

Supporting Information

Ancillary ligand enabled structural and fluorescent diversity in metal-organic frameworks: application for ultra-sensitive detection of nitrofurantoin antibiotics

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Table S1. Crystallographic Data for **FCS-4** and **FCS-5**.

| <i>Compounds</i> | <i>FCS-4</i> | <i>FCS-5</i> |
|---------------------------------------------------------|--------------------------------------------------------------------------------|--------------------------------------------------------------------|
| Empirical formula | C ₄₄ H ₃₄ N ₂ O ₂₂ Zn ₃ | C ₂₂ H ₂₀ NO _{11.5} Zn ₂ |
| Formula mass | 1138.84 | 613.13 |
| Crystal system | monoclinic | triclinic |
| Space group | <i>P2₁/c</i> | <i>P-1</i> |
| a (Å) | 9.8772(8) | 8.2490(5) |
| b (Å) | 17.151(3) | 11.0993(6) |
| c (Å) | 13.5423(15) | 13.7359(7) |
| α (°) | 90 | 89.549(4) |
| β (°) | 97.668(9) | 86.324(4) |
| γ (°) | 90 | 72.561(5) |
| V (Å³) | 2273.6(5) | 1197.27(11) |
| Z | 2 | 2 |
| D_{calc} (g·cm⁻³) | 1.663 | 1.701 |
| Reflections collected | 14543 | 15781 |
| Data [<i>I</i>>2σ(<i>I</i>)]/parameters | 5367/322 | 5717/334 |
| Goodness-of-fit on F² | 0.955 | 1.048 |
| R₁ indices [<i>I</i>>2σ(<i>I</i>)] | 0.0848 | 0.0375 |
| wR₂ indices (all data) | 0.2201 | 0.1026 |
| Residual electron density | 0.755 | 0.879 |

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

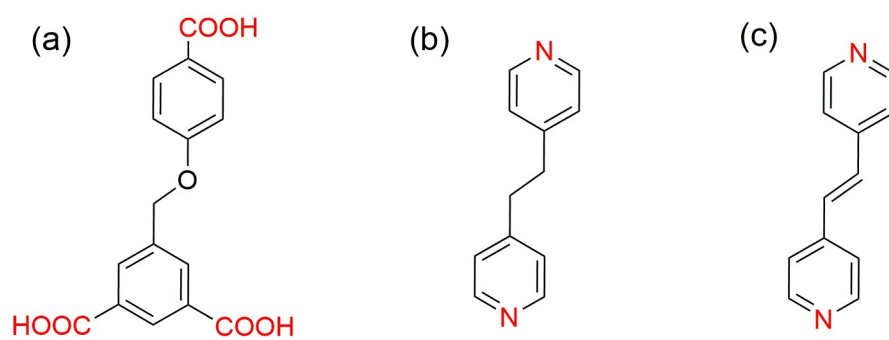


Fig. S1 Schematic illustration of (a) H₃cbbi, (b) bpe and (c) bpee ligands.

