Supporting Information for

Metal-Organic Framework-based Fluorescence Resonance Energy Transfer Nanoprobe for Highly Selective Detection of *Staphylococcus Aureus*

Jing Qiao[‡], Xuanbo Chen[‡], Xingliang Xu, Ben Fan, Ying-Shi Guan^{*}, Hong Yang^{*}, and Quan Li^{*}

Institute of Advanced Materials and School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, China

Calculation of the content of HCAA and VAN-PEG-FITC.

The HCAA content in HCAA@UiO-66 was determined according to the absorbance of HCAA and UiO-66. We can use the following equations to calculate the amount of HCAA:

 $A_{270} = \varepsilon_{\text{UiO-66, 270}} \times C_{\text{UiO-66}} \times b$

 $A_{325} = \varepsilon_{\text{UiO-66, 325}} \times C_{\text{UiO-66}} \times b + \varepsilon_{\text{HCAA, 325}} \times C_{\text{HCAA}} \times b$

The calibration curves of absorbance intensity of HCAA at 325 nm and UiO-66 at 325 nm and 270 nm in ethanol were recorded in Fig. S1.



Fig. S1 Calibration curves of absorbance in ethanol of (A) HCAA at 325 nm, (B) UiO-66 at 325 nm, and (C) 270 nm.



Fig. S2 Absorbance of HCAA@UiO-66 in ethanol.

According to the calibration curves shown in Figure S1 and the absorbance values at 270 nm and

325 nm in Figure S2, the following equations can be obtained:

$$A_{270} = 3.037 = 7.198 \times C_{\text{UiO-66}}$$

 $A_{325} = 1.569 = 3.775 \times C_{\text{UiO-66}} + 23.87 \times C_{\text{HCAA}}$

Therefore, C_{UiO-66} and C_{HCAA} were calculated to be 0.42 mg/mL and 0.00022 mg/mL, respectively, which means that HCAA possessed a proportion of 0.52% in the UiO-66.

The VAN-PEG-FITC content in VAN-PEG-FITC/HCAA@UiO-66 composite was calculated by the difference between the actual dosage and the amount in the supernatant. By using the following equation to calculate the amount of FITC:

$$A_{450} = \varepsilon_{\rm FITC} \times C_{\rm FITC} \times b$$

The calibration curves of absorbance intensity of FITC at 450 nm in saline (pH=7.2) were made in Figure S4.



Fig. S3 Calibration curve of absorbance in saline (pH=7.2) of FITC at 450 nm.



Fig. S4 Absorbance of supernatant of free VAN-PEG-FITC.

8 mg of HCAA@UiO-66 and 1.6 mg VAN-PEG-FITC were mixed in 10 mL saline to give the composite. The absorbance of the centrifugated supernatant at 450 nm was measured to be 0.31556 (Fig. S5). According to the calibration curve shown in Fig. S4 and the absorbance value at 450 nm from Fig. S5, the following equation can be obtained:

 $A_{450} = 0.31566 = 8722.8 \times C_{\text{FITC}} - 0.05835$

Therefore, C_{FITC} was calculated to be 4.29×10^{-5} mmol/mL, indicating the amount of VAN-PEG-

FITC in the supernatant was 1.5578 mg. This shows that $0.0422 \text{ mg} (1.16 \times 10^{-5} \text{ mmol})$ of VAN-PEG-FITC was coated on 8 mg HCAA@UiO-66, which embedded $0.00432 \text{ mg} (1.96 \times 10^{-4} \text{ mmol})$ of HCAA. Furthermore, the molar ratio of FRET donor (HCAA) and acceptor (FITC) (D/A) could be calculated at 16.9.



Fig. S5 Synthesis of VAN-PEG-FITC.



Fig. S6 ¹H NMR spectrum of VAN-PEG-FITC (600MHz, DMSO-d₆).



Fig. S7 MALDI-TOF-MS spectrum of VAN-PEG-FITC (A) and FTIR spectra of HCAA@UiO-66, PEG-FITC, PEG-FITC/HCAA@UiO-66, VAN-PEG-FITC, VAN-PEG-FITC/HCAA@UiO-66 (B).



Fig. S8 (a) SEM and (b) TEM images of synthesized UiO-66.



Fig. S9 Fluorescence lifetimes at 440 nm in HCAA@UiO-66 and VAN-PEG-FITC/HCAA@UiO-66.



Fig. S10 I_{440}/I_{520} values of VAN-PEG-FITC/HCAA@UiO-66 and its diluents. Insert Photographs of the probe suspension under a UV lamp of 365 nm.



Fig. S11 Emission spectra of HCAA@UiO-66 (0.25 mg/mL) mixing with PEG-FITC (ranging from 0 to 0.1 mg/mL).



Fig. S12 The plot of fluorescence ratio I_{440}/I_{520} values against PEG-FITC concentration.



Fig. S13 I_{440}/I_{520} values of PEG-FITC/HCAA@UiO-66 after co-incubating with *S. aureus* and interfering bacteria.



Fig. S14 CLSM images of *S. aureus* and interfering bacteria after treatment with PEG-FITC/HCAA@UiO-66.