A new pyromellitic acid and 3,5-bis(benzoimidazo-1-ly)pyridine based Zn(II)-MOF as prospective turn-off-on sensor for tetracycline

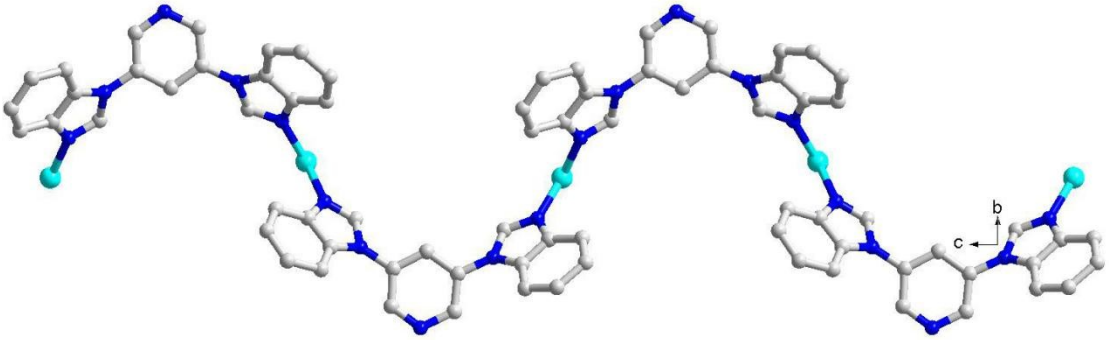

Fig. S1 view of the 1D chain built by N-donors and metal centers