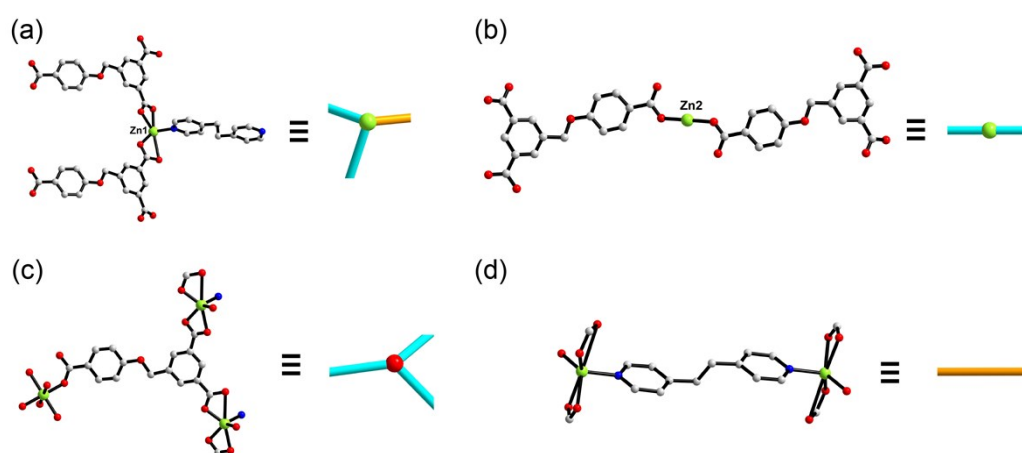


Fig. S2 (a) Zn1 atom as a trinode; (b) Zn2 atom as a dinode; (c) cbbi³⁻ ligand as a trinode; (d) bpe ligand as a linker.

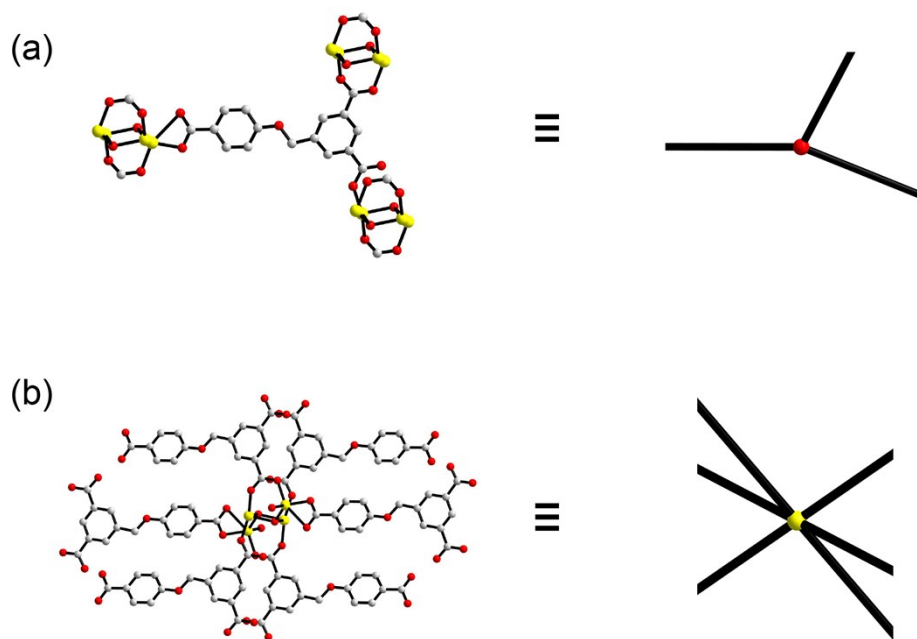


Fig. S3 (a) cbbi^{3-} ligand as a trinode; (b) tetranuclear zinc atoms as a hexanode.

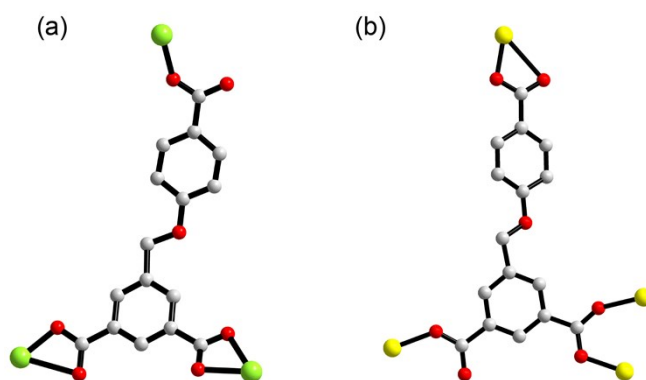


Fig. S4 Coordination modes of cbbi^{3-} ligands in (a) FCS-4 and (b) FCS-5.

