Supplementary information

A novel 3D Cd-based luminescent coordination polymer for selective sensing of 4-NP and NZF

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Table S1. Crystallographic data for **1**.

Complex	**1**
Empirical formula	$C_{140}H_{112}Cd_7N_{847}$
Formula weight	3445.25
Crystal system	triclinic
Space group	*P-1*
a [Å]	10.8154(6)
b [Å]	17.0791(11)
c [Å]	17.5910(10)
α [°]	82.238(3)
β [°]	84.722(3)
γ [°]	87.293(3)
V [Å^3]	3203.9(3)
Z	1
*D*c / (g·cm^{-3})	1.786
F(000)	1720.0
μ(Mo *K*α) / mm^{-1}	1.237
Reflections collected	48426
θ range for data collection / (°)	2.779-25.436
Independent reflections (R_{int})	11761 (0.1070)
Data / restraints / parameters	11761/100/945
Gof	1.017
R_1, wR_2 [I>2σ(I)]^{ab}	0.0598, 0.1234
R_1, wR_2 (all data)^a	0.1246, 0.1530
Largest diff. Peak and hole[e·Å^{-3}]	1.89 and -2.75
CCDC number	1886813

Table. S2 Selected bond lengths/Å and bond angles/°for complex (**1**).

Complex **1**					
Cd1-O1	2.281(5)	Cd2-O2	2.331(6)	Cd1-O21^B	2.327(15)
Cd1-O2	2.274(8)	Cd2-O11	2.238(5)	Cd1-O21A^B	2.347(18)
Cd1-O3^A	2.328(6)	Cd2-O18	2.295(8)	Cd3-O16^E	2.448(5)
Cd1-O10^B	2.271(5)	Cd2-O19	2.277(8)	Cd3-N4^D	2.212(7)
Cd2-O21^C	2.364(16)	Cd3-O7	2.364(6)	Cd3-O6	2.640(5)
Cd4-O1^F	2.279(5)	Cd4-O12^F	2.225(6)	Cd2-O23^C	2.701(16)
Cd4-O9^B	2.381(5)	Cd2-O21A^C	2.57(2)	Cd3-O15^E	2.407(5)
Cd4-O9^G	2.381(5)	Cd4-O12	2.225(6)	Cd3-O6^D	2.388(5)
Cd4-O1	2.279(5)	Cd2-O1	2.227(6)		
Cd2-Cd1-Cd4	64.156(16)	O10^B-Cd1-O21A^B	102.3(5)	O7-Cd3-O6^D	126.94(18)

