

Supporting Information

Single-phase white light material and antibiotic detection of lanthanide metal-organic framework

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Reference

Materials and Physical Measurements

All reagents and solvents were purchased from commercial sources and used directly without further purification. Terbium(III) nitrate hexahydrate ($\text{Tb}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$), Europium(III) nitrate hexahydrate ($\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$) and Lanthanum(III) nitrate hexahydrate ($\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$) were purchased from Shanghai Yien Chemical Technology Co., Ltd., 4,4',4''-nitrotribenzoic acid (H_3TCA) was purchased from Yanshen Science and Technology Co., Ltd., Chinese Academy of Sciences of Jilin Province, Nitrofurazone (NZF), nitrofurantoin (NFT), azithromycin (AZM), clarithromycin (CLR), roxithromycin (ROX), sulfamonomethoxine (SMM) and ciprofloxacin hydrochloride (CPFX-HCl) were purchased from Shanghai Macklin Biochemical Co. Ltd.

Powder X-ray diffraction (PXRD) data was obtained by Rigaku Miniflex 600 X-Ray Diffractometer, with Cu Ka radiation at 40 kV and 15 mA at room temperature. Fourier transform infrared (FT-IR) spectra were recorded on Brooktensar-27 infrared spectrometer during the range of 4000 to 400 cm^{-1} . Ultraviolet-visible absorption spectra (UV-vis) were measured with a Shimadzu UV-2700 spectrophotometer. Fluorescence spectra were achieved through a Shimadzu RF-6000 spectrophotometer. Thermogravimetric analyses (TGA) were taken on the Rigaku Thermal plus EVO2 TG-DTA 8122 instrument under oxygen stream with a heating rate of 10 $^{\circ}\text{C} \cdot \text{min}^{-1}$. N_2 adsorption/desorption isotherms were measured at 77 K using an ASAP2020M instrument. Elemental analyses (C, H, and N) were performed with a Vario EL cube elemental analyzer.

X-ray Crystal Structure Analysis

X-ray single crystal diffraction data of **HNU-82-84** were measured and obtained on a Bruker APEX-II CCD with nitrogen-flow temperature controller using graphite monochromatic Mo K α radiation ($\lambda=0.71073$ Å) at 150 K. The single crystal structure of **HNU-82-84** was reduced by the Bruker SHELXTL. The structure was solved by the direct method and refined by the full-matrix least-squares method on F² using the SHELXTL crystallographic software package.¹ All H atoms were placed geometrically for **HNU-82-84** and all nonhydrogen atoms were refined using anisotropic thermal parameters. The final formula of **HNU-82-84** was determined by single-crystal structure, and the crystallographic data was shown in Table S1 in the ESI. The CCDC numbers of **HNU-82-84** are 2225974, 2225976, 2225977.

Table S1. The crystal data of **HNU-82-84**.

Complex	HNU-82	HNU-83	HNU-84
Empirical formula	C ₂₄ H ₂₉ N ₂ O ₁₂ Tb	C ₂₄ H ₂₉ N ₂ O ₁₂ Eu	C ₂₄ H ₂₉ N ₂ O ₁₂ La
Formula weight	696.41	689.45	676.4
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P2₁/n</i>	<i>P2₁/n</i>	<i>P2₁/n</i>
<i>a</i> (Å)	9.2557	9.2570	9.3685
<i>b</i> (Å)	12.8698	12.8401	12.8587
<i>c</i> (Å)	23.7286	23.8208	24.1274
α (°)	90	90	90
β (°)	94.905	95.633	96.179
γ (°)	90	90	90
<i>V</i> (Å ³)	2816.2	2817.69	2889.66
<i>Z</i>	4	4	4
<i>D</i> _{calcd} (g cm ⁻³)	1.643	1.625	1.555
μ (Mo K α) (mm ⁻¹)	12.907	16.492	11.970
<i>F</i> (000)	1392	1384	1360
<i>R</i> _{int}	0.0649	0.0632	0.0390
<i>R</i> ₁ ^a [I>2 δ (I)]	0.0591	0.0604	0.0669
<i>wR</i> ₂ ^b (all data)	0.1616	0.1546	0.1854
Goof on F ²	1.103	1.080	1.097

$$R_1 = \sum(|F_o| - |F_c|) / \sum|F_o|; wR_2 = \{ \sum w(|F_o|^2 - |F_c|^2)^2 / \sum w(|F_o|^2)^2 \}^{1/2}.$$

