Supporting Information

Lanthanide-based Nanocomposites for Photothermal Therapy under Near Infrared Laser: Relationship between Light and Heat, Bio-stability and Reaction Temperature

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The following formula is used to calculate the light-to-heat conversion efficiency[1]:

$$\sum_i \mathrm{m}_i C_{p,i} \frac{dT}{dt} = Q_{NC} + Q_{Dis} - Q_{Surr} \quad (S1)$$

where m and C_p are the mass and heat capacity of water, respectively, T is the solution temperature, Q_{NC} is the energy inputted by NCs, QD is the baseline energy inputted by the sample cell, and Q_{Surr} is heat conduction away from the system surface by air.

$$Q_{NC} = I(1-10^{-A_{980}})\eta \quad (S2)$$

where I is incident laser power, η is the conversion efficiency from incident laser energy to thermal energy, and A_{980} is the absorbance of the simple at wavelength of 980 nm.

$$Q_{Surr} = hS(T - T_{Surr}) \quad (S3)$$

where h is heat transfer coefficient, S is the surface area of the container, and T_{Surr} is the ambient temperature of the surroundings.

$$Q_{NC} + Q_{Dis} = Q_{Surr-Max} = hS(T_{Max} - T_{Surr}) \quad (S4)$$

Through the formulas (S1), (S2), (S3), and (S4) above, the light-to-heat conversion efficiency is obtained as follows:

$$\eta = \frac{hS(T_{Max} - T_{Surr}) - Q_{Dis}}{I(1-10^{-A_{980}})} \quad (S5)$$

Observing formula (S5), to get the value of light-to-heat conversion efficiency, only the value of *hS* needs to be calculated, while other values can be obtained during the experiment. The value of hS can be obtained through the following formulas:

$$\theta = \frac{T - T_{Surr}}{T_{Max} - T_{Surr}} \quad (S6) \qquad \tau_s = \frac{\sum_i m_i C_{p,i}}{hS} \quad (S7) \qquad \frac{d\theta}{dt} = \frac{1}{\tau_s}\left[\frac{Q_{NC} + Q_{Dis}}{hS(T_{Max} - T_{Surr})} - \theta\right] \quad (S8)$$

$$dt = \tau_s \frac{d\theta}{\theta} \quad (S9) \qquad t = -\tau_s \ln\theta \quad (S10)$$

In general, the light emitted by the laser is converted into heat by the photothermal material and the sample cell, that is, Q_{NC} and Q_{Dis} above. Part of the generated heat is absorbed by the solution, which causes the temperature to rise, and the other part diffuses into the air. Due to the limitation of the experimental condition, we assume that all the heat released by the material is absorbed by the solution. The simplified equation is shown as follows:

$$\eta = \frac{cm(T_s - T_p)}{P\Delta t} \quad (S11)$$

c and *m* respectively represent the specific heat capacity and mass of water, *Ts* represents the temperature change of the composite material aqueous solution, *Tp* refers to the temperature change of the pure aqueous solution, and *P* refers to the temperature of the 980 nm laser during irradiation.

