

## Functionalized $\text{Cu}_3\text{BiS}_3$ nanoparticles for dual-modal imaging and targeted photothermal/photodynamic therapy

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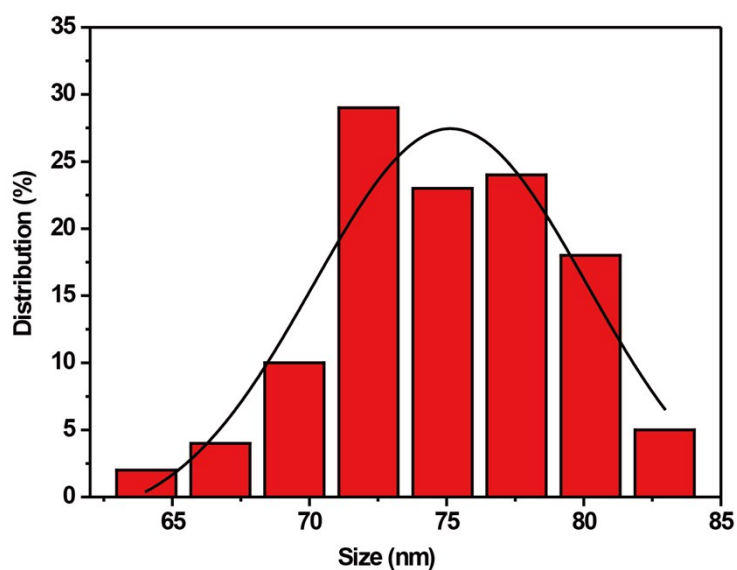


Fig. S1. Size distribution data of hydrophobic  $\text{Cu}_3\text{BiS}_3$  NPs.

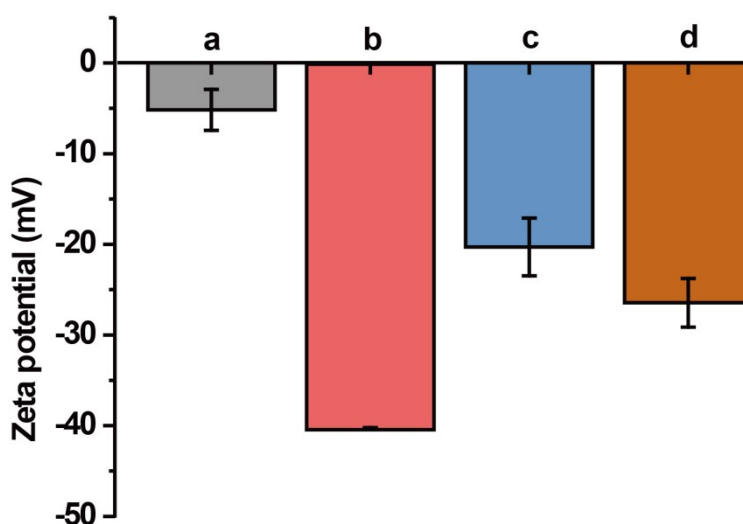


Fig. S2. Zeta potentials of  $\text{Cu}_3\text{BiS}_3$ -DSPE-PEG(- $\text{NH}_2$ ) (a),  $\text{Cu}_3\text{BiS}_3$ -PEG-(Ce6) (b),  $\text{Cu}_3\text{BiS}_3$ -PEG-(Ce6- $\text{Gd}^{3+}$ ) (c) and  $\text{Cu}_3\text{BiS}_3$ -PEG-(Ce6- $\text{Gd}^{3+}$ )-FA (d).

