Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

A ultrastable cucurbit[6]uril-based multifunctional supramolecular assembly for efficient detection of nitroaromatic compounds and antibiotics

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

Compound	
Empirical formula	$C_{144}H_{136}N_{76}O_{56}S_4Zn_2$
Formula weight	4086.26
Crystal system	Monoclinic
Space group	C2/m
a (Å)	31.654(5)
b (Å)	20.851(3)
c (Å)	15.488(2)
α (°)	90
β (°)	94.774(5)
γ (°)	90
V (Å^3)	10186(3)
Z	2
D_c/(g cm^{-3})	1.332
μ /(mm^{-1})	1.486
F(000)	4208.0
θ range (°)	5.08 - 101.482
R_{int}	0.0752
Parameters	655
T (K)	170
goodness of fit	1.127
Limiting indices	-31 ⩽ h ⩽ 29
	-20 ⩽ k ⩽ 20
	-15 ⩽ l ⩽ 15
R indices [I > 2σ(I)]	R1=0.1130,wR2=0.3023
R indices (all data)	R1=0.1248,wR2=0.3129

Table S2 Performance of reported MOFs for detecting TNP

MOFs	Solvent	K_{sv} (M^{-1})	detection limit	References
$\{[Zn_8(L)_6(\mu_3\text{-}OH)_4(H_2O)_6]\cdot(DMF)\cdot(H_2O)_{2.5}\}_n$	DMSO	2.5×10^4	—	[30]
$\{[Zn_3(mtrb)_3(btc)_2]\cdot 3H_2O\}_n$	MeOH	3.26×10^4	0.26 μM	[31]
$\{[Cd_3(SDB)_3(TIB)](H_2O)_2(1,4\text{-dioxane})(G)x\}_n$	H_2O	2.43×10^4	0.15 μM	[32]
$\{[Zn_2(L)(DMF)_3]\cdot 2DMF\cdot 2H_2O\}$	DMF	2.61×10^4	0.64 ppm	[33]
$\{[Cd_4(L)_2(L_2)_3(H_2O)_2](8DMF)(8H_2O)\}_n$	EtOH	3.89×10^4	1.98 ppm	[34]
1	H_2O	2.86×10^4	71 ppb	This work

Table S3 Performance of reported MOFs for detecting OTC and TC

MOFs	Solvent	K_{sv}	LOD	Species	Ref.
$[Zn_3(L)_2(1,4\text{-bimb})_3]_n$	H_2O	$1.99 \times 10^5\ M^{-1}$	0.15 μM	TC	[35]
$[Zn(bpydb)(bimmb)_{0.5}]_n$(1)	H_2O	$1.28 \times 10^5\ M^{-1}$	104 ppb	TC	[36]
$\{[Zn_2(bpydb)_2(bimb)]\cdot[Zn(bpydb)(bimb)]\cdot H_2O\}_n$(2)		$7.96 \times 10^4\ M^{-1}$	168 ppb		
ROD-Zn1	H_2O	$2.75 \times 10^4\ M^{-1}$	0.11 μM	TC	[37]
ROD-Zn2		$2.67 \times 10^4\ M^{-1}$	0.12 μM		
$[Tb(HL)L(H_2O)]_n$	H_2O	$2.18 \times 10^4\ M^{-1}$	1.95 nM	OTC	[38]
		$1.39 \times 10^4\ M^{-1}$	2.77 nM	TC	
1	H_2O	$3.59 \times 10^4\ M^{-1}$	153 ppb	OTC	This work
		$5.99 \times 10^4\ M^{-1}$	148 ppb	TC	