O1-Cd1-Cd2	39.17(15)	O20-Cd1-Cd2	142.26(19)	O7-Cd3-O6	50.72(17)
O1-Cd1-Cd4	31.74(13)	O20-Cd1-Cd4	80.09(19)	O7-Cd3-O15^{E}	141.76(18)
O1-Cd1-O3^{A}	74.7(2)	O20-Cd1-O1	103.2(2)	O7-Cd3-O16^{E}	88.89(18)
O1-Cd1-O21^{B}	157.7(4)	O20-Cd1-O2	171.5(3)	O15^{E}-Cd3-O6	166.03(17)
O1-Cd1-O21A^{B}	166.2(5)	O20-Cd1-O3^{A}	83.1(3)	O15^{E}-Cd3-O16^{E}	54.03(18)
O2-Cd1-Cd2	41.78(15)	O20-Cd1-O21^{B}	94.0(4)	O11-Cd2-O18	82.2(2)
O2-Cd2-Cd1	40.53(19)	O2-Cd2-O21A^{C}	82.0(4)	N1-Cd3-O6^{D}	84.4(2)
O2-Cd2-O21^{C}	78.3(4)	O11-Cd2-Cd1	91.76(15)	C54^{E}-Cd3-C13	141.1(2)
O2-Cd2-O23^{C}	117.6(3)	O11-Cd2-O2	88.5(2)	Cd1-Cd4-Cd1^{F}	180.0
N1-Cd3-O6	83.5(2)	O20-Cd1-O21A^{B}	81.9(5)	O1^{F}-Cd4-Cd1^{F}	31.78(12)
N1-Cd3-O7	88.5(3)	O21^{B}-Cd1-Cd2	123.0(3)	O1-Cd4-Cd1^{F}	148.22(12)
N1-Cd3-O15^{E}	90.0(2)	O21^{B}-Cd1-Cd4	170.4(3)	O1^{F}-Cd4-Cd1	148.22(12)
N4^{D}-Cd3-O7	95.4(3)	O21^{B}-Cd1-O3^{A}	93.6(4)	O1-Cd4-Cd1	31.78(12)
N4^{D}-Cd3-O15^{E}	92.0(2)	O21^{B}-Cd1-O21A^{B}	12.2(6)	O1-Cd4-O1^{F}	180.0
N4^{D}-Cd3-O16^{E}	87.0(2)	O21A^{B}-Cd1-Cd2	135.2(4)	O1^{F}-Cd4-O9^{B}	90.87(19)
N4^{D}-Cd3-N1	171.0(2)	O21A^{B}-Cd1-Cd4	159.9(4)	O1-Cd4-O9^{G}	90.87(19)
Cd1-Cd4-Cd1^{6}	180.0	O1-Cd2-Cd1	40.31(13)	O1-Cd4-O9^{B}	89.13(19)
N4^{D}-Cd3-O6	92.6(2)	O1-Cd2-O2	80.7(2)	O1^{F}-Cd4-O9^{G}	89.13(19)
N4^{D}-Cd3-C54^{E}	88.6(2)	O1-Cd2-O11	90.1(2)	N1-Cd3-O16^{E}	101.2(2)
O2-Cd1-O3^{A}	105.2(3)	O1-Cd2-O18	167.5(3)	N4^{D}-Cd3-O6^{D}	86.7(2)
O2-Cd1-O21^{B}	84.2(4)	O1-Cd2-O19	94.3(2)	O1^{F}-Cd4-Cd1^{F}	31.78(12)
O2-Cd1-O21A^{B}	96.0(5)	O1-Cd2-O21^{C}	102.1(4)	O1-Cd4-Cd1^{F}	148.22(12)
O3^{A}-Cd1-Cd2	87.02(19)	O1-Cd2-O23^{C}	89.5(4)	O1^{F}-Cd4-Cd1	148.22(12)
O3^{A}-Cd1-Cd4	93.16(16)	O1-Cd2-O21A^{C}	112.5(4)	O1-Cd4-Cd1	31.78(12)
O3^{A}-Cd1-O21A^{B}	93.4(5)	O12^{F}-Cd4-Cd1^{F}	94.90(15)	O1-Cd4-O1^{F}	180.0
O10^{B}-Cd1-Cd2	93.02(15)	O12^{F}-Cd4-O1	85.9(2)	O1^{F}-Cd4-O9^{B}	90.87(19)
O10^{B}-Cd1-Cd4	66.81(16)	O12-Cd4-O1	94.1(2)	O1-Cd4-O9^{7}	90.87(19)
O10^{B}-Cd1-O1	91.09(19)	O12^{F}-Cd4-O1^{F}	94.1(2)	O1-Cd4-O9^{B}	89.13(19)
O10^{B}-Cd1-O2	89.4(2)	O12-Cd4-O1^{F}	85.9(2)	O1^{F}-Cd4-O9^{G}	89.13(19)
O10^{B}-Cd1-O3^{A}	157.4(3)	O12^{F}-Cd4-O9^{G}	92.1(2)	O9^{B}-Cd4-Cd1^{F}	122.65(15)
O10^{B}-Cd1-O20	83.1(3)	O12-Cd4-Cd1	94.90(15)	O9^{G}-Cd4-Cd1	122.65(15)
O10^{B}-Cd1-O21^{B}	105.2(4)	O12-Cd4-Cd1^{F}	85.10(15)	O9^{G}-Cd4-Cd1^{F}	57.35(15)
O12^{F}-Cd4-O12	180.0	O12-Cd4-O9^{G}	87.9(2)	O9^{B}-Cd4-Cd1	57.35(15)
Cd2-O1-Cd1	100.5(2)	O12^{F}-Cd4-O9^{B}	87.9(2)	O9^{B}-Cd4-O9^{G}	180.0
Cd2-O1-Cd4	120.7(2)	O12-Cd4-O9^{B}	92.1(2)	O12-Cd4-Cd1	94.90(15)
Cd4-O1-Cd1	116.5(2)	O12^{F}-Cd4-O12	180.0	O12-Cd4-Cd1^{F}	85.10(15)
Cd1-O2-Cd2	97.7(3)	Cd2-O1-Cd1	100.5(2)	O12^{F}-Cd4-Cd1	85.10(15)
Cd3^{D}-O6-Cd3	103.78(18)	Cd2-O1-Cd4	120.7(2)	O12^{F}-Cd4-Cd1^{F}	94.90(15)
O9^{B}-Cd4-Cd1^{F}	122.65(15)	Cd4-O1-Cd1	116.5(2)	O12^{F}-Cd4-O1	85.9(2)
O9^{G}-Cd4-Cd1	122.65(15)	O12^{F}-Cd4-Cd1	85.10(15)	O12-Cd4-O1	94.1(2)
O9^{G}-Cd4-Cd1^{F}	57.35(15)	N4^{D}-Cd3-O15^{E}	92.0(2)	O12^{F}-Cd4-O1^{F}	94.1(2)
O9^{B}-Cd4-Cd1	57.35(15)	N4^{D}-Cd3-O16^{E}	87.0(2)	O12-Cd4-O1^{F}	85.9(2)
O9^{B}-Cd4-O9^{G}	180.0	N4^{D}-Cd3-N1	171.0(2)	O12^{F}-Cd4-O9^{G}	92.1(2)
N4^{D}-Cd3-O6	92.6(2)	O12-Cd4-O9^{B}	92.1(2)	O12-Cd4-O9^{G}	87.9(2)

