

Supporting Information for

Lanthanide Organic Framework as a Reversible Luminescent Sensor for Sulfamethazine Antibiotics

Kui Ren[†], Wu-Shun Hua, Xiao-Feng Guo[†], Hong Wang^{*}

Key Laboratory of Analytical Chemistry for Biology and Medicine (Ministry of Education), College of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, China

Corresponding author: Hong Wang

E-mail address: hongwang@whu.edu.cn

Tel.: +86-27-87218924; fax: +86-27-68754067

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Calculation of Limit of Detection

SMZ (0-40 μM) was added to Eu-MOF in ethanol-borate buffer (6:4, v/v) (50mM) solution and the fluorescent intensities of the resulted solutions were recorded, and a good linear relationship between the fluorescence intensity and concentrations of SMZ was obtained with slope (K) of 46.06 μM^{-1} . Standard deviation (Sb) was calculated from baseline 720-735nm of Eu-MOF. Limit of detection was calculated according to the formula: $\text{LOD} = 3S_b/K = 3 \times 10.06/46.06 = 0.6554 \mu\text{M}$.

DFT Calculation

The geometry optimizations and energies of HOMO and LUMO were performed with Gaussian 09 by Density Functional Theory (DFT) method with the B3LYP function employing 6-31G(d) basis set for all molecules.

Crystallographic data for reported Eu-MOF

CCDC 1816956 contains the supplementary crystallographic data for reported Eu-MOF in this paper. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

Table S1. Crystal data and structure refinement for Eu-MOF

Empirical formula	C ₃₀ H ₂₂ EuNO ₇ (+solvent)
Formula weight	660.44
T (K)	150.03
λ (Å)	0.71073
Crystal system	monoclinic
Space group	P21/c
Crystal colour	Colourless
a (Å)	8.0364(3)
b (Å)	16.6086(7)
c (Å)	27.1347(11)
α (°)	90
β (°)	96.8380(1)
γ (°)	90
V (Å ³)	3596.0(2)
μ (mm ⁻¹)	1.780
Dx (g cm ⁻³)	1.220
Z	4
F(0 0 0)	1312.0
Refinement method	Full-matrix least-squares on F ²
Goodness-of-fit on F2	1.052
R(reflections)	0.0340(5575)
wR2 (reflections)	0.0833(7359)
Date completeness	0.999
Theta range	2.453 to 26.406 deg

Table S2. K_{SV} of Eu-MOF with the addition of SMZ at different temperature

T	$K_{sv}(\text{L/mol})$
20°C	4.598×10^4
50°C	5.183×10^4
80°C	5.442×10^4

Table S3. ICP results of Eu-MOF and Eu-MOF after five switching process.

samples	Detection spectrum	Concentration ($\mu\text{g/mL}$)
Eu-MOF	Eu 381.967	5.2693
Eu-MOF after five switching process	Eu 381.967	6.0735

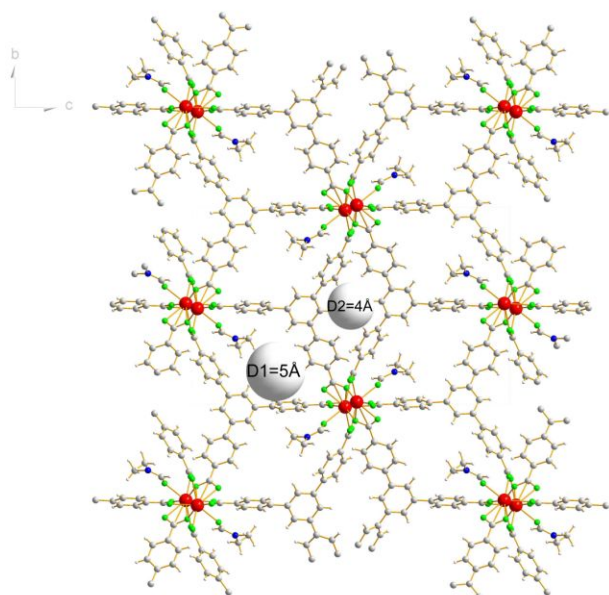


Figure S1. The Eu-MOF with two types of 2D channels.

