Supporting Information

A zinc-based metal-organic framework with triazine moiety: effective detection of antibiotics and photodeg-radation dyes in aqueous solutions

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Expermential Section

Physical measurements

Elemental analysis of C, H and N atoms was carried out on a Elemantar Vario EL analyzer. The infrared spectra (IR) were acquired by using a thermo scientific nicolet 6700 FT-IR spectrometer from 4000 to 500 cm^{-1} were registered on Avatar 360 E.S.P. using KBr pellets. The powder X-ray diffraction (PXRD) patterns of the samples were obtained using a Bruker D8 Advance powder diffractometer at 40 kV and 40 mA using Cu-Kα radiation (λ = 1.5418 Å), with a scan rate of 0.2 s per step and a step size of 0.02 (2θ). Simulation of PXRD spectra with single crystal data and diffraction crystal module of Mercury program. The thermal stability of the samples was performed on a NETZSCH STA 449 C system under a heating rate of 10 °C/min from 30 to 800 ℃ at N_2 atmosphere.

X-ray Crystallography

The single-crystal X-ray diffraction analysis of **1-Zn** was carried out on a Rigaku supernova CCD system. Confocal monochromatic Mo Kα radiation (λ = 0.71073 Å). Crystal structures were solution by SHELXS-2014 and least squares refinement by SHELXL-2014. The non-hydrogen atoms were refined with anisotropic thermal mobility coefficients. All hydrogen atoms are positioned at geometrically ideal locations and refined using the riding method. The crystallographic data for **1-Zn** are listed in Table S1. Some bond lengths and bond angles are given in Table S2.

Determination of reactive species

In order to identify the main active species, quenching experiments were performed by introducing different scavengers in the photocatalytic system, where benzoquinone (BQ, 0.2 mmol L^{-1}), isopropyl alcohol (IPA, 0.2 mmol L^{-1}) and ethylenediaminetetraacetic acid disodium salt (EDTA-2Na, 0.2 mmol L^{-1}) were used as quenchers for $\cdot O_2^-$, ·OH and h^+ species.[1,2] The electron spin resonance (ESR) spectra of ·OH and $\cdot O_2^-$ were registered on an electron paramagnetic resonance spectrometer (EMX-Plus, Bruker) using 5,5-dimethylpyrroline N-oxide (DMPO) as a sacrificial agent.

Photocatalytic activity

The photocatalytic properties of complex **1-Zn** were investigated by simulating visible light degradation of dyes under a 300 W xenon lamp with a 420 nm filter. Before light exposure, 50 mg of the photocatalyst powder was mixed in 50 ml of an aqueous solution containing Rh B and MB (10 ppm L^{-1}). At the same time, the suspension was stirred continuously for 60 min in the absence of visible light to arrive at an adsorption-desorption equilibrium. Furthermore, the photocatalytic decomposition efficiency was

analyzed through their characteristic absorption peaks at 554 nm for Rh B and 644 nm for MB. Then, all samples were exposed to visible light and taken out of the reaction solution (3 ml) every 5 min, separated the supernatant with a centrifuge at 5000 rpm, and collected for UV analysis last. Comparative experiments were carried out without **1-Zn** under the above conditions.

Table. S1 Crystallographic data and structure refinements for **1-Zn.**

Sample	**1-Zn**
Formula	$C_{48}H_{28}N_6O_{14}S_6Zn_3$
CCDC	2214180
Formula weight	1301.23
Space group	P2(1)/c
Crystal system	Monoclinic
a / Å	4.7442(2)
b / Å	31.8938(10)
c / Å	15.6270(6)
α / deg	90
β / deg	95.026(3)
γ / deg	90
V / $Å^3$	2355.44(15)
Z	2
D_{calc} (g cm^{-3})	1.835
μ / mm^{-1}	1.861
Reflections collected	9660
Independent reflections	5138
R(int)	0.0257
F (000)	1312
GOF on F^2	1.031
R_1[a] [I > 2σ(I)]	0.0647
wR_2[b] (all data)	0.1643
[a]$R_1 = \Sigma\|\|F_o\| - \|F_c\|\|/\Sigma\|F_o\|$. [b]$wR_2 = [\Sigma w (F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	

Table. S2. Selected bond lengths (Å) and angles (°) for **1-Zn**.

