

Supporting Information for

Three Multi-responsive Luminescent Zn-CPs for Detection of Antibiotics/Cations/Anions in Aqueous Media

Chuanbin Fan,^{a,b} Guimei Huang,^{a,c} Zhiyong Xing,^{a,b} Junli Wang,^{a,b} Yaqin Pang,^{a,b} Qingping Huang,^{a,b} Shifu Huang,^{a,b} Ziao Zong,^{a,b,*} Feng Guo,^{a,b,**}

- a. School of Laboratory Medicine, Youjiang Medical University for Nationalities, Baise, Guangxi, 533000, P.R. China
- b. Industrial College of Biomedicine and Health Industry, Youjiang Medical University for Nationalities, Baise, Guangxi, 533000, P.R. China
- c. School of Chemistry and Pharmaceutical Sciences, Guangxi Normal University, Guilin 541004, People's Republic of China

*Corresponding author: zongziao@126.com.

**Corresponding author: guofeng1510@yeah.net.

Materials and General Characteristics

The used materials of this work were of AR grade and purchased from commercial sources without further purification. The experimental powder X-ray diffraction (PXRD) of YMUN 6–8 samples were collected on a Rigaku Miniflex 600 instrument. A Nicolet 170SX spectrometer was employed to record the infrared (IR) spectra with KBr pellets, and the measurements were in the range of 4000–400 cm^{-1} . We used the Perkin-Elmer TG-7 thermogravimetric analyzer to conduct thermogravimetric analysis (TGA) under nitrogen condition, and the heating rate was 10 $^{\circ}\text{C min}^{-1}$ from 30 to 800 $^{\circ}\text{C}$. A Shimadzu UV-2550 spectrophotometer was used to obtain the UV–vis spectra. Luminescence spectra were collected on a Perkin Elmer LS55 spectrophotometer.

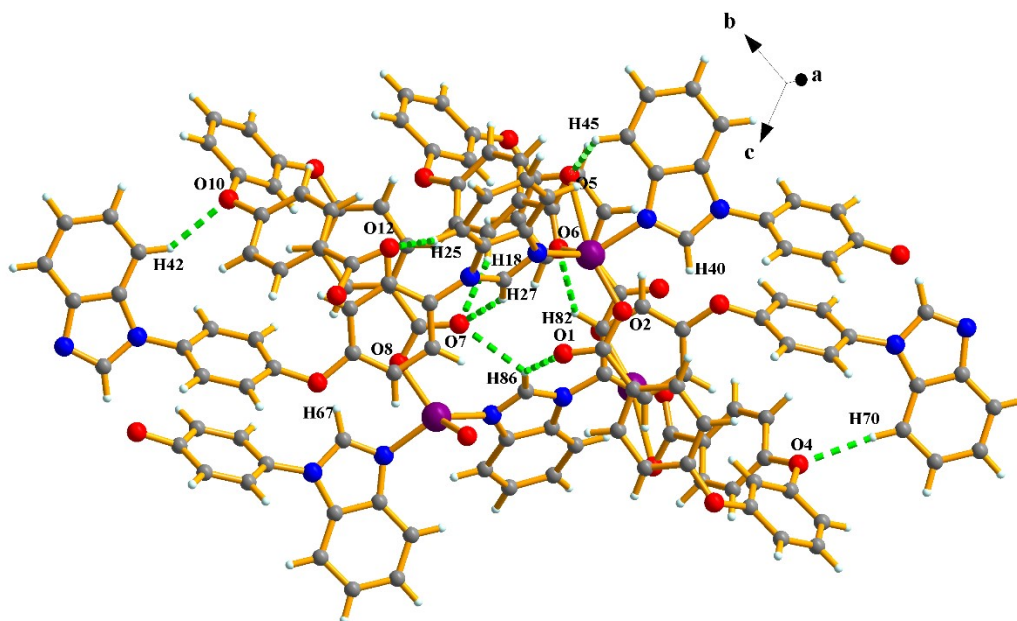


Figure S1. View of the noncovalent supramolecular interactions in YMUN 6. The weak interactions in the neighboring A and B segments by C-H \cdots O hydrogen bonding interactions (the distance of C-H \cdots O and the angle of \angle C-H \cdots O are listed in Table S2).

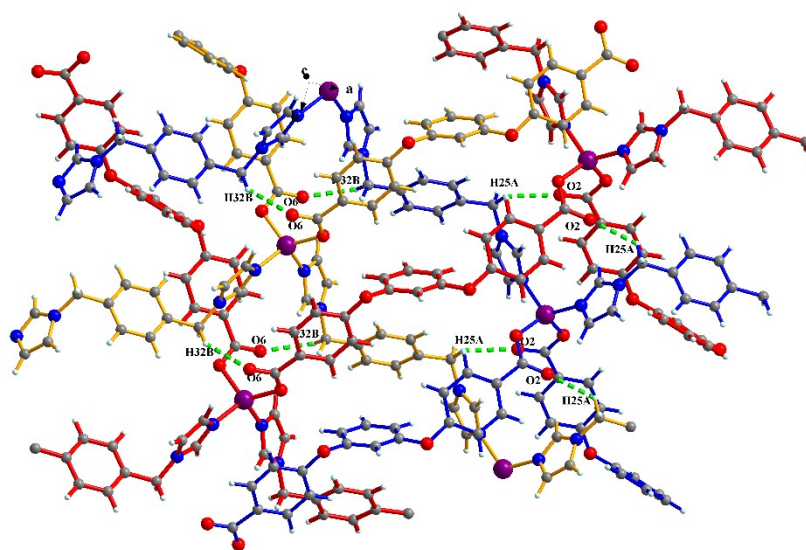


Figure S2. View of the noncovalent supramolecular interactions in YMUN 7. The neighboring 2D three-fold interpenetrated structures are interlined by C-H \cdots O hydrogen-bonding interactions (the distance of C-H \cdots O and the angle of \angle C-H \cdots O are listed in Table S2).

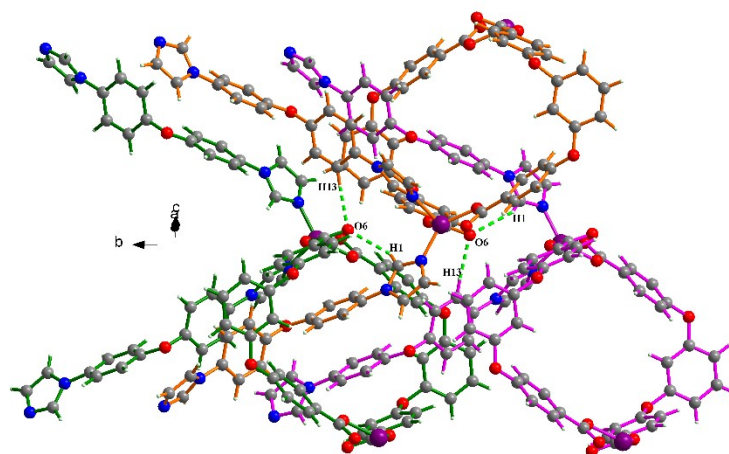


Figure S3. View of the noncovalent supramolecular interactions in YMUN **8**. The neighboring 2D three-fold interpenetrated structures are interlined by C-H \cdots O hydrogen-bonding interactions (the distance of C-H \cdots O and the angle of \angle C-H \cdots O are listed in Table S2).