N4^{D}-Cd3-O7	95.4(3)	N4^{D}-Cd3-C13	97.0(3)	O12^{F}-Cd4-O9^{B}	87.9(2)
Cd1-O2-Cd2	97.7(3)				

^{A}-X,-Y,2-Z; ^{B}1-X,1-Y,2-Z; ^{C}-1+X,-1+Y,+Z; ^{D}1-X,2-Y,1-Z; ^{E}-1+X,1+Y,+Z; ^{F}1-X,-Y,2-Z; ^{G}+X,-1+Y,+Z; ^{H}+X,1+Y,+Z;

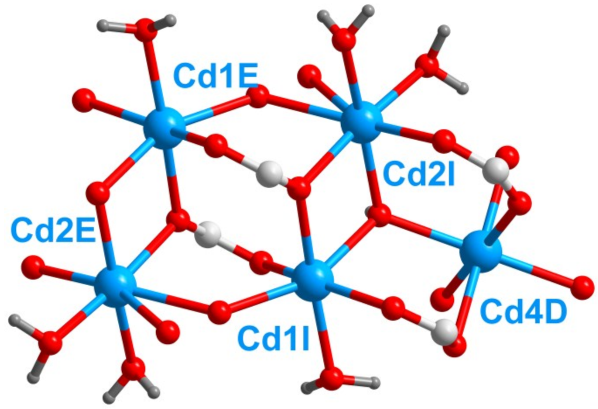

Figure S1. The 1D $\{Cd_5(COO)_8(u_3\text{-}H_2O)_2\}_n$ SBUs for **1**.

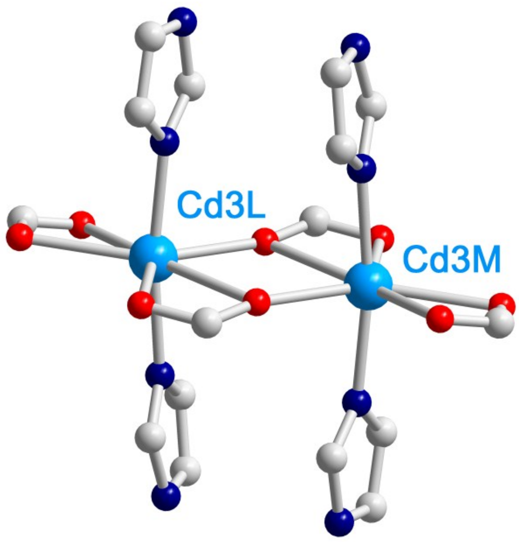

Figure S2. The binuclear paddle-wheel $\{Cd_2(COO)_4\}_n$ SBU for **1**.

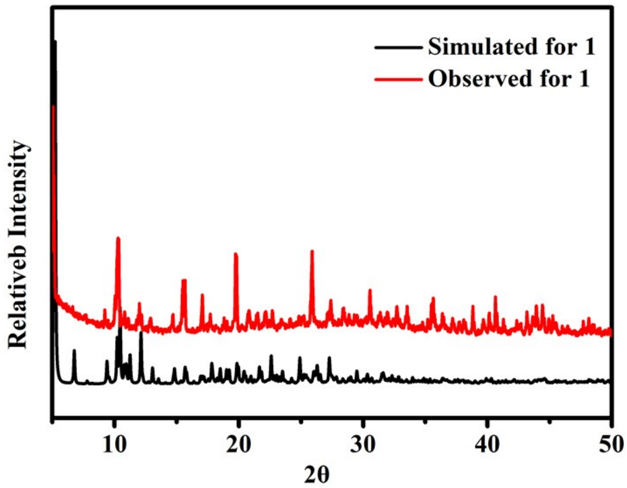

Figure S3. PXRD patterns of the series complexes. Black: Simulated from the X–ray single–crystal data; Red: observed for the as–synthesized solids.