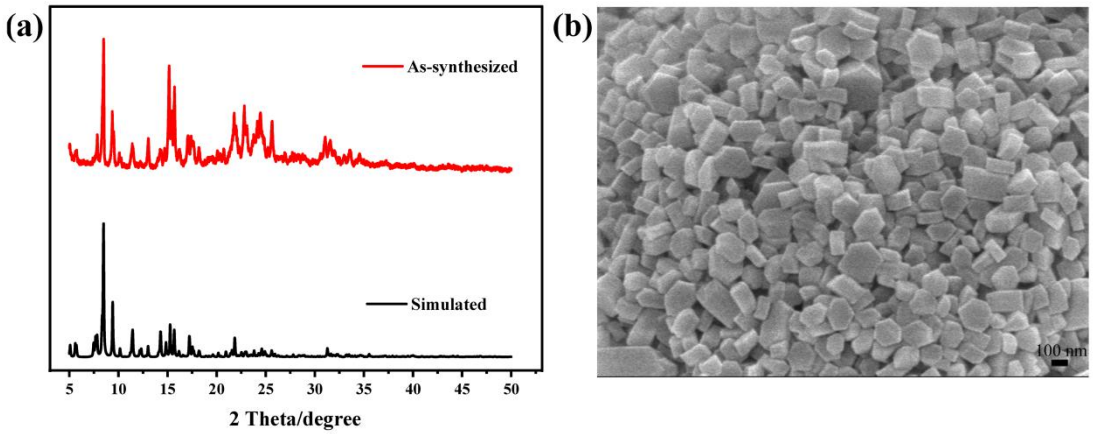


Fig. S1 (a) The PXRD pattern spectra of 1 and the simulated spectra. (b) The SEM image of the ground sample for the sensing experiment.

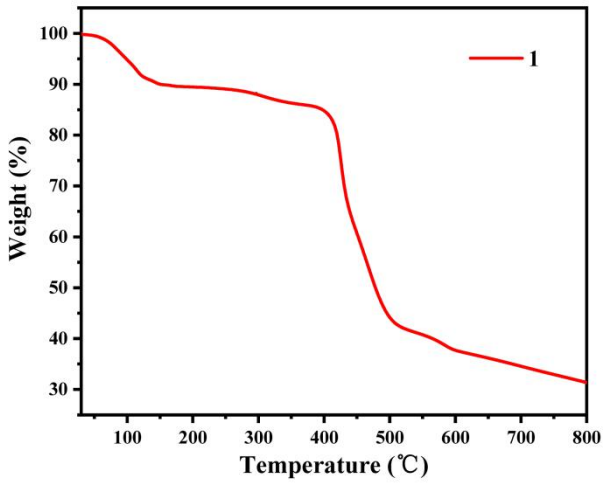


Fig. S2 TGA curves of **1** under anatmosphere of N_2 (5 ℃min^{-1})

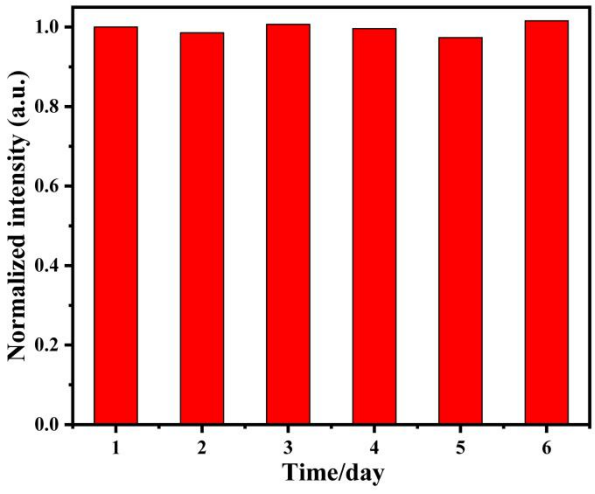


Fig. S3 Luminescence spectra of **1** dispersed in water with different times.

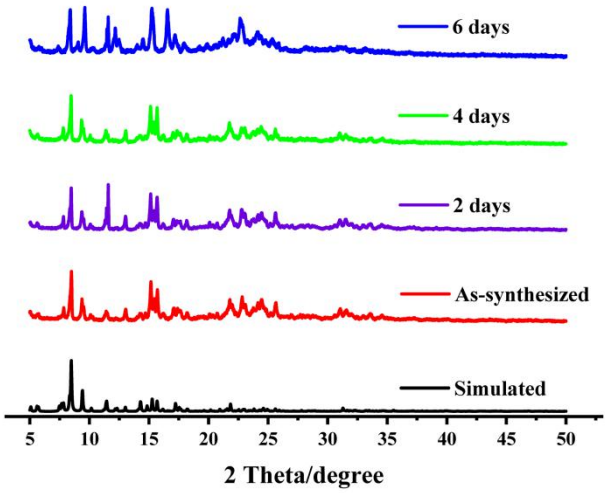


Fig. S4 PXRD patterns of 1 after soaked in water with different times.