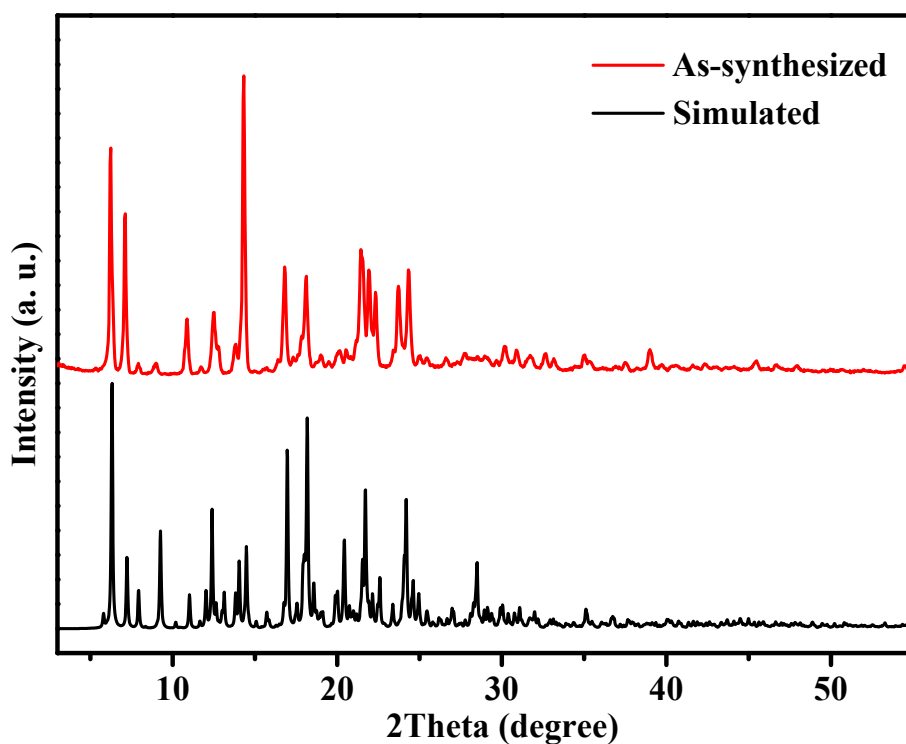


Figure S4. PXRD patterns of YMUN **6**, simulated and as-synthesized.

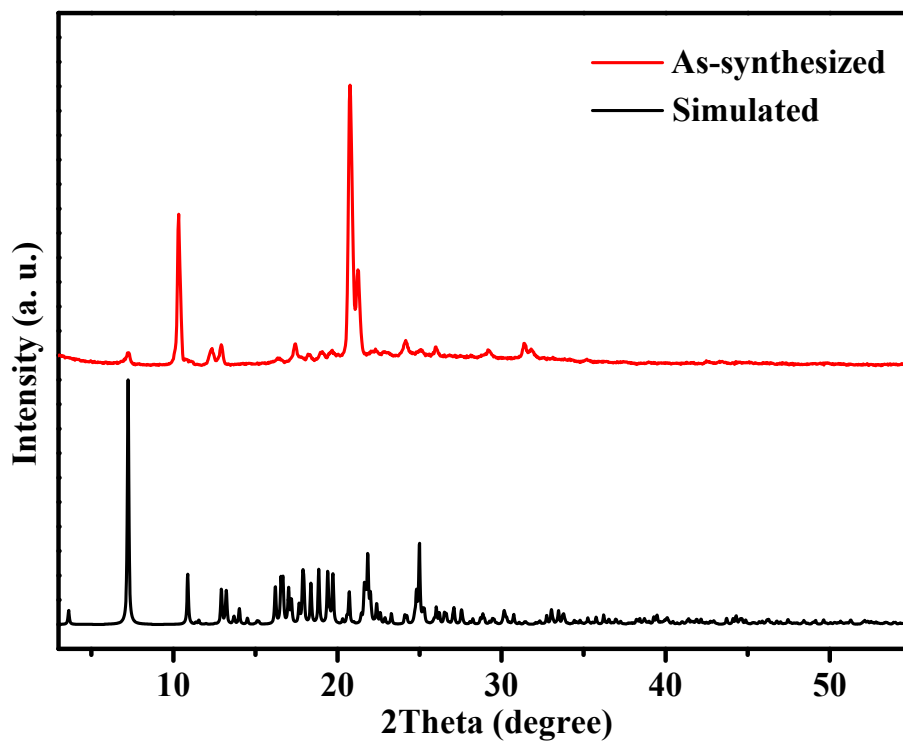


Figure S5. PXRd patterns of YMUN 7, simulated and as-synthesized.

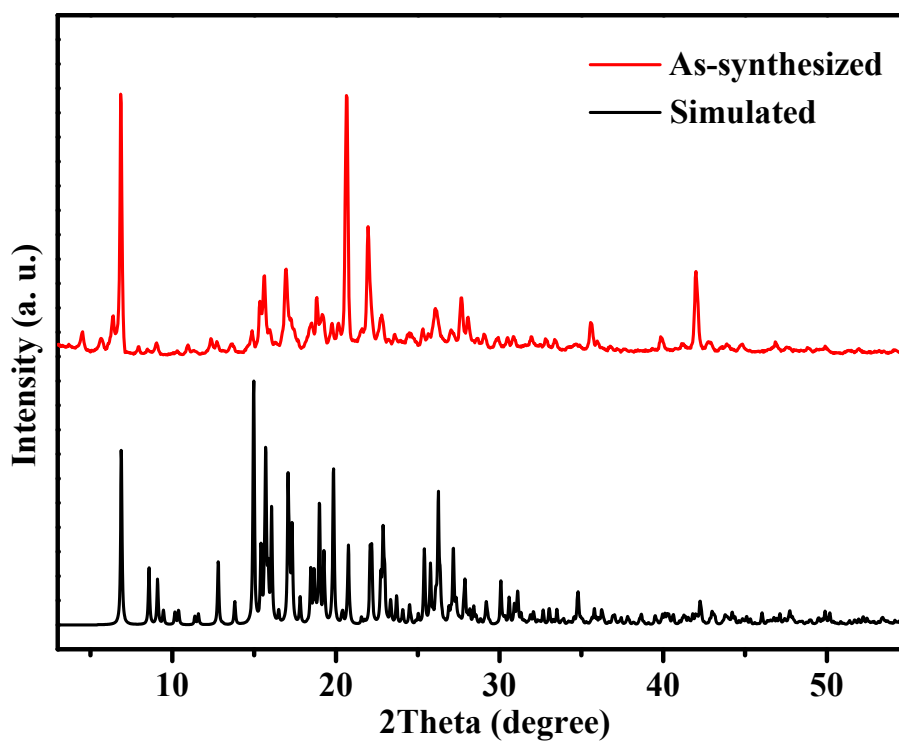


Figure S6. PXRd patterns of YMUN 8, simulated and as-synthesized.