Zn1-O1	1.943(4)	Zn2-O3	1.853(5)
Zn1-O6#1	1.963(3)	Zn2-O2w	1.985(10)
Zn1-O5#2	1.967(3)	Zn2-O1w	2.095(14)
Zn1-O4#3	1.971(3)	Zn2-O2	2.198(5)
O1-Zn1-O6#1	103.19(16)	O1-Zn1-O5#2	110.07(16)
O6#1-Zn1-O5#2	105.13(13)	O1-Zn1-O4#3	140.34(16)
O6#1-Zn1-O4#3	97.88(14)	O5#2-Zn1-O4#3	96.02(14)
O3-Zn2-O2w	145.9(4)	O3-Zn2-O1w	87.3(4)
O2w-Zn2-O1w	85.5(5)	O3-Zn2-O2	101.1(2)
O2w-Zn2-O2	83.5(4)	O1w-Zn2-O2	168.9(4)

Table. S3. HOMO and LUMO energies calculated for selected analytes and 1-Eu used at B3LYP/6-31G*level.

Analytes	**HOMO (eV)**	**LUMO (eV)**	**Band Gap (eV)**	**Ref.**
ENR	-6.264	-1.837	4.427	3
CIP	-6.274	-1.841	4.433	3
NOR	-6.450	-2.020	4.430	3
MDZ	-7.307	-2.835	4.472	4
TCH	-6.200	-3.860	2.340	4
1-Zn	-6.775	-2.609	4.166	This work

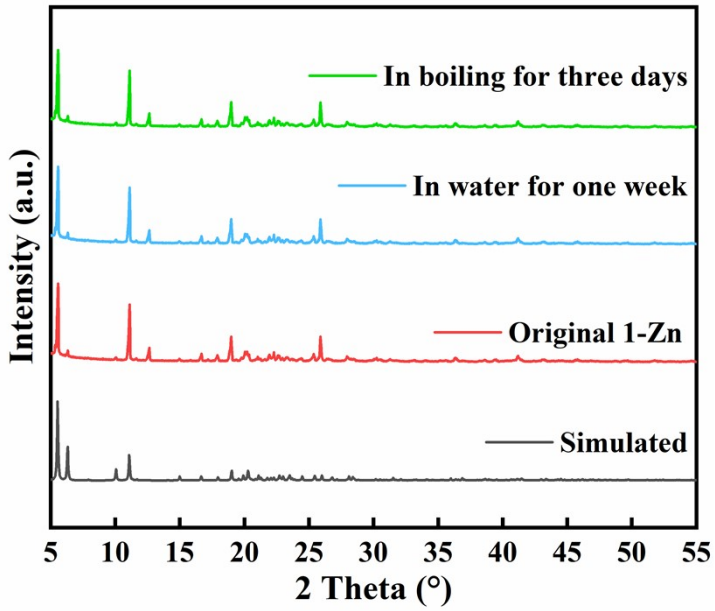

Fig. S1 The PXRD patterns of **1-Zn**.

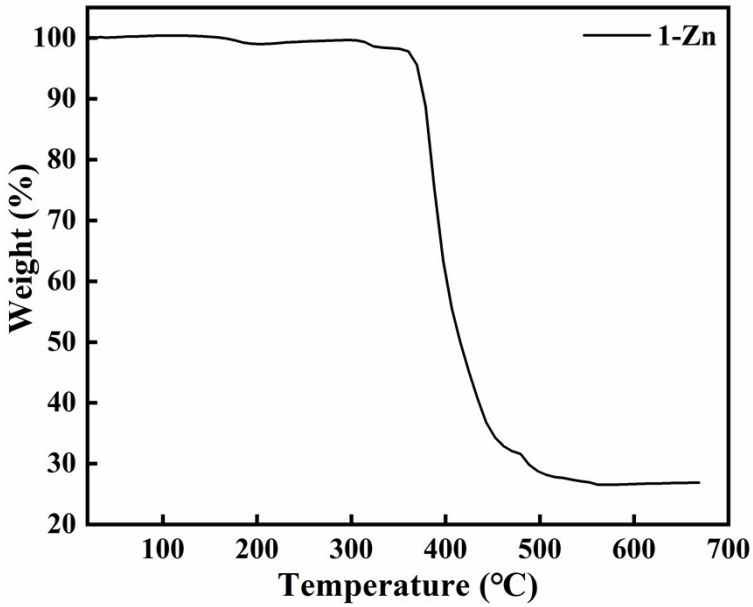

Fig. S2 Thermogravimetric analysis of **1-Zn**.