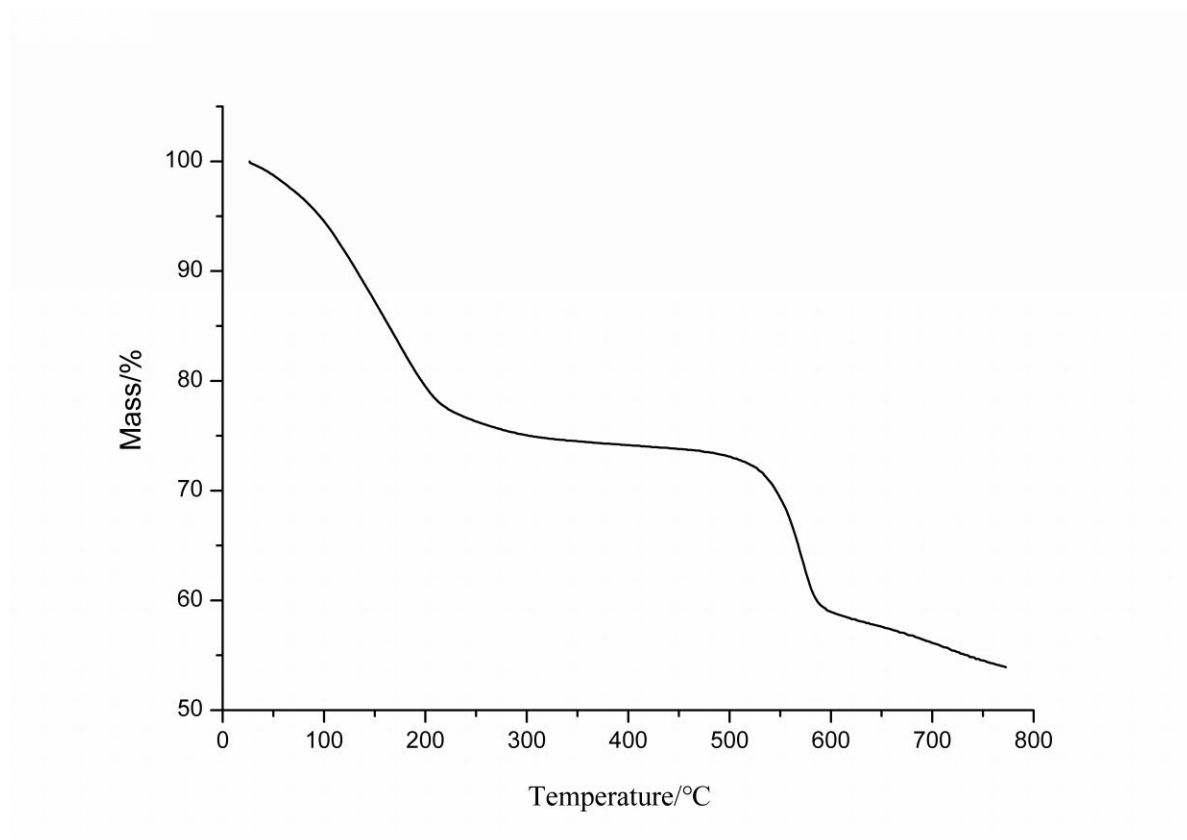


Figure S2. TGA trace of Eu-MOF in nitrogen with a heating rate of 5°C per minute.