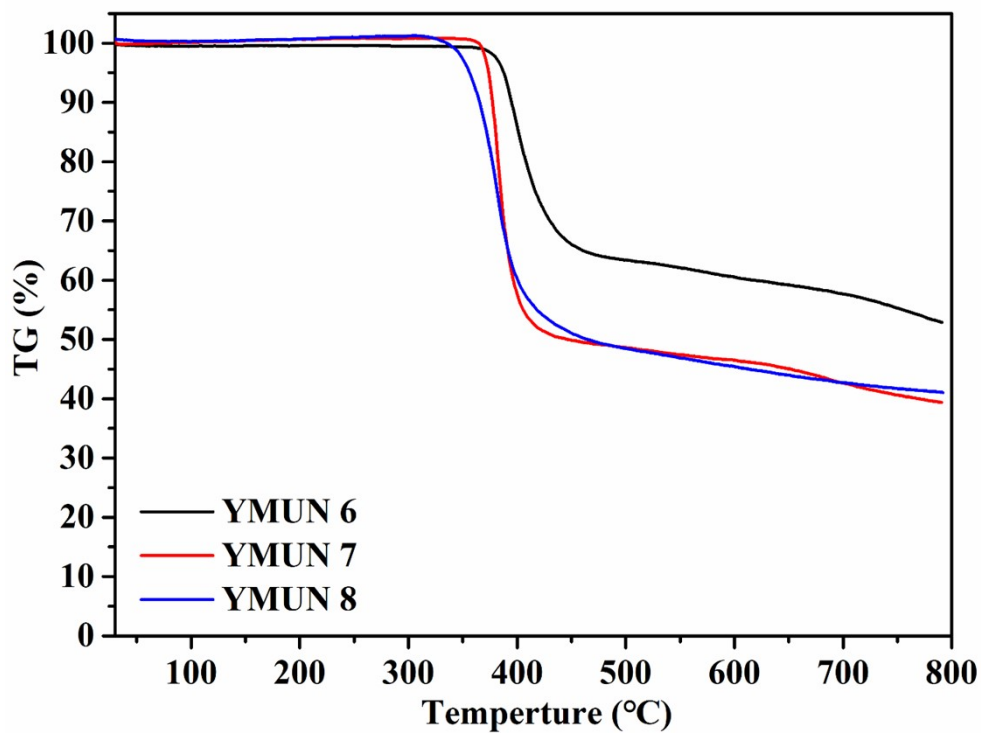


Figure S7. The TG curves of YMUN 6–8

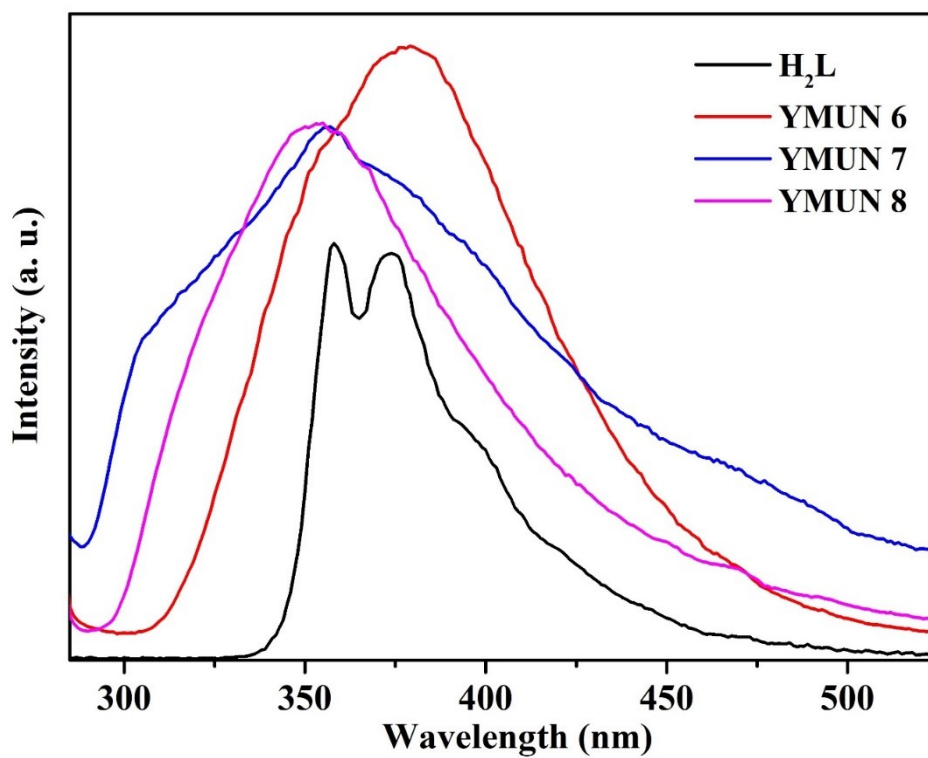


Figure S8. Photoluminescence of H₂L ligand and YMUN 6–8 at room temperature in the solid state.