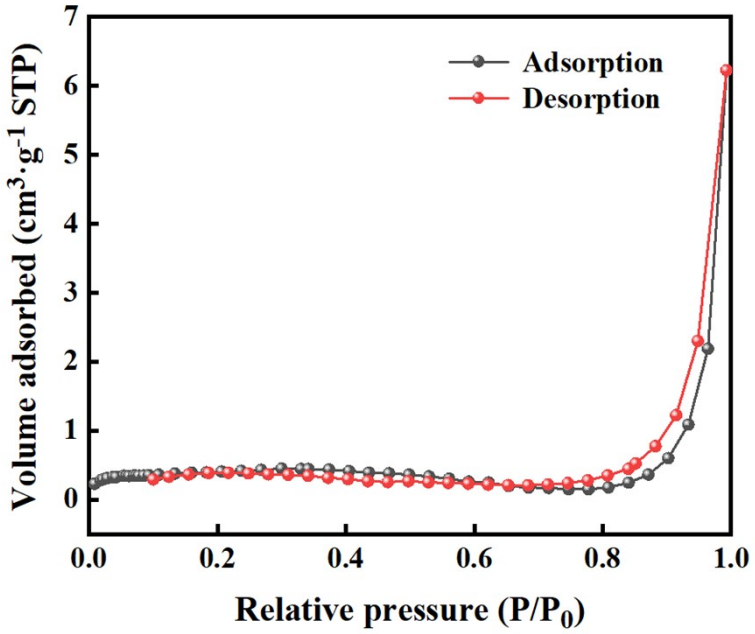

Fig. S3 N_2 adsorption isotherm of **1-Zn** at 77 K.

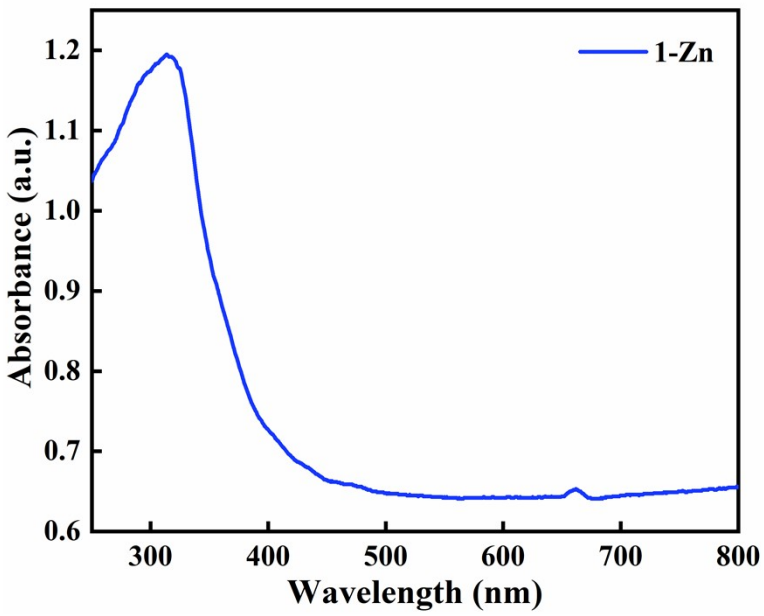

Fig. S4 UV-Vis adsorption spectrum of **1-Zn**.

