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Supplementary Materials: Polypyrrole Nanosheets Prepared by Rapid In Situ Polymerization for NIR-II Photoacoustic-Guided Photothermal Tumor Therapy

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Calculation of Photothermal Conversion Efficiency

The photothermal conversion efficiency of PPy NSs aqueous solution (100 μg/mL) was calculated using a circular quartz colorimetric dish with a diameter of 1 cm². The calculation formula of photothermal conversion efficiency (η) is:

$$\eta = \frac{hS(T_{max} - T_{surr}) - Q_s}{I(1 - 10^{-A})} \qquad \text{(Eq 1)}$$

Where h is the heat transfer coefficient, and S is surface area of laser irradiation area. Tmax is the highest steady-state temperature of nanoplates irradiated at 808/1064 nm laser, which are 58.1 °C and 62.1 °C respectively. Tsurr (25 °C) is ambient temperature. Qs represents the heat emitted from the light absorbed by the quartz sample cell itself. Using a quartz cuvette cell containing same volume of ultrapure water without any PPy nanosheets, the independently measured heat is 17.64 mW. I (1 W) is laser power. A808/1064 is the absorbance (1.05/1.06) of PPy NSs at 808/1064 nm.

Calculate hS according to the following formula:

$$hS = \frac{m_s C_s}{\tau_s} \qquad \text{(Eq 2)}$$

$$\tau_s = -\frac{t}{ln\,\theta} \qquad \text{(Eq 3)}$$

$$\theta = \frac{T - T_{surr}}{T_{max} - T_{surr}} \qquad \text{(Eq 4)}$$

ms (1 g) and Cs (4.2 J/g) are the mass and specific heat capacity of the solvent. T is PPy nanosheets temperature during cooling. τs is the sample system time constant. The temperature cooling time is fitted with a linear curve, and it can be determined to be 253.4/251.2 s at 808/1064 nm. Therefore, the 808/1064 nm laser heat conversion efficiency (η) of PPy NSs can be calculated to be 58.27%/66.01%.

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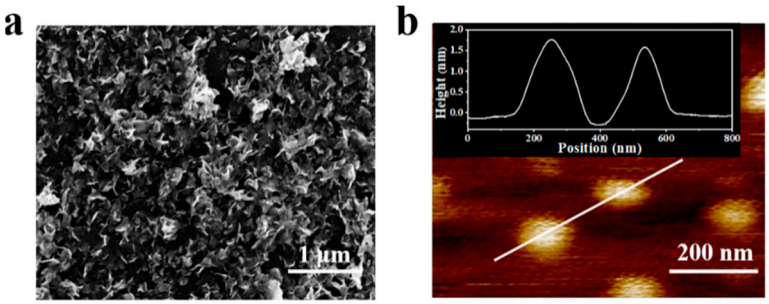

Figure S1. SEM (**a**) and AFM (**b**) images of MnO_2 NSs.

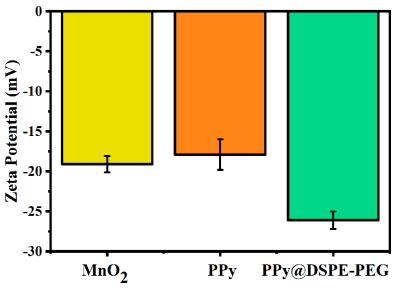

Figure S2. Zeta potential of MnO_2 NSs, PPy NSs and PPy@DSPE-PEG NSs.