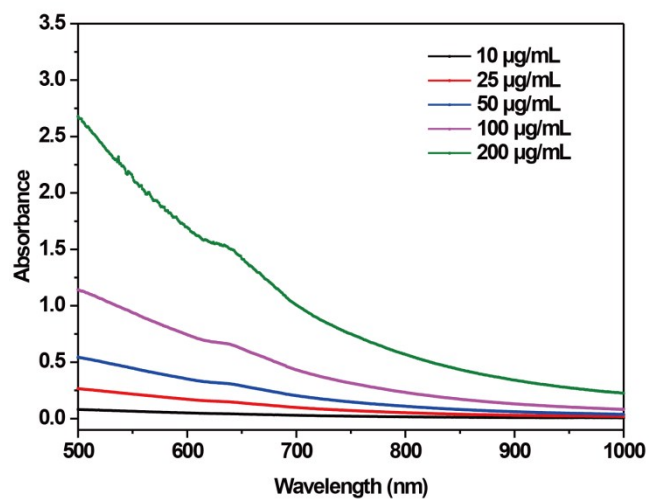


Fig. S3. Vis-NIR spectra of Cu<sub>3</sub>BiS<sub>3</sub>-PEG-(Ce6-Gd<sup>3+</sup>)-FA solutions with different concentrations.

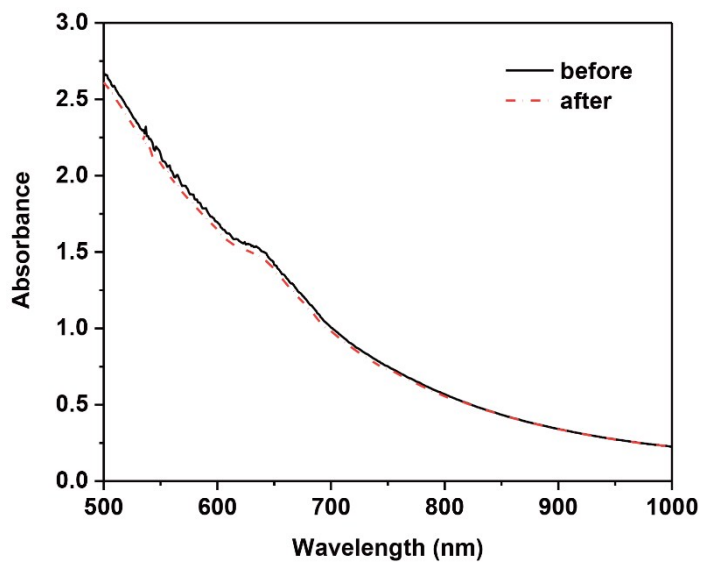


Fig. S4. Vis-NIR spectra of the Cu<sub>3</sub>BiS<sub>3</sub>-PEG-(Ce6-Gd<sup>3+</sup>)-FA solution (200 µg/mL) before laser irradiation and after 8 heating/cooling cycles.

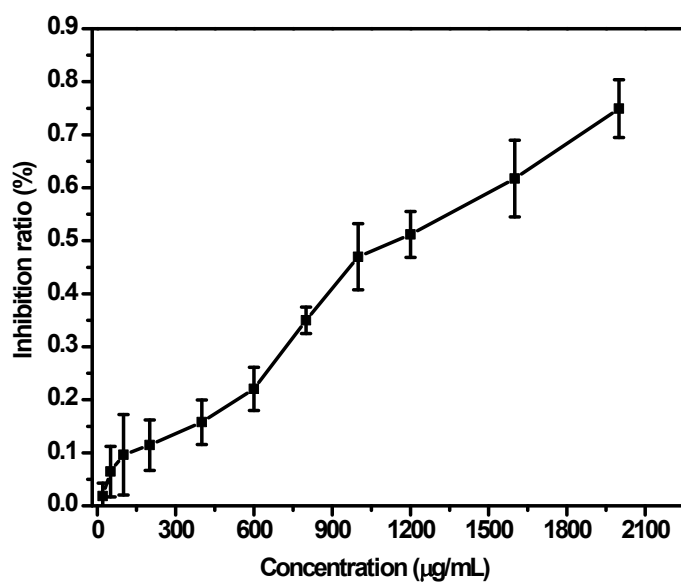


Fig. S5. The inhibition ratio (measured by MTT assay) of HeLa cells after incubation with  $\text{Cu}_3\text{BiS}_3\text{-PEG-(Ce6-Gd}^{3+}\text{)-FA}$  of different concentrations for 24 h.

