## **Supporting Information**

## Polydopamine coated multifunctional lanthanide theranostic agent for vascular malformation and tumor vessel imaging beyond 1500 nm and imaging-guided photothermal therapy

Xiaolong Li,<sup>a</sup> Mingyang Jiang,<sup>a</sup> Songjun Zeng<sup>a,\*</sup> and Hongrong Liu<sup>a,\*</sup>

<sup>a</sup> School of Physics and Electronics and Key Laboratory of Low-dimensional Quantum Structures and Quantum Control of the Ministry of Education, Synergetic Innovation Center for Quantum Effects and Applications, Hunan Normal University, Changsha, Hunan 410081 (China)

<sup>\*</sup> Address correspondence to songjunz@hunnu.edu.cn; hrliu@hunnu.edu.cn



**Figure S1**. The typical TEM and XRD results of the as-prepared NaLuF<sub>4</sub>: Yb/Er samples with/without doping Gd: (A) TEM image of NaLuF<sub>4</sub>: Gd/Yb/Er. (B) TEM image of NaLuF<sub>4</sub>: Yb/Er. (c) XRD patterns of the NaLuF<sub>4</sub>: Yb/Er (blue line), and NaLuF<sub>4</sub>: Gd/Yb/Er (red line). The inset of Figure S1B denotes the corresponding selected area electron diffraction pattern.



Figure S2. The XPS pattern of the as-prepared NaLuF<sub>4</sub>: Gd/Yb/Er NRs and NRs@PDA and

XPS N1s spectrum of NRs@PDA (the inset).



Figure S3. FTIR spectra of OA-NaLuF<sub>4</sub>: Gd/Yb/Er NRs and NRs@PDA nanocrystals. The weak absorption peaks at 2926 and 2855 cm<sup>-1</sup> are attributed to the asymmetric and symmetric stretching vibrations of the  $-CH_2$  bond, respectively. The broader and stronger band centered at 3435 cm<sup>-1</sup> is originated from the O-H group. The characteristic peaks at 1577 cm<sup>-1</sup> and

 $1496 \text{ cm}^{-1}$  are associated to the PDA.



**Figure S4.** The emission spectra of (A) IR-26 and (B) NRs@PDA and the absorption spectra of (C) IR-26 and (D) NRs@PDA. The optical density (OD) in each absorption spectrum of IR-26 and NRs@PDA presents the absorbance value at 808 nm and 980 nm, respectively.



**Figure S5.** Photo-stability curve and in *vitro* phantom imaging (the inset picture) of NaLuF<sub>4</sub> NRs@PDA in water and PBS under continuous 980 nm laser irradiation with a power density

of 0.6 W cm<sup>-2</sup> at different time points.



Figure S6. (A) The *in vitro* phantom imaging of ICG and NRs@PDA solutions after irradiation of 808 nm and 980 nm laser with different times, respectively. (B) The corresponding NIR-II fluorescent intensity.



Figure S7. In vitro HeLa cells viability after incubated with various concentrations of NaLuF4

NRs@PDA for 24 h at 37 °C under 5% CO<sub>2</sub>.



Figure S8. The time-dependent average signal intensity changes in liver and heart sites of

tumor mouse.



**Figure S9.** The corresponding NIR-II fluorescent intensity of the liver and tumor after 60 h intravenous injection with NaLuF<sub>4</sub> NRs@PDA under 980 nm laser excitation.



Figure S10. Ex vivo bioimaging of the isolated organs, including heart, liver, spleen, lung,

and kidney after 3 and 7 days injection with NaLuF<sub>4</sub> NRs@PDA.



**Figure S11.** (A) Time dependent NaLuF<sub>4</sub> NRs@PDA contents in blood (based on the tested fluorescence intensity). The inset presents the corresponding *in vitro* NIR-II imaging of blood after intravenous injection of NaLuF<sub>4</sub> NRs@PDA in 24 h under 980 nm laser excitation (100 mW/cm<sup>2</sup>). (B) Digital photography, *in vitro* imaging of feces from un-injected and injected

mouse.



Figure S12. (A) A time course of high-magnification tumor vascular imaging with FOV of 26  $mm \times 21 mm$ . (B) and (C) Cross-sectional intensity profiles along the colour lines marked in

(A). The scale bar is 2 mm.



Figure S13. (A) High-magnification NIR-II vessel image of mouse abdomen under the 980 nm laser excitation (FOV: 21 mm × 26 mm, 512 × 640 pixels, 41 µm/pixel). (C) A typical abdomen vessel image taken from (A). (B) and (D) The corresponding zoom-in images of the chosen vessels. (E) and (F) Cross-sectional intensity profiles measured along the colorized lines from the images of (B) and (D), respectively. All scale bars are 2 mm.



Figure S14. In vitro thermal images based on NRs@PDA solution with different

concentrations under the irradiation of 808 nm laser.



Figure S15. H&E stained main tissues collected from control and experiment mouse injected

with NRs@PDA solution for 3 and 7 days.