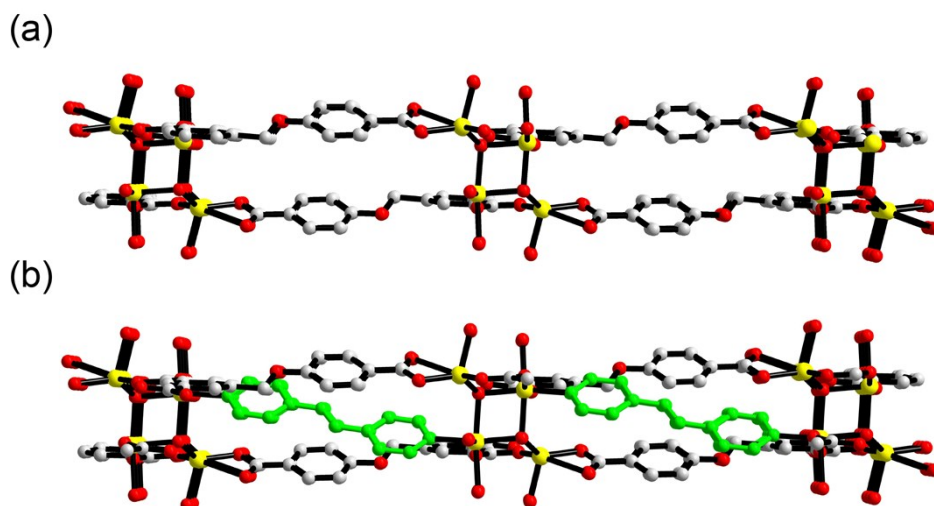


Fig. S5 Double-layer structure of FCS-5 (a) without and (b) with bpee ligand.

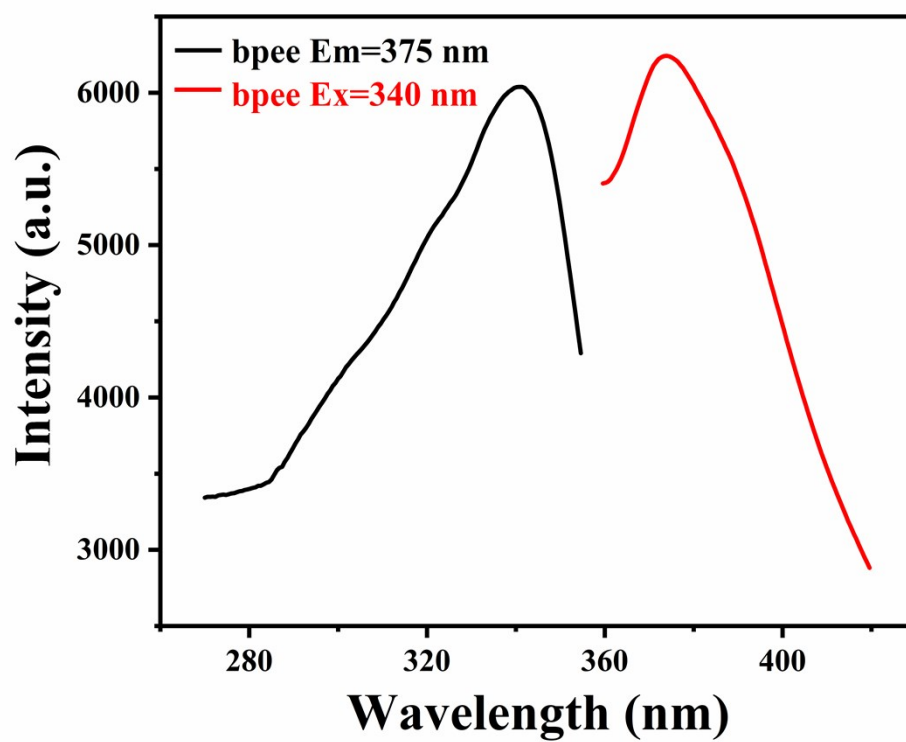


Fig. S6 The solid-state fluorescence spectrum of free ligand bpee.