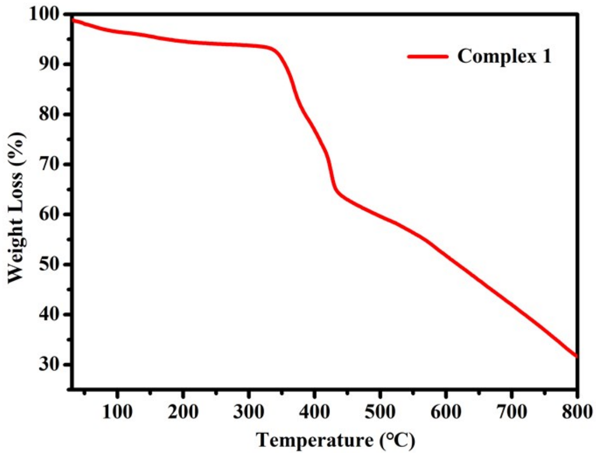

Figure S4. The TG curve of complex **1**.

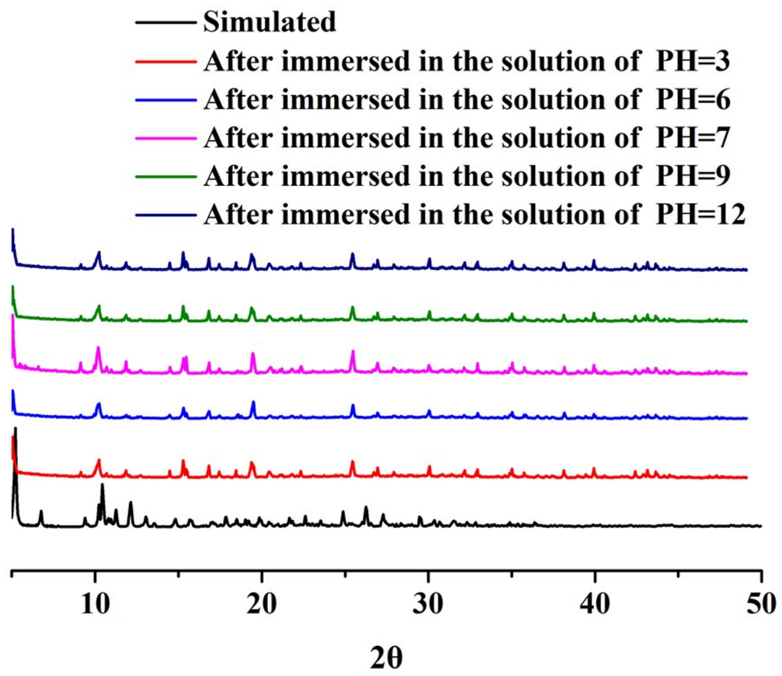

Figure S5. PXRD patterns of **1** after being immersing in water solution for various conditions.

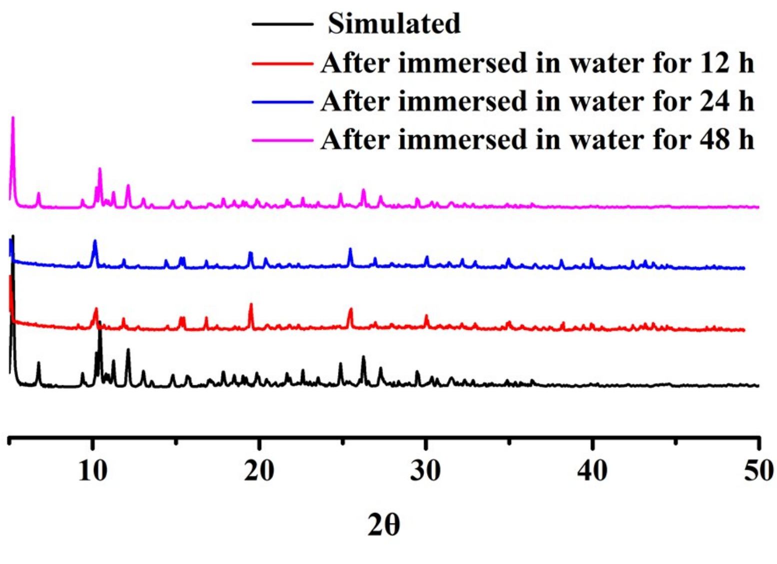

Figure S6. PXRD patterns of **1** after being immersing in water solution for various conditions.