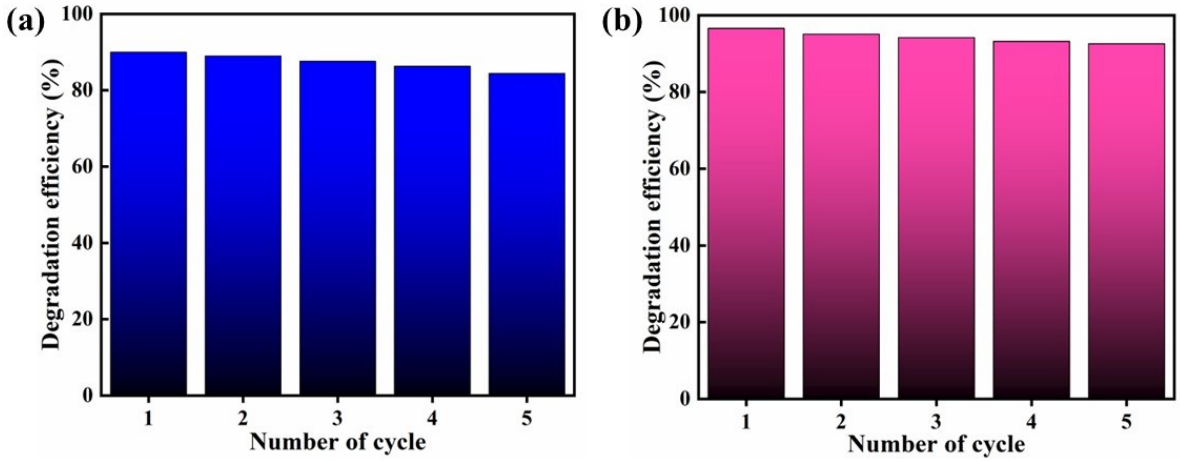

Fig. S5 The recycling performance of **1-Zn** for **(a)** Rh B and **(b)** MB.

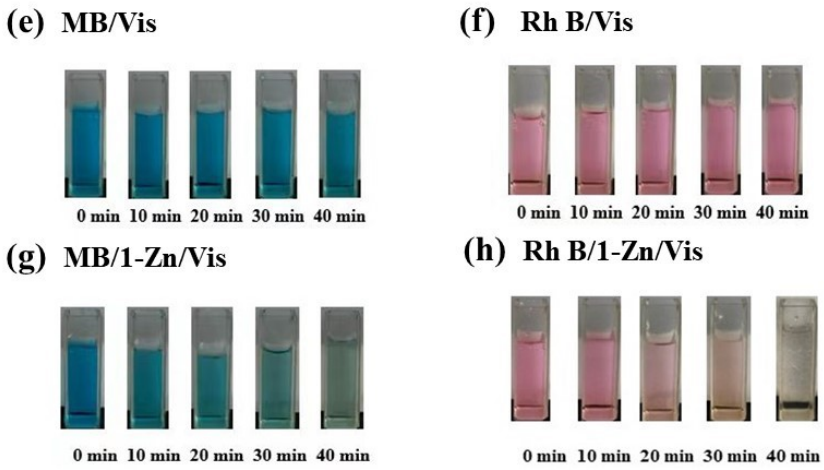

Fig. S6 Comparison of photocatalytic activity under different experimental environments.

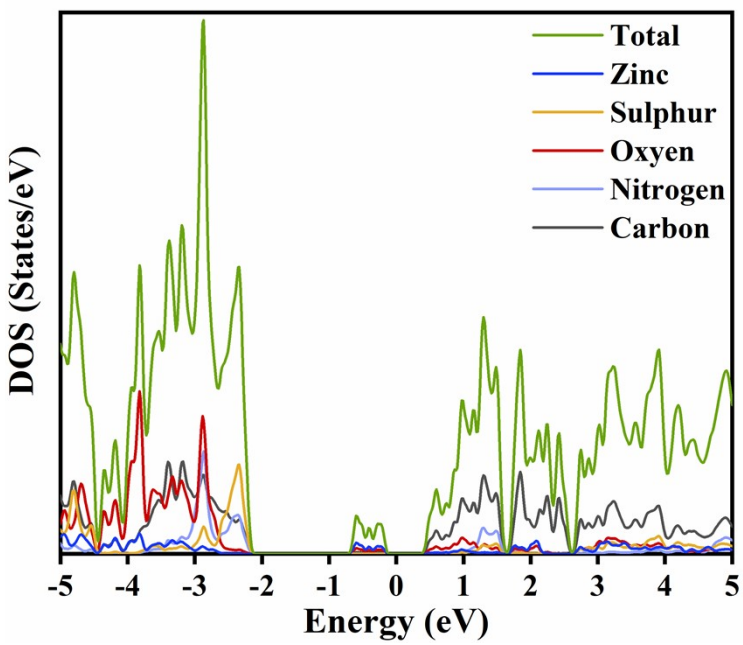

Fig. S7 The DOS and partial DOS plots for **1-Zn**.

