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Supplementary data

Design and synthesis of Zr-IR825 nanoparticles for photothermal therapy of tumor cells

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1. Experimental section

1.1. Chemical reagents

3-(4-carboxybenzyl)-2-((E)-2-((E)-3-((E)-2-(3-(4-carboxybenzyl)-1,1-dimethyl-1,3-dihydro-2H-benzo[e] indol-2-ylidene)ethylidene)-2-chlorocyclohex-1-en-1-yl)vinyl)-1,1-dimethyl-1H-benzo[e] indol-3-ium bromide (IR825, 95%) was purchased from Shanghai Yuanye Bio-Technology Co., Ltd.; Polyvinylpyrrolid one (PVP-K30, analytical grade) was purchased from Shanghai McLin Biochemical Technology Co., Ltd.; $ZrOCl_2 \cdot 8H_2O$ (analytical grade) was purchased from Shanghai McLin Biochemical Technology Co., Ltd.; N,N-Dimethylformamide (DMF, superior grade), and Triethylamine ($C_6H_{15}N$, analytical grade) were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd.; Cell-Counting-Kit-8 (CCK-8, analytical grade), Calcein-AM, and Propidium iodide (PI, analytical grade) were provided by Biotium Biotechnology Co., Ltd.

1.2. Characterization instruments

The morphology of the materials was characterized using a JSM-7500F field emission scanning electron microscope (SEM) from Japan Electron Optics Laboratory (JEOL); the particle size and Zeta potential of the nanomaterials were measured using a NANOTRAC WAVE II dynamic light scattering instrument from Microtrac, USA; elemental chemical state analysis was performed using an AXIS Supra X-ray photoelectron spectrometer (XPS) from Shimadzu, Japan; Fourier-transform infrared (FT-IR) spectra were obtained using a Spectrum Two spectrometer from PerkinElmer, USA; UV-visible absorption

spectra were measured using a UV-2600 spectrophotometer from Shimadzu, Japan; cell viability was measured using a Multiskan MK3 microplate reader from Thermo Fisher Scientific, USA.

2. Supplementary figures

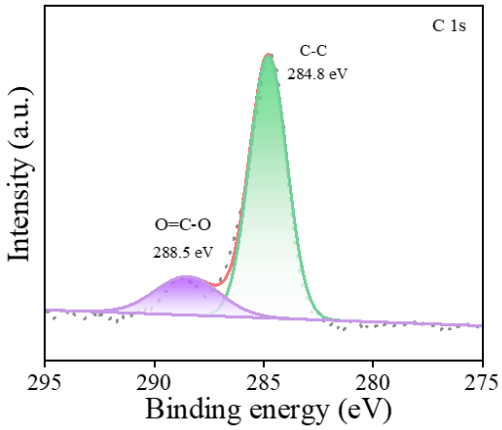

Figure S1. High-resolution C 1s spectrum of Zr-IR825 nanoparticles.

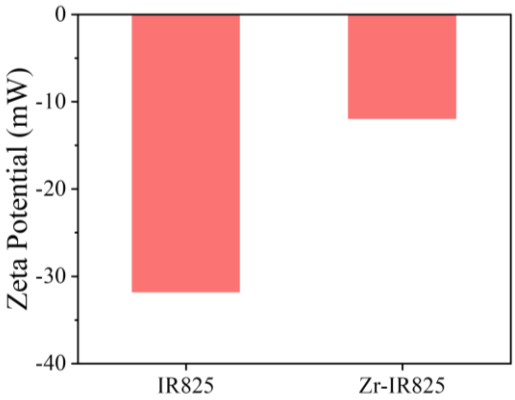

Figure S2. Zeta potential of IR825 and Zr-IR825 nanoparticles.

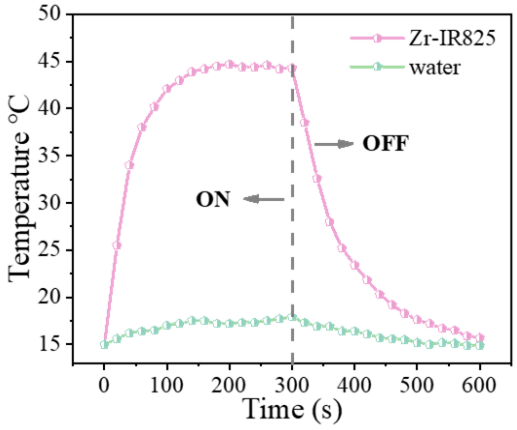

Figure S3. Heating and cooling curves of Zr-IR825 nanoparticles and water during laser on/off cycles.

