# Supporting Information

## Synergistic antibacterial effect of quaternary ammonium functionalized metal-organic framework

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### 1.1 General Procedure for the construction and characterization of materials

#### 1.1.1 Experimental materials and analytical instruments

*Pseudomonas aeruginosa* (*P. aeruginosa*, ATCC27853) and MRSA (ATCC 43300) were obtained from ATCC (American Type Culture Collection). UV-vis absorption spectra were recorded using a Varian Cary 300 UV-visble spectrophotometer. Dynamic light scattering (DLS) was carried out using a LA-300 DLS Nano-Analyzer. Energy dispersive spectroscopy (EDS) analysis was performed using a HITACHI S-4800 scanning electron microscope (SEM) equipped with an Oxford X-max spectrometer. Fourier-transform infrared spectroscopy (FT-IR) was performed on NEXUS 470. The morphology of the samples was analyzed by a HITACHI S-4800 SEM and a JEM-2010 transmission electron microscope (TEM). The surface compositions of the samples were measured by X-ray photoelectron spectroscopy (XPS, Versa Probe PHI 5000).

#### 1.1.2 Preparation of the Fe-TBP-QAS nanoparticles.

$Fe(NO_3)_3 \cdot 9H_2O$ (10g) and $Na(OOCCH_3) \cdot 3H_2O$ (12 g) were dissolved in 10 mL of deionized water. The solution was stirred for 24 h under room temperature. The red precipitation was filtered and washed with deionized water several times. The obtained product $[Fe_3O(OOCCH_3)_6OH] \cdot 2H_2O$ was dry in under 50 °C. then, to a 50 mL glass vial was added 10 mL of $Fe_3O(OAc)_6(H_2O)_3(OAc)$ solution (2.2 mg $mL^{-1}$ in DMF), 5.0 mL of TCPP solution (2.6 mg $mL^{-1}$ in DMF), and 2 mL of formic acid. After the resulting mixture was dissolved via sonication, the vial was placed oven at 90 °C for 18 hours. The precipitate was collected by centrifugation (12000 G) and washed with DMF and ethanol to obtained product Fe-TBP nanoparticles. Finally, to deionized water of Fe-TBP (3 mL, 2 mg $mL^{-1}$), DBCO (30 μL, 50 mM) was added. The resulting mixture was sonicated for 5 min, then stirred at room temperature for 12 h in the dark to produce the Fe-TBP/DBCO. The precipitate was collected by centrifugation and washed with deionized water. Then, the precipitate was redispersed in deionized water, and QAS were added, and DBCO and QAS was synthesized as described previously[1]. After ultrasonic dispersion for several minutes, the mixture was stirred for 6 hours in

the dark. The **Fe-TBP-QAS** was collected by centrifugation and washed several times with deionized water.

### 1.1.3 UV-vis absorption spectroscopy.

Test solutions of TCPP (20 μM)、Fe-TBP (10 μg $mL^{-1}$) and the Fe-TBP-QAS (10 μg $mL^{-1}$) were prepared in Tris-HCl buffer (0.01 M, pH 7.4), and the UV-vis absorption spectra of the solutions were obtained on Varian Cary 300 UV-vis spectrophotometer.

### 1.1.4 Determination of Dynamic Light Scattering and zeta potential.

The size and zeta potential change of Fe-TBP (10 μg $mL^{-1}$)、Fe-TBP-DBCO (10 μg $mL^{-1}$) and the Fe-TBP-QAS (10 μg $mL^{-1}$) solution were analyzed on a Horiba LA-300 DLS nano-analyzer.

### 1.1.5 Determination of suface area of Fe-TBP-QAS

The nitrogen adsorption isotherms analysis determined the Brunauer Emmett Teller (BET) surface area of Fe-TBP-QAS (100 mg).

### 1.1.6 Scanning electron microscope and X-ray photoelectron spectroscopy.

A droplet of Fe-TBP (10 μg $mL^{-1}$)、Fe-TBP-DBCO (10 μg $mL^{-1}$) and the Fe-TBP-QAS (10 μg $mL^{-1}$) suspension onto 200 mesh holey carbon copper grids. Then, images were recorded by a HITACHI S-4800 scanning electron microscope. And the surface compositions of the samples were measured by X-ray photoelectron spectroscopy (XPS, Versa Probe PHI 5000).

### 1.1.7 Detection of reactive oxygen species (ROS).

The Fe-TBP-QAS nanomaterials suspension was prepared with a dose of 10 μg/mL (final concentration) and 5,5-dimethyl-1-pyrroline-N-oxide (DMPO) was added (final concentration= 40 μM). The mixed solution was exposed to light (650 nm, 1 W $cm^{-2}$) for 20 min, and the spectrum was recorded by electron spin resonance (ESR) spectroscopy.