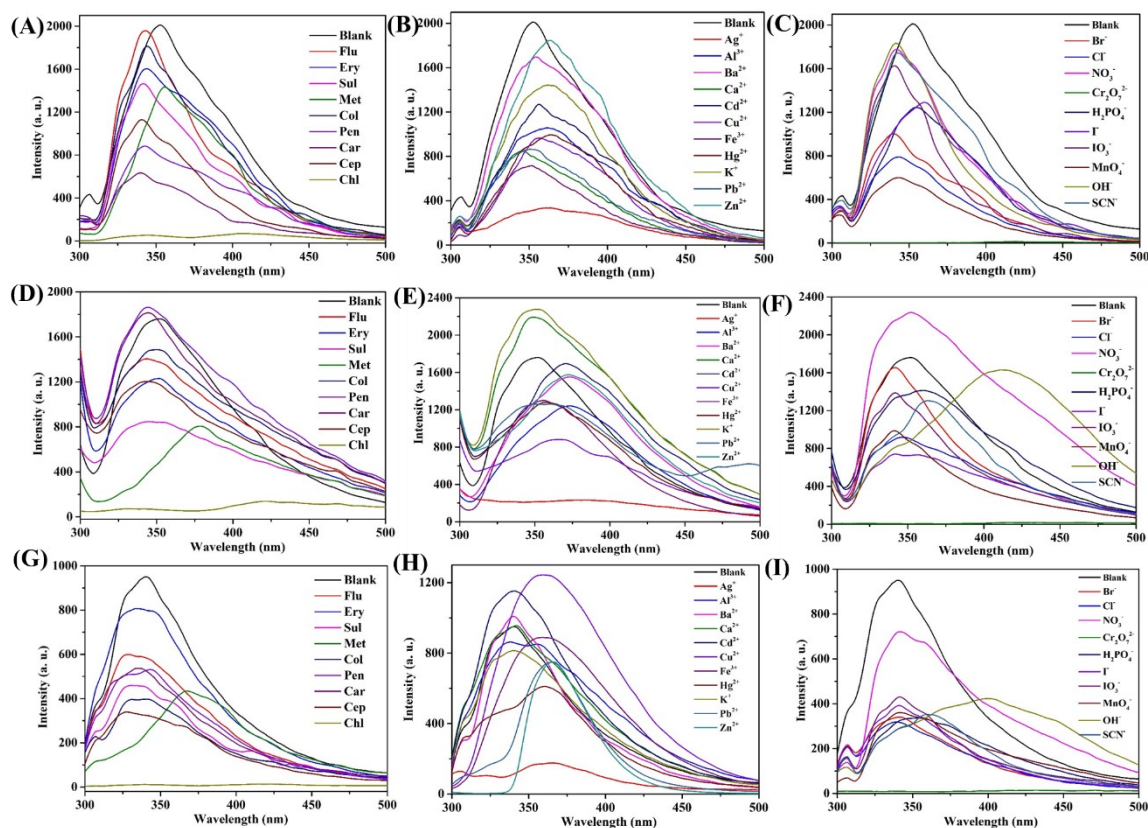


Figure S9. (A)-(C) Fluorescence spectra of **YMUN 6** powder and **YMUN 6** powder introduced into different antibiotics (0.5 mM), metal ions (1.0 mM), and cations (1.0 mM) in the aqueous solution at room temperature ($\lambda_{\text{ex}} = 275$ nm). (E)-(G) Fluorescence spectra of **YMUN 7** powder and **YMUN 7** powder introduced into different antibiotics (0.5 mM), metal ions (1.0 mM), and cations (1.0 mM) in the aqueous solution at room temperature ($\lambda_{\text{ex}} = 271$ nm). (G)-(I) Fluorescence spectra of **YMUN 8** powder and **YMUN 8** powder introduced into different antibiotics (0.5 mM), metal ions (1.0 mM), and cations (1.0 mM) in the aqueous solution at room temperature ($\lambda_{\text{ex}} = 275$ nm).

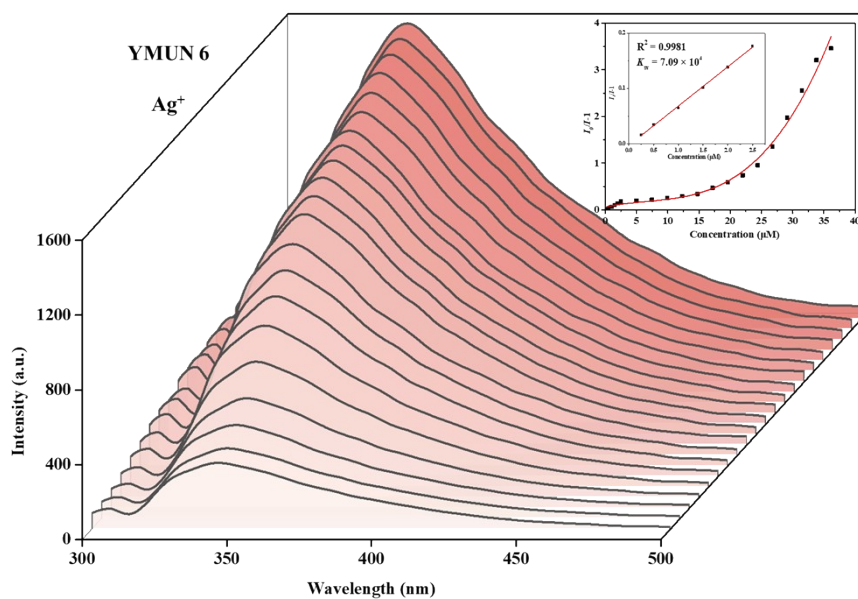


Figure S10. The fluorescence intensity trend spectra and the $S-V$ linear relationship curve of YMUN 6 after adding Ag^+ solution.

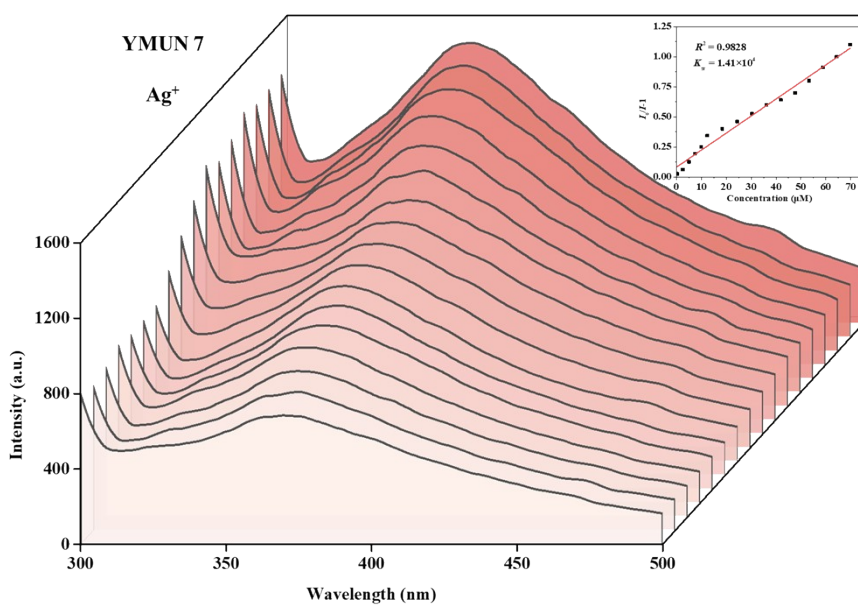


Figure S11. The fluorescence intensity trend spectra and the $S-V$ linear relationship curve of YMUN 7 after adding Ag^+ solution.

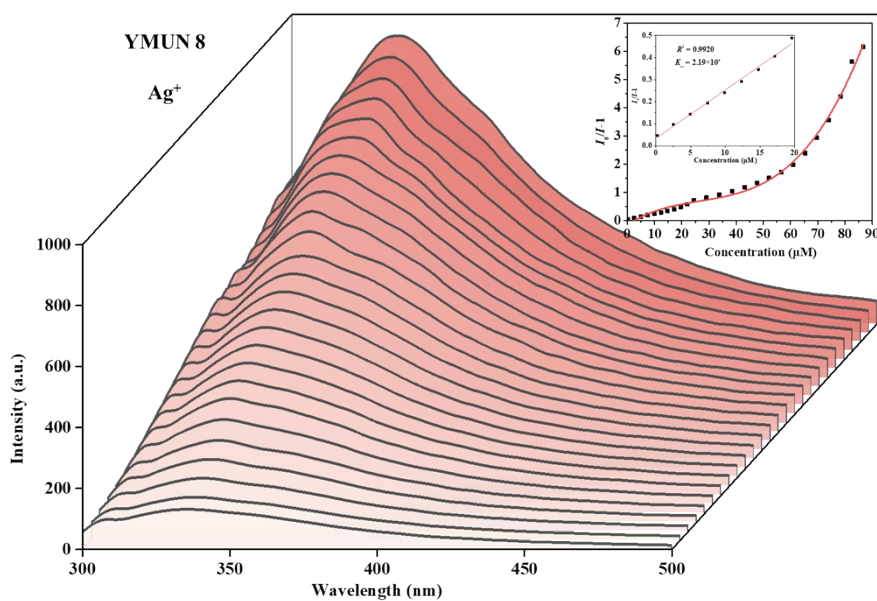


Figure S12. The fluorescence intensity trend spectra and the $S-V$ linear relationship curve of YMUN 8 after adding Ag^+ solution.