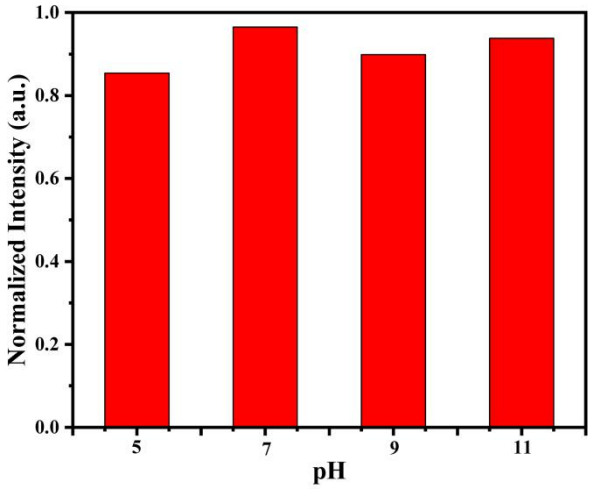


Fig. S5 Luminescence spectra of **1** dispersed in aqueous solution with different pH value.

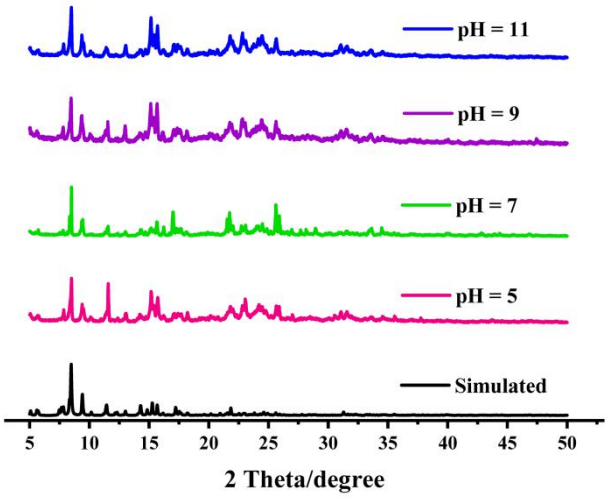


Fig. S6 PXRD patterns of 1 after soaked in aqueous solution with different pH value.

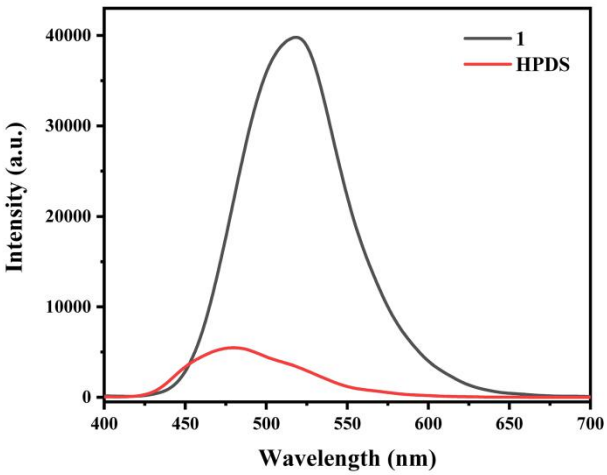


Fig. S7 The luminescent spectrum of **1** and HQDS in solid states.

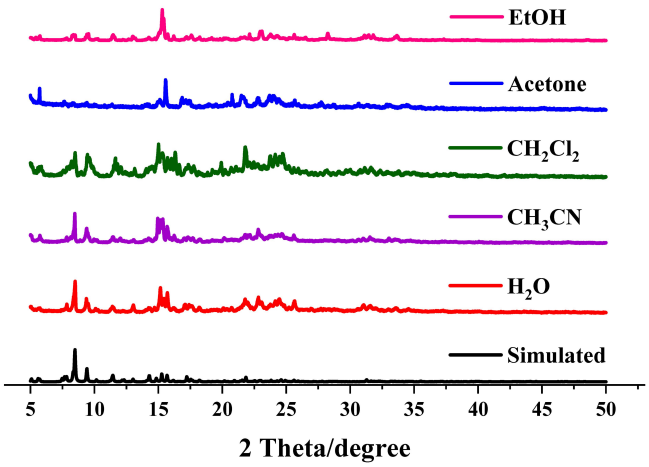


Fig. S8 PXRD patterns of **1** after soaked in common solvents.

