

Supporting Information

Structurally controllable Cd(II)-based luminescent metal-organic frameworks for efficient detection of antibiotics in water

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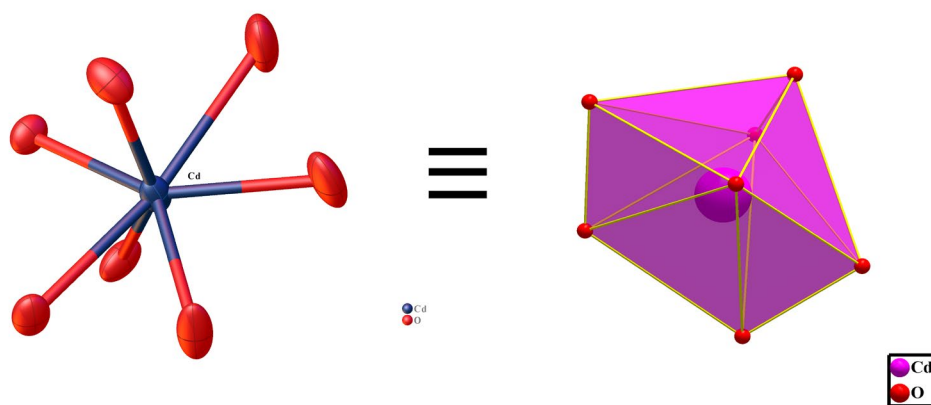


Fig. S1. The coordination mode of Cd^{2+} ions in **FCS-8**.

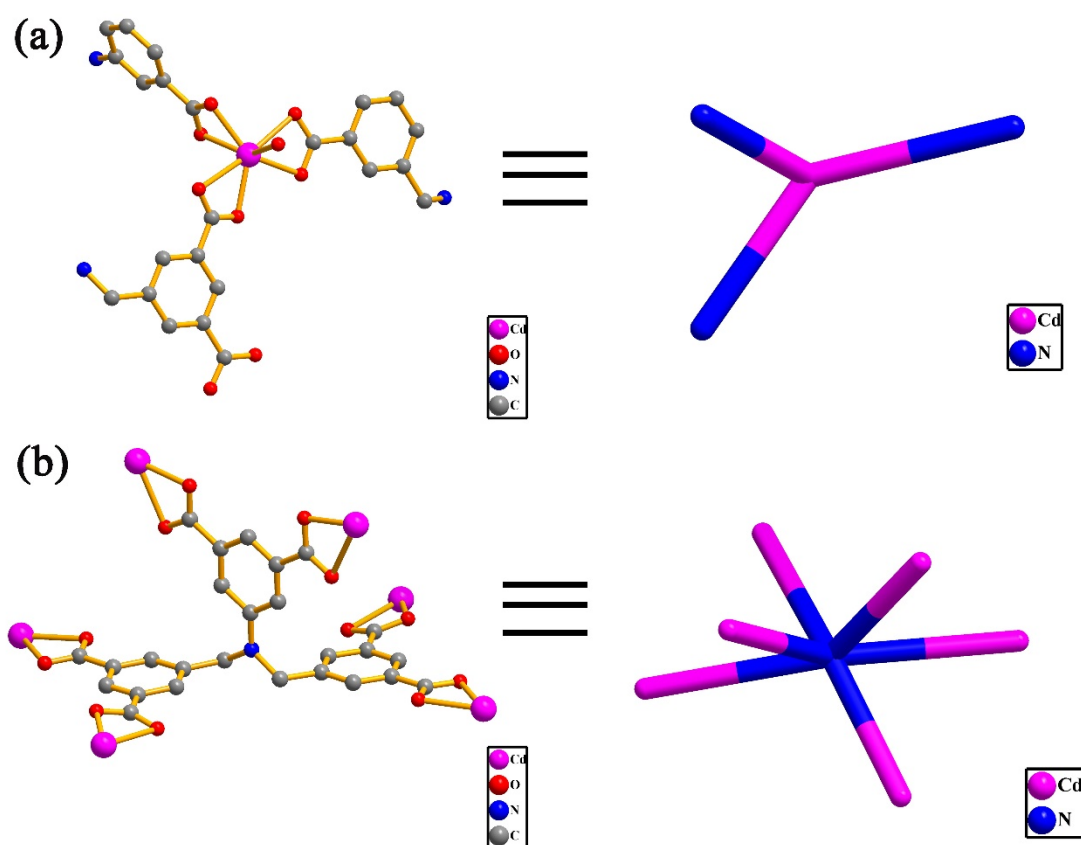


Fig. S2. (a) Cd^{2+} ions as 3-c nodes and (b) bmipia^{6-} ligand as 6-c nodes in **FCS-8**.

