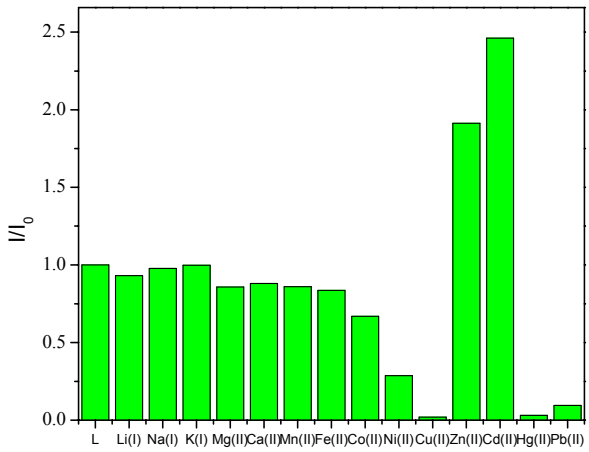

Fig. S7 Fluorescence response of **L** (1.0×10^{-5} M, CH_3OH) to different ions (1.0×10^{-4} M), λ_{ex}=340 nm.

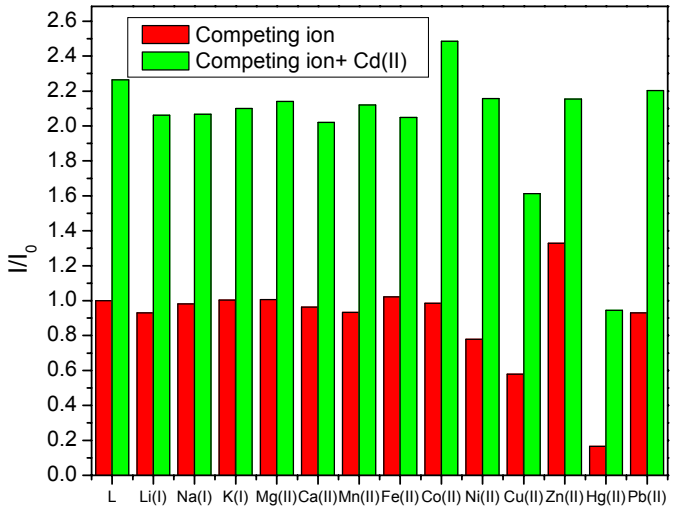

Fig. S8 Fluorescence response of **L** (1.0×10^{-5}M, CH_3OH) to Cd(II) in the presence of competing metal ions (1.0×10^{-5} M), λ_{ex}=340 nm.

i H. A. Benesi and J. H. Hildebrand, *J. Am. Chem. Soc*., 1949, **71**, 2703.
ii C. D. Gutsche, M. Iqbal and I. Alam, *J. Am. Chem. Soc*., 1987, **109**, 4314.