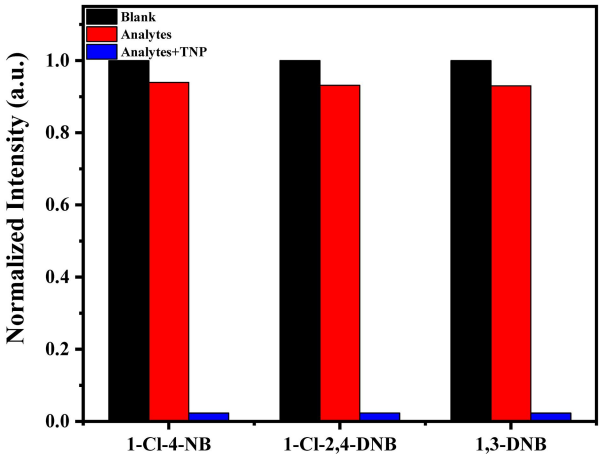
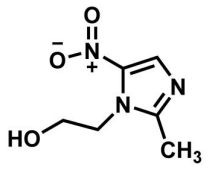
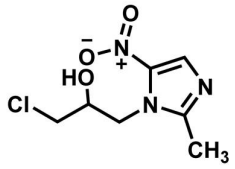


Fig. S9 Relative intensities of **1** to various NACs. The black bars represent the

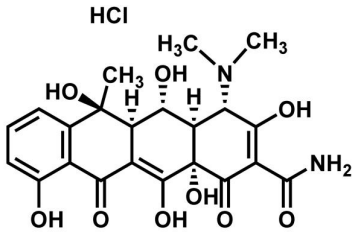
emission intensities of **1** in water, the red bars represent the emission intensities of **1** in the individual aqueous solutions of NACs (1 mM), and the blue bars represent a change of the emission intensities upon subsequent addition of TNP (1 mM) to the above NACs solutions.