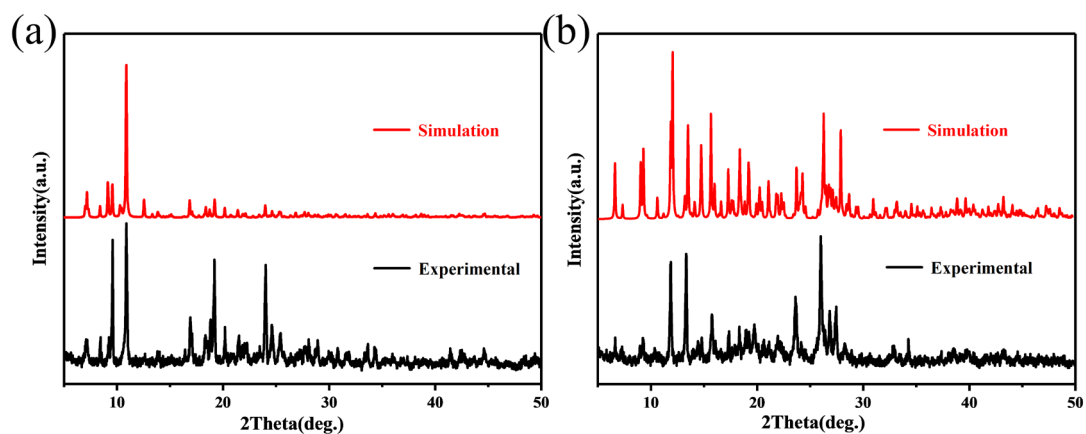


Fig. S3. The powder X-ray diffraction patterns of FCS-7 (a) and FCS-8 (b).

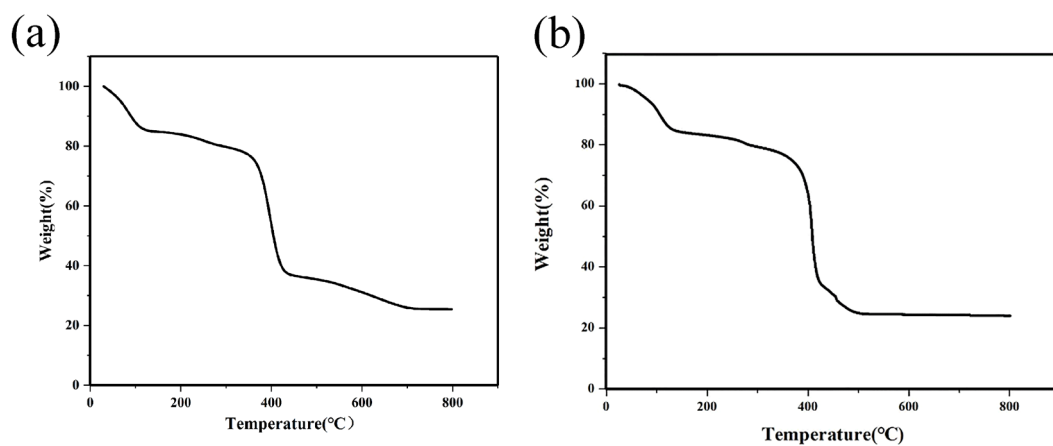


Fig. S4. The thermogravimetric analyses for FCS-7 (a) and FCS-8 (b).

