Electronic Supporting Information (ESI)

Materials and instruments

All purchased starting materials and solvents were used without further purification. ¹H NMR spectra were obtained using Bruker Avance 500 MHz spectrometers. Chemical shifts are reported as δ in ppm and are internally referenced to tetramethylsilane (TMS, 0.0 ppm for ¹H) or dimethyl sulfoxide-d6 (DMSO-d6, 2.5 ppm for ¹H). Infrared spectroscopy (IR) spectra were recorded on Nicolet iS5 with pressed KBr pellets. UV-vis absorption spectra were taken on PerkinElmer Lambda 750. The powder XRD patterns were collected in the $2\theta = 3^{\circ}-50^{\circ}$ range on a Bruker D8 ADVANCE X-ray diffractometer with the operating power set to 40 kV/40 mA at room temperature. All TGA experiments were performed under a N₂ atmosphere from 30-650 °C at a rate of 10 °C min⁻¹ using a GA-500 instrument. Brunauer Emmett Teller (BET) specific surface area obtained by N₂ adsorption experiment on a Micrometric ASAP 2020 V4.01 instrument. Fluorescence spectra were recorded on a Perkin-Elmer LS55 spectrofluorometer. Solid fluorescence quantum yields were determined with a Horiba Jobin Yvon Fluorolog-3 spectrofluorimeter. Time-resolved fluorescence measurements were performed using a Life-Spec-ps fluorescence lifetime analytical spectrometer (Edinburgh Instruments).

Determination of TMPyPE content

The content of cationic TMPyPE can be determined *via* ¹H-NMR and UV–vis spectroscopy analysis. The ¹H NMR study was performed to determine the amount of TMPyPE within per $[Zn_8(Ad)_4(BPDC)_6O]$ unit (Fig. S1). 8 mg of activated sample was completely dissolved in 500 µL of DMSO-*d6* and 20 µL of D₂SO₄. ¹H NMR (500 MHz) spectra of dissolved sample was collected at room temperature. The integration

for one set of the adenine hydrogens was set as 1 (for the $[Zn_2(Ad)_1(BPDC)_{1.5}O_{0.25}]$ unit). We then integrated the methyl peak for TMPyPE cation, which shows that each $[Zn_8(Ad)_4(BPDC)_6O]$ unit contains 0.5 TMPyPE.





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Fig. S1 ¹H NMR spectra (500 MHz) of (A) TMPyPE dissolved in DMSO- d_6 and (B) activated TMPyPE@bio-MOF-1 dissolved in DMSO- d_6 and D₂SO₄.

In order to verify the results of ¹H NMR analysis, the amount of TMPyPE also be determined by UV-vis spectroscopy. The absorbance of different concentration of TMPyPE in DMF solution was measured and repeated three times, and then the average values were calculated. Therefore, the relationship for the intensity-concentration of TMPyPE in DMF solution could be obtained (Fig. S2). Activated sample (about 1.5 mg) was dissolved in 1 mL DMF solution containing $20\mu L D_2SO_4$ to become clear solution. The obtained solution was diluted 20 times. The absorbance

of the solution was measured, and the concentration was calculated by equation: y = 36.60008x + 0.00112 (y represents the absorbance and x is the concentration of TMPyPE). Then the amount of TMPyPE in TMPyPE@bio-MOF-1 was calculated to be 0.180 mg. Assuming the number of replaced cations is n, the chemical formula for dried TMPyPE-included compound is $Zn_8(C_5H_4N_5)_4(C_{14}H_8O_4)_6O(Me_2NH_2)_{2.4n}(C_{50}H_{44}N_4)_n$, whose molecular weight is 2516.78 + 46.09(2-4n) + 700.36n. In this compound, the mass content of TMPyPE cations is expressed as $R = m_{TMPyPE}/m_{TMPyPE@bio-MOF-1} = 700.36n/[2516.78 + 46.09(2-4n) + 700.36n]$ (R is the mass fraction of cationic TMPyPE in the composite TMPyPE@bio-MOF-1). Determined through the above procedure, R = 0.1200. Therefore, the value of n can be derived as 0.49, which is similar to the result of ¹H NMR analysis.



Fig. S2 The absorbance-concentration diagram and the fitted curve for TMPyPE DMF solution.



Fig. S3 The partial enlargement of Fig. 2B (A) and the PXRD patterns of activated TMPyPE@bio-MOF-1 (black), activated TMPyPE@bio-MOF-1 after being soaked in aqueous solutions with PH value of 3 (red), 6 (blue) and 9 (green) (B).



Fig. S4 SEM image of TMPyPE@bio-MOF-1 (powder product is on the top and crystal product is on the bottom).



Fig. S5 TGA plots of TMPyPE@bio-MOF-1 and activated TMPyPE@bio-MOF-1.



Fig. S6 FTIR spectra of TMPyPE, TMPyPE@bio-MOF-1 and bio-MOF-1.



Fig. S7 Solid-state PL spectra of bio-MOF-1 and TMPyPE (λ_{ex} = 300 nm).



Fig. S8 Solid-state PL spectra of TMPyPE@bio-MOF-1 and activated TMPyPE@bio-MOF-1 (λ_{ex} = 365 nm).



Fig. S9 (A) Emission spectra of TMPyPE DMF solution (10⁻⁶ mol L⁻¹) and the filtrate after suspending the activated TMPyPE@bio-MOF-1 in DMF for 24 h excited at 365 nm. (B) Emission spectra of TMPyPE in water (10⁻⁶ mol L⁻¹) and the filtrate after suspending the activated TMPyPE@bio-MOF-1 in water for 24 h excited at 365 nm.



Fig. S10 (A) The fitting plot of the I_0/I of activated TMPyPE@bio-MOF-1 with the increasing concentration of NFZ at low concentration range. (B) The fitting plot of the

 I_0/I of activated TMPyPE@bio-MOF-1 with the increasing concentration of NFT at low concentration range.



Fig. S11 (A) Emission spectra of activated TMPyPE@bio-MOF-1 suspension upon addition of nitrofurazone (NFZ) aqueous solution (0.222 mM). (B) The

fitting plot of the I_0/I of activated TMPyPE@bio-MOF-1 suspension with the increasing concentration of NFZ at low concentration range.



Fig. S12 (A) Emission spectra of activated TMPyPE@bio-MOF-1 suspension upon addition of nitrofurantoin (NFT) aqueous solution (0.225 mM). (B) The fitting plot of

the I_0/I of activated TMPyPE@bio-MOF-1 suspension with the increasing concentration of NFT at low concentration range.









Wavelength (nm)



Fig. S13 Emission spectra of activated TMPyPE@bio-MOF-1 suspension dispersed in water upon addition of different antibiotics of MDZ, CAP, STZ, SDZ, SMZ, NFX, EM and AMX aqueous solution (1 mM).



Fig. S14 Stern-Volmer (SV) plots for antibiotics aqueous solution.



Fig. S15 PXRD patterns of activated TMPyPE@bio-MOF-1 (blue) and activated TMPyPE@bio-MOF-1 after being soaked in NFZ (red) and NFT (black), respectively.



Fig. S16 Spectral overlap between the absorption spectra of antibiotics aqueous solution and the emission spectrum of activated TMPyPE@bio-MOF-1 aqueous suspension.





Fig. S17 Emission spectra (λ_{ex} =440 nm) of activated TMPyPE@bio-MOF-1 suspension upon addition of NFZ (A) and NFT (C) aqueous solution (1 mM). Stern–Volmer plot of NFZ (B) and NFT (D).



Fig. S18 HOMO and LUMO energies for TMPyPE and selected antibiotics.