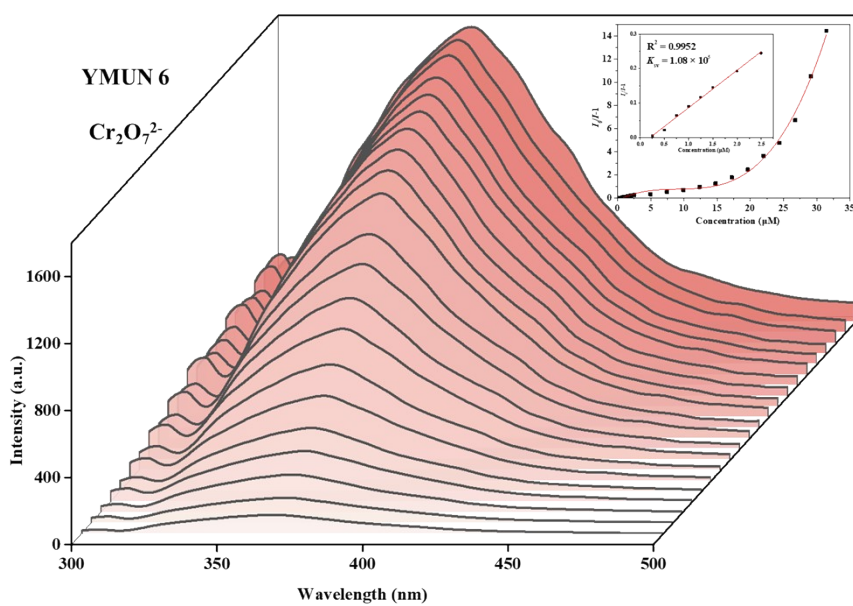


Figure S13. The fluorescence intensity trend spectra and the $S-V$ linear relationship curve of YMUN 6 after adding $\text{Cr}_2\text{O}_7^{2-}$ solution.

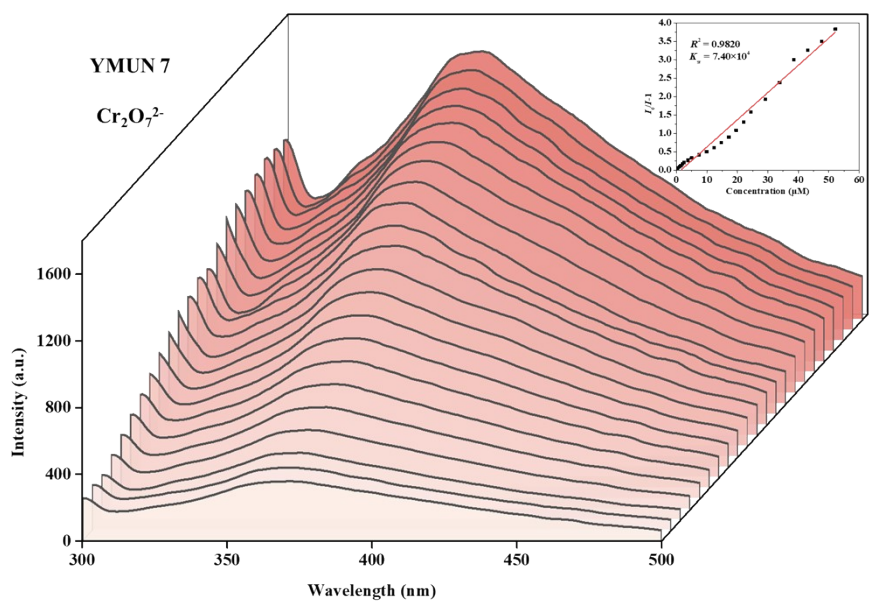


Figure S14. The fluorescence intensity trend spectra and the $S-V$ linear relationship curve of YMUN 7 after adding $\text{Cr}_2\text{O}_7^{2-}$ solution.

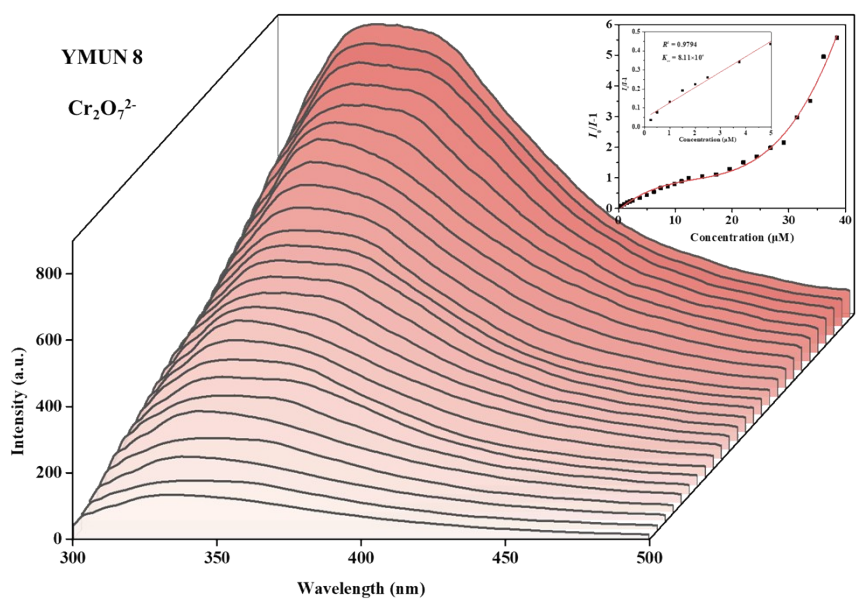


Figure S15. The fluorescence intensity trend spectra and the $S-V$ linear relationship curve of YMUN 8 after adding $\text{Cr}_2\text{O}_7^{2-}$ solution.