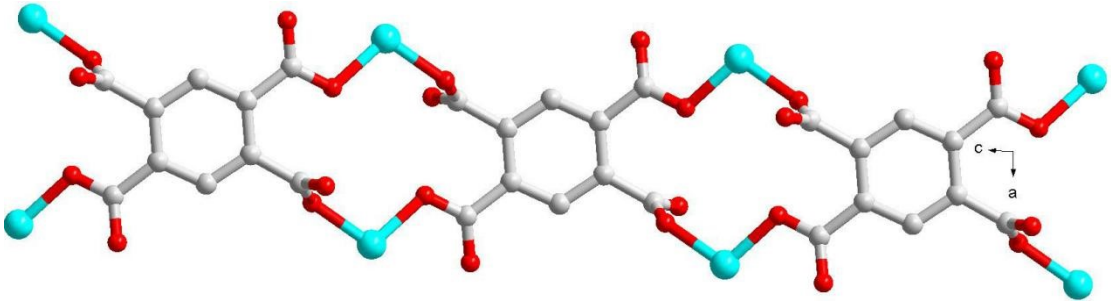

Fig. S2 view of the 1D chain built by carboxylate ligands and metal centers

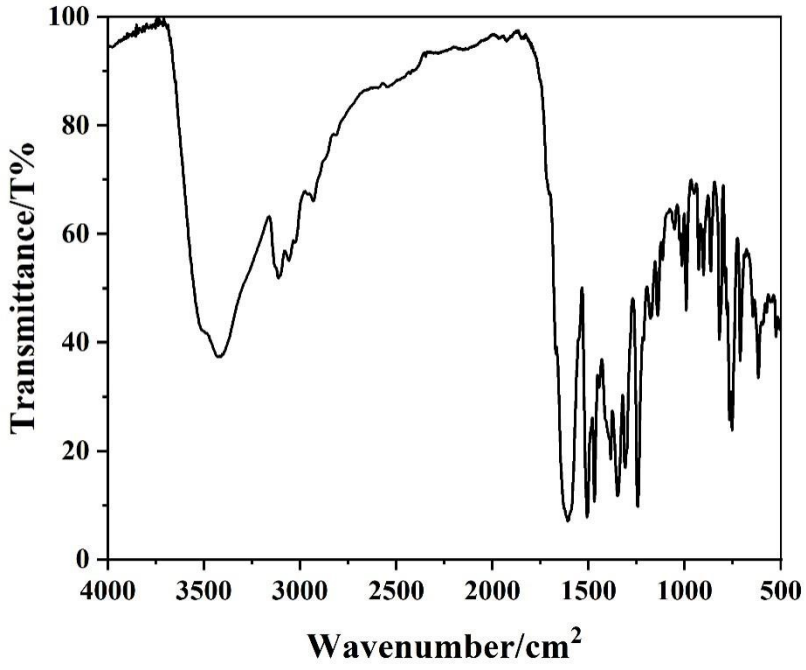

Fig. S3 View of the IR

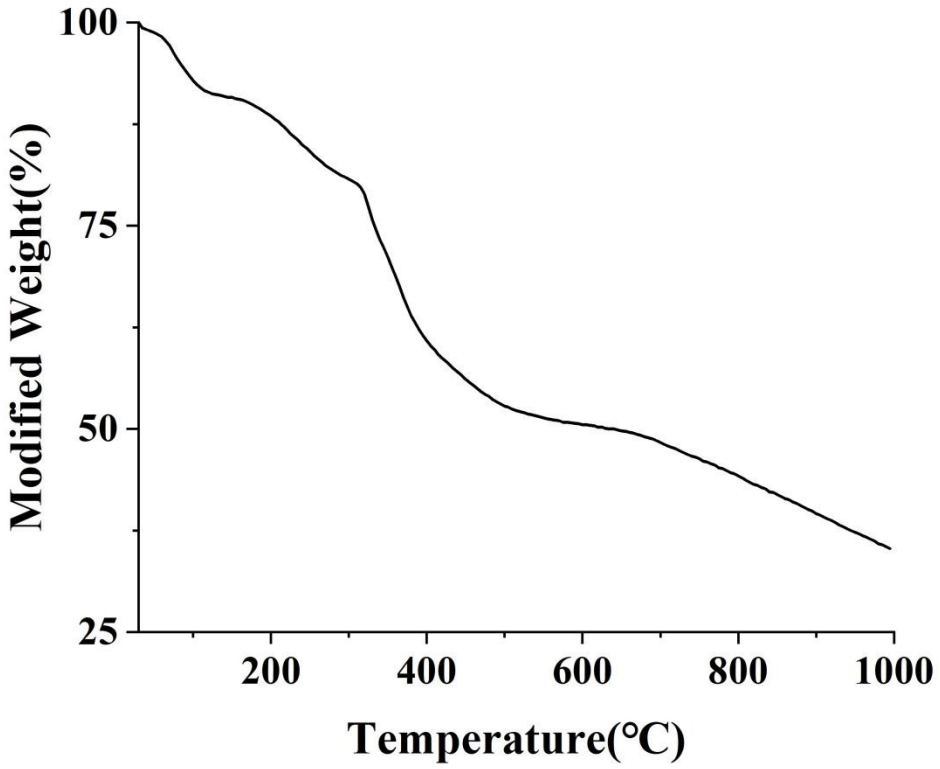

Fig. S4 view of the TGA