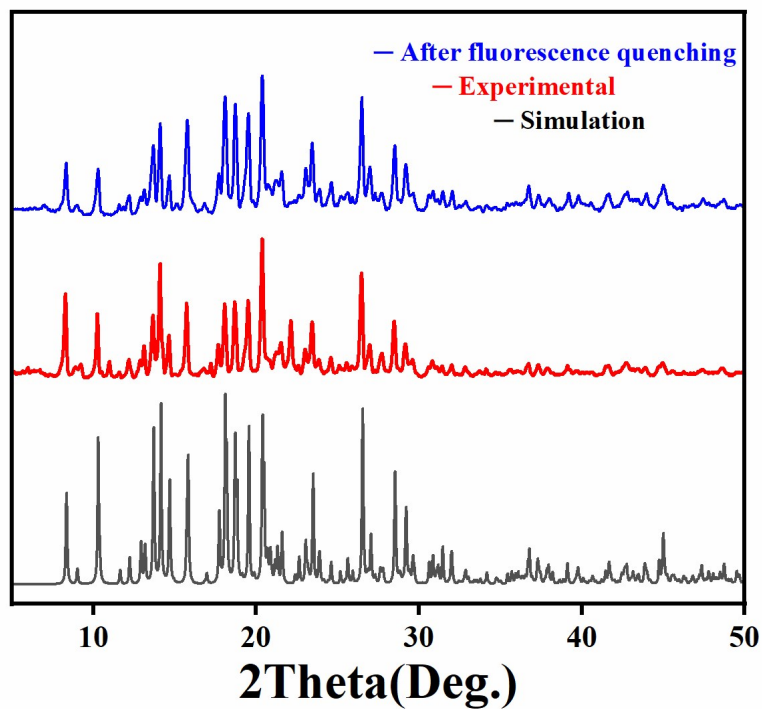


Fig. S7 The stimulated and experimental PXR D patterns of FCS-4 before and after the fluorescence quenching experiments.

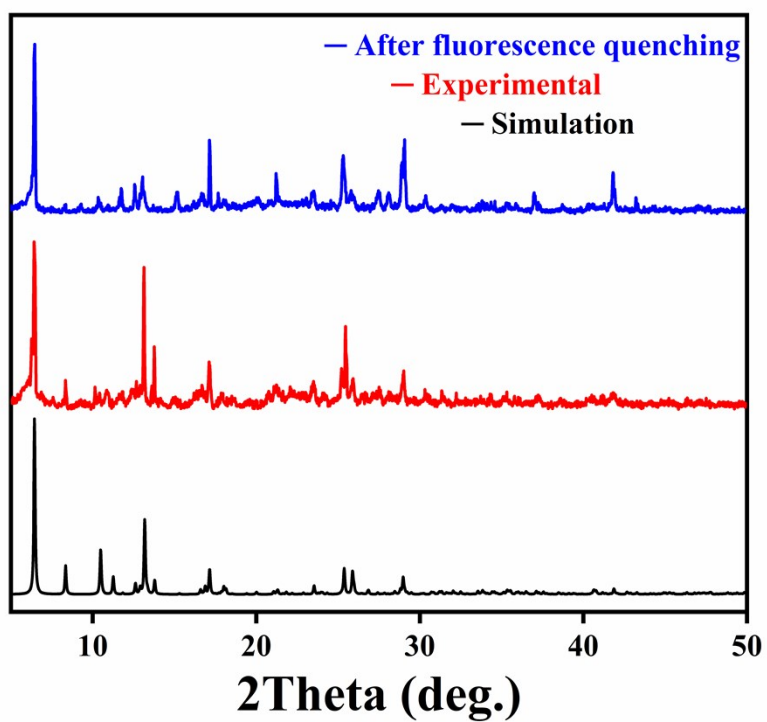


Fig. S8 The stimulated and experimental PXR D patterns of FCS-5 before and after the fluorescence quenching experiments.