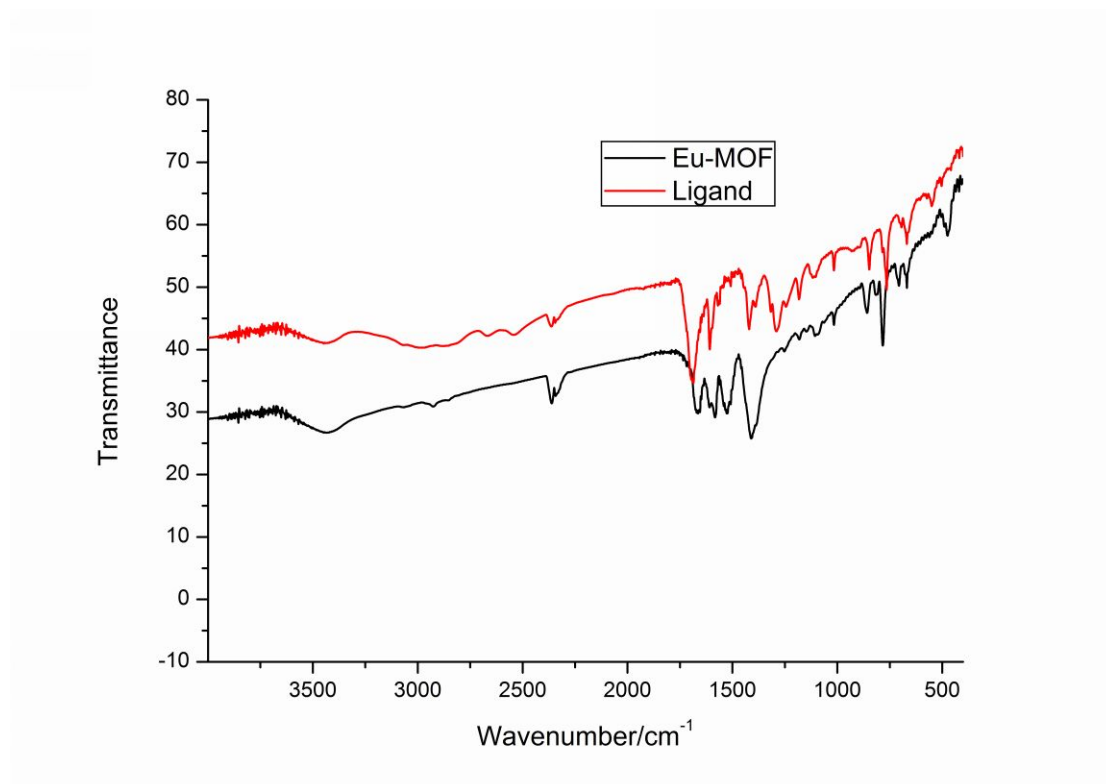


Figure S3. The IR spectra of H₃BTB ligand and MOF

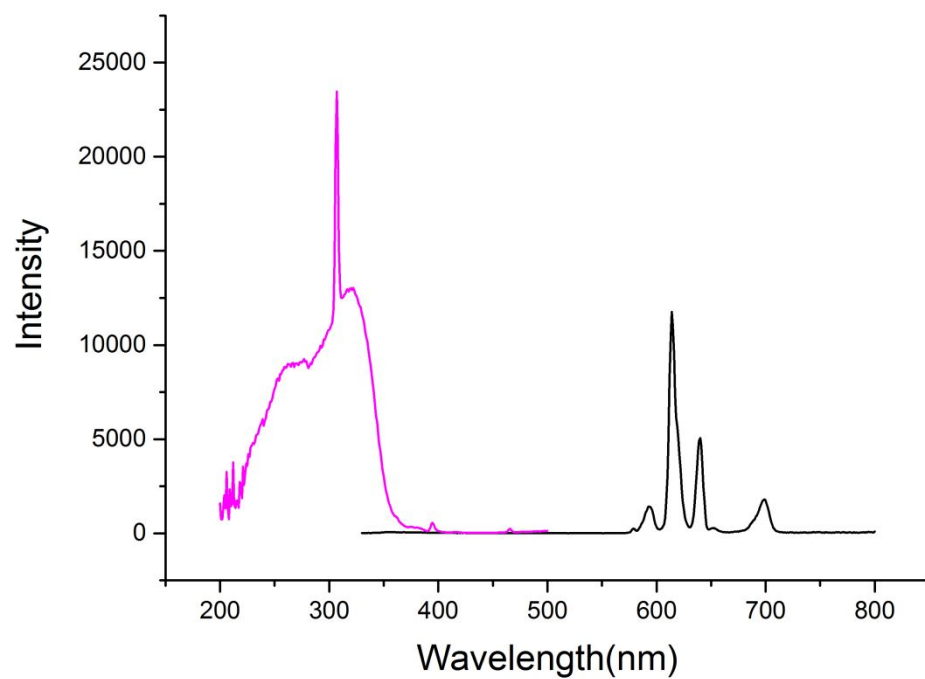


Figure S4. The emission and excitation spectra of Eu-MOF

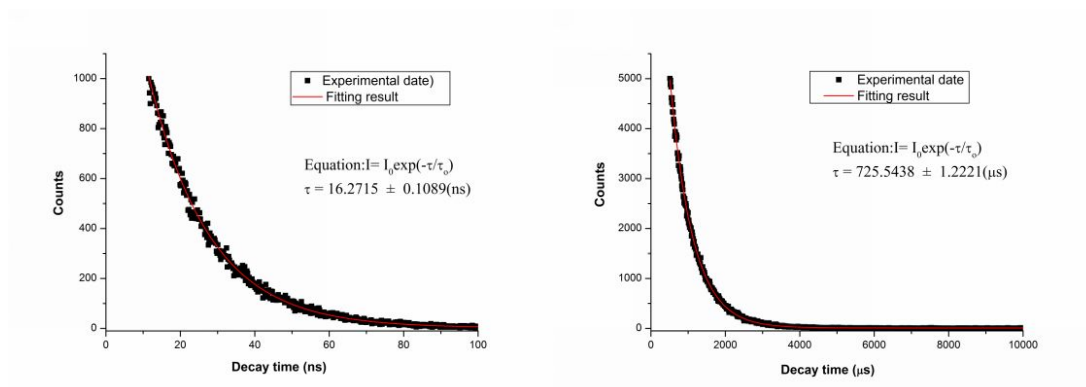


Figure S5. The luminescence decay curves of pure ligand (left) and Eu-MOF (right)

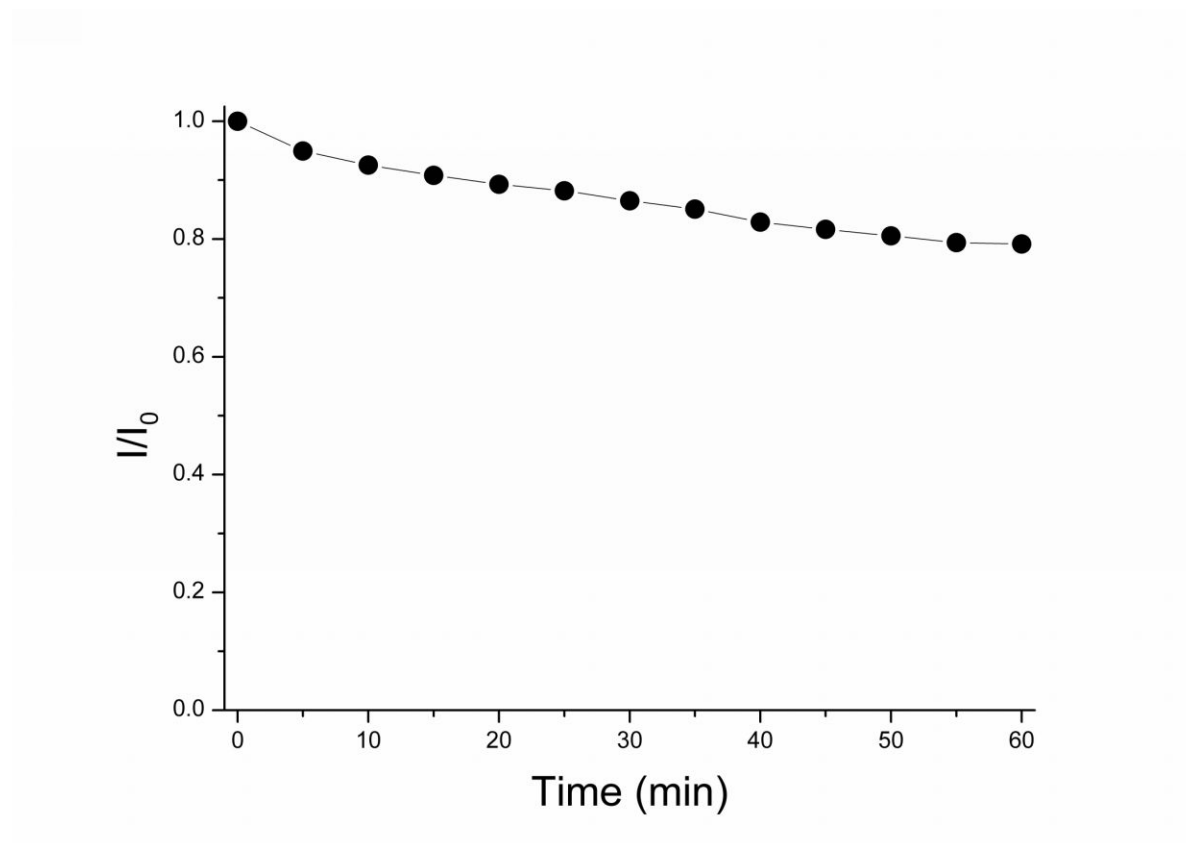


Figure S6. Time dependent fluorescence intensity of Eu-MOF within 60 min. Wavelength: 614 nm.