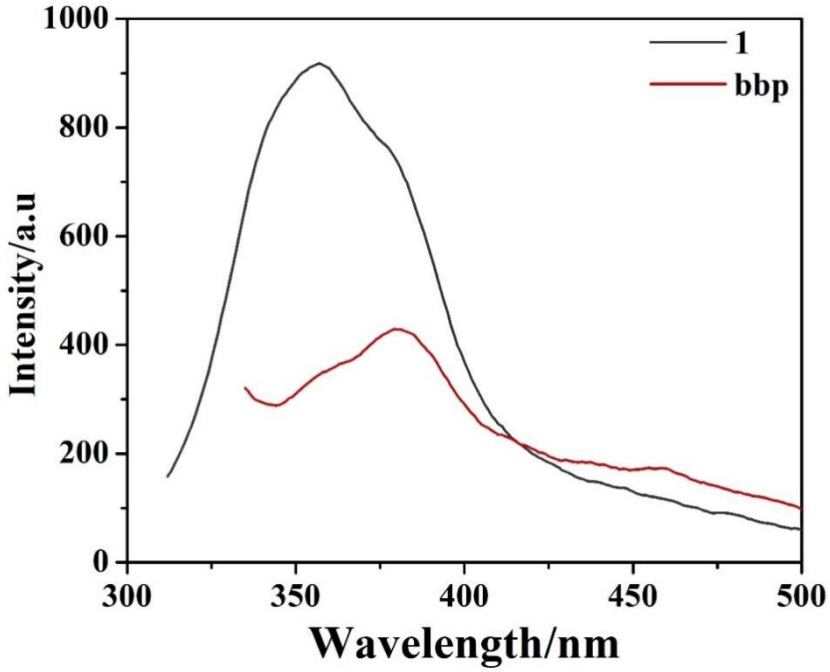

Fig. S5 Emission spectra for 1 and bbp ligand.

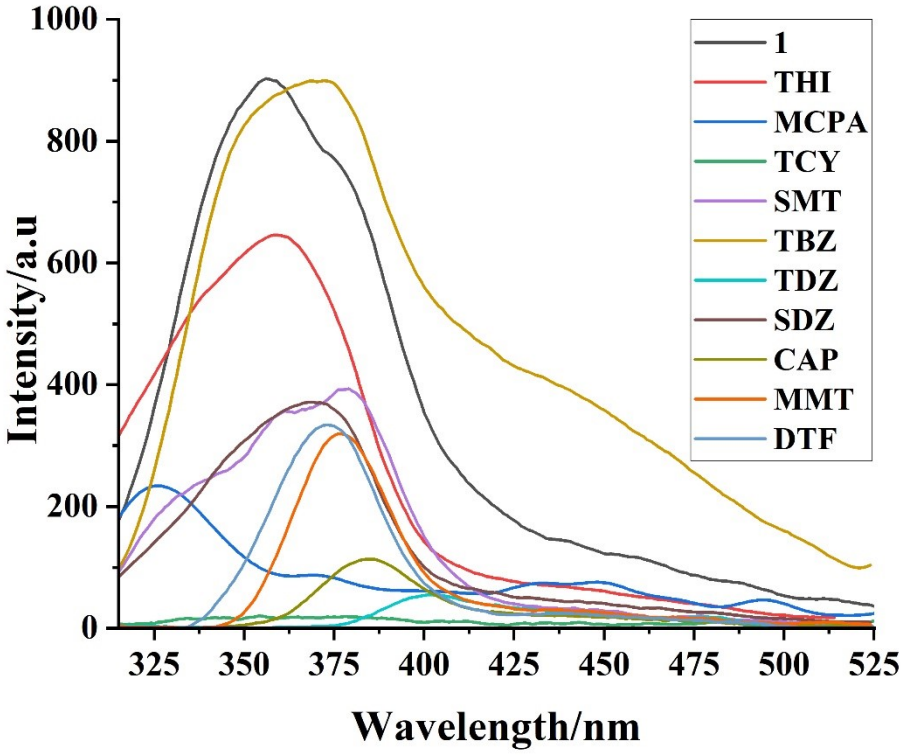

Fig. S6 Emission spectra of 1 in pure form as well as in the presence of different antibiotics.