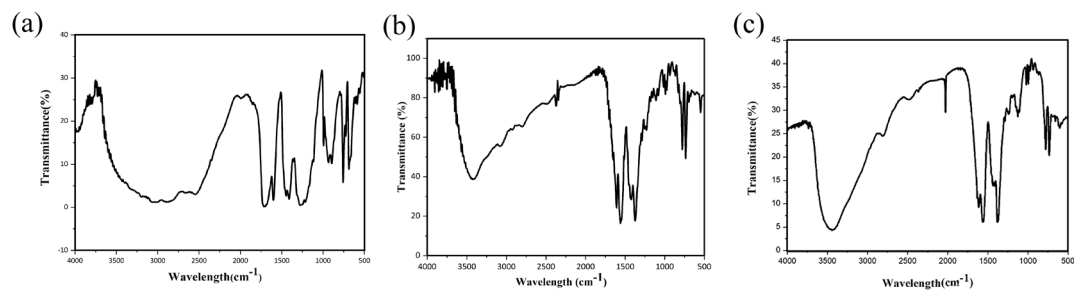


Fig. S5. The infrared spectra of L (a), FCS-7 (b) and FCS-8 (c).

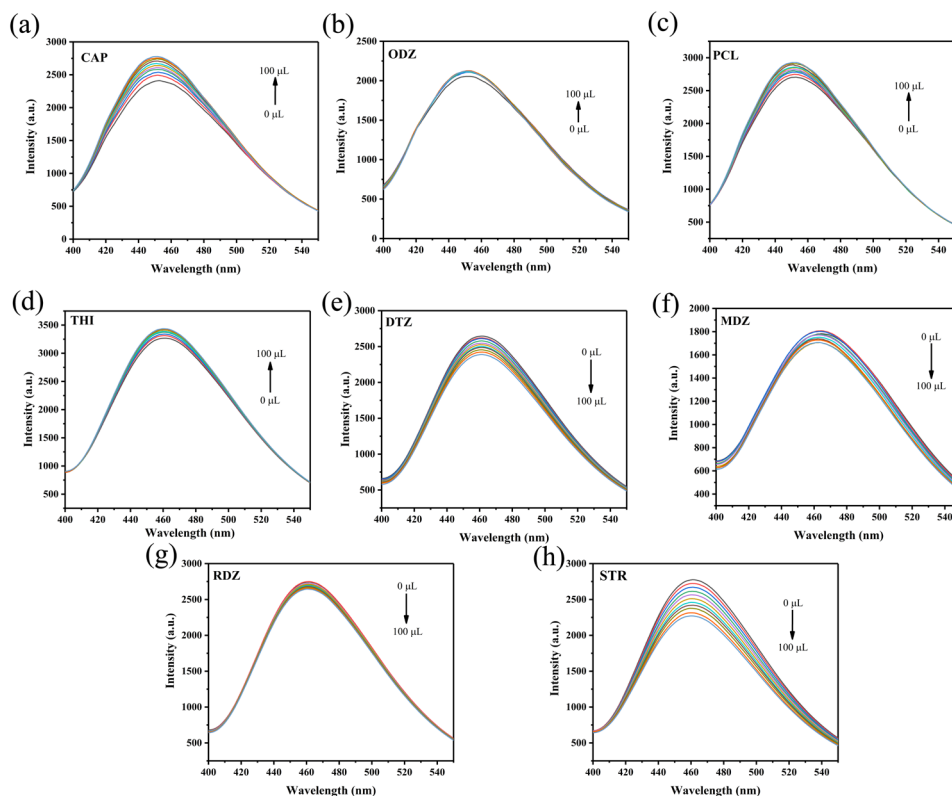


Fig. S6. The fluorescence titration of **FCS-7** with the gradual addition of CAP(a), ODZ(b), PCL(c), THI(d), DTZ(e), MDZ(f), RDZ(g) and STR(h).

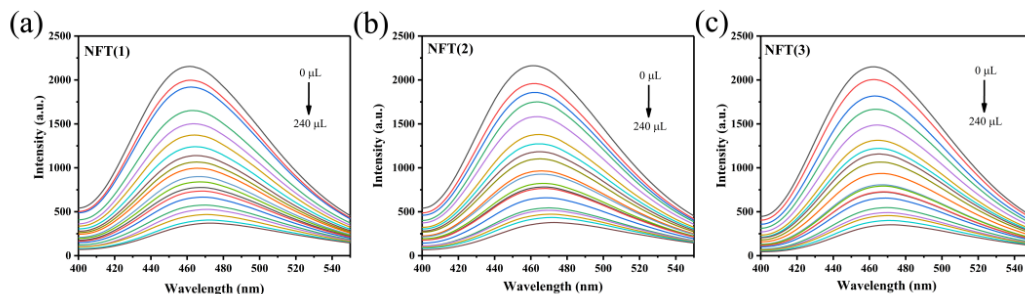


Fig. S7. The three fluorescence titrations of **FCS-7** with gradual addition of NFT.