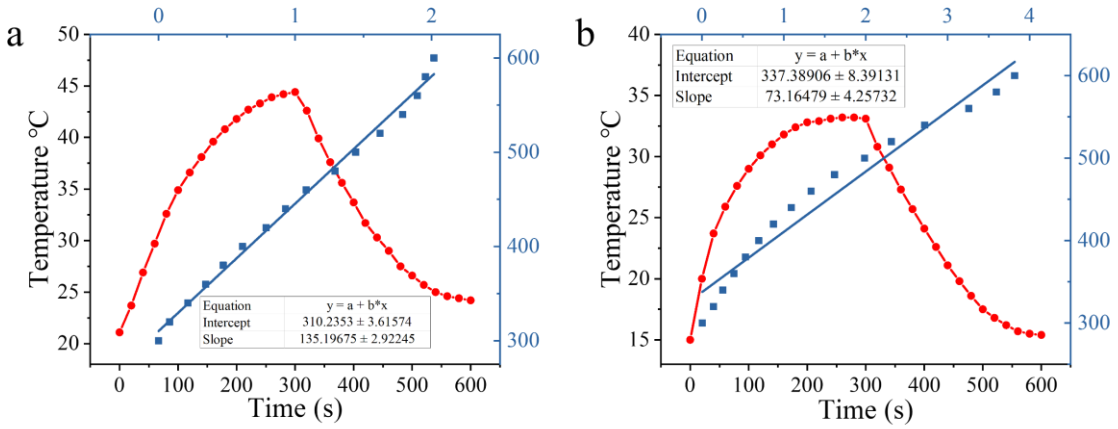

Figure S4. Heating and cooling curves of IR825 **(a)** and ICG **(b)** during laser on/off cycles, along with their time constants (τs).

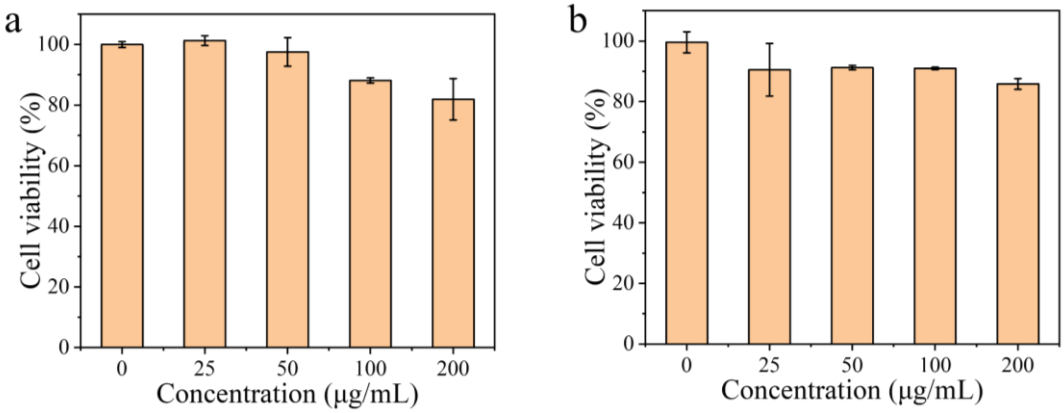

Figure S5. Cell viability of 4T1 cells **(a)** and L929 cells **(b)** after co-incubation with Zr-IR825 nanoparticles for 48 h.

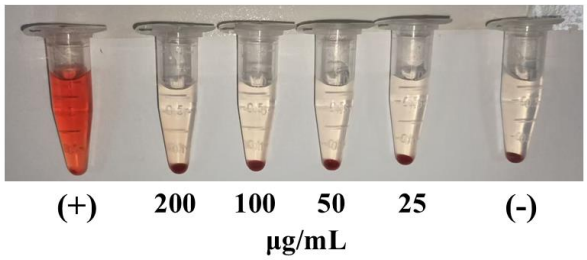

Figure S6. Photographs of the mixed solution in a plastic tube.