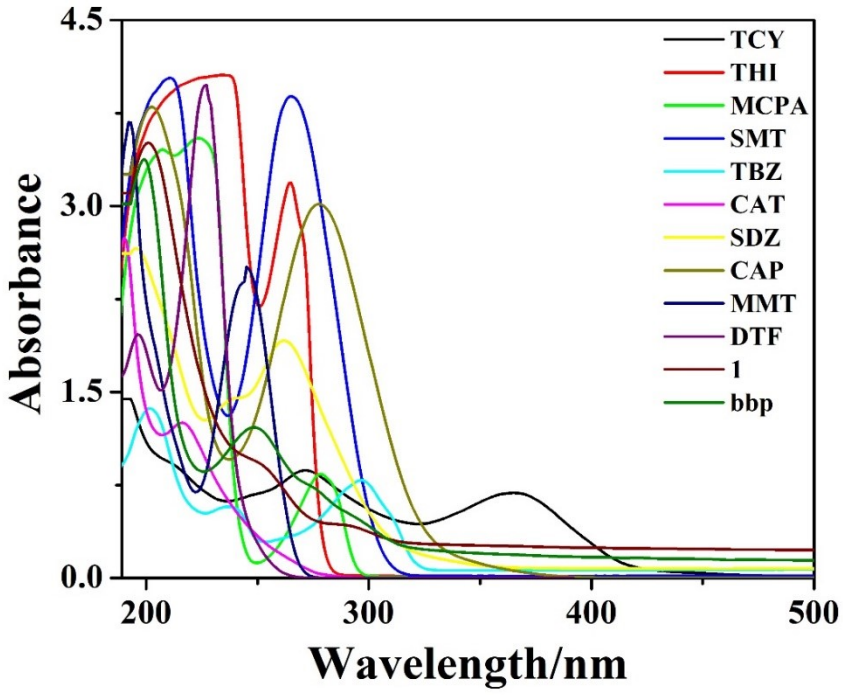

Fig. S7 UV-Vis. spectra of 1, bbp and different antibiotics.

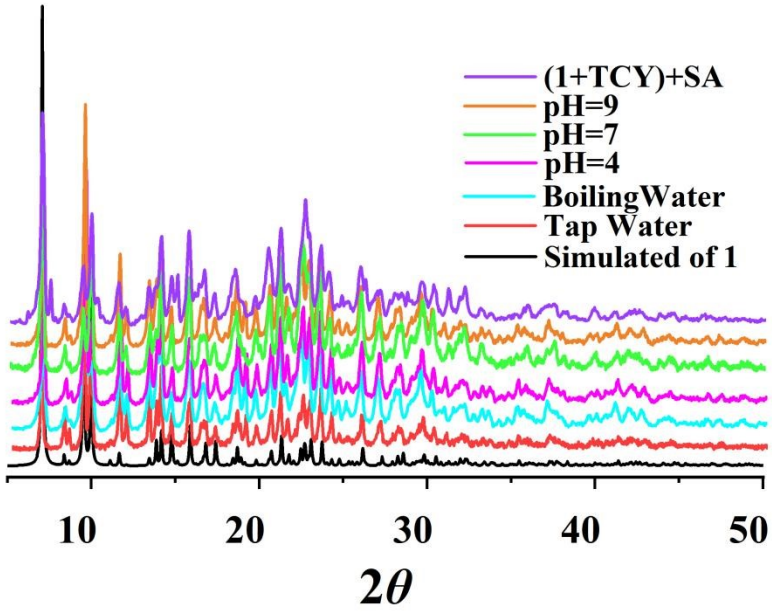

Fig. S8 Simulated and Experimental (under different conditions) PXRD plots for 1.