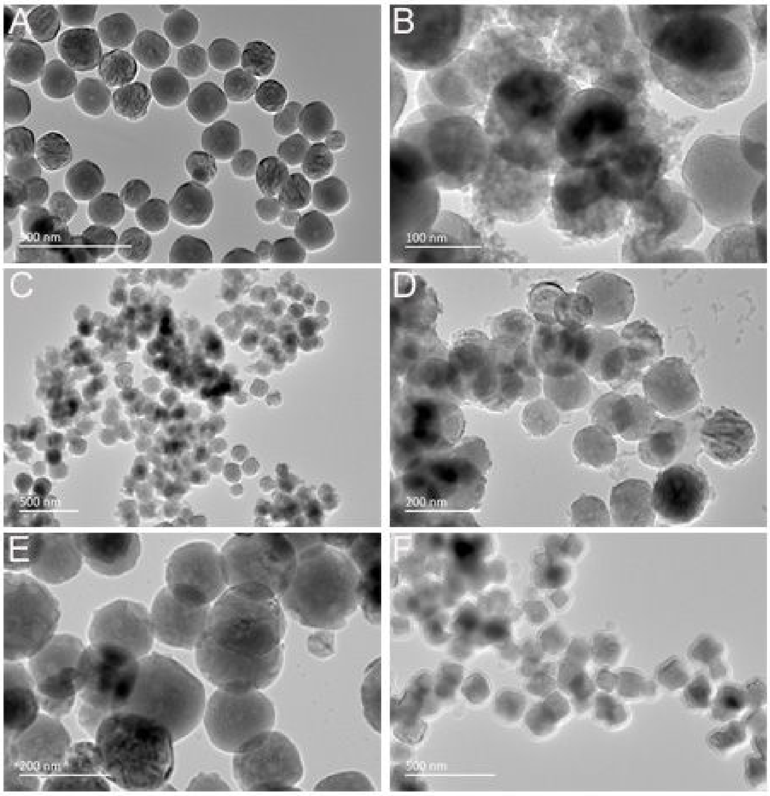

Figure S1. TEM images of (A) UCNP, (B) UCNP@CuS, (C) UCNP@MnO_2, (D) UCNP@PPy, (E) UCNP@Dp, and (F) UCNP@C.

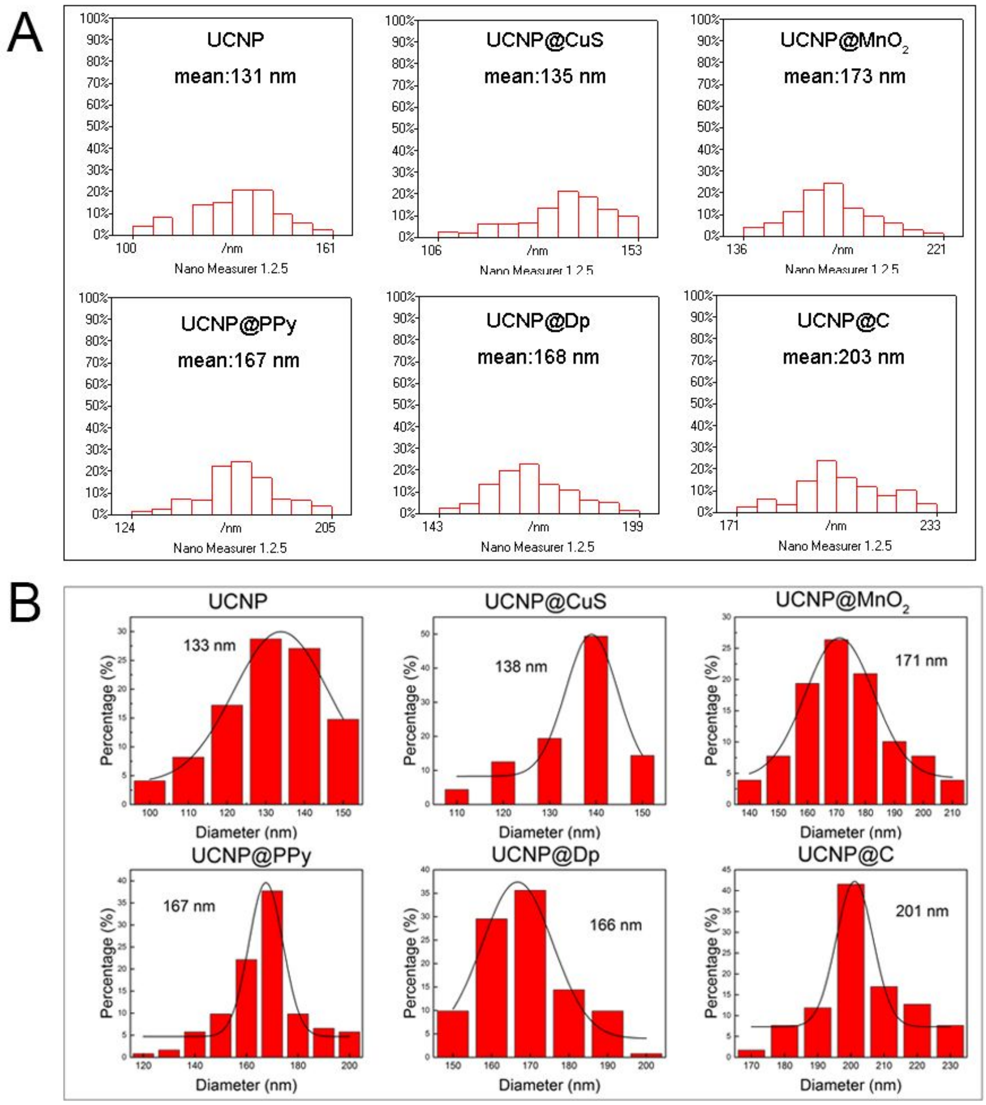

Figure S2. The (A) counts and (B) Gaussian distribution of the five PTT agents' sizes by Nanomeasure.