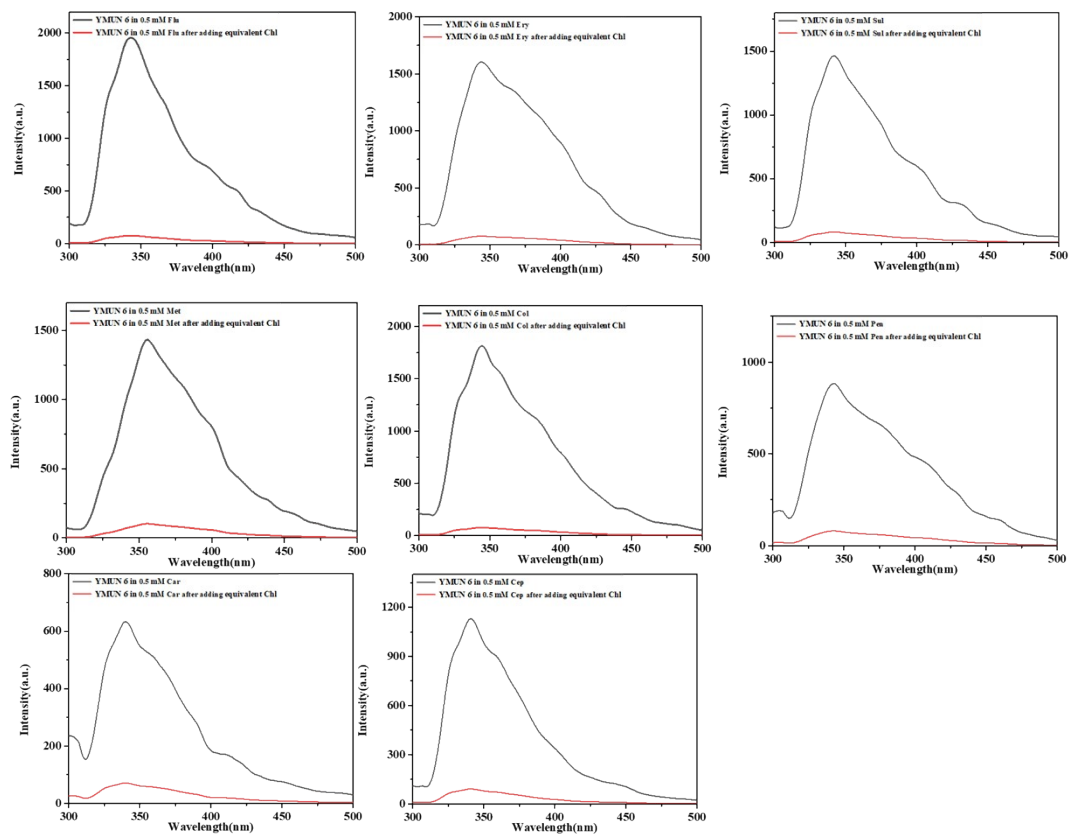


Figure S16. The fluorescence spectra of **YMUN 6** in various antibiotics (0.5 mM) (Black lines), and adding equivalent **Chl** in various antibiotics solution.

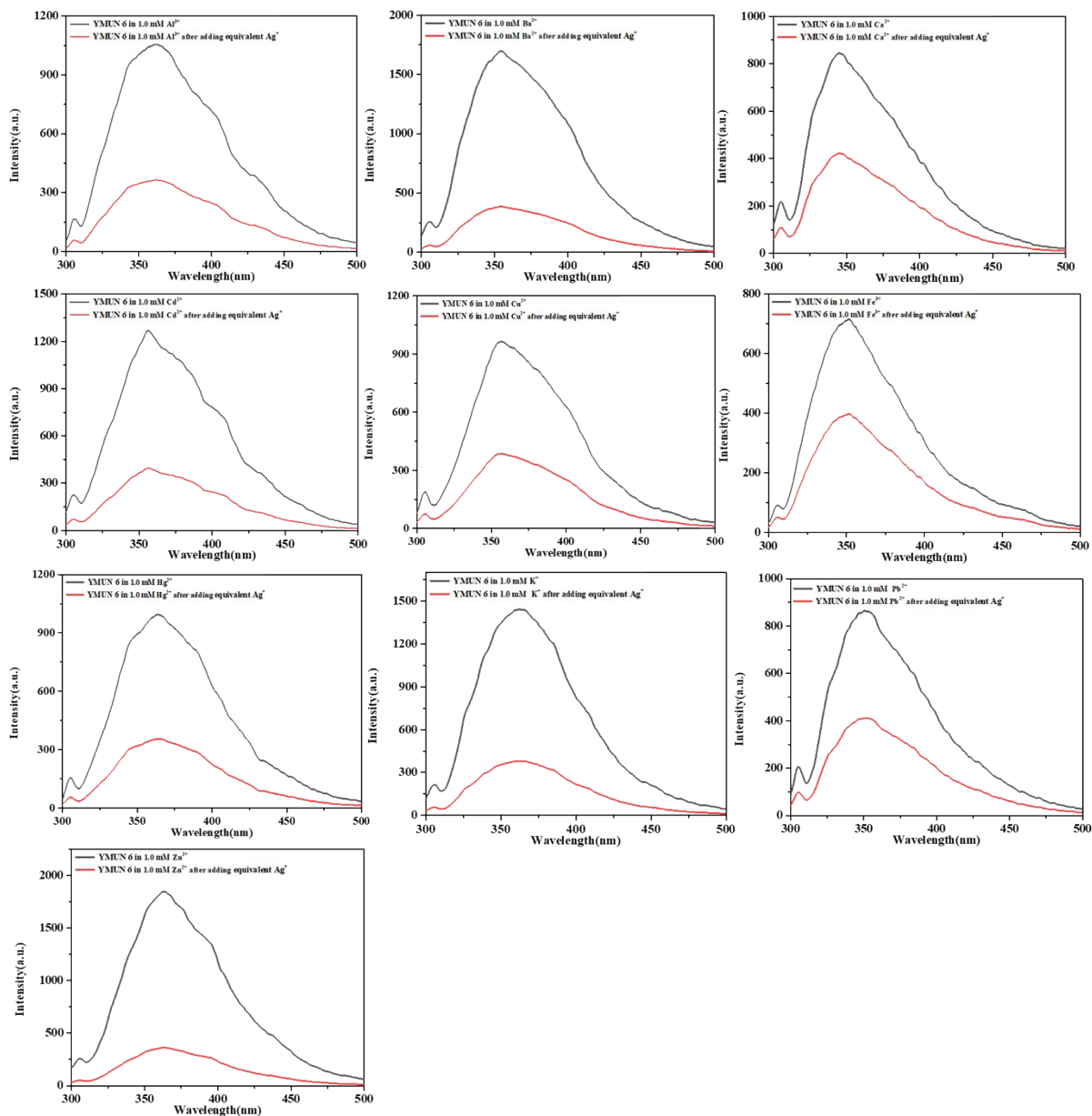


Figure S17. The fluorescence spectra of YMUN 6 in various metal ions (1.0 mM) (Black lines), and adding equivalent Ag^+ in various metal ions solution.