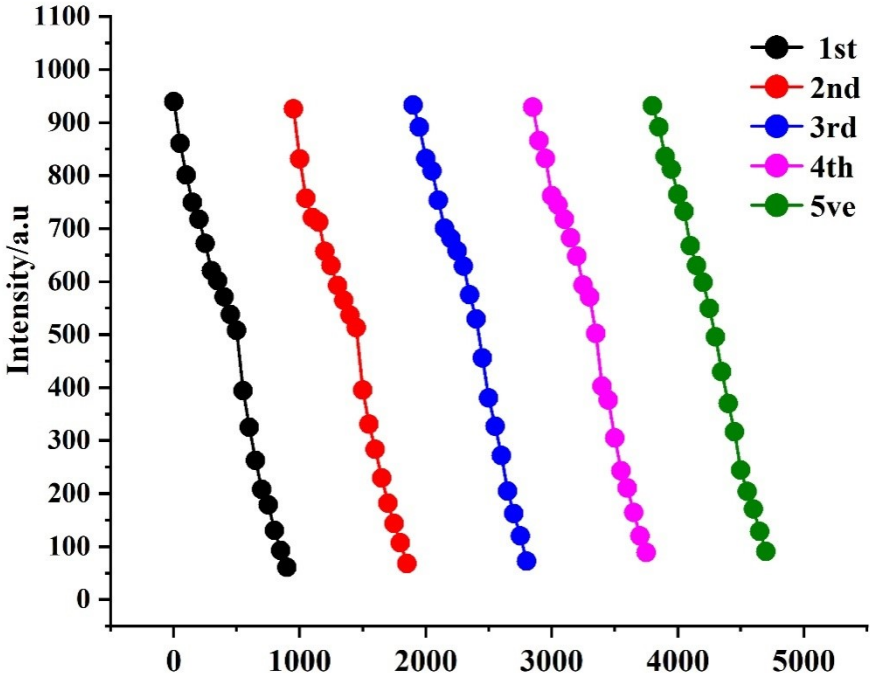

Fig. S9 Results of the recycle experiments.

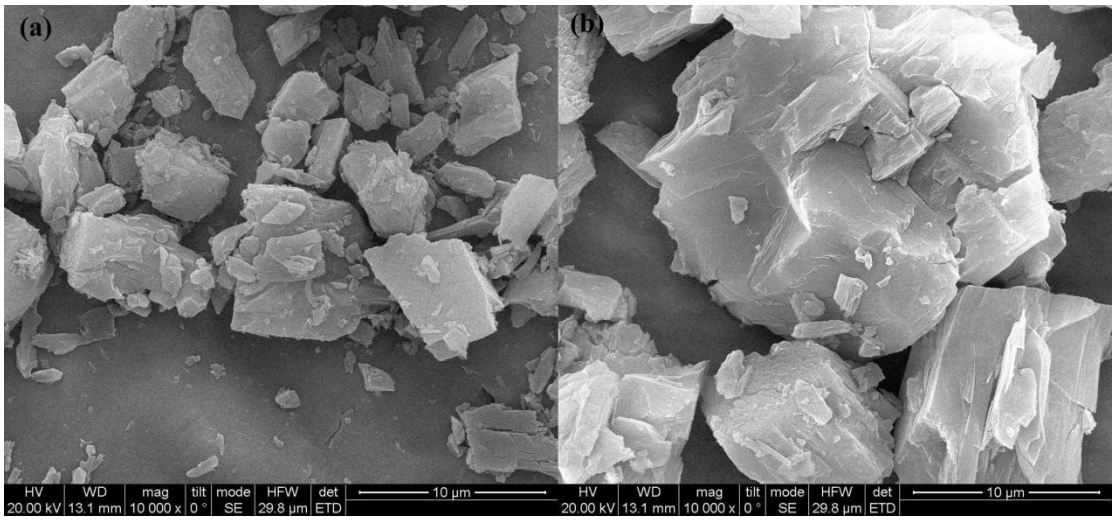

Fig. S10 SEM for the samples : (a) before sensing; and (b) after sensing TCY.