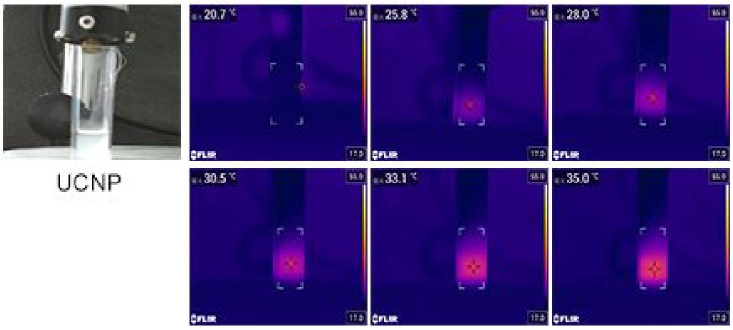

Figure S3. Infrared thermal imaging photographs of UCNP solution.

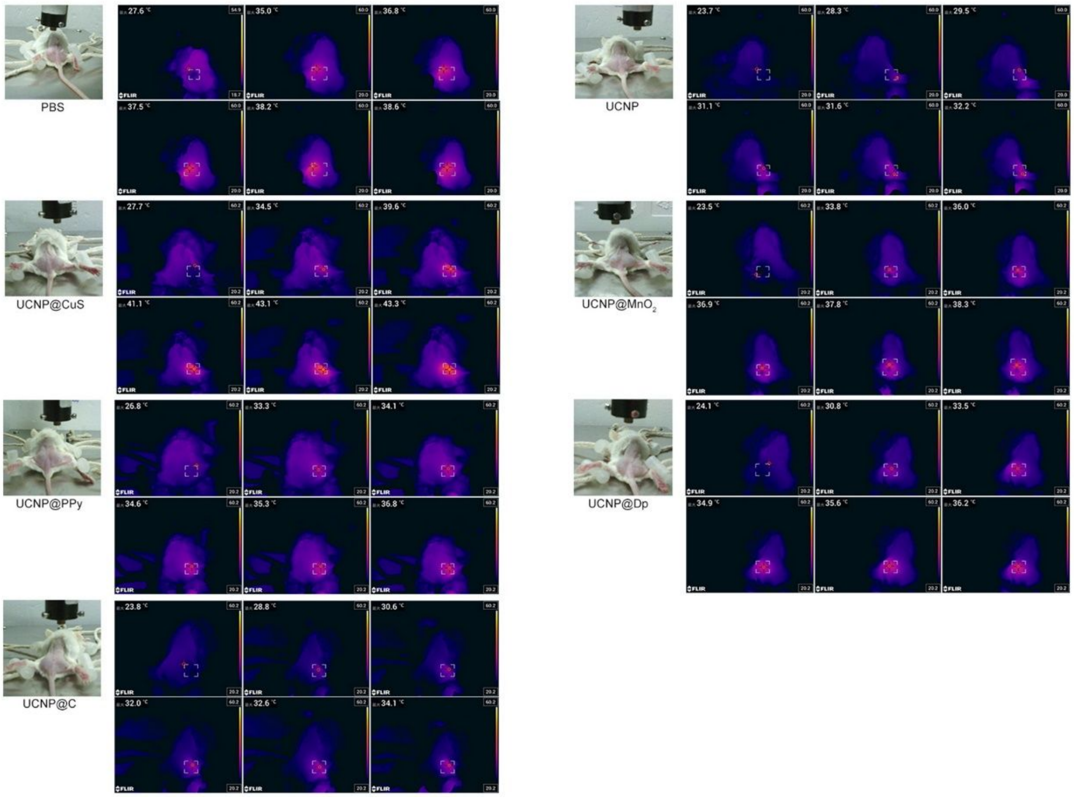

Figure S4. Infrared thermal imaging photographs of mice irradiated at different time points after injected with different materials subcutaneously (the 980 nm laser power: 0.75 w/cm^2).