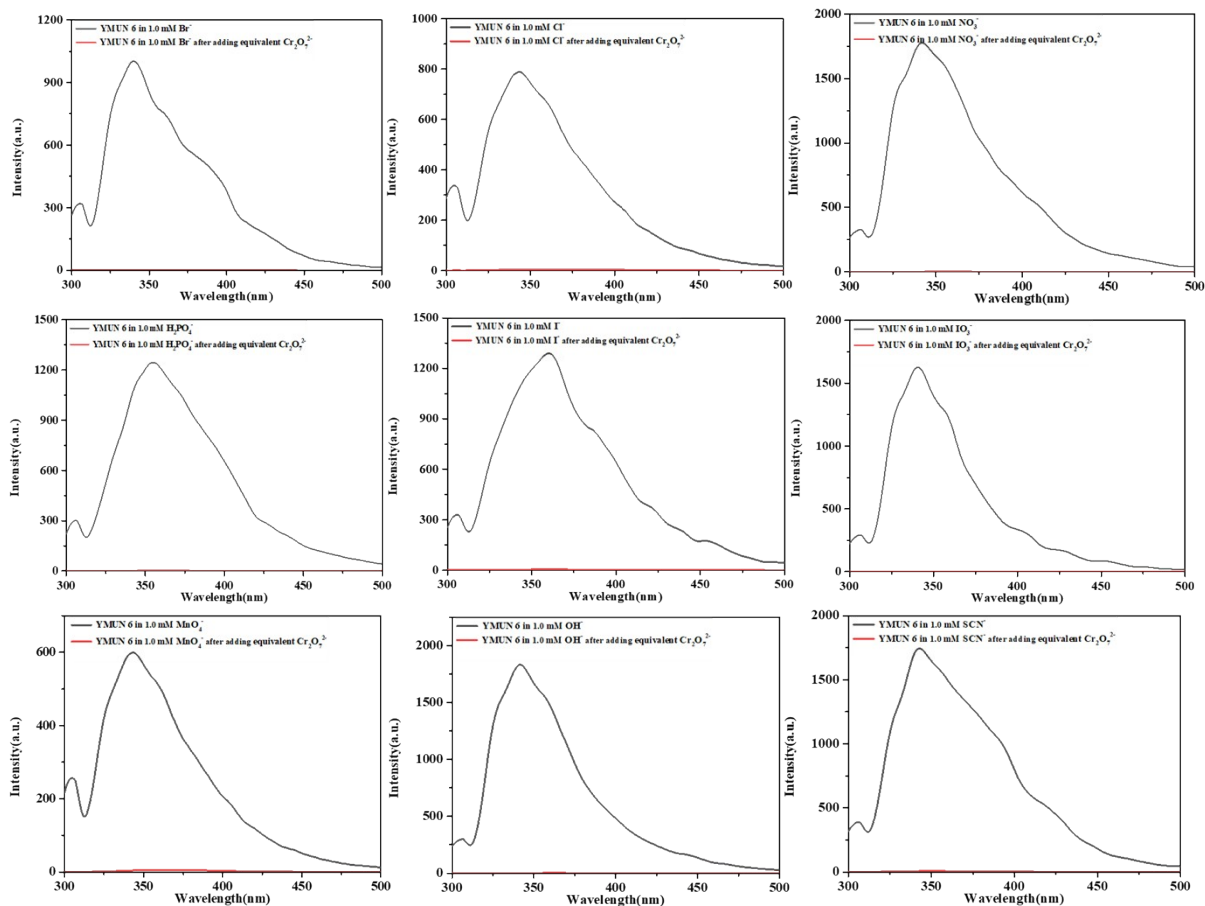


Figure S18. The fluorescence spectra of YMUN 6 in various anions (1.0 mM) (Black lines), and adding equivalent $\text{Cr}_2\text{O}_7^{2-}$ in various anions solution.

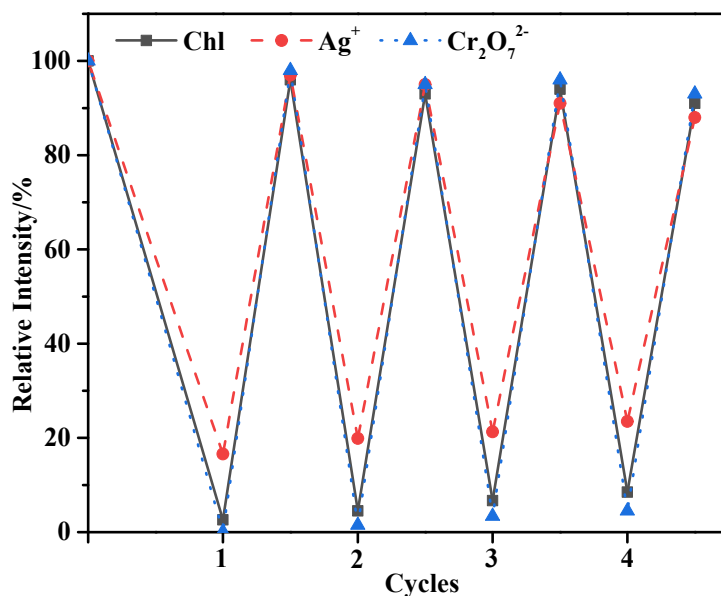


Figure S19. The recycling fluorescence intensity of YMUN 6 for Chl antibiotic, Ag^+ ion, and $\text{Cr}_2\text{O}_7^{2-}$ ion, respectively, after four times.

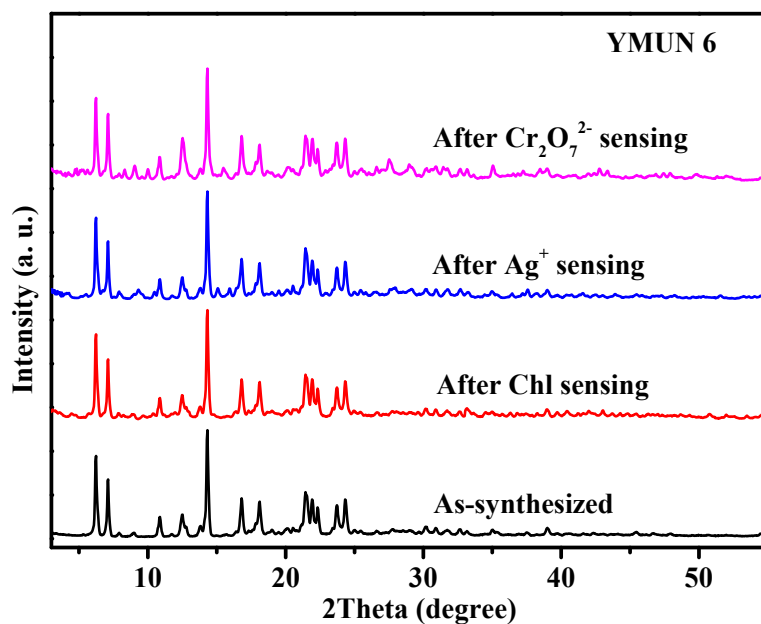


Figure S20. The comparison of PXR patterns for YMUN 6 after Chl antibiotic, Ag⁺, Cr₂O₇²⁻ ions sensing.