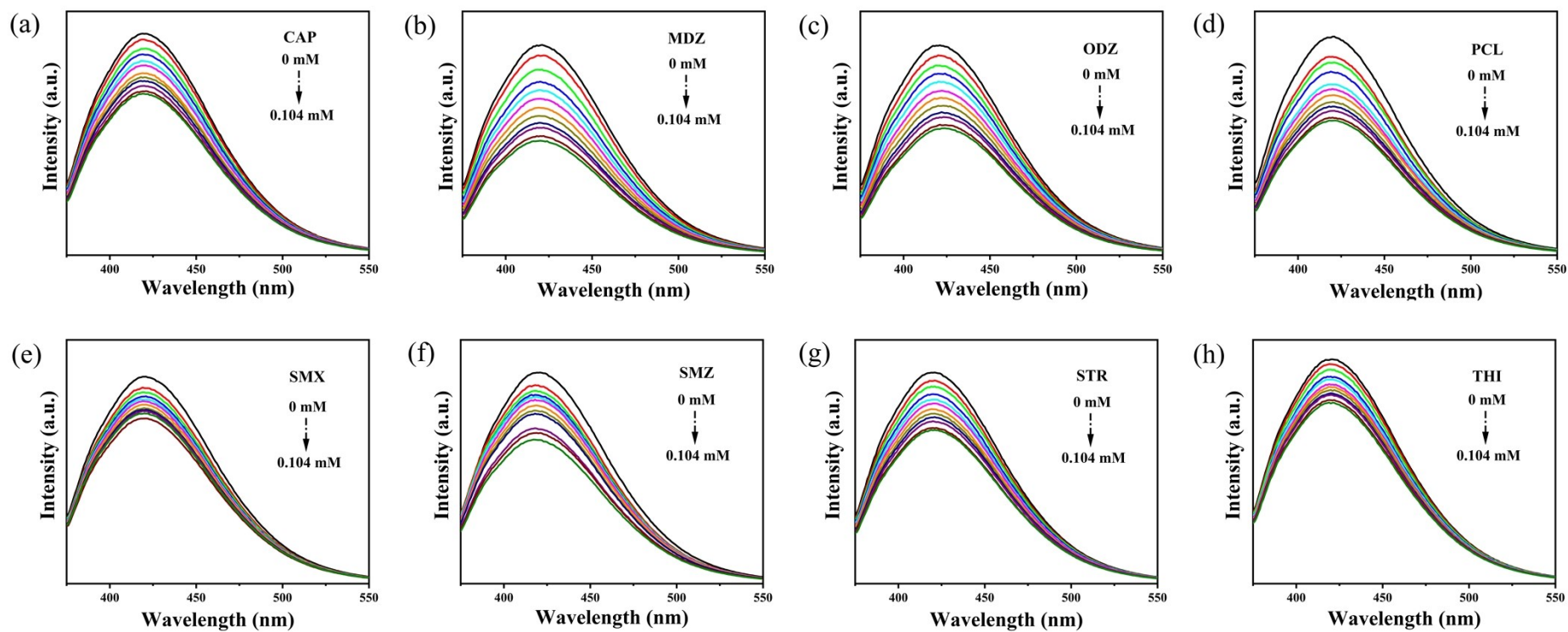


Fig. S9 The fluorescence titration of FCS-5 with gradual addition of different antibiotics.