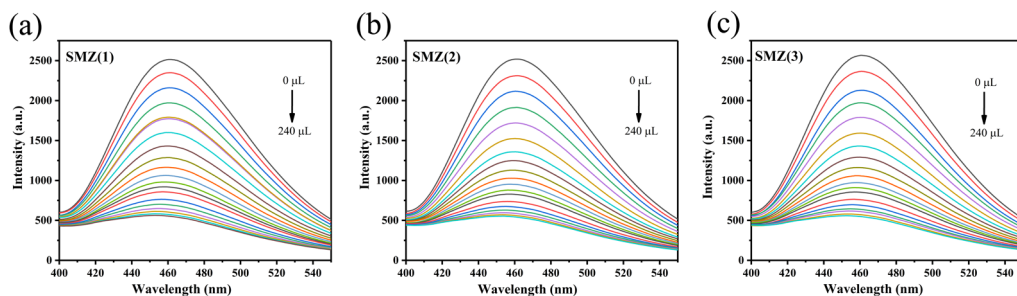


Fig. S8. The three fluorescence titrations of **FCS-7** with gradual addition of SMZ.

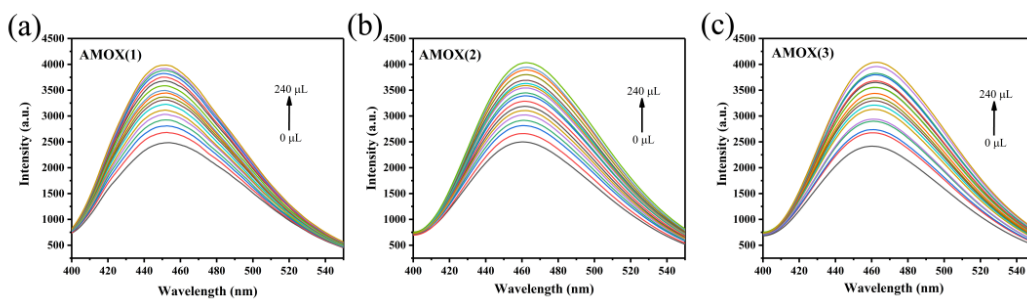


Fig. S9. The three fluorescence titrations of FCS-7 with gradual addition of AMOX.

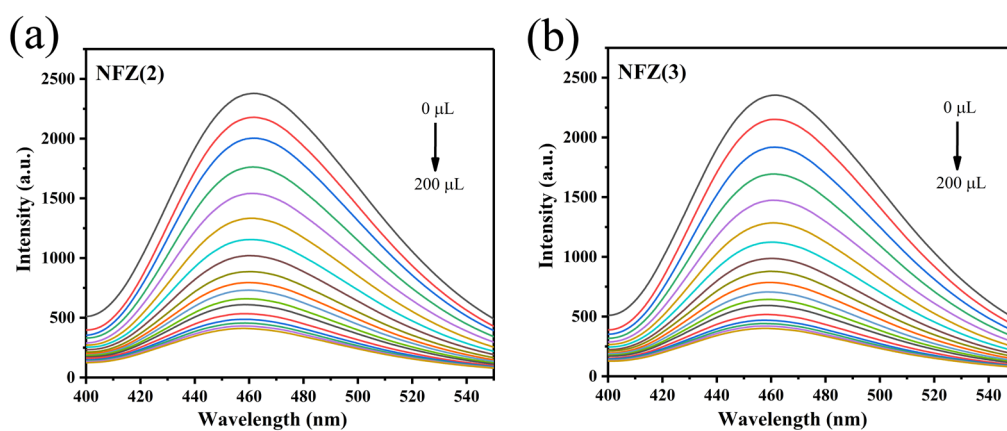


Fig. S10. The two fluorescence titrations of FCS-7 with gradual addition of NFZ.