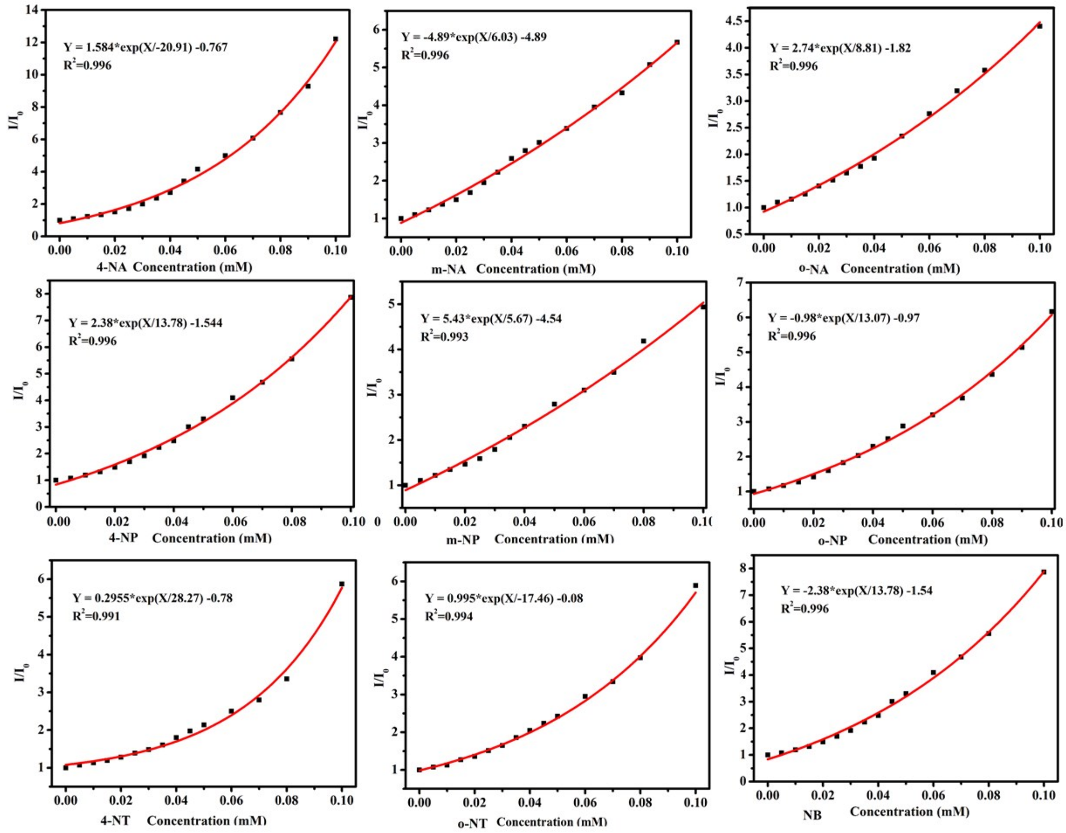

Figure S7. The K_{SV} plot for the fluorescence quenching of 4-NP, m-NP, o-NP, 4-NA, m-NA, o-NA, 4-NT, o-NT and NB to aqueous@**1** suspensions.