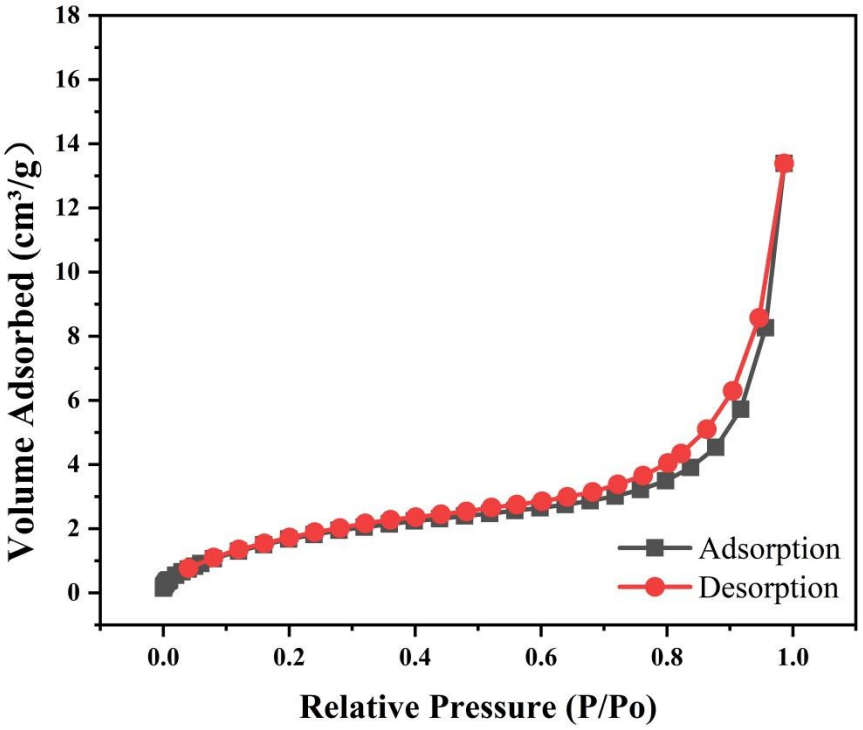

Fig. S11 Nitrogen adsorption-desorption isotherms of the as-synthesized **1**.

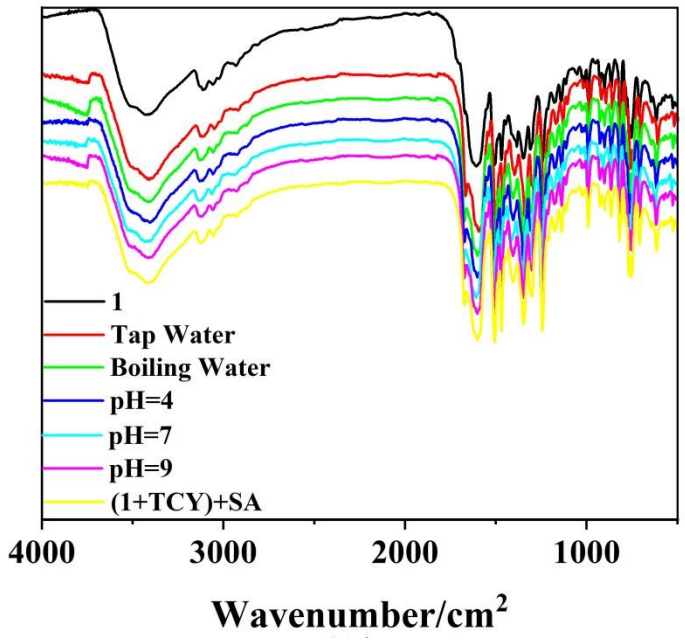

Fig. S12 The IR plots for samples of **1** under different conditions.