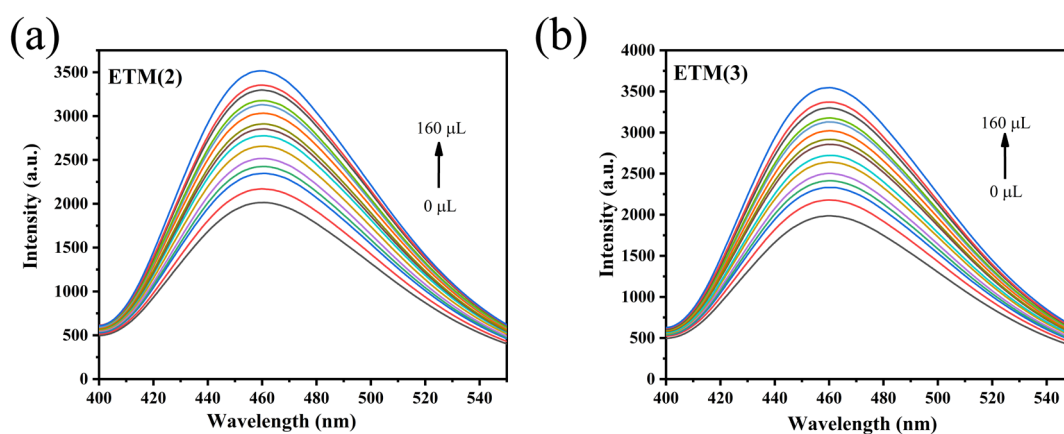


Fig. S11. The two fluorescence titrations of FCS-7 with gradual addition of ETM.

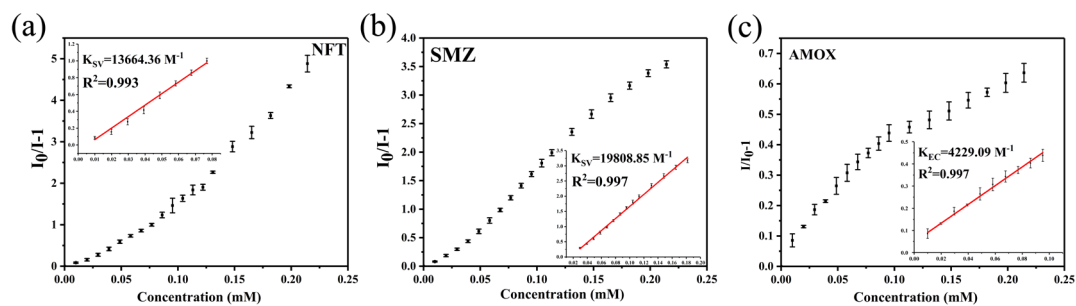


Fig. S12. Correlation curves of FCS-7 calculated by using the Stern–Volmer equation for the detection of NFT(a), SMZ(b) and AMOX(c). Inset: linear fitting plots in the low concentration region.