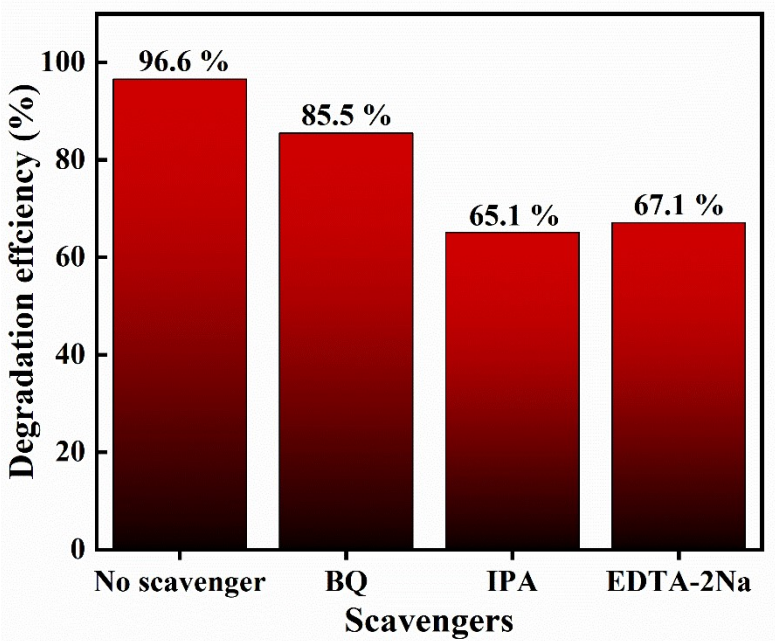

Fig. S8 Photocatalytic degradation of Rh B with the addition of different scavengers.

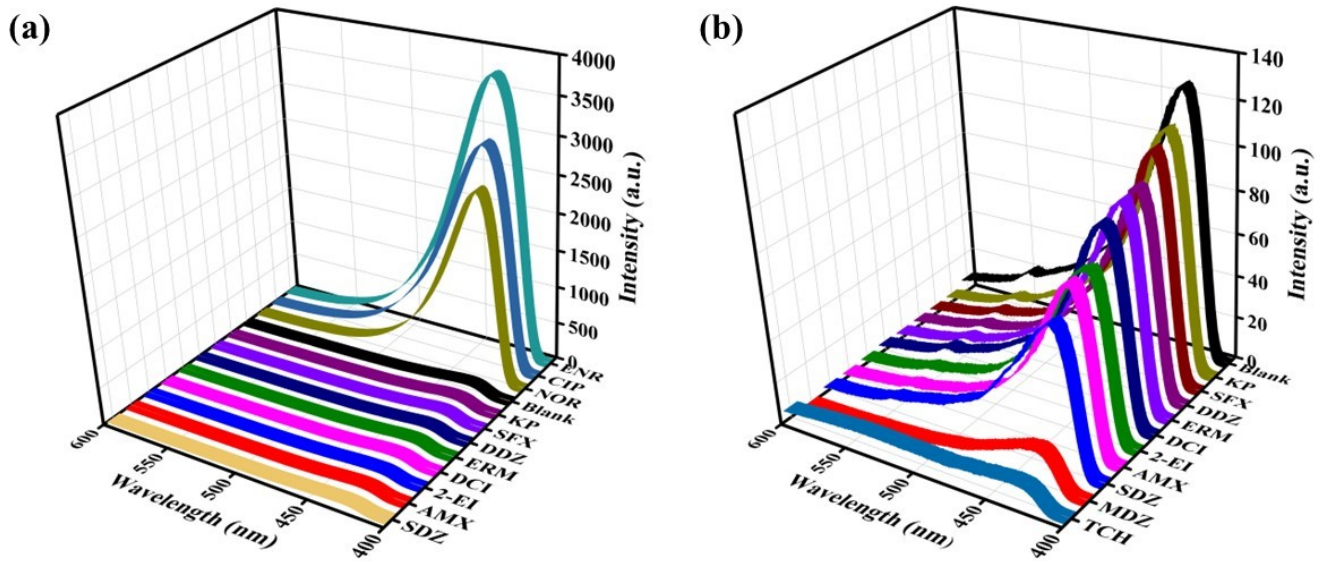

Fig. S9 Complex **1-Zn** detection of (a) fluorescence-enhanced and (b) fluorescence-diminished luminescence spectra.