### 1.1.8 Analysis of bacterial morphology by Scanning electron microscope.

*P. aeruginosa* (ATCC 27853) was grown in LB (Luria-Bertani) medium to $OD_{600}$ =

0.15, and then incubated with PBS, Fe-TBP (10 μg $mL^{-1}$), Fe-TBP-QAS (10 μg $mL^{-1}$). Then, bacteria were treated with light (650 nm, 1 W $cm^{-2}$) for 20 min. After incubation for 1 h, the resulting bacteria were collected and fixed in 2.5% glutaraldehyde in phosphate-buffered saline at overnight and then washed with PBS twice after fixation. Then, bacteria were dehydrated using an ethanol series with an increasing concentration (20%, 30%, 50%, 60%, 80%, 90%, 98%) for 5 min, and finally suspended in pure t-butanol for 15 min. Bacteria were air-dried and coated with gold for SEM imaging on a Hitachi S4800 Scanning Electron Microscope.

**1.1.9 Measurement of bacterial viability.**

The antibacterial effect of Fe-TBP (200 μg $mL^{-1}$) and Fe-TBP-QAS (200 μg $mL^{-1}$) without and with light irradiations (650 nm, 1 W $cm^{-2}$, 20 min) by plate counting method. Bacteria were seeded at a density of $10^6$ cells $mL^{-1}$ in a 96-well plate, followed by incubation with different components. Then, the suspensions were treated without and with light irradiations. Then, bacteria were further cultured with complete medium for 4 h and then the bacteria and material incubation solution was further diluted to $10^3$, $10^4$, and $10^5$ times using sterile water. Each experiment was carried out in triplicate.