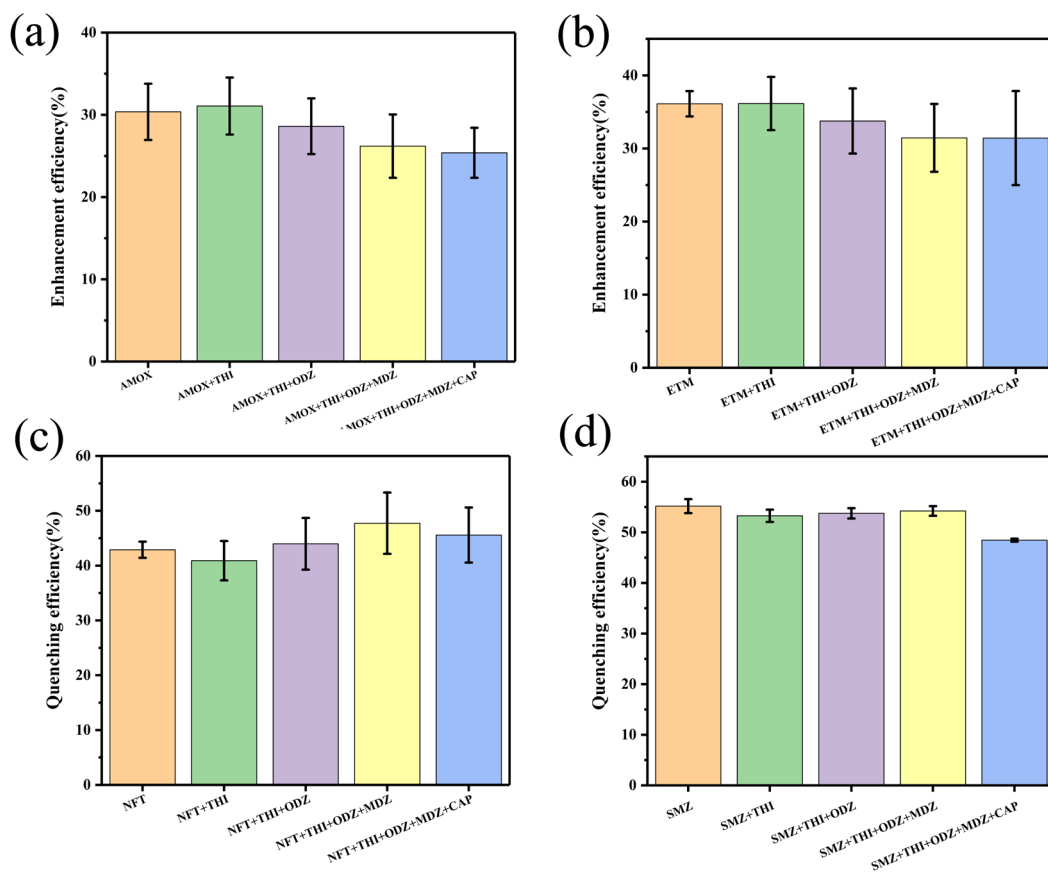


Fig. S13. The anti-interference ability of FCS-7 toward AMOX(a), ETM(b), NFT(c) and SMZ(d) in the presence of various kinds of interfering antibiotics.

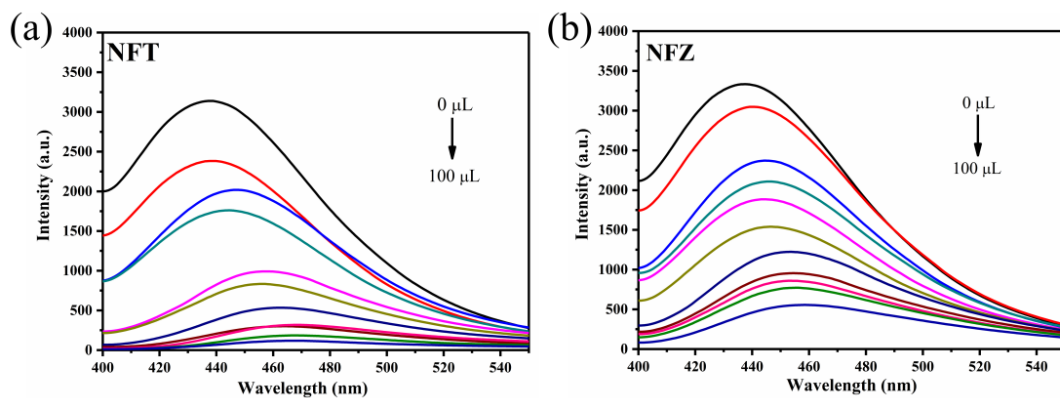


Fig. S14. The fluorescence titration of **FCS-8** with the gradual addition of (a) NFT and (b) NFZ.