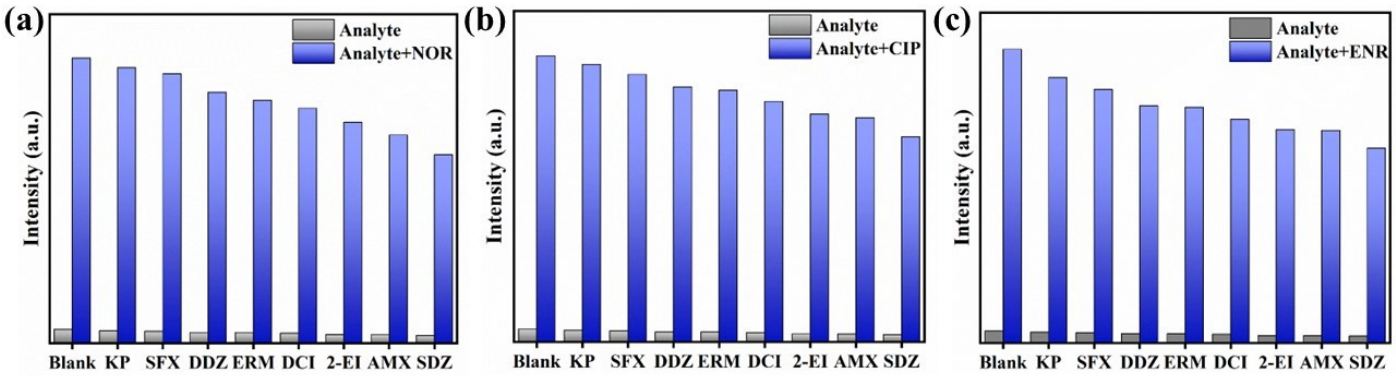

Fig. S10 the luminescent intensity of **1-Zn** dispersed in (a) NOR, (c) CIP, and (d) ENR with other competing antibiotics (10^{-4} mol L^{-1}).

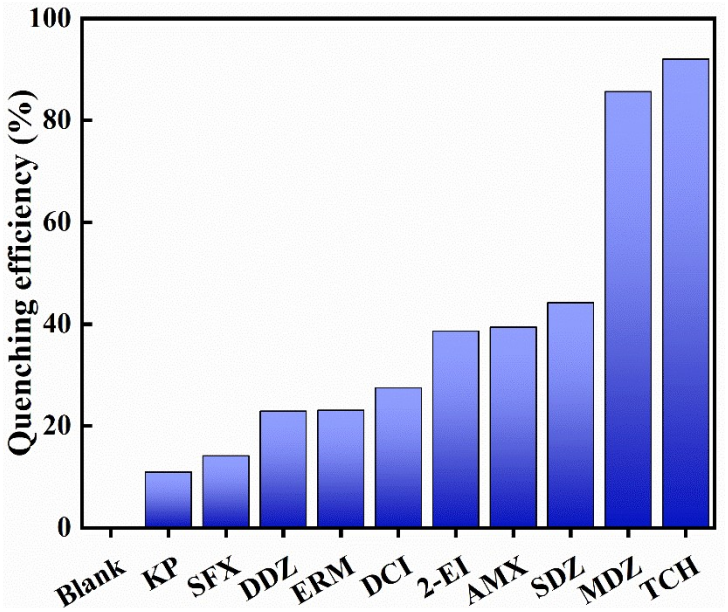

Fig. S11 Quenching efficiency of **1-Zn** in 10^{-4} mol L^{-1} of different antibiotics.