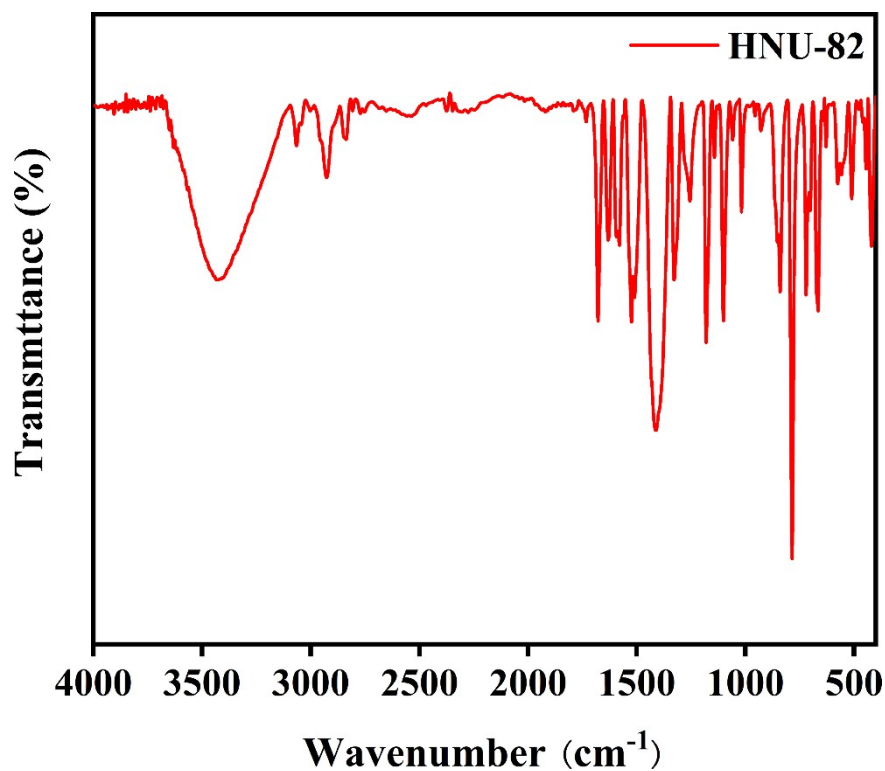


Figure S1. The IR spectrum of HNU-82.