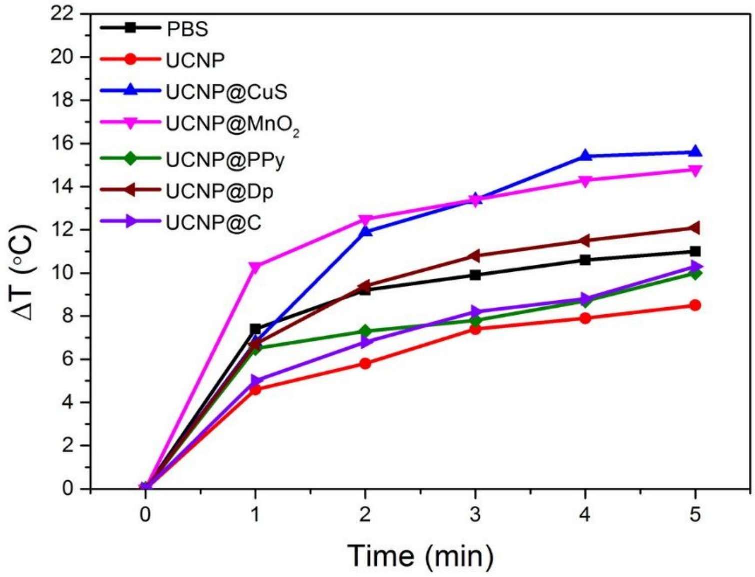

Figure S5. The temperature change curves versus irradiation time. (the 980 nm laser power: 0.75 w/cm^2).

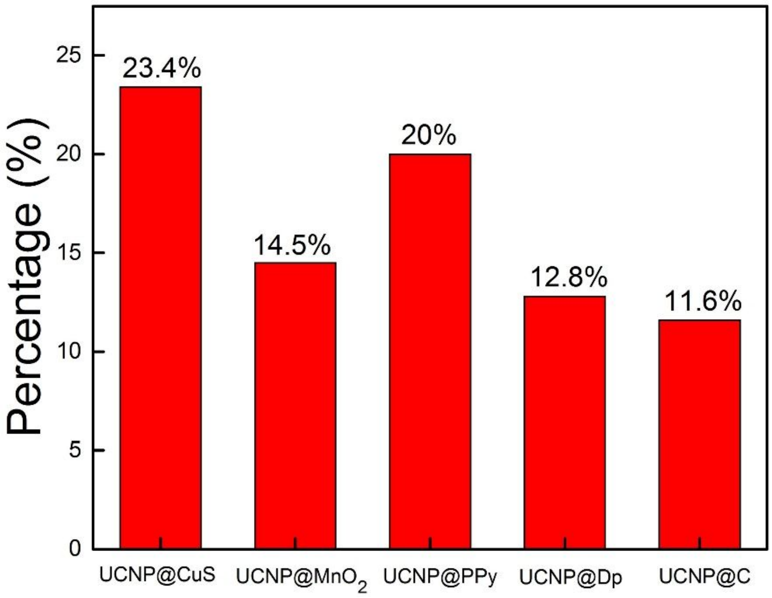

Figure S6. Photothermal efficiency of the five PTT agents under NIR laser.

Table S1. The thickness change before and after irradiation.

	Size before (nm)	Size after (nm)	Thickness before (nm)	Thickness after (nm)	Thickness change (nm)	Thickness change percent (%)
UCNP	264	199	0	0	0	0
CuS coated	549	1254	285	1055	770	270
MnO_2 coated	407	323	143	124	-19	-13
PPy coated	1109	1190	N/A	N/A	N/A	N/A
Dp coated	1897	1834	N/A	N/A	N/A	N/A
C coated	379	343	115	144	29	25