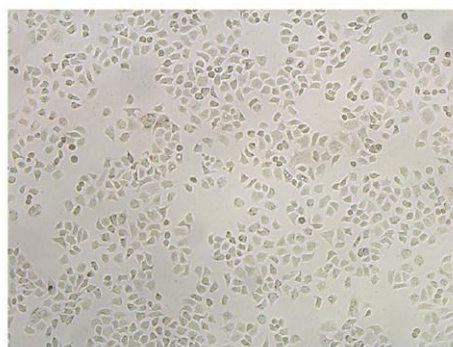


Fig. S6. Typical bright field microscopy image of trypan blue stained HeLa cells after incubation with  $\text{Cu}_3\text{BiS}_3\text{-PEG-(Ce6-Gd}^{3+}\text{)-FA}$  (100 µg/mL) for 4 h.

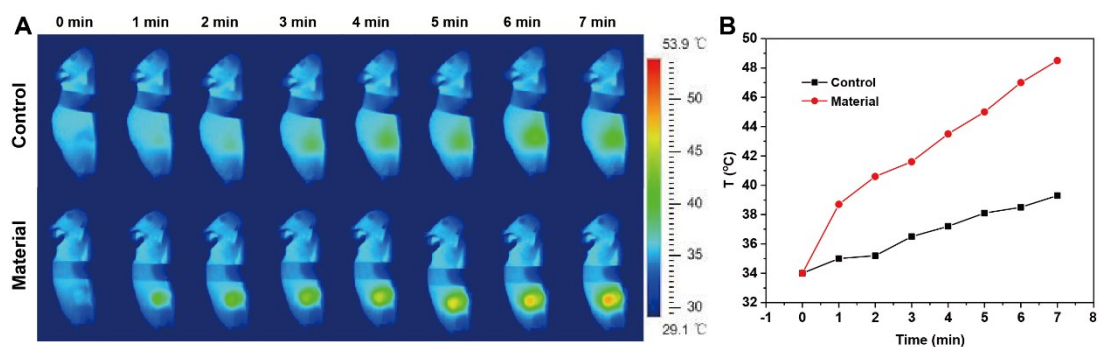


Fig. S7 (A) NIR thermal images of HeLa tumour-bearing mice intravenously injected with either PBS (Control) or  $\text{Cu}_3\text{BiS}_3\text{-PEG-(Ce6-Gd}^{3+}\text{)-FA}$  (Material) and then exposed to the NIR laser irradiation (808 nm, 0.5 W/cm<sup>2</sup>); (B) The temperature changes of the tumours based on infrared thermal imaging data in (A).

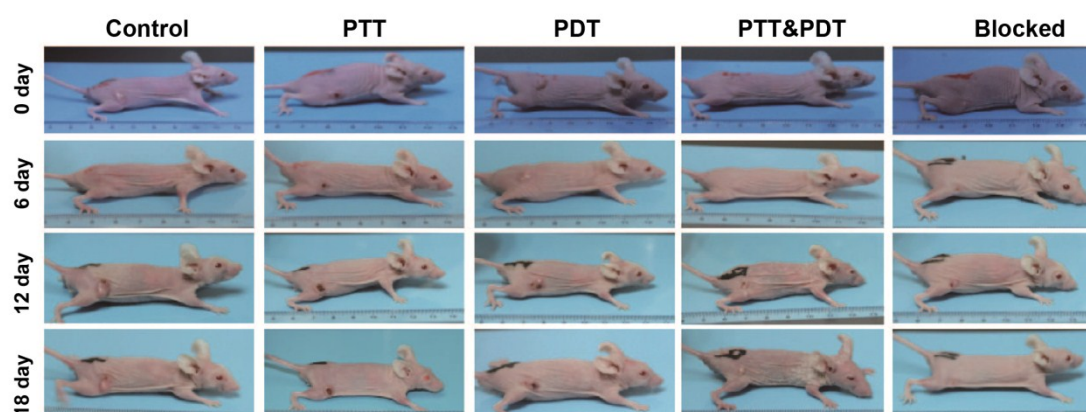


Fig. S8. Representative photographs of HeLa tumor-bearing nude mice obtained from each treated group.