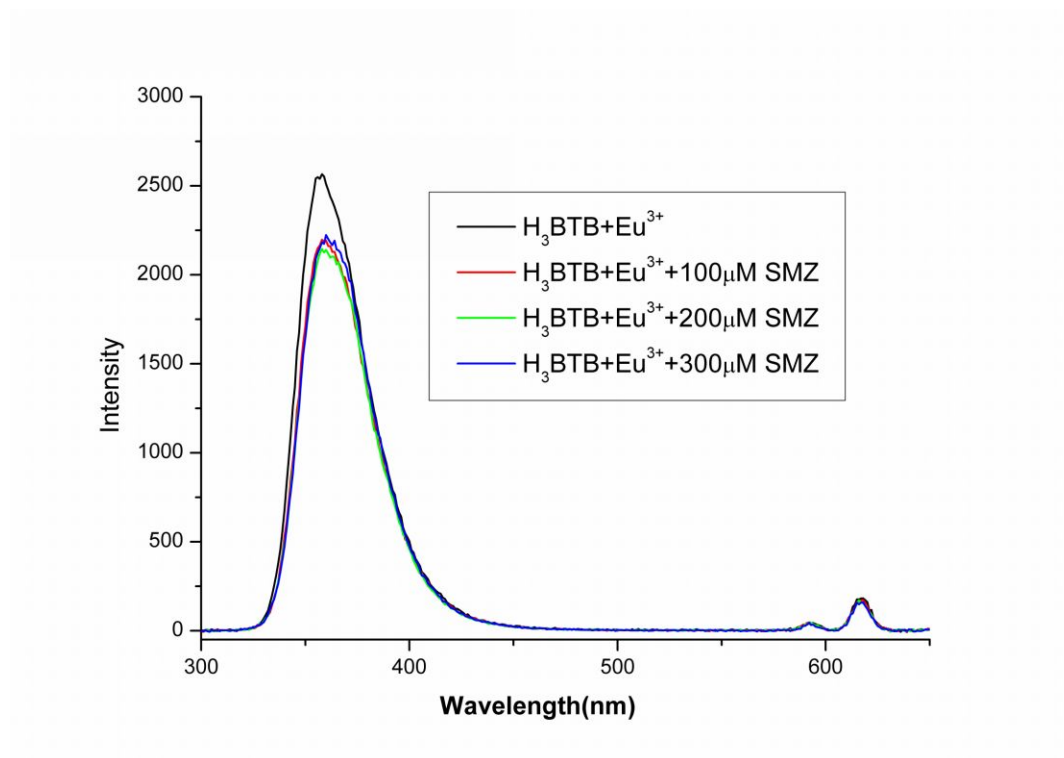


Figure S7. Fluorescence response (ex=287) of ligand (H₃BTB) mixed with Eu ions upon the addition of SMZ (0, 100, 200, 300 μM)

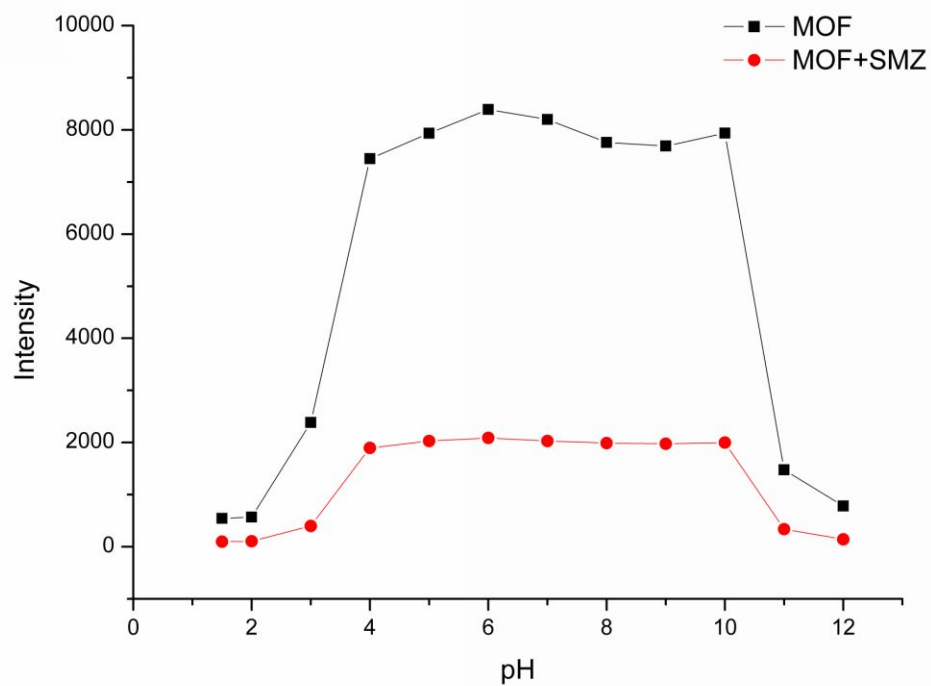


Figure S8. Fluorescence intensity of Eu-MOF and Eu-MOF with SMZ in ethanol-borate buffer (6:4, v/v) (50mM) at different pH.

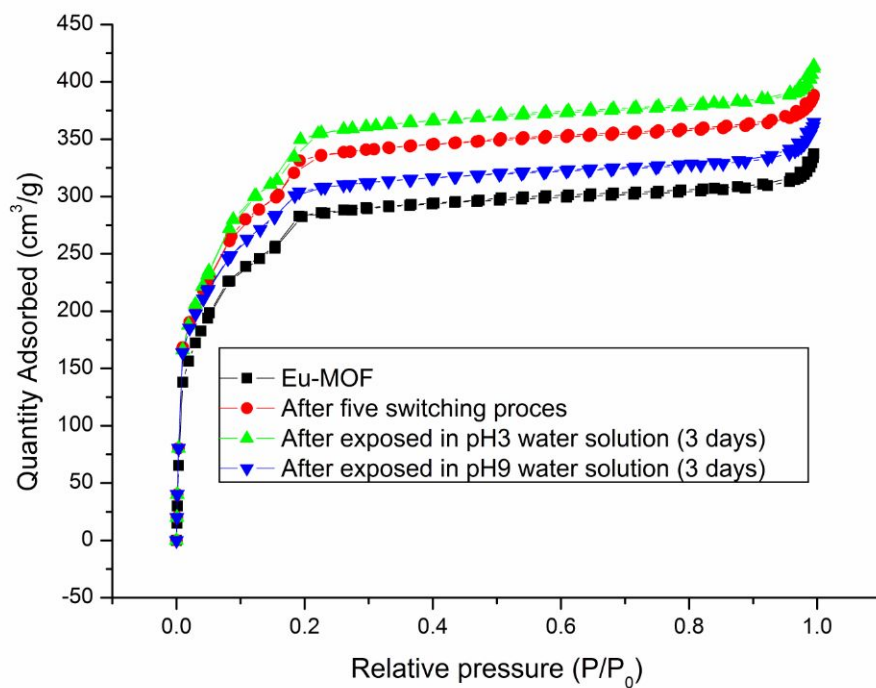


Figure S9. The nitrogen adsorption isotherms indicated the chemical stability of Eu-MOF after five switching process with SMZ and after exposed in different pH water solution (3 days).