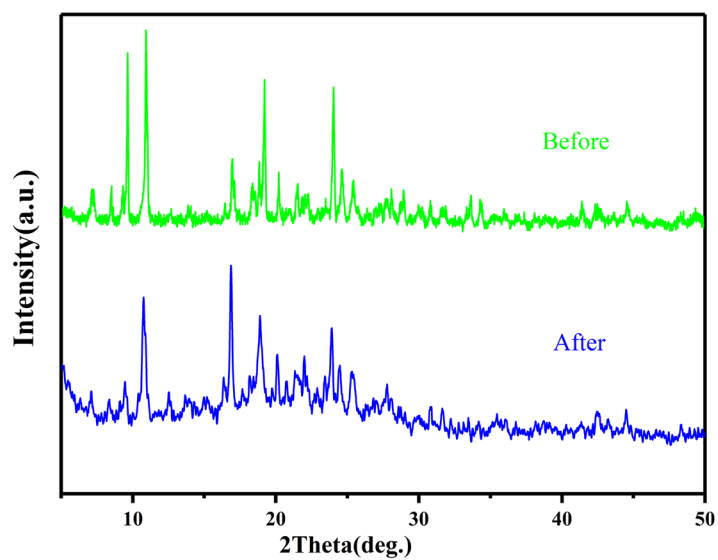


Fig. S15. The Powder X-ray diffraction patterns of **FCS-7** before and after the fluorescence quenching experiment induced by NFZ.

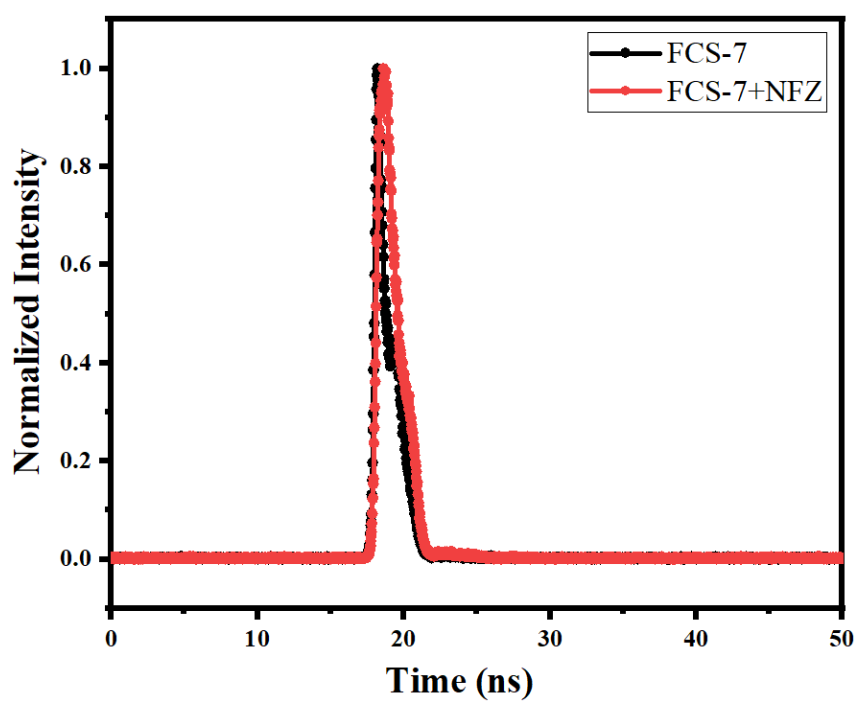


Fig. S16. Time-resolved fluorescence decay of FCS-7 before (black) and after (red) the addition of NFZ.