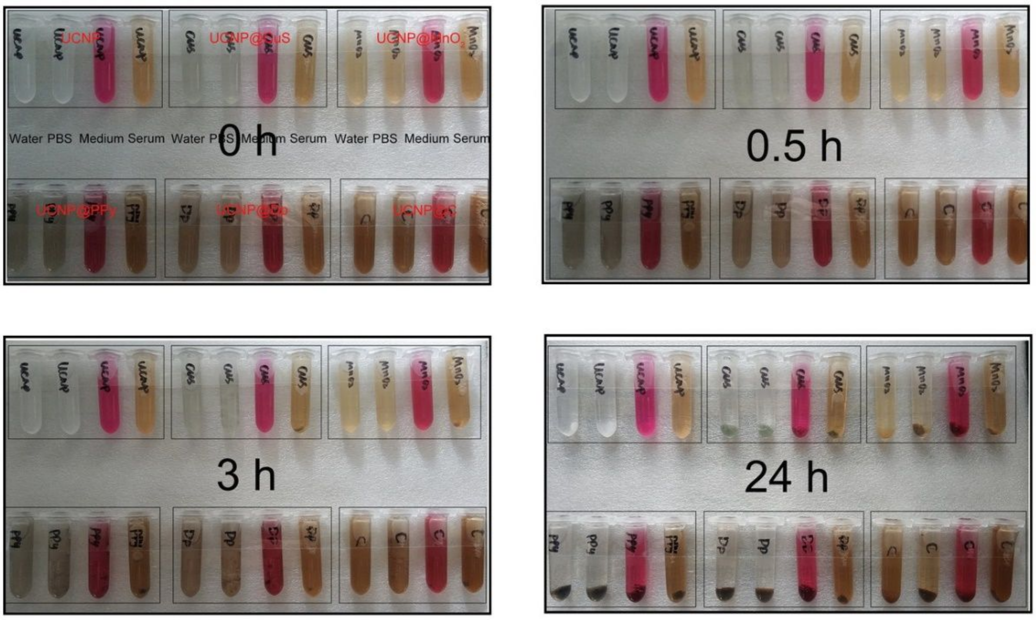

Figure S7. Photographs of the materials (UCNP, UCNP@CuS, UCNP@MnO_2, UCNP@PPy, UCNP@Dp and UCNP@C) at different time points when dissolved in water, PBS, culture medium and serum, respectively.

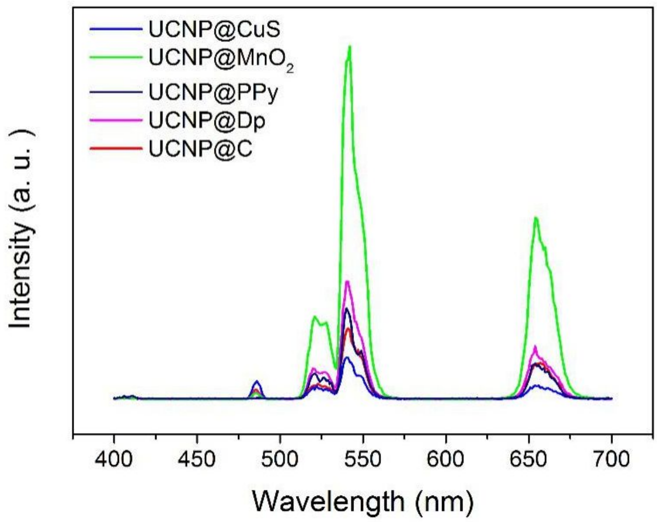

Figure S8. UCL spectra of different materials under 980 nm lase irradiation.