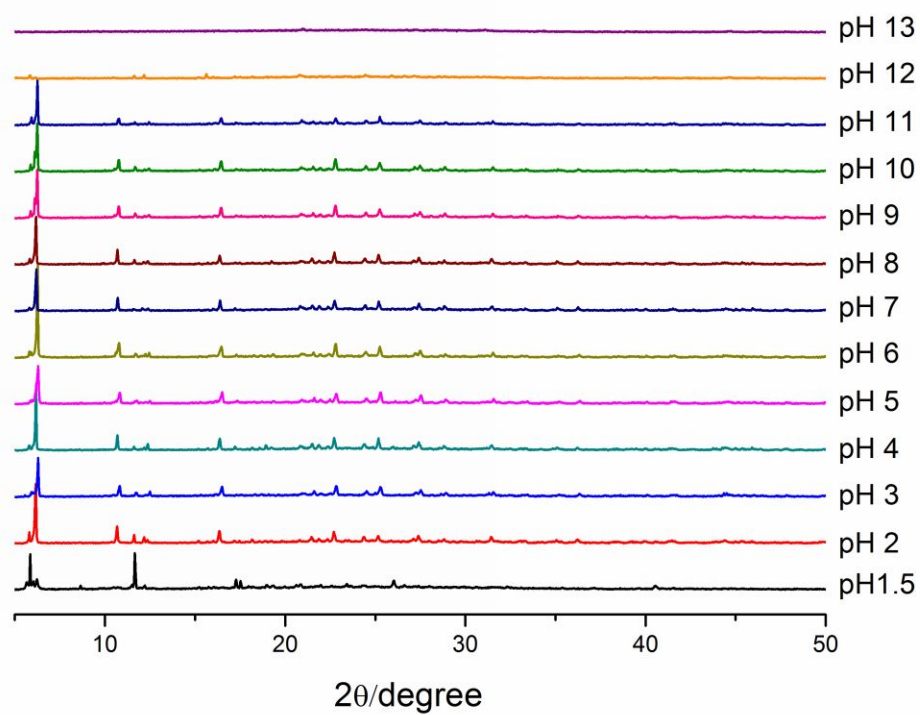


Figure S10. PXRD patterns of Eu-MOF after 72 hours of immersion in water at different pH

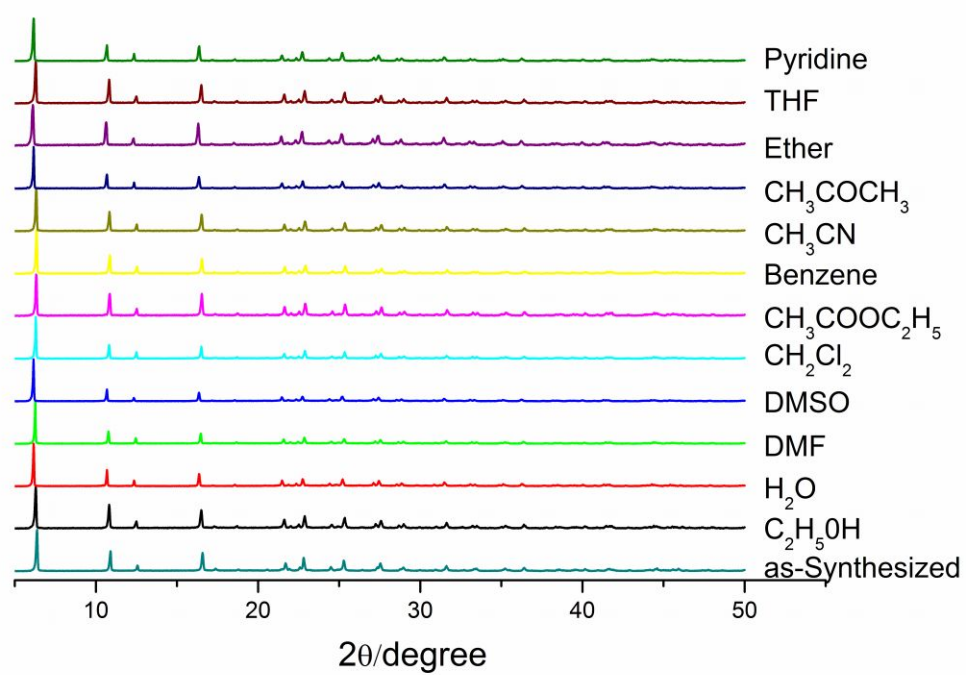


Figure S11. PXRD patterns of Eu-MOF after 72 hours of immersion in various solvents.