## 1.2 Additional experimental details figures

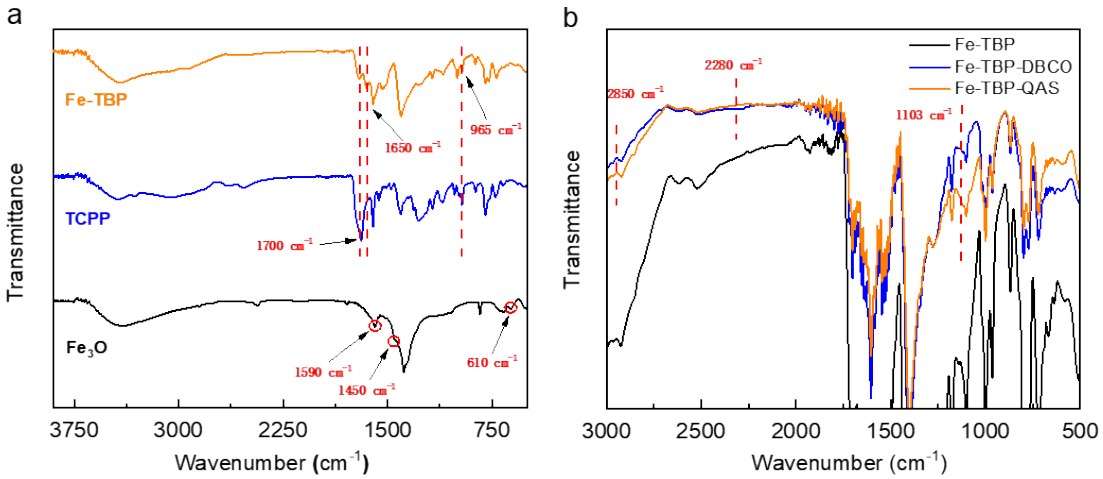


**Figure S1.** FTIR spectra of (a) $Fe_3O$、TCPP、Fe-TBP and (b) Fe-TBP-DBCO、Fe-TBP-QAS.

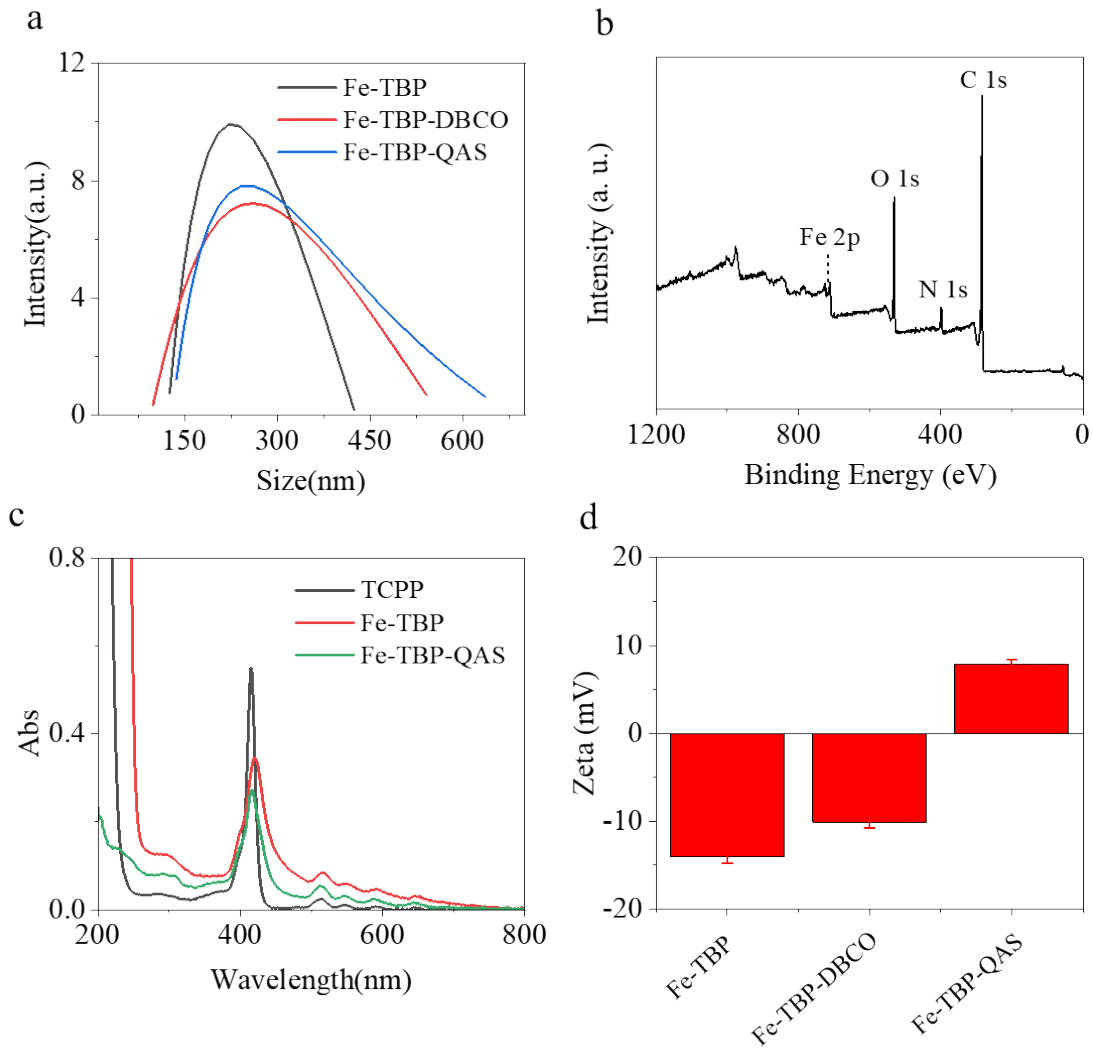


**Figure S2.** (a) Dynamic light scattering of Fe-TBP (10 μg $mL^{-1}$), Fe-TBP-DBCO (10 μg $mL^{-1}$) and Fe-TBP-QAS (10 μg $mL^{-1}$) in Tris-HCl (0.01 M, pH 7.4) buffer solution. (b) X-ray photoelectron spectroscopy (XPS) spectra of Fe-TBP-QAS (10 μg $mL^{-1}$). (c) UV-vis absorbance spectral changes of TCPP (10 μg $mL^{-1}$), Fe-TBP (10 μg $mL^{-1}$) and Fe-TBP-QAS (10 μg $mL^{-1}$) in Tris-HCl (0.01 M, pH 7.4) buffer solution. (d) the zeta potential of Fe-TBP (10 μg $mL^{-1}$), Fe-TBP-DBCO (10 μg $mL^{-1}$) and Fe-TBP-QAS (10 μg $mL^{-1}$) in Tris-HCl (0.01 M, pH 7.4) buffer solution.