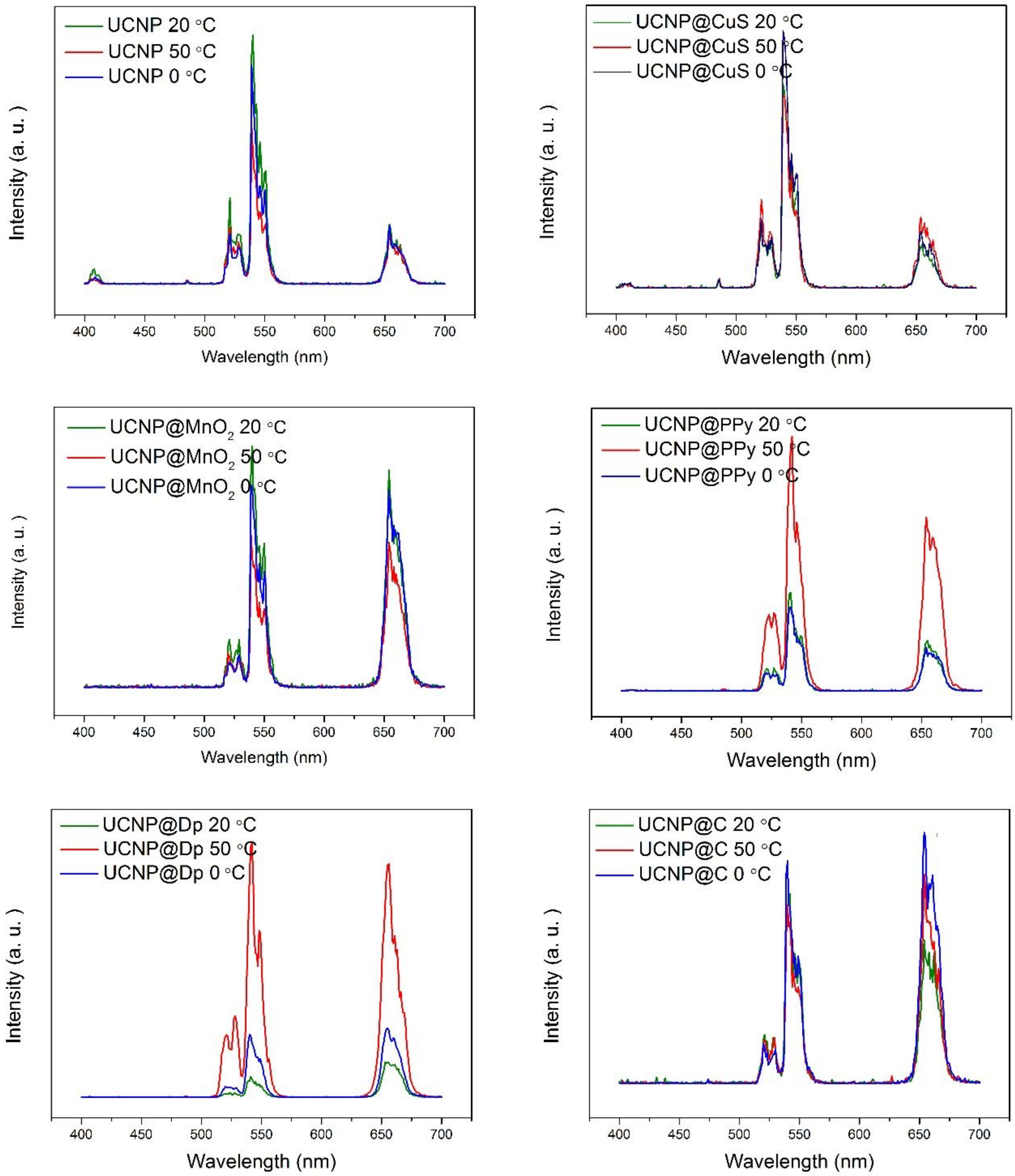

Figure S9. UCL spectra of UCNP, UCNP@CuS, UCNP@MnO$_2$, UCNP@PPy, UCNP@Dp, and UCNP@C at different detection temperature.

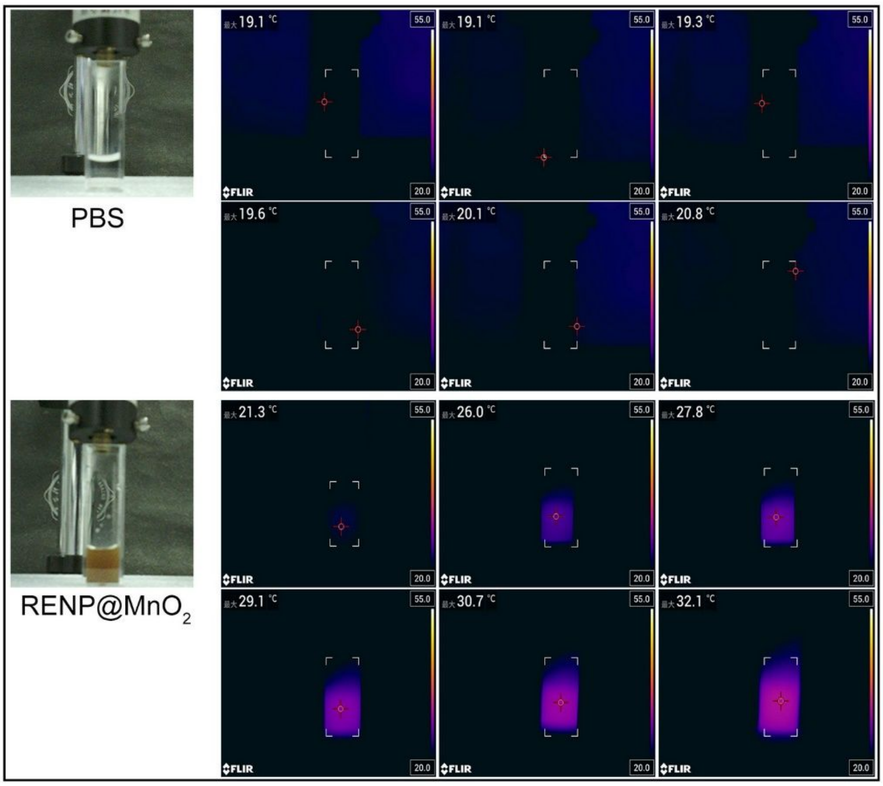

Figure S10. Infrared thermal images of PBS and RENP@MnO_2 under 808 nm laser.