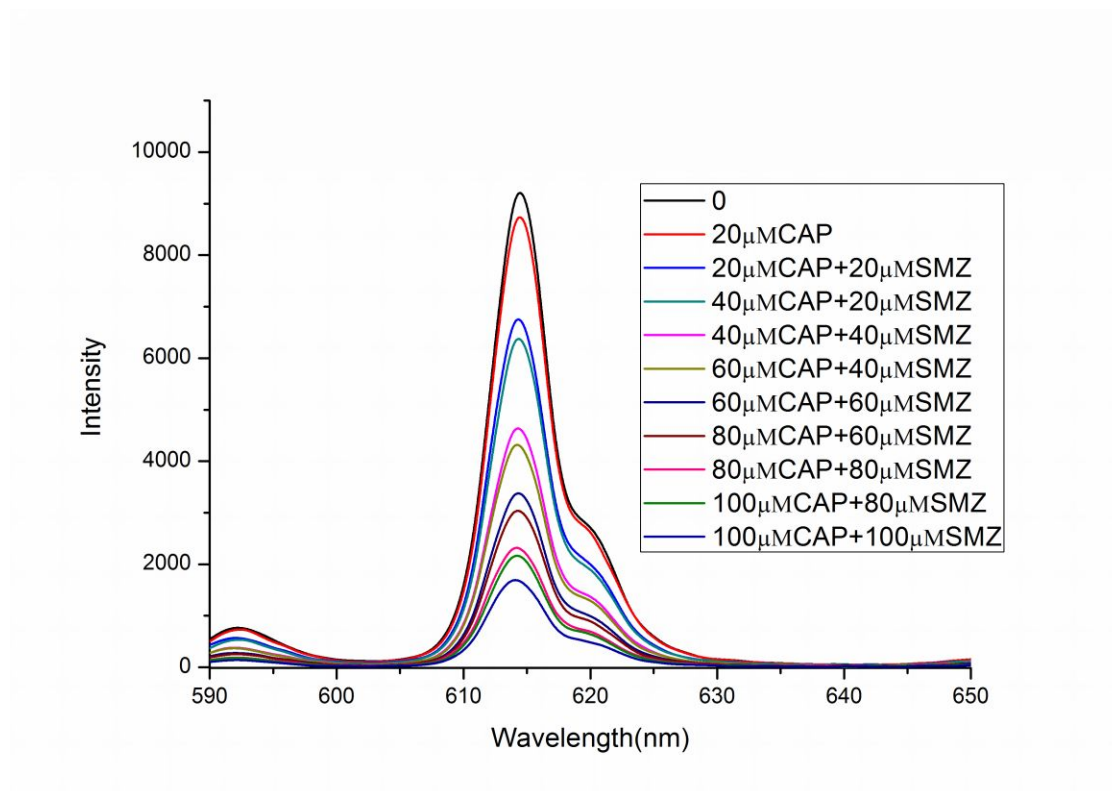


Figure S12. Fluorescence spectra of Eu-MOF upon addition of CAP followed by SMZ.

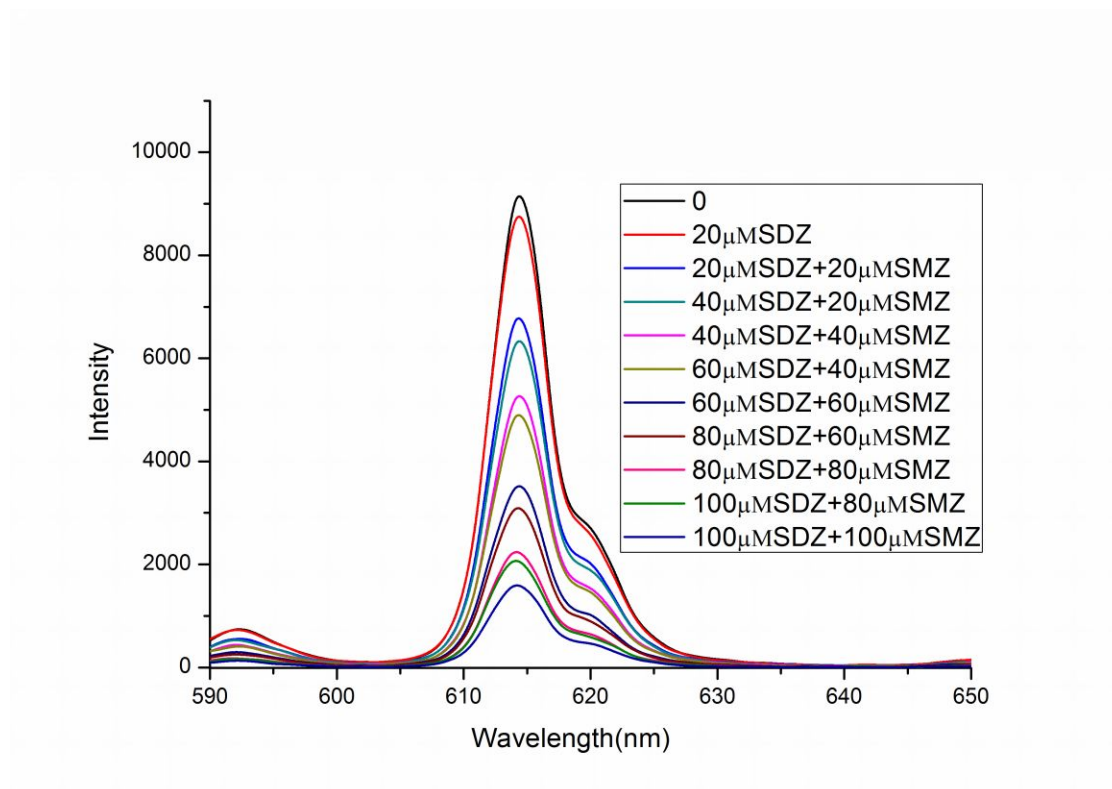


Figure S13. Fluorescence spectra of Eu-MOF upon addition of SDZ followed by SMZ.