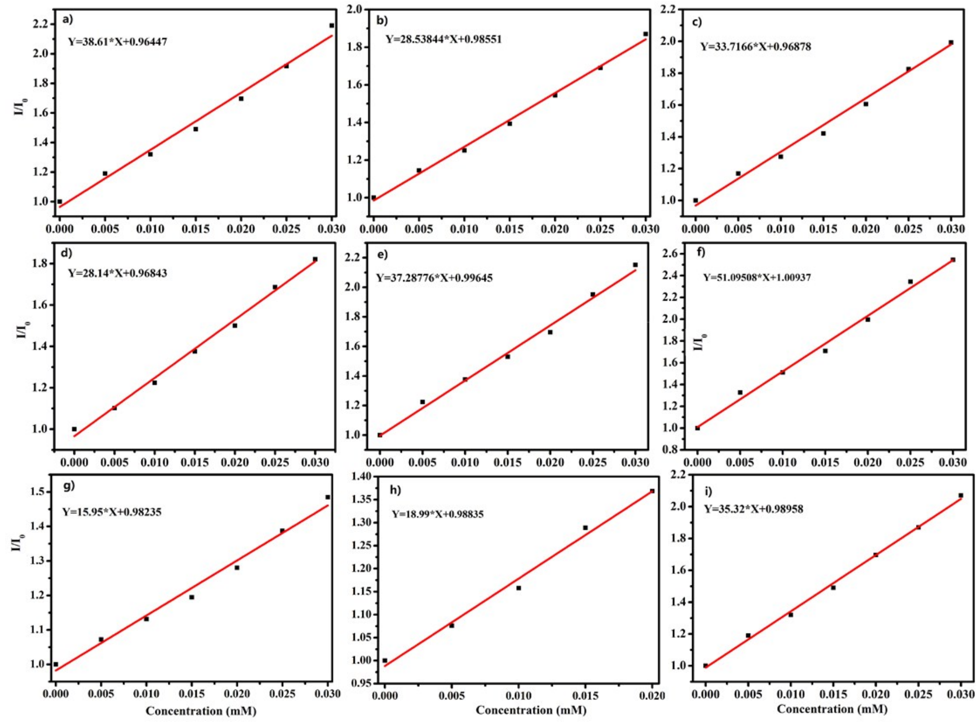

Figure S8. The K_{SV} plot for the fluorescence quenching of 4-NP (a), m-NP(b), o-NP(c), 4-NA(d), m-NA(e), o-NA(f), 4-NT(g), o-NT(h) and NB(i) to aqueous@**1** suspensions at low concentration.

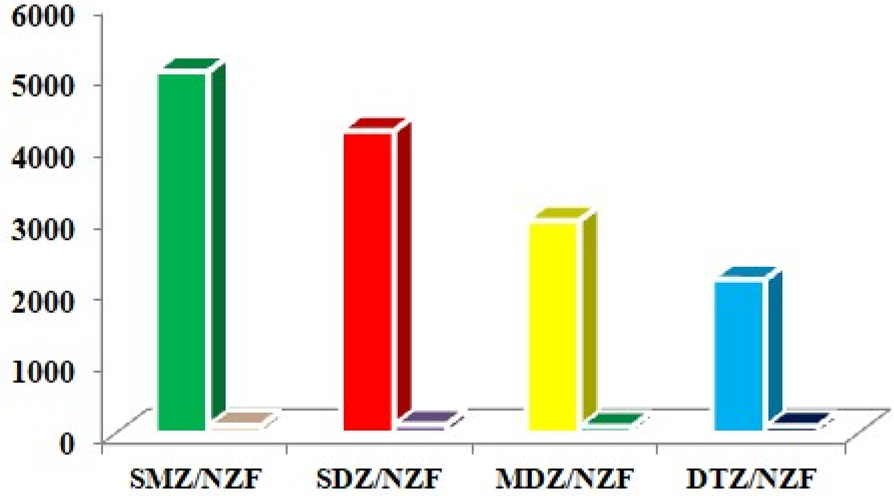

Figure S9. Comparison of the luminescence intensity of **1** in DMF suspension with the introduction of other antibiotic.

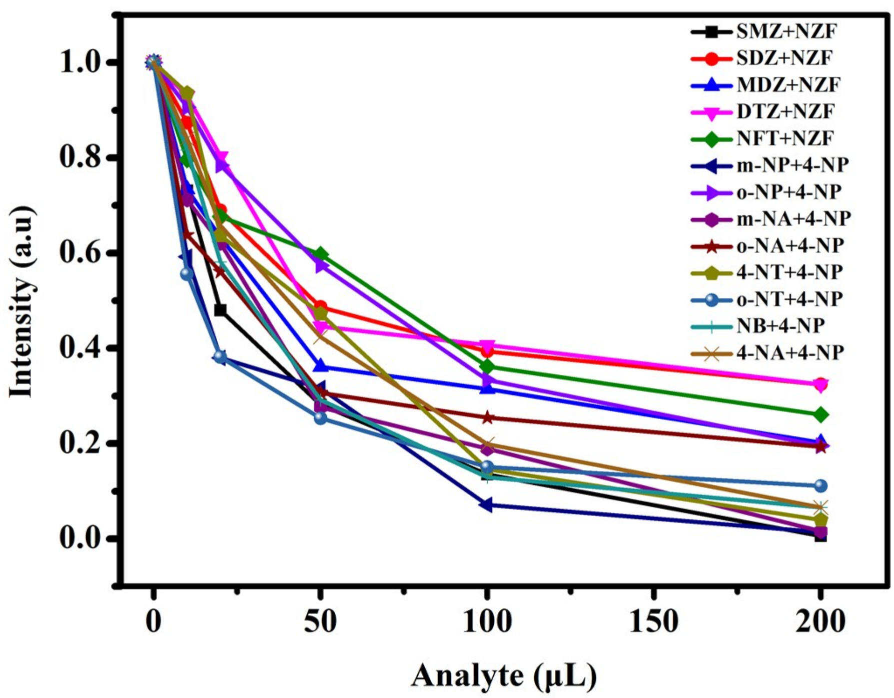

Figure S10. the selective detection of 4-NP/NZF (f) on LCP 1 in the presence of various analyte in water system.