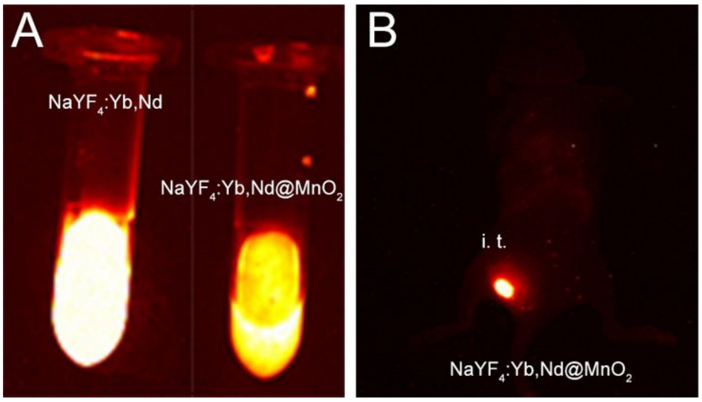

Figure S11. The imaging phostograph of (A) $NaYF_4$:Yb,Nd and $NaYF_4$:Yb,Nd@MnO_2 in the tubes under 808 nm laser and (B) in the mice after injection with $NaYF_4$:Yb,Nd@MnO_2 in the tumor focus (i. t.). (Power: 1.0 W/cm^2)

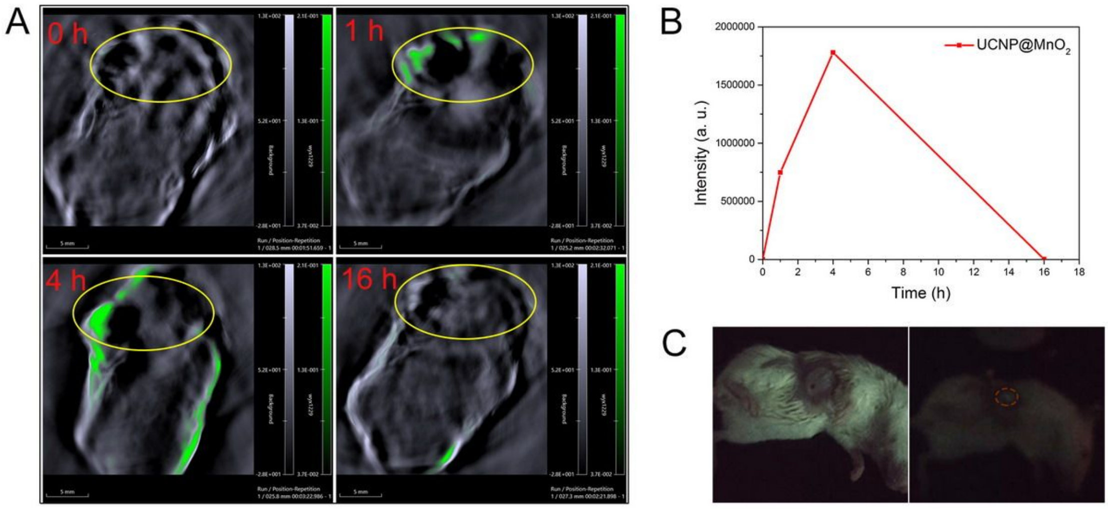

Figure S12. (A) Photoacoustic imaging photographs and (B) quantification curve in the tumor site at different time points. (C) UCL imaging of UCNP@MnO_2 in mice.

References:

(1) Tian, Q.; Jiang, F.; Zou, R.; Liu, Q.; Chen, Z.; Zhu, M.; Yang, S.; Wang, J.; Wang, J.; Hu, J., Hydrophilic Cu9S5 nanocrystals: a photothermal agent with a 25.7% heat conversion efficiency for photothermal ablation of cancer cells in vivo. *ACS nano* **2011,** 5, 9761-9771.