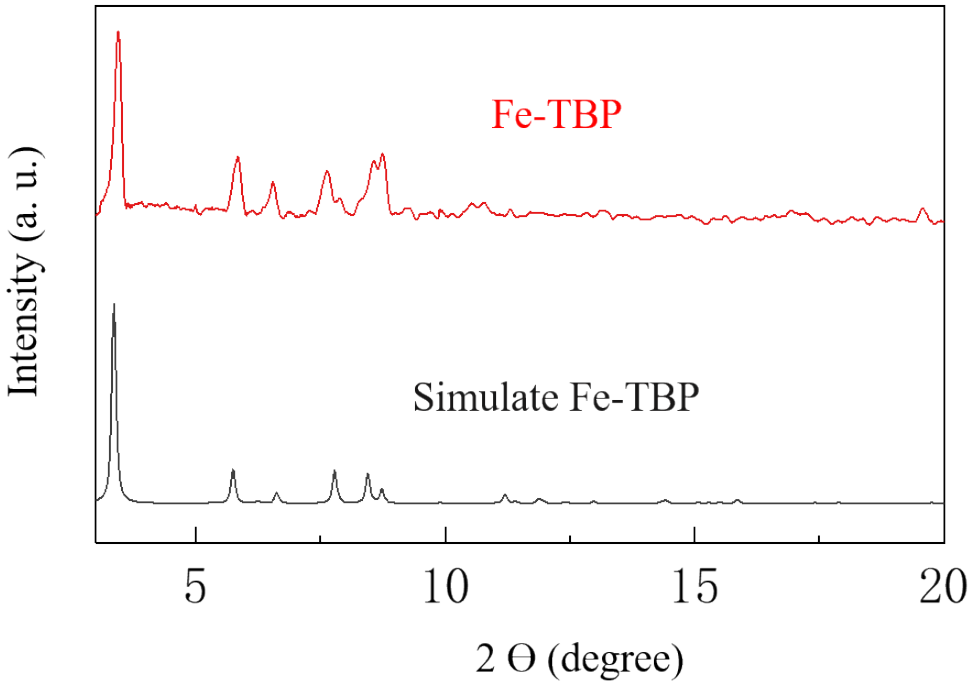


**Figure S3.** PXRD patterns of synthetic Fe-TBP and simulated Fe-TBP at 77K.

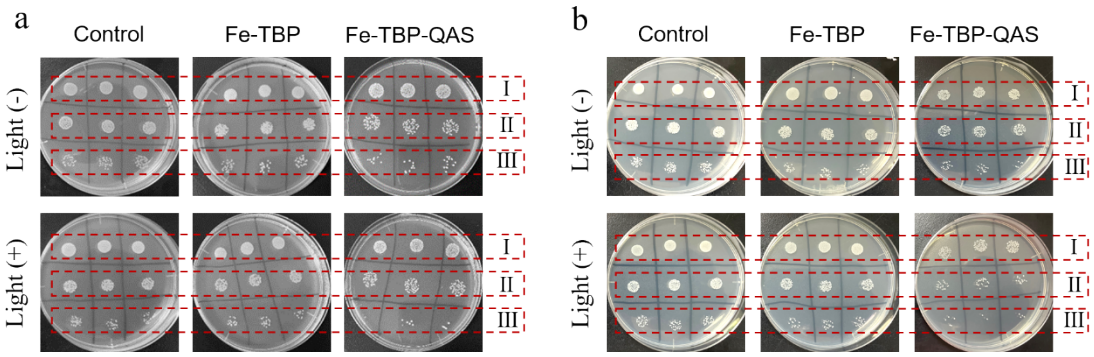


**Figure S4.** Bacterial cultures of (a) *P. aeruginosa* (ATCC 27853) and (b) MRSA (ATCC 43300) without and with treatment with Fe-TBP and Fe-TBP-QAS. I: Bacteria and material incubating solution diluted $10^3$ times; II: Bacteria and material incubating solution diluted $10^4$ times; III: Bacteria and material incubating solution diluted $10^5$ times.

**Table1**. Minimum inhibitory concentration (MIC) and Minimum bactericidal concentration (MBC) of the Fe-TBP-QAS for *P. aeruginosa* and MRSA

| | *P. aeruginosa*（ATCC 27853） | | MRSA (ATCC 43300) | |
|---|---|---|---|---|
| Sample | MIC (μg /mL) | MBC (μg /mL) | MIC (μg /mL) | MBC (μg /mL) |
| Fe-TBP-QAS | 512 | 1024 | 512 | 1024 |

## 1.3 Additional references

1. H.-Y. Fan, S. K. Kawade, A. K. Adak, C. Cho, K.-T. Tan, C.-C. Lin. Silver-Coated $Cu_2O$ Nanoparticle Substrates for Surface Azide–Alkyne Cycloaddition. *ACS Applied Nano Materials* **2021.** *4* (2), 1558-1566.