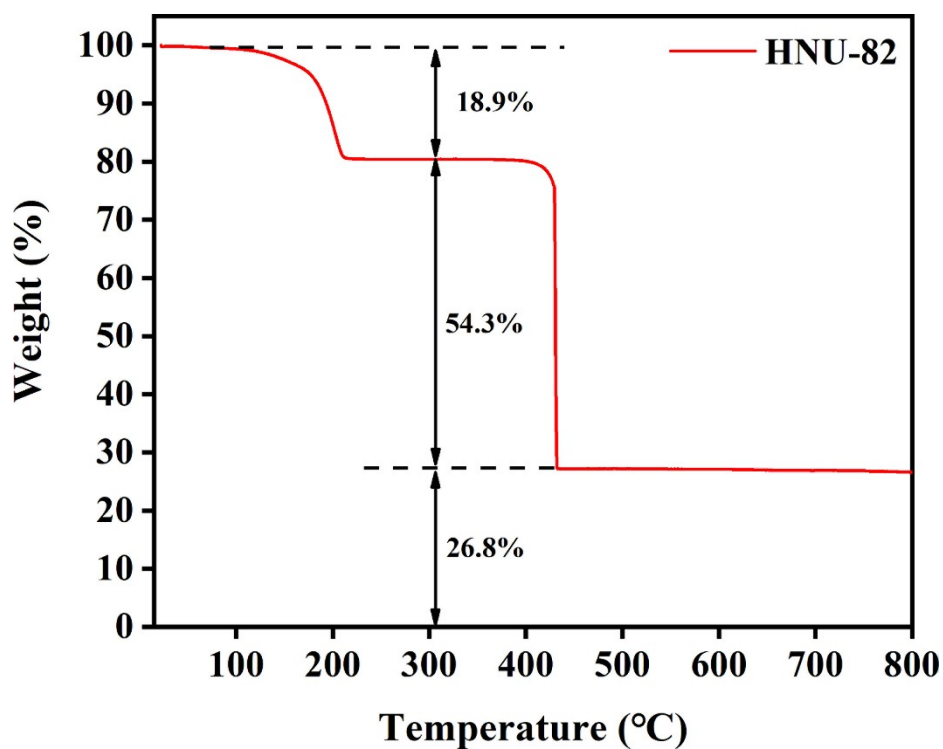


Figure S2. The TG plot of HNU-82.

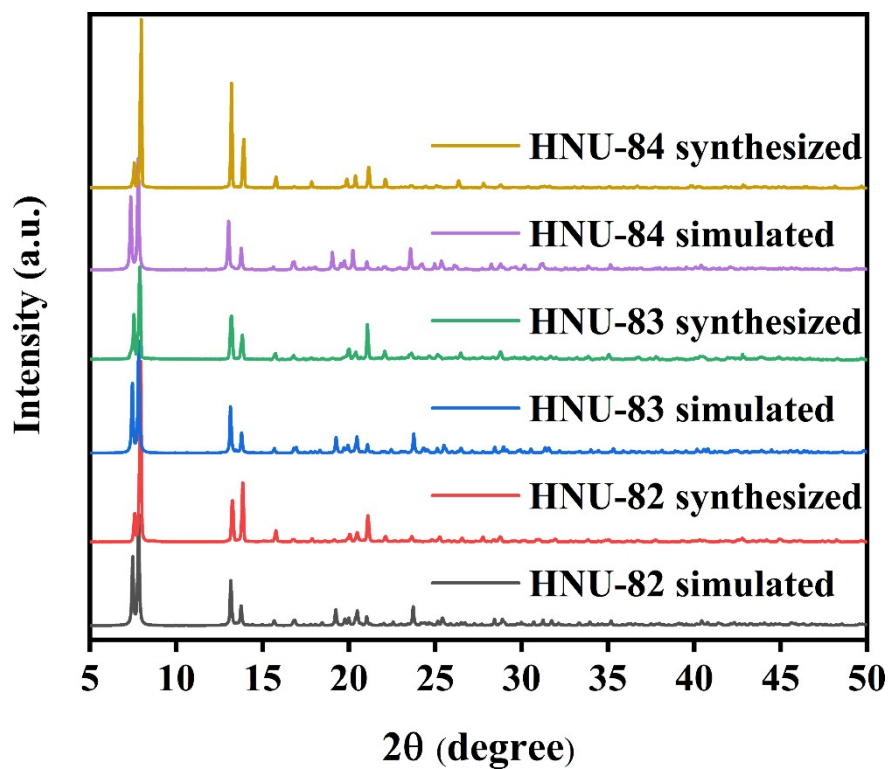


Figure S3. The PXRD pattern of HNU-82-84.