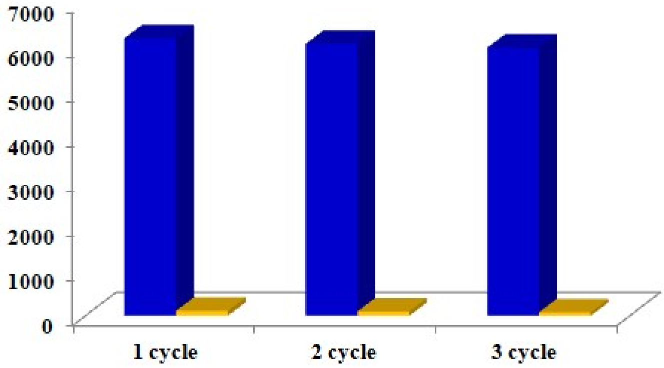

Figure S11. The results of **1** for three continuous cycles.

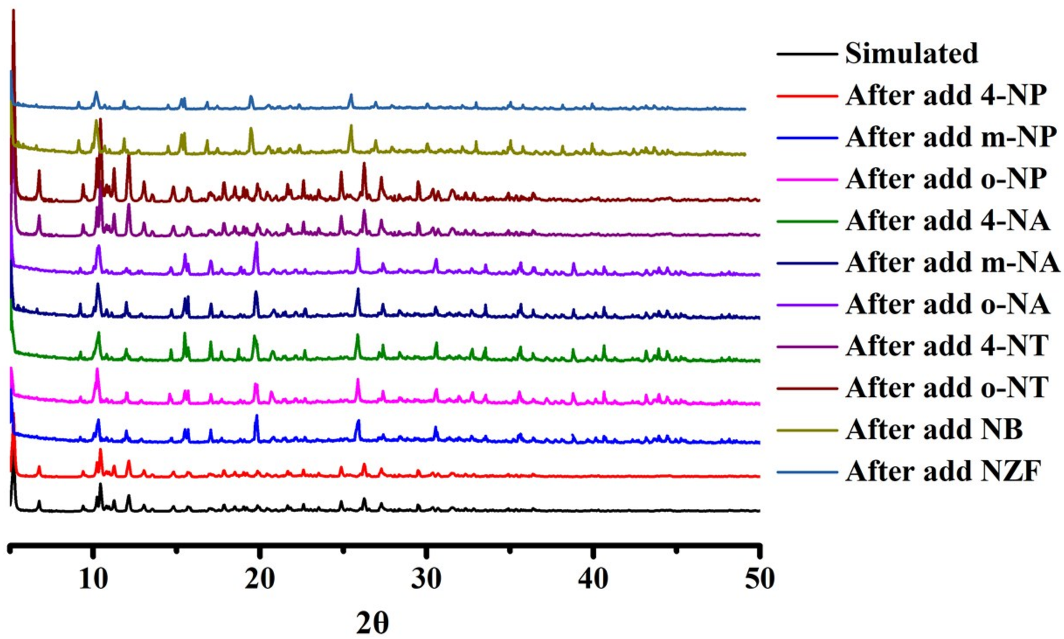

Figure S12. The PXRD patterns of **1** for the simulated, as-synthesized and after immerging in NACs and antibiotic.