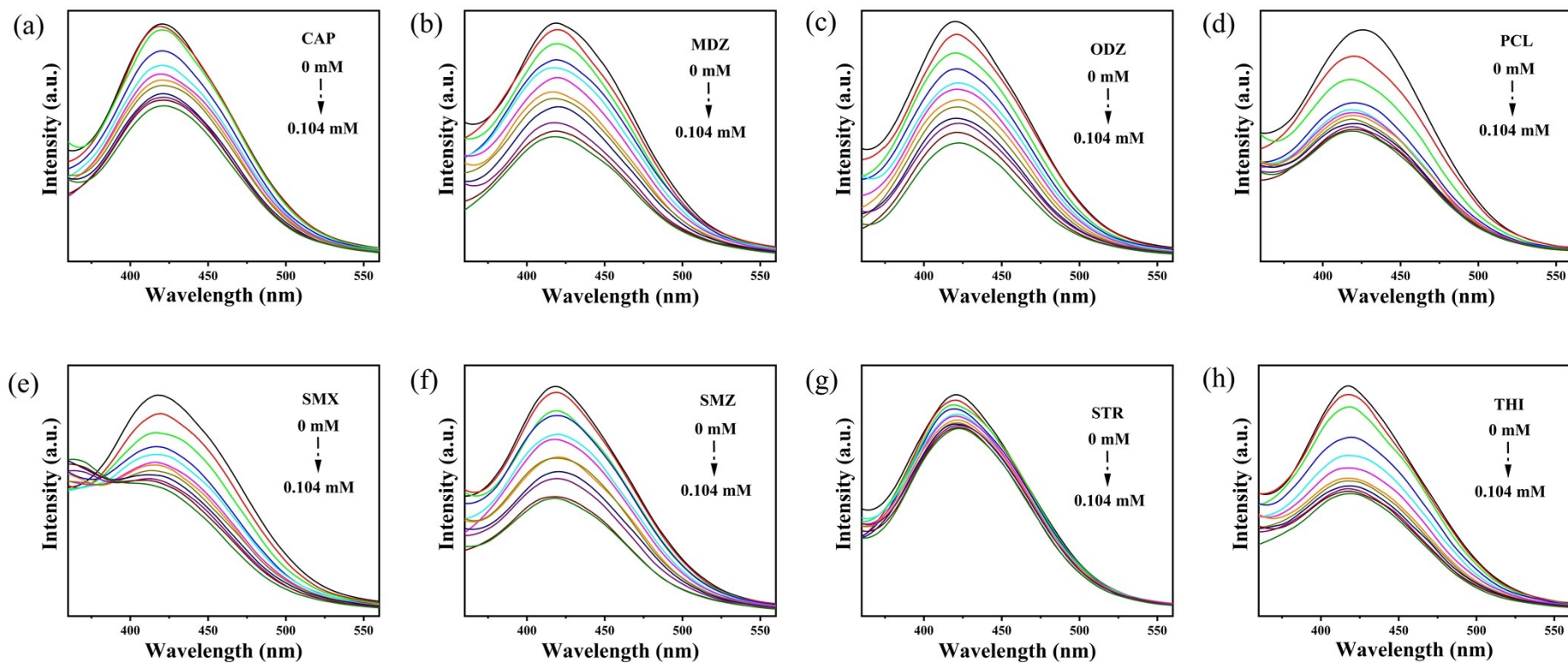


Fig. S10 The fluorescence titration of FCS-4 with gradual addition of different antibiotics.

