## **Supporting Information**

## NaGdF4:Nd@NaGdF4 Core-Shell Down-Conversion Nanoparticles as NIR-II Fluorescent Probes for Targeted Imaging of Bacteria

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**Figure S1.** (a) TEM image of NaGdF<sub>4</sub>:5%Nd core NPs. (b) Size distribution of NaGdF<sub>4</sub>:5%Nd core NPs obtained by Gaussian fitting of particle size statistical software.



Figure S2. X-ray diffraction patterns of OA-capped DCNPs, PAA-DCNPs, and DCNPs-Van.



**Figure S3.** X-ray diffraction patterns of NaGdF<sub>4</sub>:5%Nd and NaGdF<sub>4</sub>:xNd@NaGdF<sub>4</sub> (x = 1, 3, 5, 8, 10%) NPs.

Space group	x = 0%	x = 5%	x = 10%	
	P6 <sub>3</sub> /m	P6 <sub>3</sub> /m	P6 <sub>3</sub> /m	
a (Å)	6.020	6.048	6.055	
b (Å)	6.020	6.048	6.055	
c (Å)	3.601	3.612	3.615	
V (Å <sup>3</sup> )	113.018	114.420	114.780	
$\chi^2$		3.571	2.731	
R <sub>wp</sub> (%)		8.982	8.244	
$R_{p}(\%)$		6.889	6.389	

**Table S1.** Refined structural parameters of NaGdF<sub>4</sub>:xNd@NaGdF<sub>4</sub> (x = 0, 5, 10%) NPs.



**Figure S4.** Luminescence intensity of DCNPs-Van as a function of irradiation time upon 808 nm excitation (300 mW/cm<sup>2</sup>).



Figure S5. FTIR spectra of (1) OA-DCNPs, (2) PAA-DCNPs, (3) PAA, (4) DCNPs-Van, and (5) Van.

Compared with OA-DCNPs, the absorption bands around 2926 and 2854 cm<sup>-1</sup> corresponding to C-H stretching vibrations decrease and the O-H stretching band around 3434 cm<sup>-1</sup> increases in PAA-DCNPs and DCNPs-Van. Since OA on the surface of DCNPs is replaced by PAA, the characteristic vibration band of C=O at  $\sim$ 1719 cm<sup>-1</sup> increases in PAA-DCNPs. After covalent coupling with vancomycin, the absorption bands of functional groups of vancomycin appears in DCNPs-Van.



**Figure S6.** Quantification of vancomycin. (a) UV-Vis absorbance spectra of concentration-dependent vancomycin and (b) corresponding calibration curve.



**Figure S7.** NIR-II images of (a)  $10^7$  CFU/mL *E. coli* + different concentrations of *S. aureus* suspensions, and (c)  $10^7$  CFU/mL *S. aureus* + different concentrations of *E. coli* suspensions upon 808 nm excitation (300 mW/cm<sup>2</sup>); luminescence response of (b)  $10^7$  CFU/mL *E. coli* + different concentrations of *S. aureus* suspensions, and (d)  $10^7$  CFU/mL *S. aureus* + different concentrations of *E. coli* suspensions.



**Figure S8.** NIR-II images of (a) *B. subtilis* suspensions, (d) *E. faecalis* suspensions and (g) *P. aeruginosa* suspensions upon 808 nm excitation (300 mW/cm<sup>2</sup>); luminescence response of (b) *B. subtilis* suspensions, (c) *B. subtilis* original supernatants, (e) *E. faecalis* suspensions, (f) *E. faecalis* original supernatants, (h) *P. aeruginosa* suspensions, and (i) *P. aeruginosa* original supernatants at different bacterial concentrations. The insets of (b) and (e) show a linear relationship between the luminescence response and the logarithm of bacterial concentrations from 10<sup>4</sup> to  $10^7$  CFU/mL.

Fig. S8b (inset) shows a linear relationship between the luminescence response and the logarithm of the concentration of *B. subtilis* suspensions in the concentrations range from  $10^4$  to  $10^7$  CFU/mL with a slope of 4.86 and a correlation coefficient of 0.995; Fig. S8e (inset) shows a linear relationship between the luminescence response and the logarithm of the concentration of *E. faecalis* suspensions,  $10^4$  to  $10^7$  CFU/mL, with a slope of 3.74 and a correlation coefficient of 0.997.



Figure S9. (a) NIR-II images of DCNPs-Van covered by pork muscle tissues with various thicknesses upon 808 nm excitation ( $300 \text{ mW/cm}^2$ ). (b) NIR-II signal intensity from DCNPs-Van covered by tissues with different temperatures as a function of different depths.

1 min	2 min	3 min	4 min	5 min	High
15 min	30 min	2 h	6 h	10 h	
				- 13	Low

**Figure S10.** NIR-II imaging of healthy mice after intravenous injection of DCNPs-Van at different time intervals upon 808 nm excitation (300 mW/cm<sup>2</sup>).