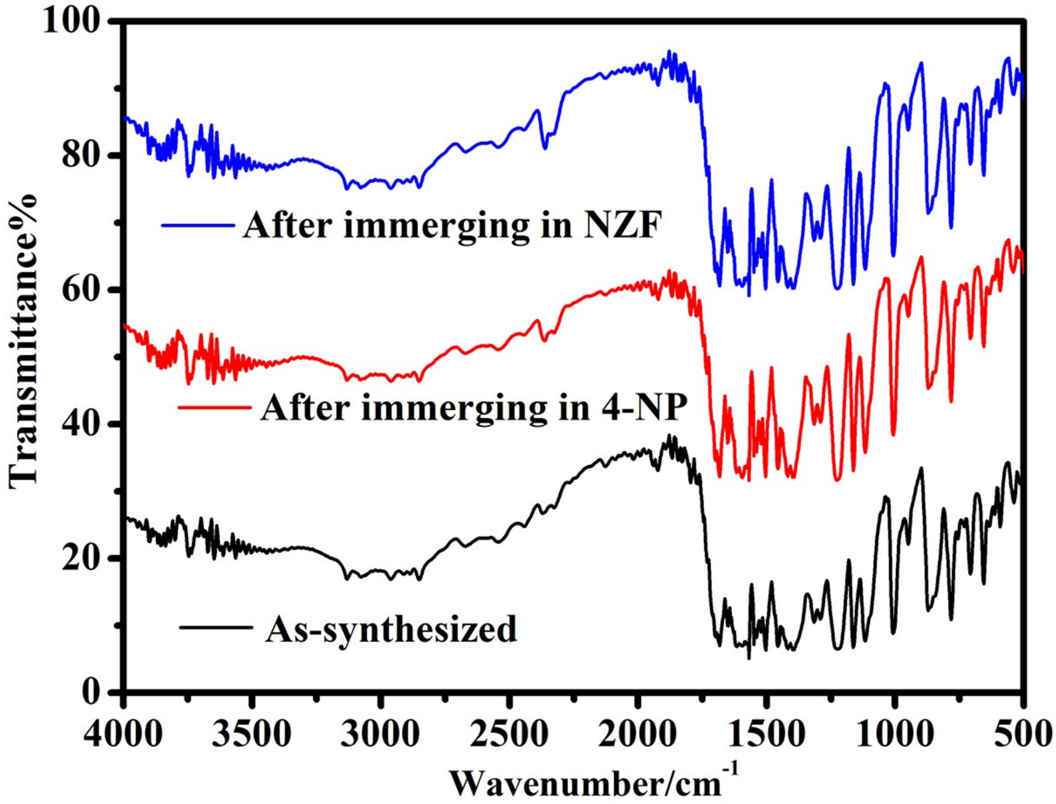

Figure S13. The IR patterns of **1** for the, as-synthesized and after immerging in 4-NP and NZF .

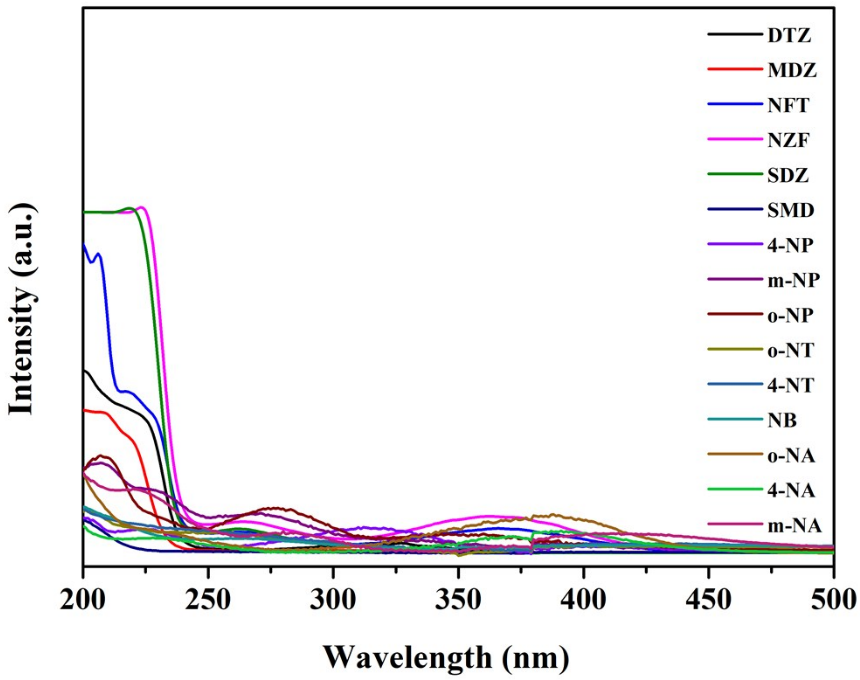

Figure S14. The UV spectra of NACs and antibiotic.

Table S3. Summary of LCPs for detecting 4-NP and NZF.

Molecular Formula	analyte	Quenching Constant (Ksv/M^{-1})	detection limit (DL)	Ref.
$\{[Cd_2(obtz)(Meip)_2]\cdot H_2O\}_n$	4-NP	0.113×10^3	NA	24
$\{[Cd(obtz)(ndc)]\cdot 0.5H_2O\}_n$	4-NP	0.117×10^3	NA	24
$\{[Eu_2(TDC)_3(CH_3OH)_2]\cdot CH_3OH\}_n$	NZF	1.6×10^4	NA	*25*