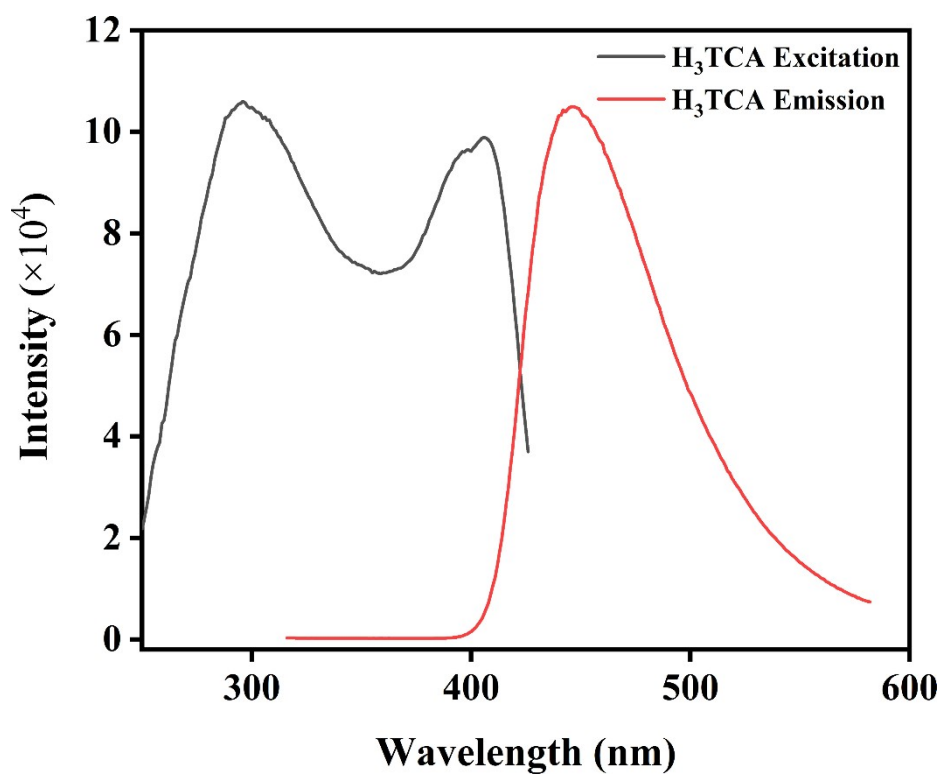


Figure S4. Fluorescence excitation and emission spectra of H₃TCA.

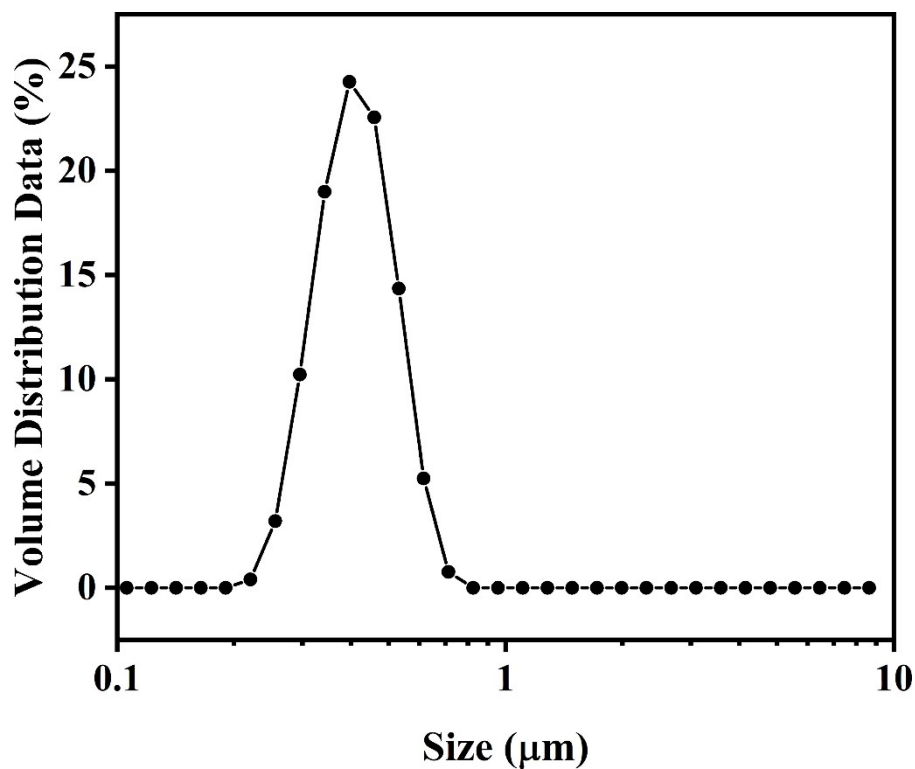


Figure S5. Particle size distribution of HNU-82.