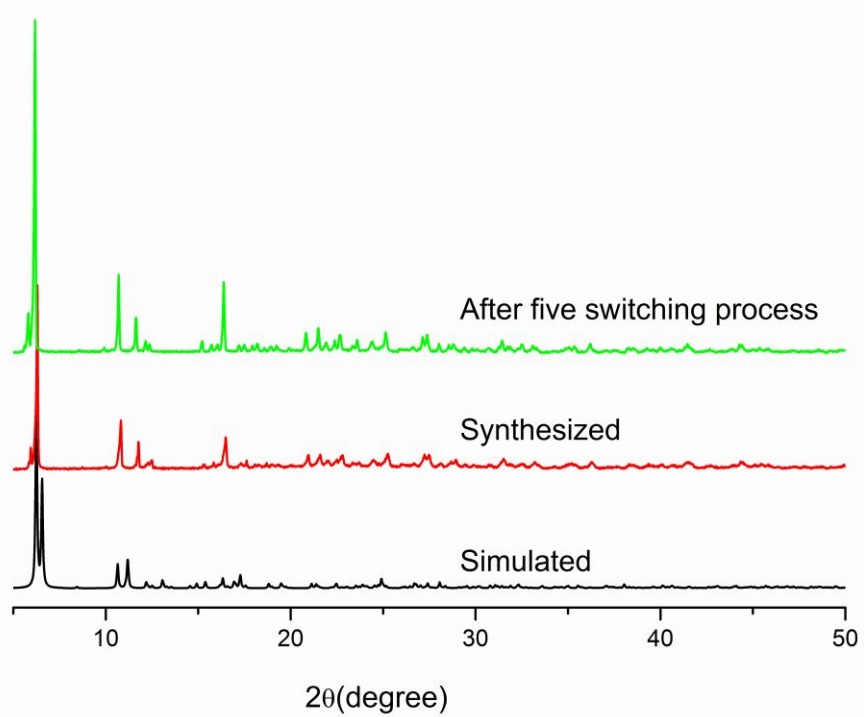


Figure S14. PXRD of Eu-MOF after five switching process.

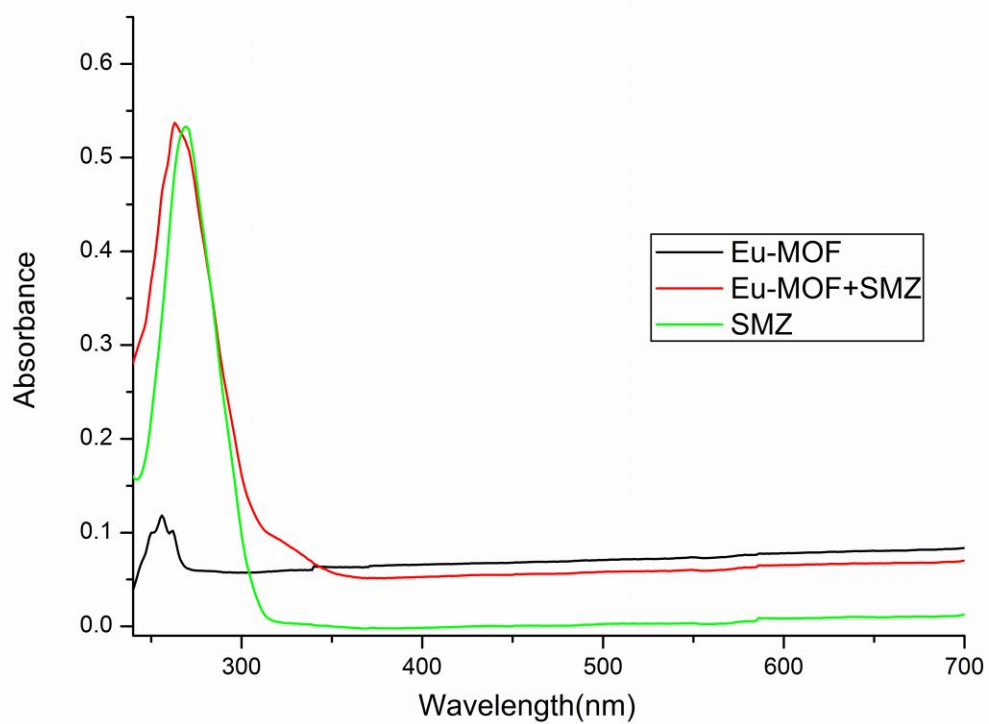


Figure S15. UV/Vis absorption spectra of Eu-MOF, SMZ and the mixture of SMZ and Eu-MOF.

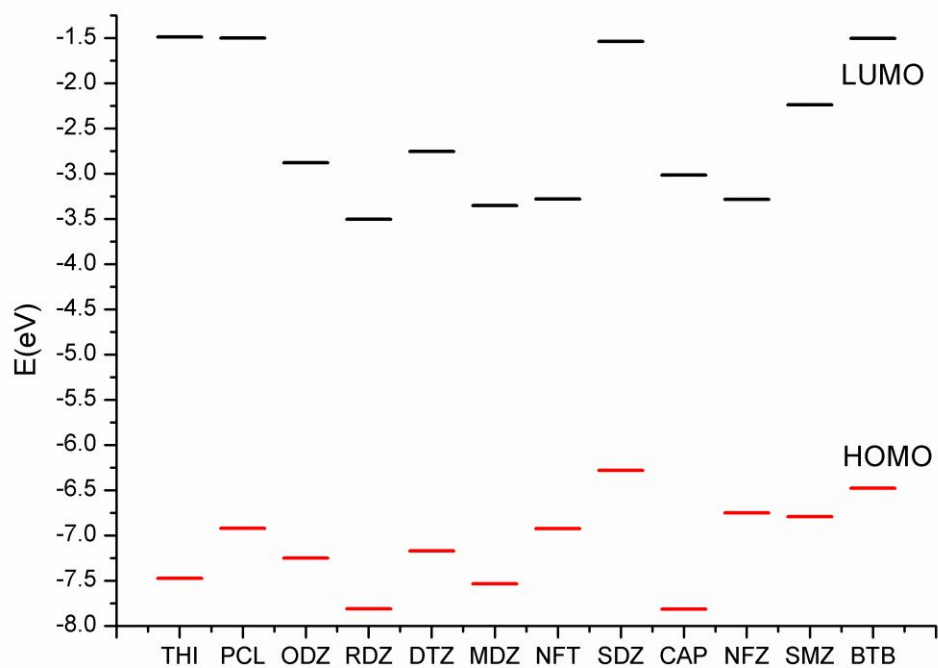


Figure S16. HOMO and LUMO energy levels of the analytes and the H₃BTB calculated by density functional theory (DFT) at B3LYP/6-31G(d) basis set.