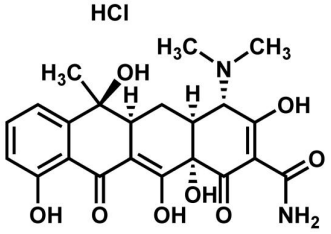
MDZ



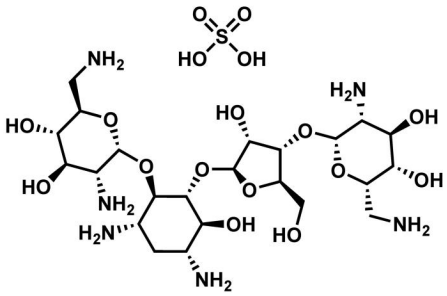
ODZ



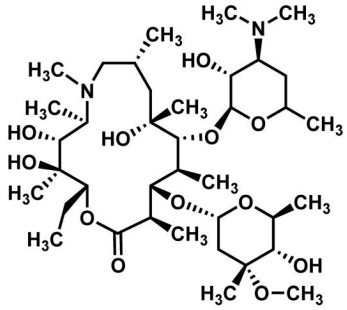
OTC



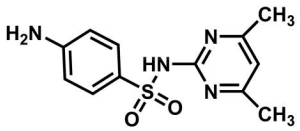
TC



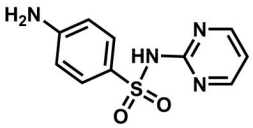
NEO



AZM



SDZ



SMZ

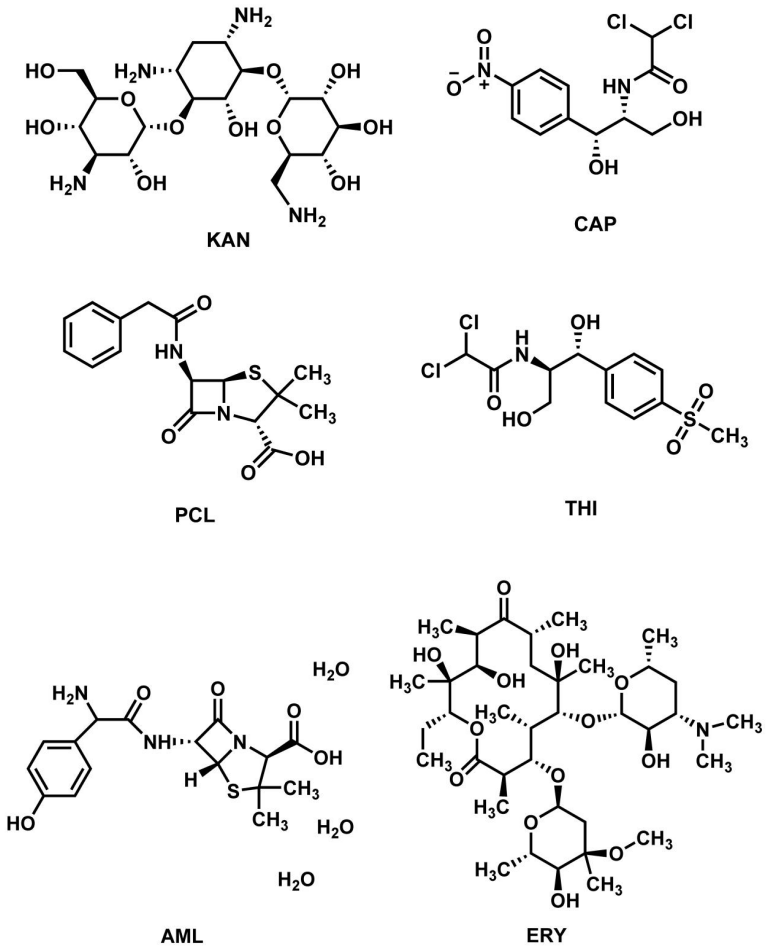


Fig. S10 Selected molecular structures of antibiotic substances.

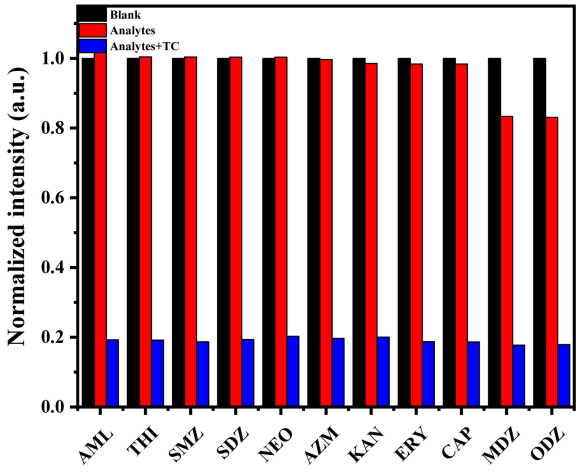


Fig. S11 Relative intensities of **1** to various antibiotics. The black bars represent the emission intensities of **1** in water, the red bars represent the emission intensities of 1 in the individual aqueous solutions of antibiotics (1 mM), and the blue bars represent

a change of the emission intensities upon subsequent addition of TC (1 mM) to the above antibiotics solutions.

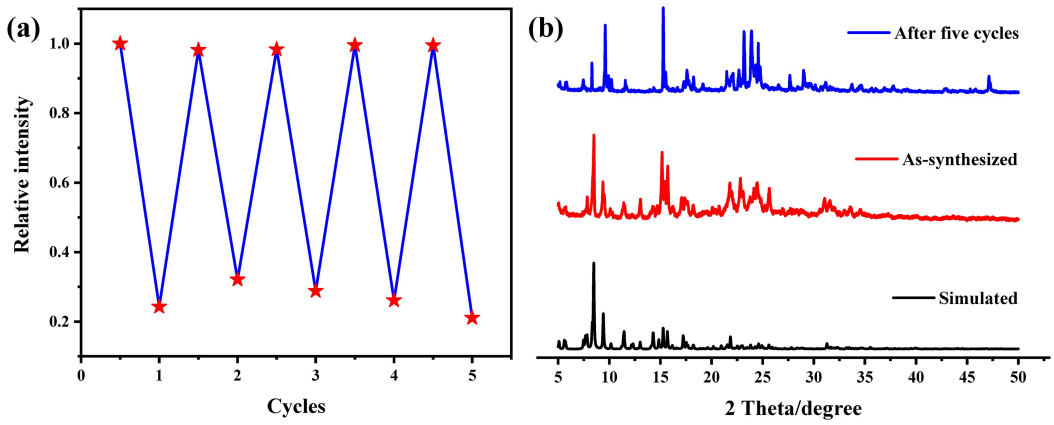


Fig. S12. (a) The recyclability tests of **1** in water. (b) The PXRD patterns of **1** after five cycles.