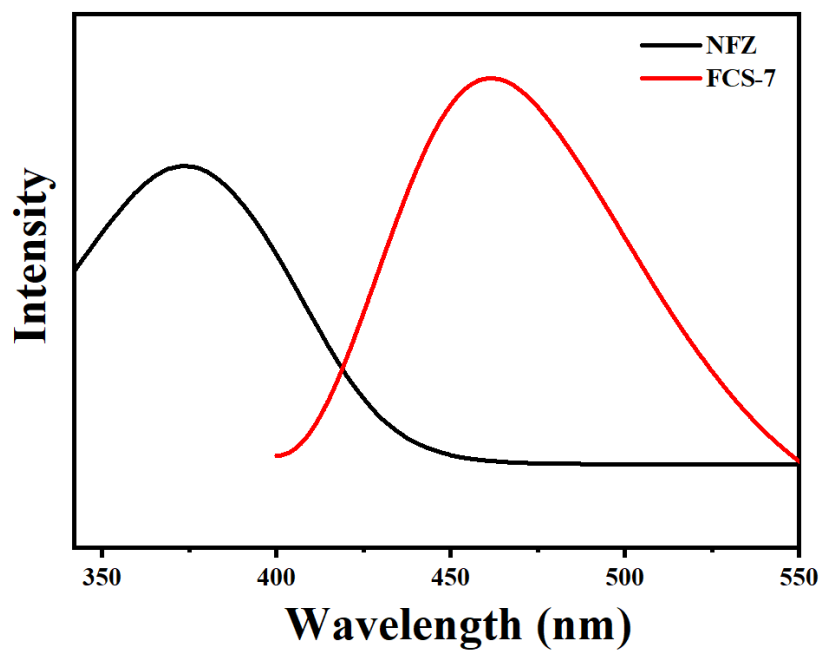


Fig. S17. UV-vis absorption spectra of NFZ and the normalized emission spectra of FCS-7 in water.

Table S1. Crystallographic data and structure refinement parameters for **FCS-7** and **FCS-8**.

Compounds	FCS-7	FCS-8
Empirical formula	C ₅₂ H ₄₆ O ₄₄ N ₂ Cd ₄ Na ₂	C ₅₂ H ₆₆ O ₄₂ N ₂ Cd ₄
Formula weight	1897.08	1840.66
Temperature	273.15 K	100.15 K
Crystal system	monoclinic	orthorhombic
Space group	C2/c	Ccce
a (Å)	18.813(6)	20.2245(10)
b (Å)	17.151(5)	24.9058(10)
c (Å)	25.366(8)	17.2568(8)
α (°)	90	90.00
β (°)	104.339(13)	90.00
γ (°)	90	90.00
Z	4	4
D_c/(g cm⁻³)	1.589	1.407
F(000)	3750.0	3680.0
θ range (°)	3.9 to 55.348	5.19 to 60.992
Reflections collected	80239	38610
Data / restraints / parameters	9123/2/443	6601 / 24 / 281
Goodness-of-fit on F²	1.066	1.099
R1 indices(I > 2 σ (I))	0.0517	0.0553
wR₂ indices(all date)	0.1672	0.1609

$$^a R = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^b wR(F^2) = [\sum (w(F_o^2 - F_c^2)^2) / \sum (w(F_o^2)^2)]^{1/2}.$$

Table S2. Comparison of the proposed detection method in this study with other literature.

Complexes	Objective	LDR	Ksv	LOD	Ref.
[Cd(mba)(bpdb) _{0.5}]	NFZ	1-10 μ M	81498 M ⁻¹	0.123 μ M	[1]
[Zn(L ¹) _{0.5} (L ²) _{0.5} (H ₂ O)]·DMF	NFZ	0-29.1 μ M	52000 M ⁻¹	19.6 μ M	[2]
{[Cd(L) _{0.5} (bpe) _{0.5} (H ₂ O)]·x(solv)}	NFZ	0-90 μ M	35000 M ⁻¹	0.33 μ M	[3]
{[Zn(TTPA)]·1.5DMA} _n	NFZ	0-50 μ M	23500 M ⁻¹	6.57 μ M	[4]
Zr ₆ O ₆ (OH) ₂ (TDCA) ₄ (CH ₃ COO) ₂	NFZ	0.7-250.4 μ M	--	0.25 μ M	[5]
[Cd(L ₁)(1,4-NDA)] _n	NFZ	0-100 μ M	3854 M ⁻¹	2.02 μ M	[6]
ssDNA	NFZ	1.25-160 ng/mL	--	1.13 ng/mL	[7]
WO ₃ /CuMnO ₂	NFZ	0.015-32 μ M	--	1.19 nM	[8]
O-AgNPs	NFZ	1-500 μ M	--	1.88 μ M	[9]
FCS-7	NFZ	3-40 μ M	121170.44 M ⁻¹	92 μ g·L ⁻¹	This work

Table S3. HOMO and LUMO energies for H₆bmipia and NFZ calculated by density functional theory (DFT) with B3LYP/6-31+G* basis set.

Compound	HOMO (eV)	LUMO (eV)	Band Gap (eV)
H ₆ bmipia	-6.2015	-2.3179	3.8836
NFZ	-6.6963	-3.2462	3.61022

References

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