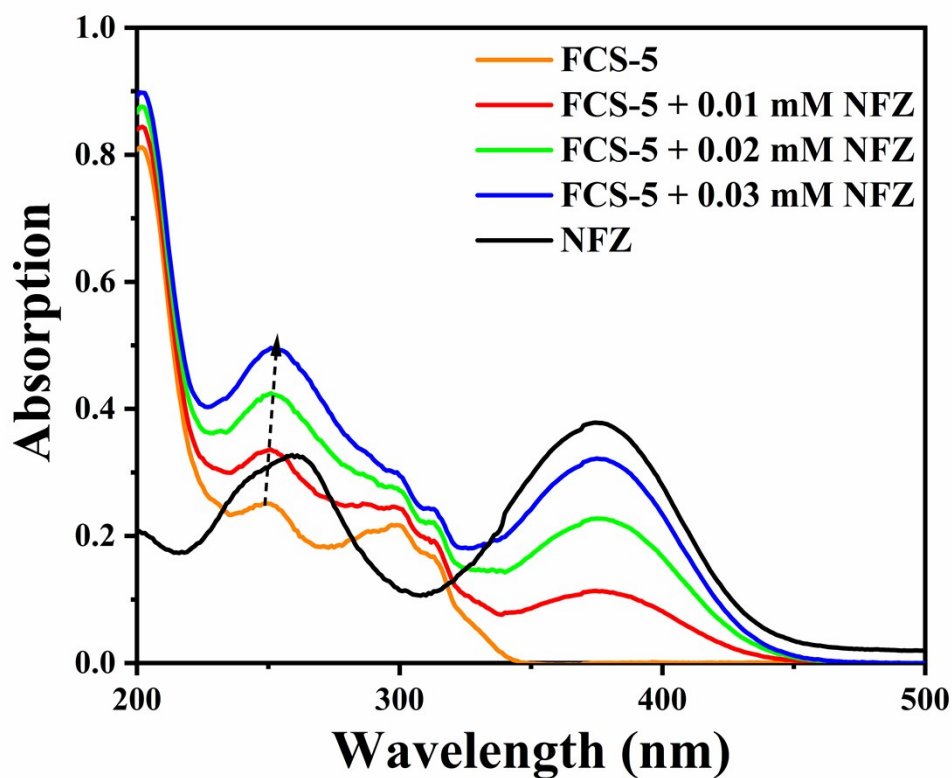


Fig. S11 UV-Vis spectra of FCS-5 before and after the addition of NFZ.

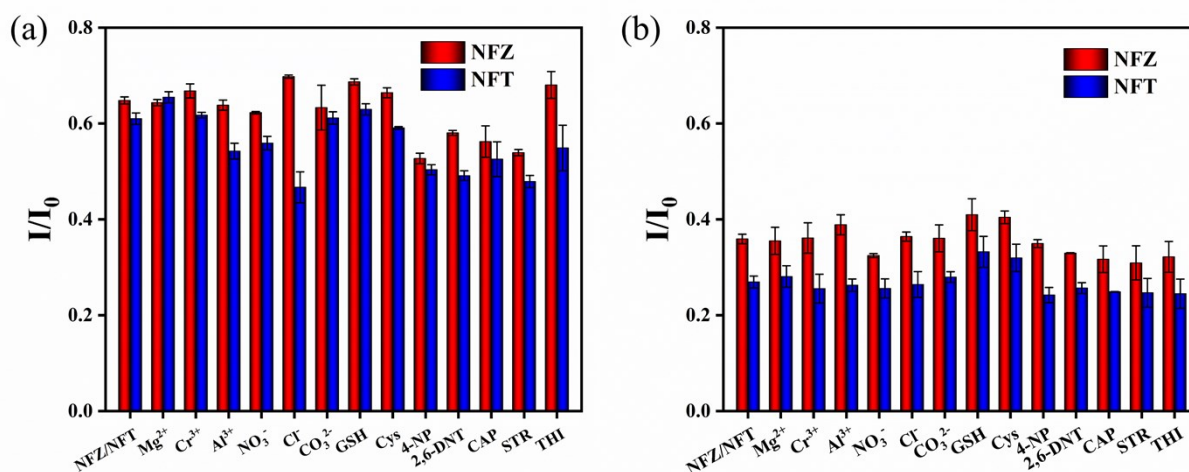


Fig. S12 Anti-interference ability of (a) FCS-4 and (b) FCS-5 toward NFZ/NFT (0.05 mM) in the presence of various kinds of interfering substances (0.25 mM).

Equation S1: Fitted curves of (1) **FCS-4** and (2) **FCS-5**.

(1) $y=128.0\exp(-x/19.39)-5.14$

(2) $y=176.6 \exp(-x/10.27)+1.64$