

Supporting information

A cucurbit[6]uril-based supramolecular assembly test strip for immediate detection of nitrofuran antibiotics in water

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Table S1. Crystal data and structure refinement for **1**

Compound	1
Empirical formula	C ₉₆ H ₇₂ CdN ₂₄ O ₂₀
Formula weight	1994.17
Crystal system	Monoclinic
Space group	C2/c
a (Å)	17.938(11)
b (Å)	21.945(14)
c (Å)	25.620(16)
α (°)	90
β (°)	106.696(2)
γ (°)	90
V (Å ³)	9660(11)
Z	4
D _v /g cm ⁻³)	1.371
μ / (mm ⁻¹)	0.308
F(000)	4096.0
θ range (°)	4.96-56.724
R _{int}	0.0334
Parameters	636
T (K)	273.15
goodness of fit	1.112
Limiting indices	-23 ≤ h ≤ 23 -29 ≤ k ≤ 29 -34 ≤ l ≤ 34
R indices [I > 2σ(I)]	R ₁ =0.0354,wR ₂ =0.0855
R indices (all data)	R ₁ =0.0388,wR ₂ =0.0915

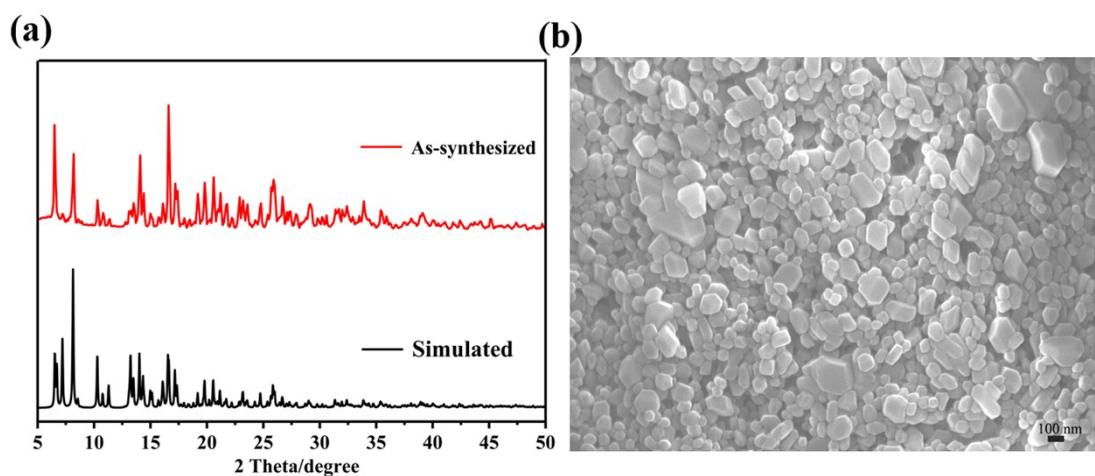


Fig. S1. (a) The PXRD pattern spectra of 1 and the simulated spectra. (b) The SEM image of the ground sample for the sensing experiment.

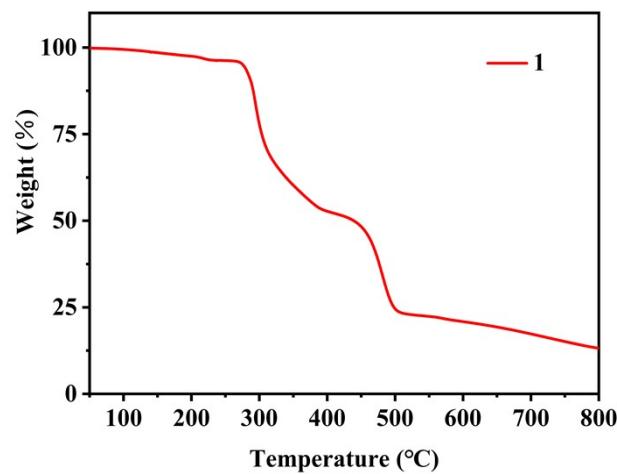


Fig. S2. The TGA curve of 1.