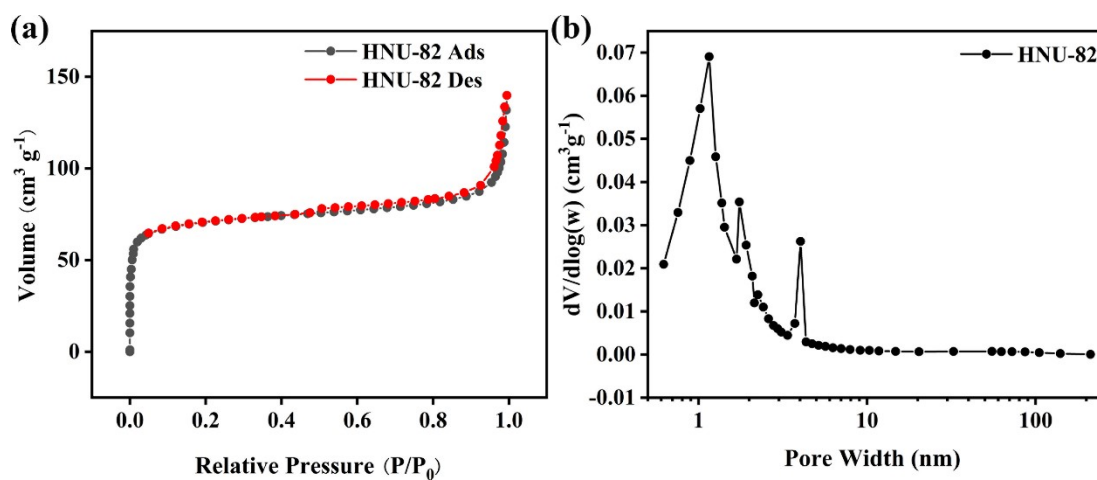


Figure S6. N₂ adsorption-desorption isotherms (a) and the pore size distribution (b) of HNU-82.

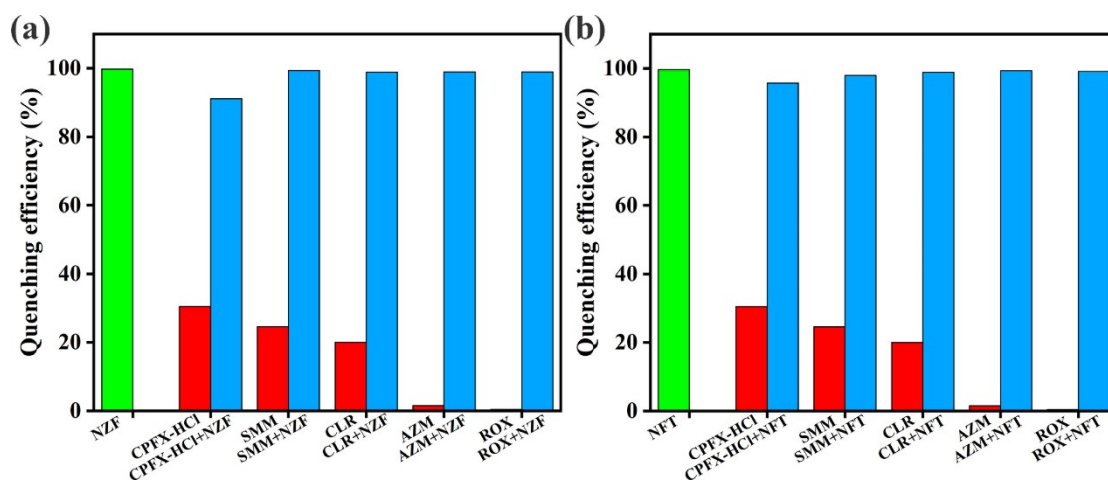


Figure S7. Anti-interference test of HNU-82 against NZF and NFT antibiotic assays.