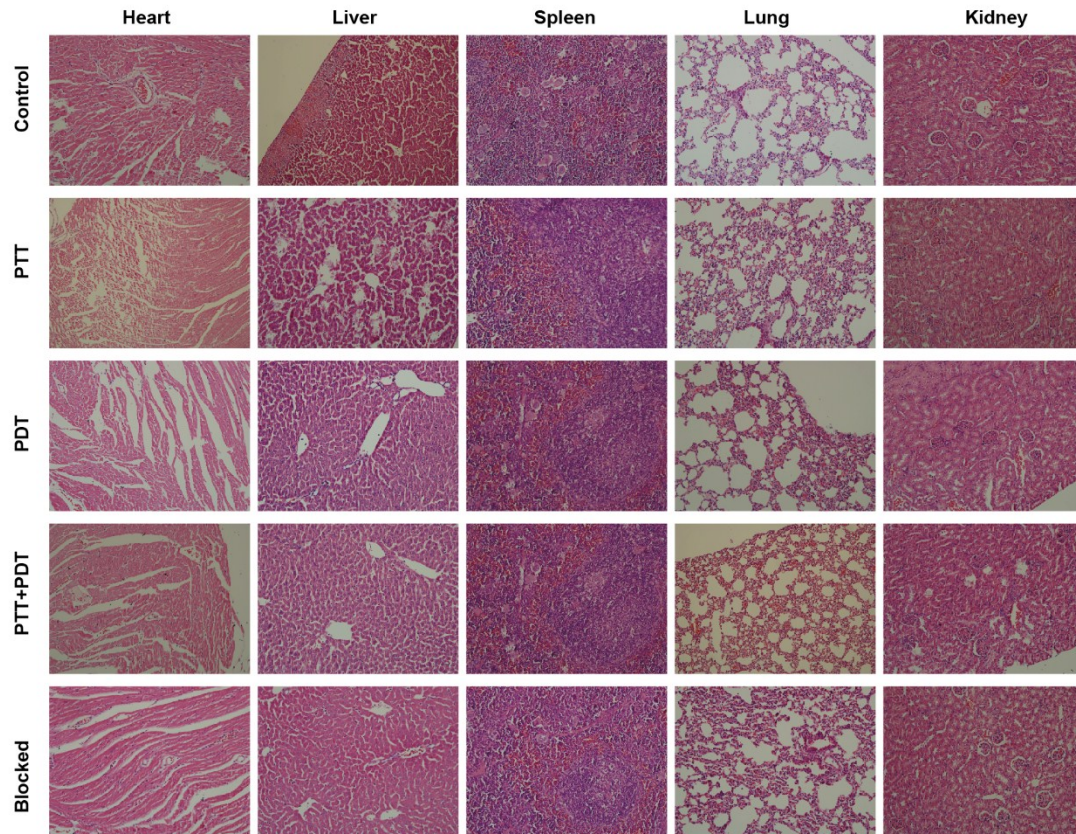


Fig. S9. Representative H&E histopathological images of major organs after various treatments.

**The full name and units of the blood indexes shown in Figure 6D:**

ALT: alanine aminotransferase (U/L)

AST: aspartate aminotransferase (U/L)

ALP: alkaline phosphatase (U/L)

CREA: creatinine ( $\mu\text{M}$ )

BUN: blood urea nitrogen (mM)

MCH: mean corpuscular hemoglobin (pg)

MCV: erythrocyte mean corpuscular volume (fl)

HGB: Hemoglobin (g/L)

WBC: white blood cell ( $10^9/L$ )

HCT: Red blood cell specific volume (%)

RBC: red blood cell ( $10^{12}/L$ )

MCHC: mean corpuscular hemoglobin concentration (g/L)