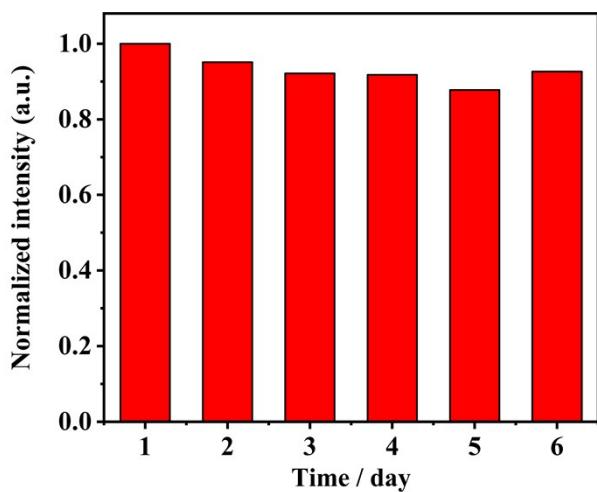


Fig. S3 Luminescence spectra of **1** dispersed in water with different times.

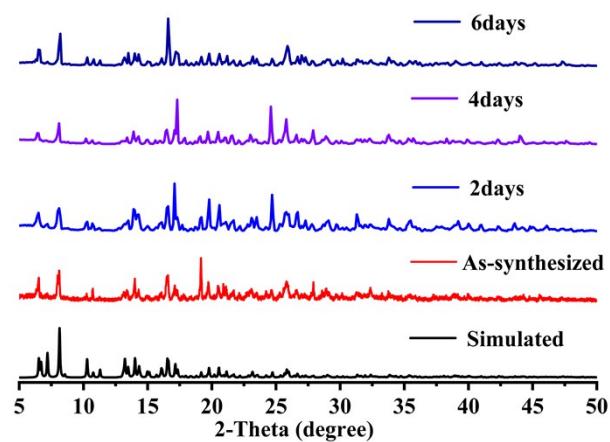


Fig. S4 PXRD patterns of **1** after soaked in water with different times.

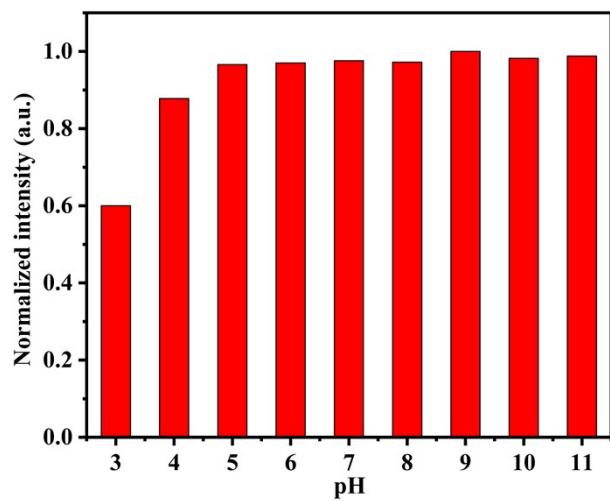


Fig. S5 PXRD patterns of **1** in aqueous solution with different pH value.

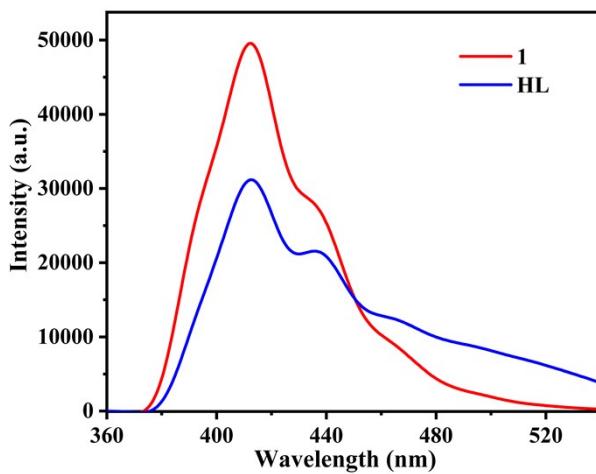


Fig. S6. The emission spectra of free HL ligand and **1**.

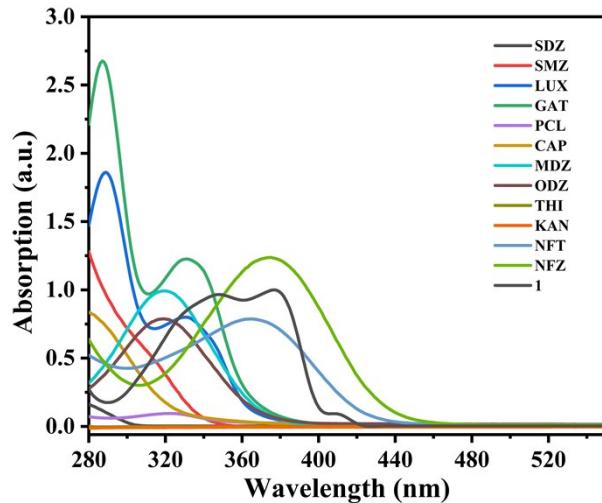


Fig. S7. The UV–vis spectra of the antibiotics and the excitation spectra of **1**.