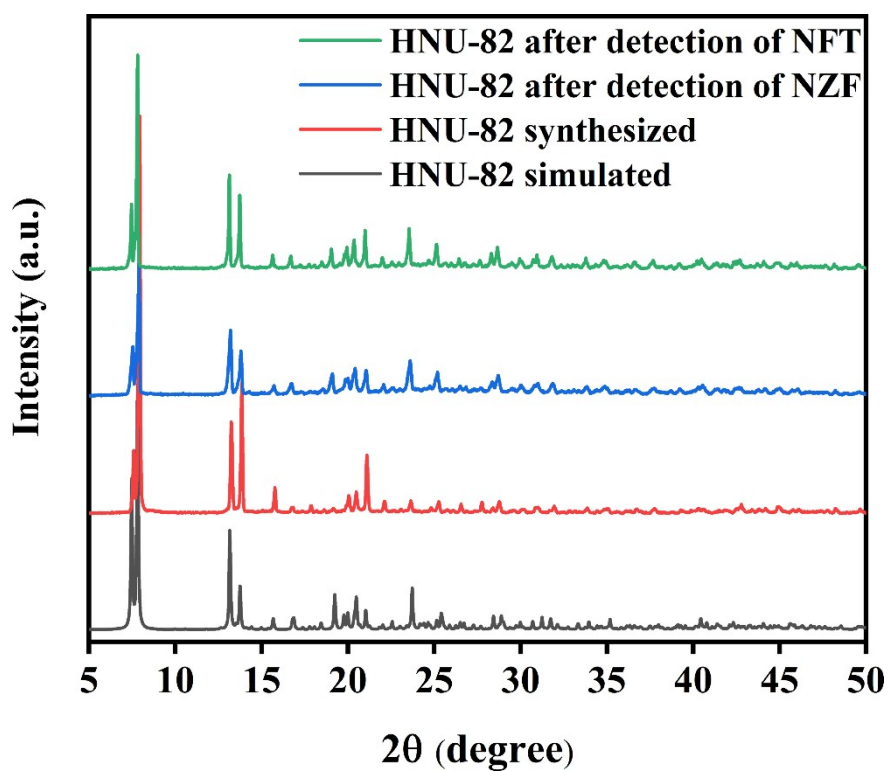


Figure S8. PXRD spectra of HNU-82 before and after detection of NZF and NFT.