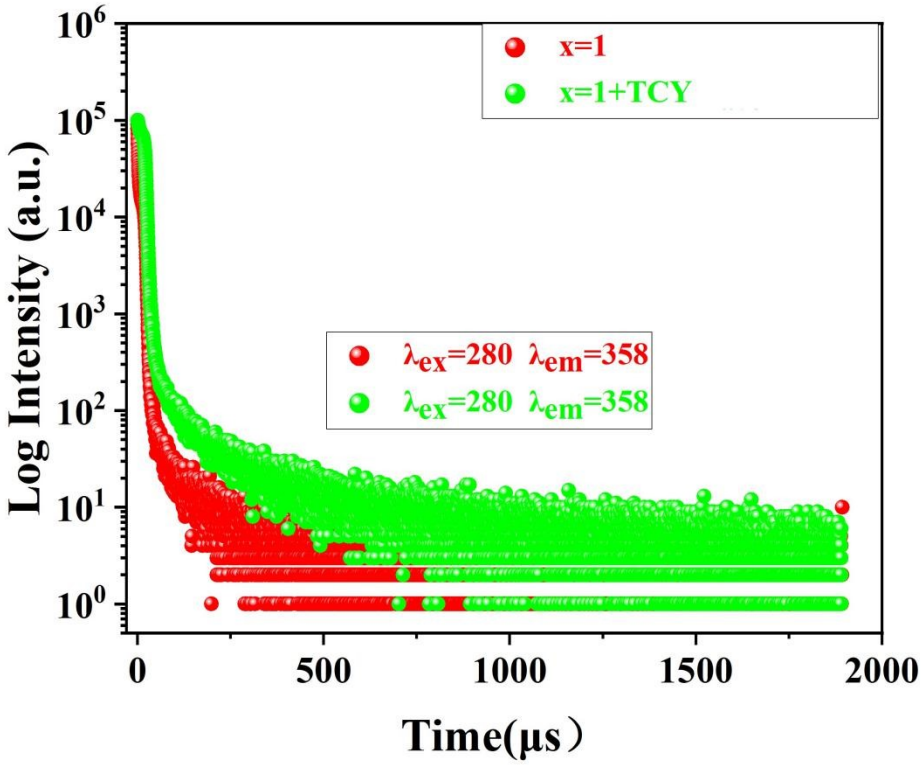

Fig. S13 fluorescence lifetime for **1** and **1**+TCY

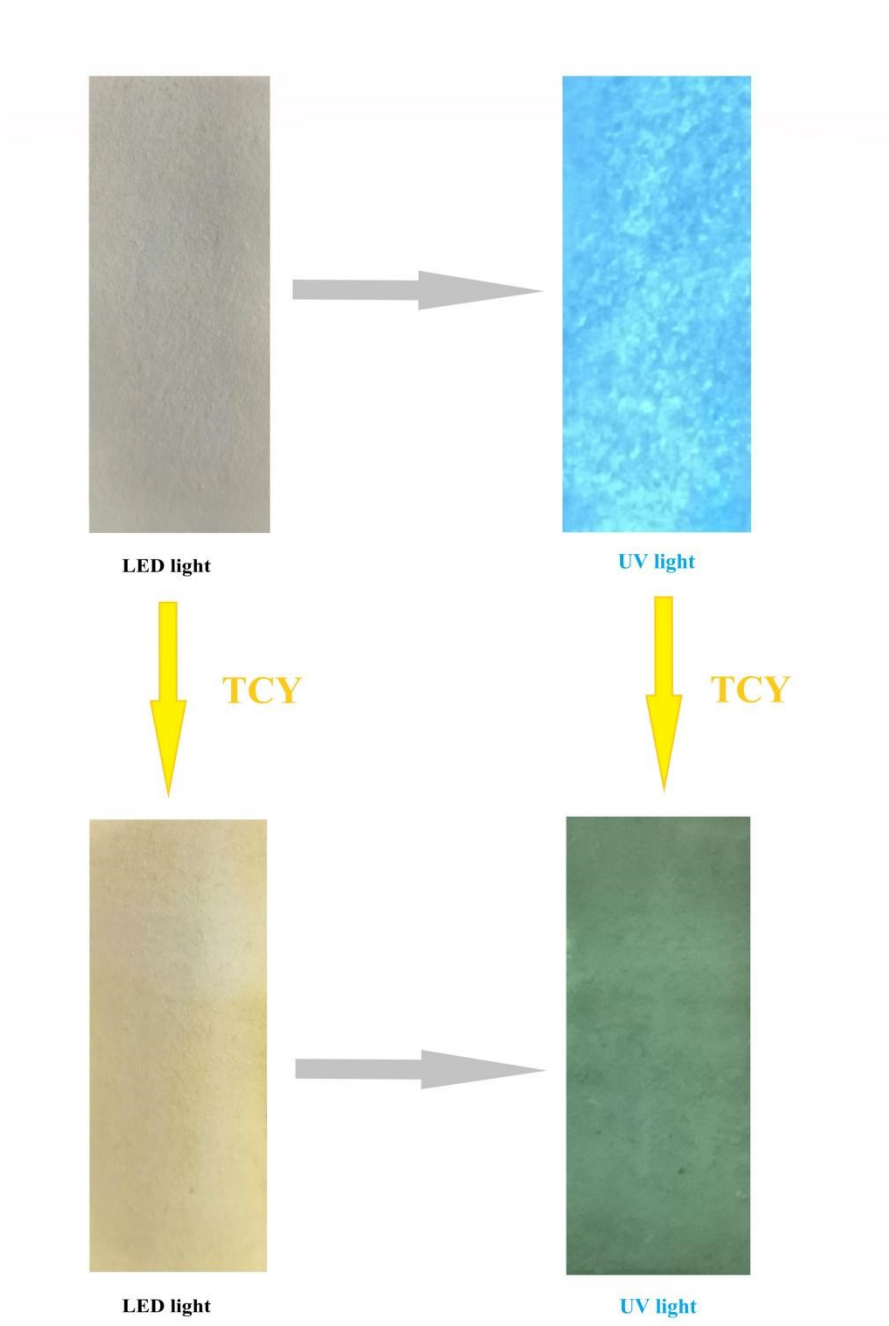

Fig. S14 (left) Optical image of the CP 1 test paper after immersion in TCY solutions under natural light; (right) optical image of the **1** test paper after immersion in TCY solutions under 365 nm ultraviolet light.

Table S1. Crystallographic data and structure refinement details for 1

Parameter	1
Formula	$C_{48}H_{28}N_{10}O_8Zn_2$, $2(H_2O)$
Formula weight	1039.57
Crystal system	Monoclinic
Space group	C2/c
a, Å	17.731(6)
b, Å	17.610(6)
c, Å	18.563(6)
α, °	90
β, °	93.025(6)
γ, °	90
V, Å ^{3}	5788(3)
Z	4
ρ_{calcd}, g/cm^3	1.193
μ, mm^{-1}	0.885
F(000)	2120
θ Range, deg	1.6-28.3
Reflection Collected	16928
Independent reflections (R_{int})	0.056
Reflections with $I > 2\sigma(I)$	4190
Number of parameters	316
R_1, wR_2 ($I > 2\sigma(I)$)*	0.0489，0.1321