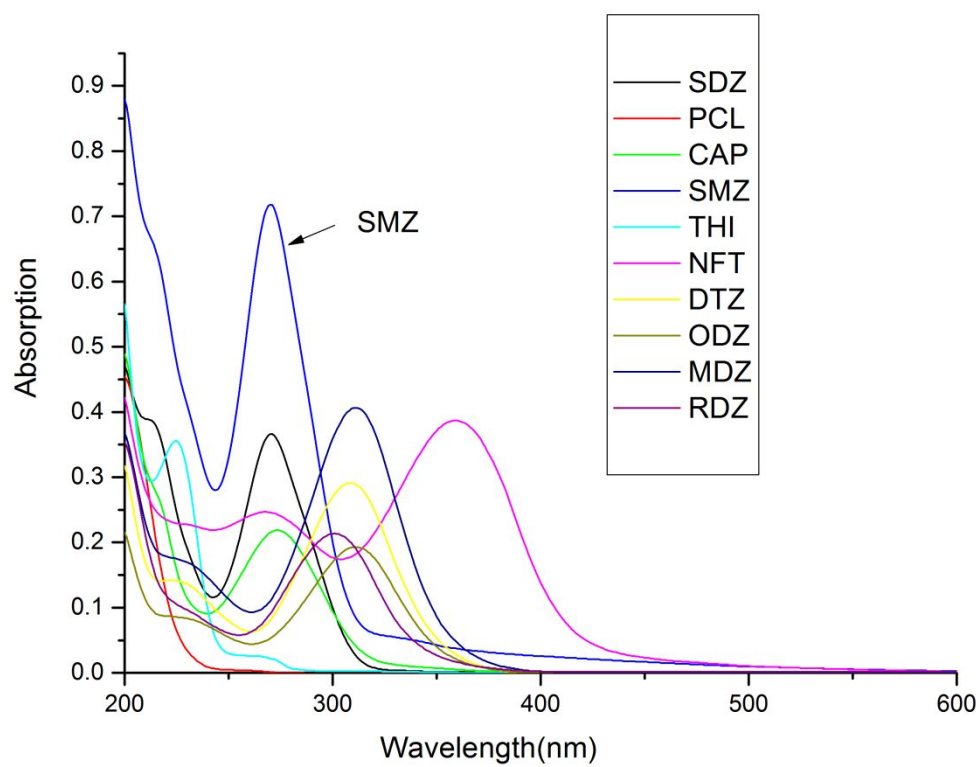


Figure S17. UV/Vis absorption spectra of different antibiotics. Concentrations: 20 µM.

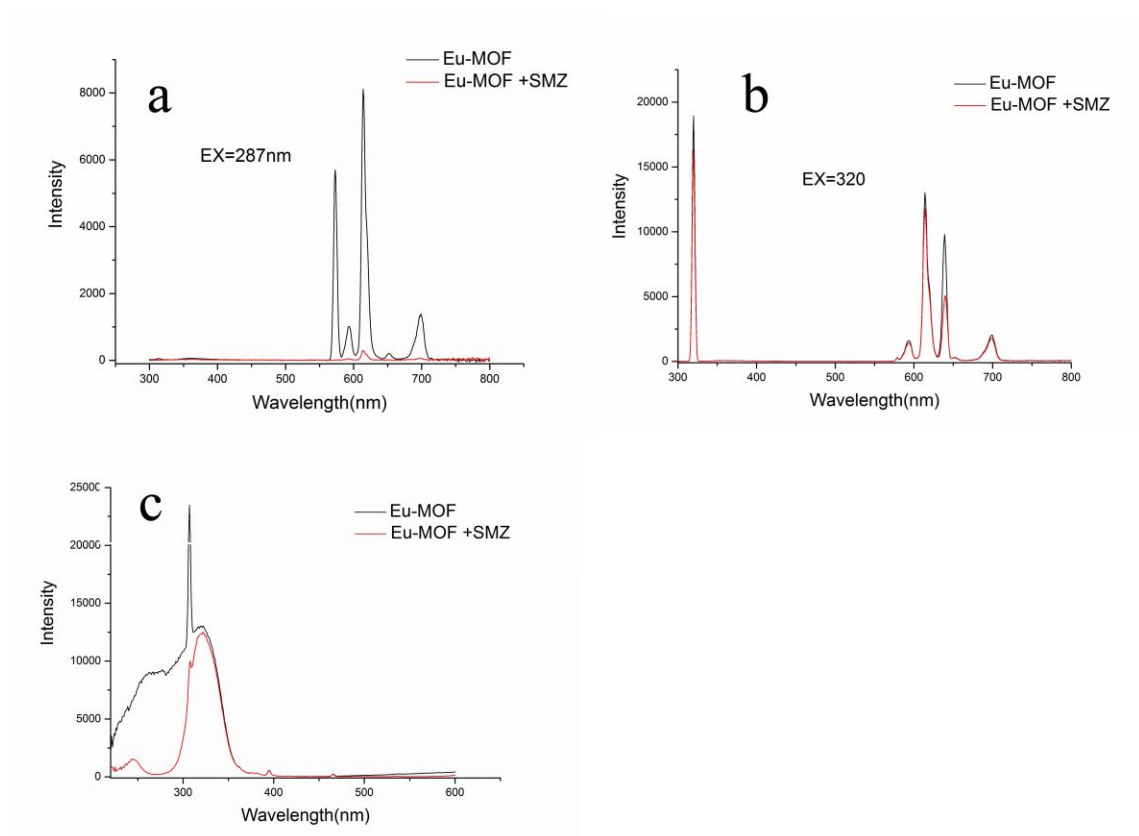


Figure S18. Fluorescence spectra of the Eu-MOF in ethanol-borate buffer (6:4, v/v) (50mM pH=7) solution upon addition of SMZ.