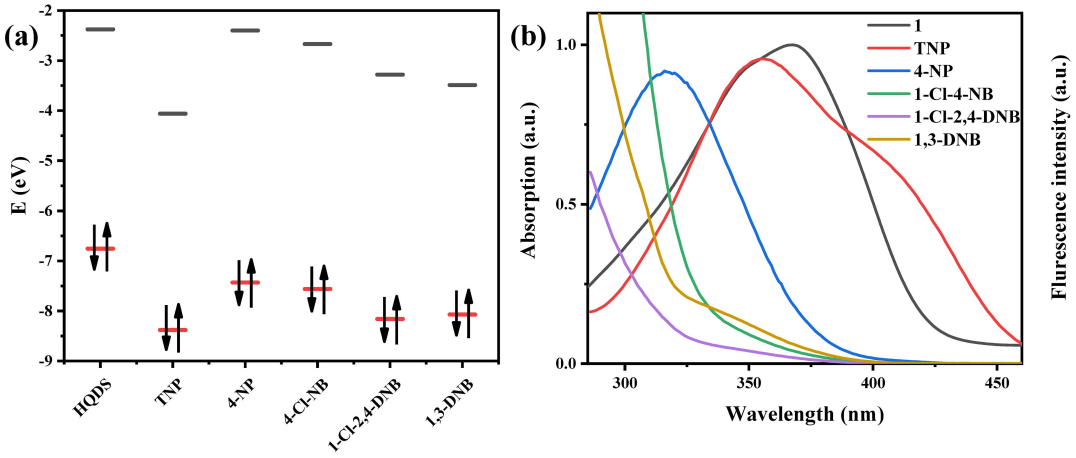


Fig. S13 (a) Theoretical HOMO and LUMO energies for HQDS, 4-NP and TNP; (b) UV-vis absorption spectra of 4-NP and TNP and emission spectra of **1** in water.

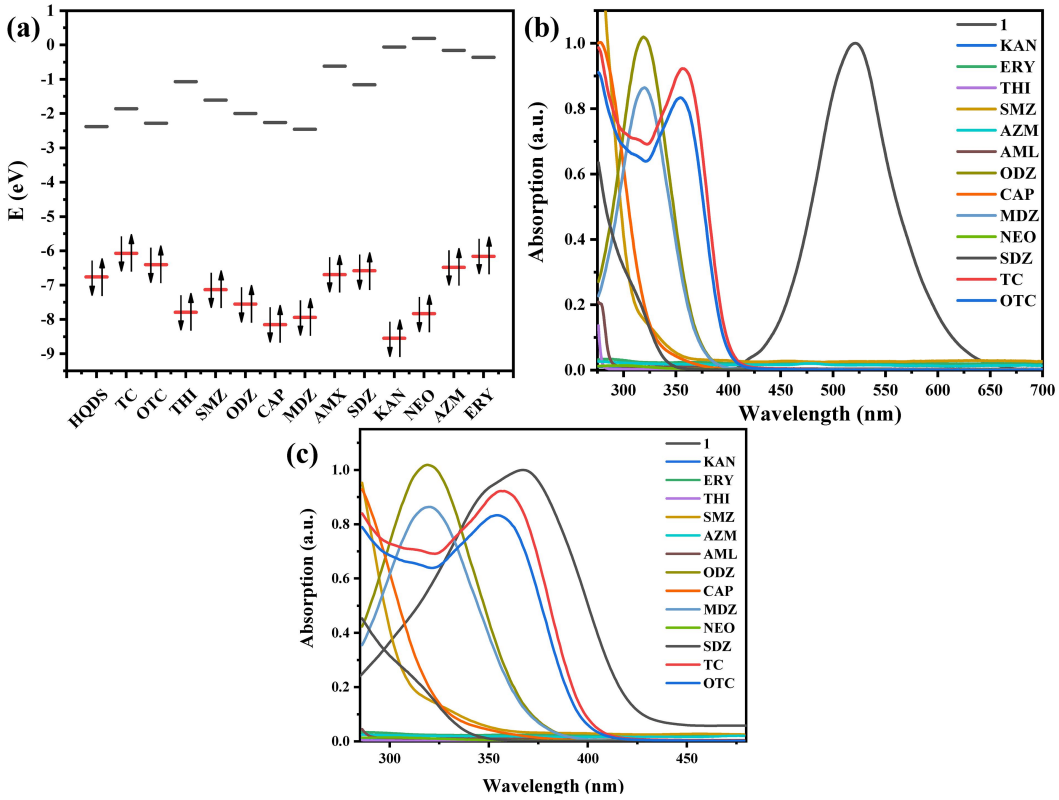


Fig. S14 (a)Theoretical HOMO and LUMO energies for HQDS, OTC and TC; (b) UV-visible spectra of antibiotics in water; (c) UV-vis absorption spectra of OTC and TC and excitation spectra of **1** in water.