R_1, wR_2 (all data)**	0.0907，0.1509

Table S2. Selected bond distances (Å) and angles (deg) for **1-2**

1			
Zn(01)-O(1)	1.937(2)	Zn(01)-N(1)	2.002(3)
Zn(01)-N(5)#1	1.998(3)	Zn(01)-O(4)#2	1.994(2)
1			
O(1)-Zn(01)-N(1)	120.99(11)	O(1)-Zn(01)-N(5)#1	107.99(11)

O(1)-Zn(01)-O(4)#2	104.48(10)	N(1)-Zn(01)-N(5)#1	111.16(12)
O(4)#2-Zn(01)-N(1)	94.51(11)	O(4)#2-Zn(01)-N(5)#1	117.58(11)

Symmetry Codes: #1= x,1-y,-1/2+z; #2= x,1-y,1/2+z

Table S3. Selected hydrogen bond distances (Å) and angles (deg) for **1**

Contact	Distance, Å			Angle
D–H···A	D–H	H···A	D···A	D–H···A, deg
1				
O(5)-H(5A)···O(3)	0.8600	2.0600	2.855(4)	153.00
O(5)-H(5B)···O(1)	0.8400	2.2700	3.110(4)	175.00
C(3)-H(3)···O(2)	0.9300	2.4800	2.794(4)	100.00
C(6)-H(6)···O(4)	0.9300	2.4800	2.973(4)	114.00
C(8)-H(8)···O(2)	0.9300	2.5500	3.262(5)	134.00
C(14)-H(14)···O(2)	0.9300	2.4800	3.239(5)	139.00
C(20)-H(20)···O(3)	0.9300	2.4700	3.341(6)	156.00