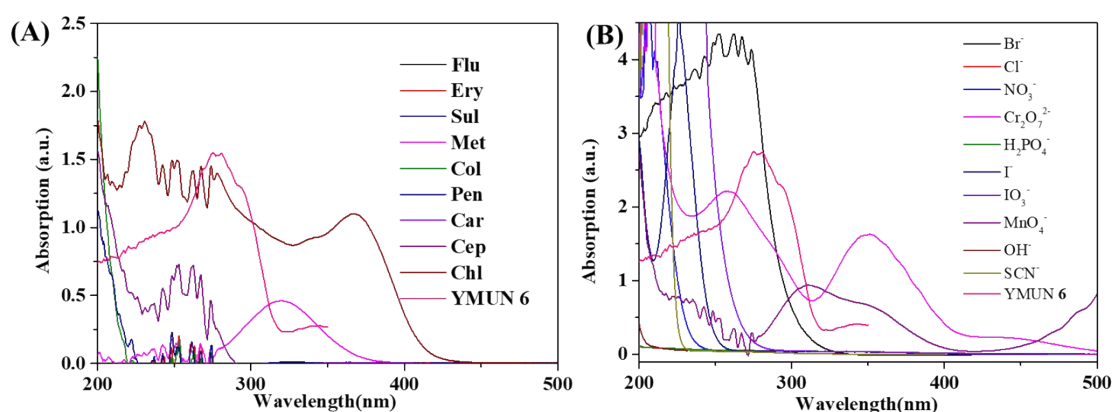


Figure S21. The UV-vis spectra of Chl antibiotic/Cr₂O₇²⁻ ion in aqueous solutions and the excitation spectrum of YMUN 6.

Table S1 Selected bond lengths (Å) and angles (°) for YMUN 6–8.

YMUN 6			
Zn1—O2	1.968 (2)	Zn2—O8 ⁱⁱⁱ	1.956 (2)
Zn1—O6 ⁱ	1.956 (2)	Zn2—O11	1.931 (2)
Zn1—N4 ⁱⁱ	2.022 (3)	Zn2—N8 ^{iv}	2.033 (3)
Zn1—N1	2.004 (3)	Zn2—N5	2.023 (3)
O2—Zn1—N4 ⁱⁱ	91.51 (11)	O6 ⁱ —Zn1—N1	98.39 (11)
O2—Zn1—N1	107.74 (11)	N1—Zn1—N4 ⁱⁱ	124.10 (12)
O6 ⁱ —Zn1—O2	117.63 (10)	O8 ⁱⁱⁱ —Zn2—N8 ^{iv}	115.24 (11)

O6 ⁱ —Zn1—N4 ⁱⁱ	118.40 (11)	O8 ⁱⁱⁱ —Zn2—N5	91.15 (11)
O11—Zn2—O8 ⁱⁱⁱ	122.29 (11)	C1—O2—Zn1	120.1 (2)
O11—Zn2—N8 ^{iv}	95.87 (11)	C47—O8—Zn2 ⁱⁱⁱ	115.4 (2)
O11—Zn2—N5	114.58 (11)	C66—O11—Zn2	122.4 (2)
N5—Zn2—N8 ^{iv}	119.90 (12)	C20—O6—Zn1 ⁱ	113.9 (2)
C87—N8—Zn2 ⁱⁱ	135.7 (2)	C46—N4—Zn1 ^{iv}	133.8 (2)
C86—N8—Zn2 ⁱⁱ	117.6 (2)	C40—N4—Zn1 ^{iv}	118.9 (2)
C21—N1—Zn1	137.2 (2)	C67—N5—Zn2	117.6 (2)
C27—N1—Zn1	116.9 (2)	C68—N5—Zn2	130.2 (2)

Symmetry codes: (i) $-x, -y, -z$; (ii) $x, y-1, z-1$; (iii) $-x+1, -y+1, -z+1$; (iv) $x, y+1, z+1$.

YMUN 7

Zn2—O5 ⁱ	1.977 (2)	Zn1—O1 ^{iv}	1.961 (2)
Zn2—O5	1.977 (2)	Zn1—O1	1.961 (2)
Zn2—N4 ⁱⁱ	2.026 (2)	Zn1—N1 ^{iv}	2.012 (3)
Zn2—N4 ⁱⁱⁱ	2.026 (2)	Zn1—N1	2.012 (3)
O5 ⁱ —Zn2—O5	115.21 (14)	N4 ⁱⁱ —Zn2—N4 ⁱⁱⁱ	108.02 (14)
O5 ⁱ —Zn2—N4 ⁱⁱⁱ	118.02 (10)	O1 ^{iv} —Zn1—O1	119.21 (14)
O5 ⁱ —Zn2—N4 ⁱⁱ	99.20 (9)	O1 ^{iv} —Zn1—N1 ^{iv}	102.48 (10)
O5—Zn2—N4 ⁱⁱ	118.02 (10)	O1—Zn1—N1 ^{iv}	108.57 (10)
O5—Zn2—N4 ⁱⁱⁱ	99.20 (9)	O1 ^{iv} —Zn1—N1	108.57 (10)
O1—Zn1—N1	102.48 (10)	N1 ^{iv} —Zn1—N1	116.23 (15)
N1 ^{iv} —Zn1—N1	116.23 (15)	C21—O5—Zn2	110.49 (19)
C21—O5—Zn2	110.49 (19)	C1—O1—Zn1	112.8 (2)
O1—Zn1—N1	102.48 (10)	C35—N4—Zn2 ^v	129.1 (2)
C24—N1—Zn1	132.5 (2)	C22—N1—Zn1	121.6 (2)

Symmetry codes: (i) $-x+1, y, -z+3/2$; (ii) $-x+1, y-3, -z+3/2$; (iii) $x, y-3, z$; (iv) $-x+2, y, -z+3/2$; (v) $x, y+3, z$.

YMUN 8

Zn1—O3	1.952 (2)	Zn1—N1	2.030 (3)
Zn1—O7 ⁱ	1.974 (2)	Zn1—N4 ⁱⁱ	2.048 (3)
O3—Zn1—O7 ⁱ	113.32 (11)	O7 ⁱ —Zn1—N1	95.75 (11)
O3—Zn1—N1	137.25 (12)	O7 ⁱ —Zn1—N4 ⁱⁱ	93.57 (11)

O3—Zn1—N4 ⁱⁱ	106.48 (11)	N1—Zn1—N4 ⁱⁱ	101.99 (12)
C19—O3—Zn1	104.9 (2)	C1—N1—Zn1	117.6 (3)
C38—O7—Zn1 ⁱ	120.6 (2)	C2—N1—Zn1	136.4 (2)
C18—N4—Zn1 ⁱⁱⁱ	122.2 (2)	C17—N4—Zn1 ⁱⁱⁱ	132.6 (3)

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $x+1/2, -y+1/2, z+1/2$; (iii) $x-1/2, -y+1/2, z-1/2$.

Table S2 Hydrogen bond distances (Å) and angles (°) of **YMUN 6–8**

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠DHA
YMUN 6				
C18-H18···O7	0.95	2.54	3.441(4)	159
C25-H25···O12	0.95	2.27	3.080(5)	143
C27-H27···O7	0.95	2.32	3.149(4)	145
C42-H42···O10	0.95	2.33	3.141(5)	143
C45-H45···O5	0.95	2.54	2.932(6)	105
C70-H70···O4	0.95	2.37	3.308(5)	171
C82-H82···O6	0.95	2.46	3.099(5)	124
C86-H86···O1	0.95	2.33	3.134(4)	142
C86-H86···O7	0.95	2.49	3.113(5)	123
YMUN 7				
C25-H25A···O2	0.99	2.47	3.061(4)	117
C32-H32B···O6	0.99	2.53	3.009(4)	109
YMUN 8				
C1-H1···O6	0.95	2.43	3.226(5)	141
C13-H13···O6	0.95	2.20	3.153(4)	178