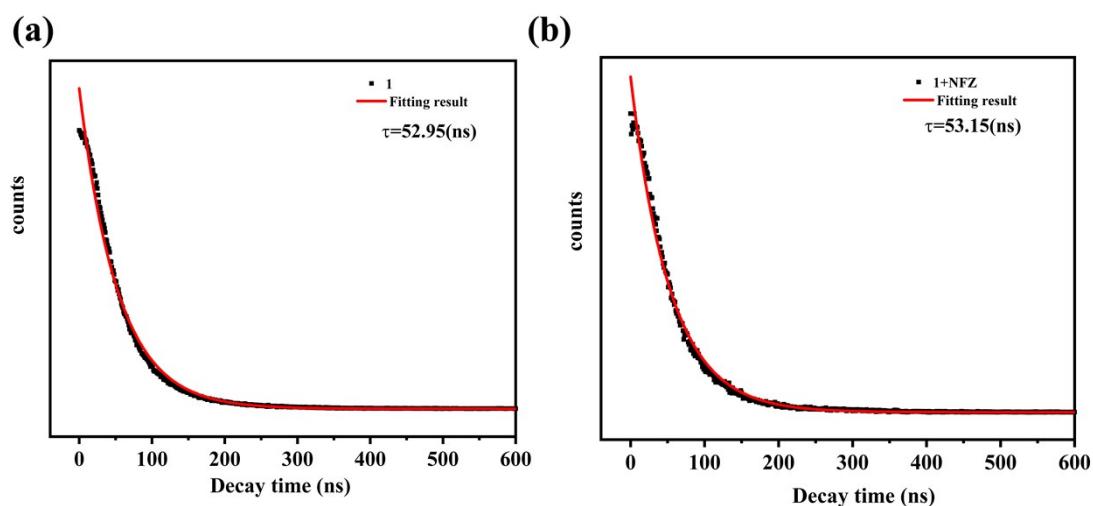


Fig. S8. The decay time of **1** and NFZ-treated samples.

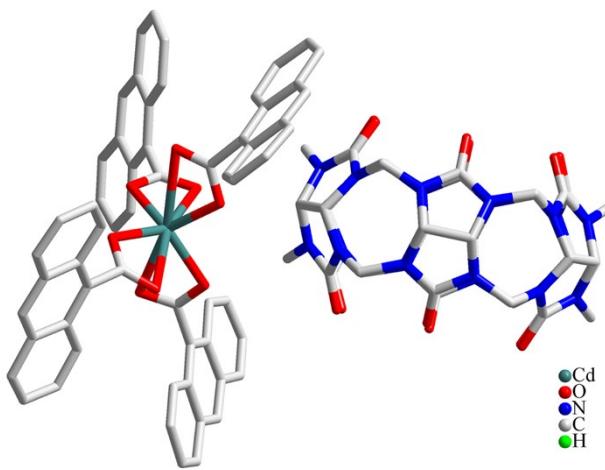


Fig. S9. The asymmetric structure unit of **1**.

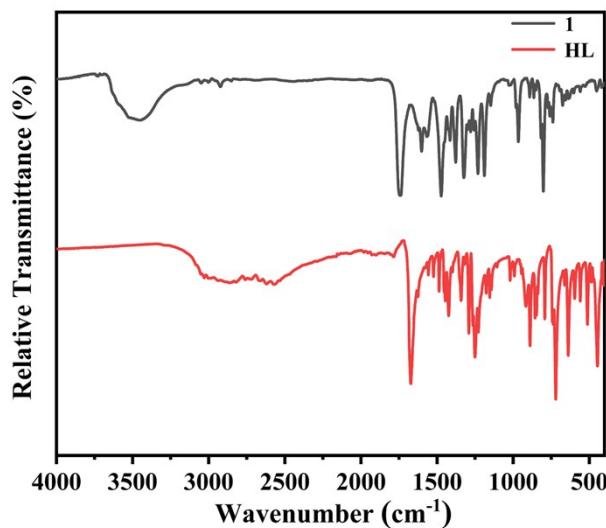


Fig. S10. The FI-TR spectrum of the free HL ligand and the as-synthesized **1**.