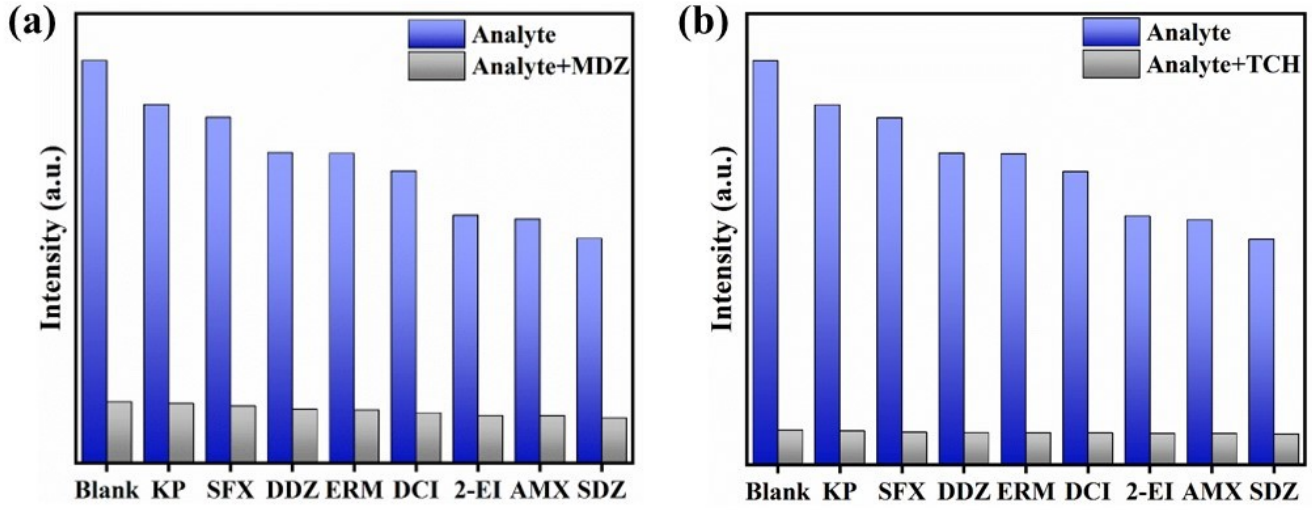

Fig. S12 the luminescent intensity of **1-Zn** dispersed in (a) MDZ and (b) TCH with other competing antibiotics (10^{-4} mol L^{-1}).

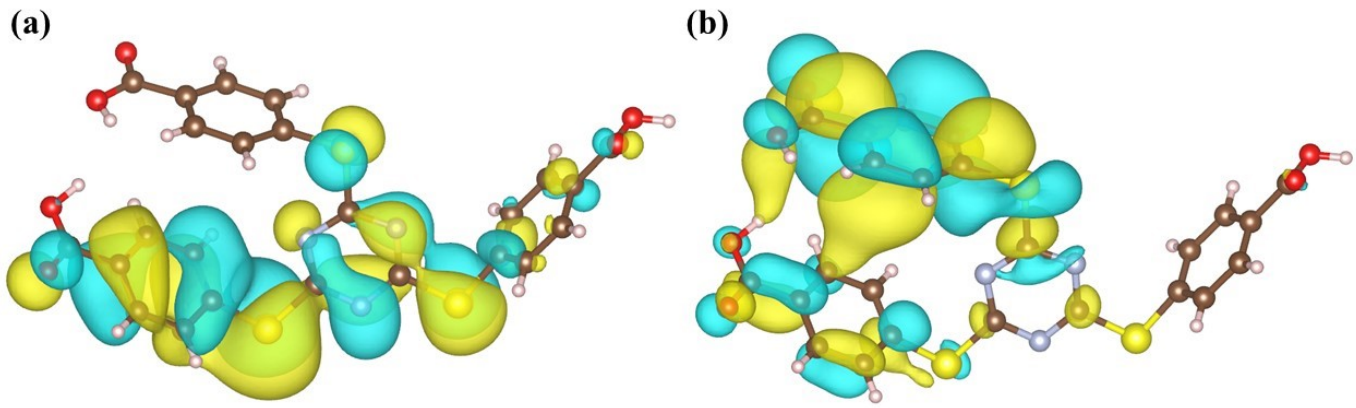

Fig. S13 The (a) LUMO and (b) HOMO level of **1-Zn**.

References

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