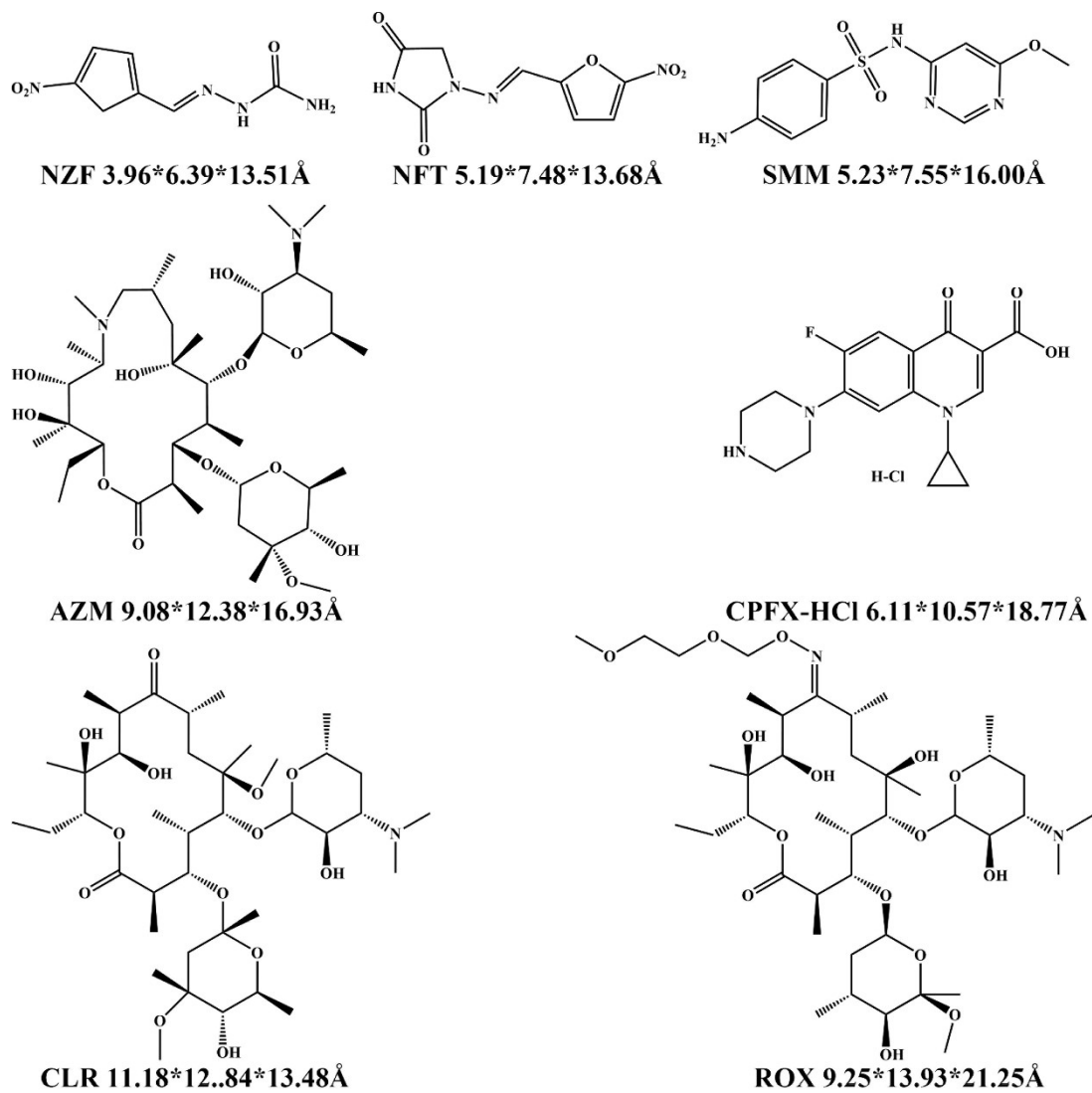


Figure S9. Antibiotic chemical structural formula and molecular size.

Table S2. The space group and Ln-O connection mode of reported results and this work.

CCDC	Empirical Formula	Space group	Ln-O	reference s
2110293-5-6(La, Eu, Tb)	C ₂₅ H ₂₁ LnN ₂ O ₇	<i>P-1</i>	7(6TCA ³⁻ ,1DMF)	3
841880(Eu)	C ₆₃ H ₄₂ Eu ₃ N ₃ O ₂₁ ,	<i>P2₁/c</i>	9(6TCA ³⁻ ,1H ₂ O)	4
807487(Tb)	C ₂₄ H ₁₉ N ₂ O ₇ Tb	<i>P-1</i>	8(6TCA ³⁻ ,1DMF)	5
1910649(Tb)	C ₂₁ H ₁₂ NO ₆ Tb	<i>C2/c</i>	8(6TCA ³⁻)	6
1052119(La)	C ₂₁ H ₁₄ LaNO ₇	<i>R32</i>	9(6TCA ³⁻ ,1H ₂ O)	7
1444538 (La)	C ₃₃ H ₃₉ LaN ₄ O ₉	<i>Pbca</i>	9(3TCA ³⁻ ,3DMF)	8
2225974-6-7(Tb, Eu, La)	C ₂₄ H ₂₉ N ₂ O ₁₂ Tb	<i>P2₁/n</i>	8(5TCA ³⁻ ,2H ₂ O)	This work

Table S3. The quantum yields of reported results and this work.

Material	λ (nm)	CIE (x,y)	QY (%)	CCT (K)	references
La _{0.9} Tb _{0.093} Eu _{0.007} (cpioa)	365	(0.319, 0.331)	54.74	6162	9
Ln@bio-MOF-1	365	(0.328,0.338)	52.9	4725	10
1-Eu _{0.0855} Gd _{0.6285} Tb _{0.2860}	390	(0.34, 0.33)	22.4	5645	11
Eu _{0.5} Tb _{0.5} -nanopaper@FB	254	(0.34, 0.36)	16.3	5336	12
Eu _{0.045} Tb _{0.955} -CPOMBA	365	(0.326, 0.343)	15	5733	13
HMA-Tb ₁₀ Eu ₁	350	(0.33, 0.34)	11.41	-	14
LnMOF-12	345	(0.332, 0.333)	11.22	-	15

Eu _{0.015} Tb _{0.037} La _{0.148} TCA	365	(0.319,0.344)	10.57	5645	This work
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