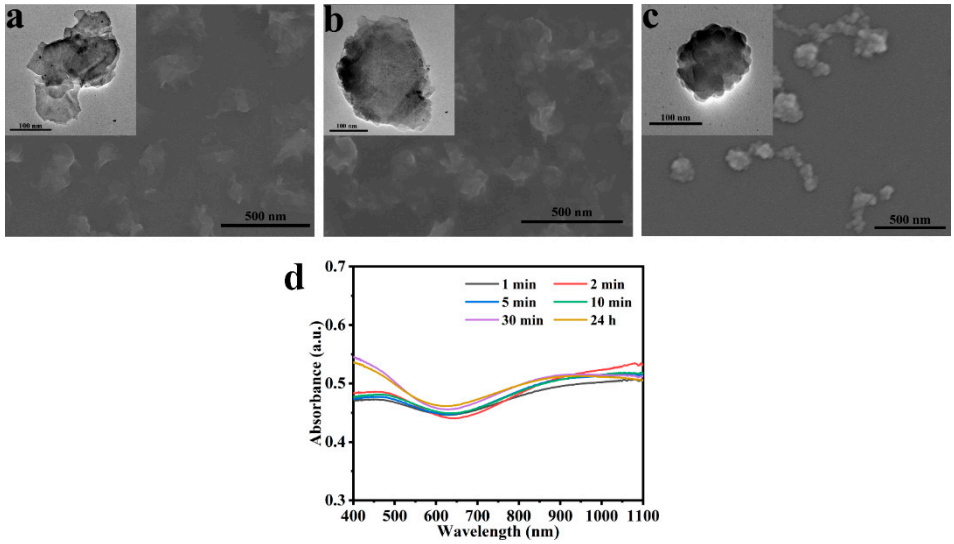

Figure S3. Morphology of PPy NSs reacted with different time (**a**) 2 min, (**b**) 30 min, (**c**) 24 h detected by SEM and TEM (insert pictures). (**d**) UV-Vis-NIR absorption spectra of PPy NSs under different synthetic time.

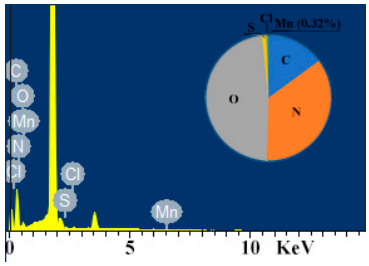

Figure S4. EDS spectrum of PPy NSs.

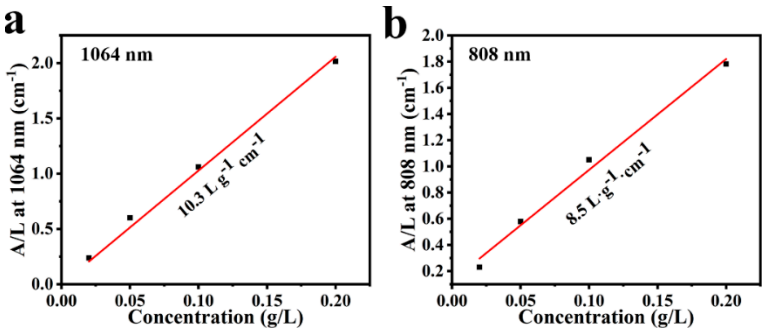

Figure S5. Extinction coefficient of PPy NSs under 1064 nm (**a**) and 808 nm (**b**) laser irradiation.

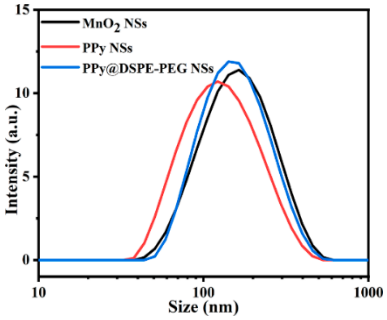

Figure S6. DLS profiles of MnO_2 NSs, PPy NSs and PPy@DSPE-PEG NSs.

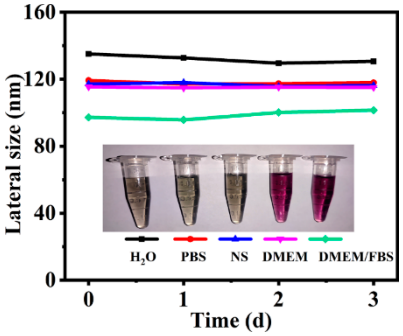

Figure S7. DLS profiles of PPy@DSPE-PEG NSs in different buffer solutions.

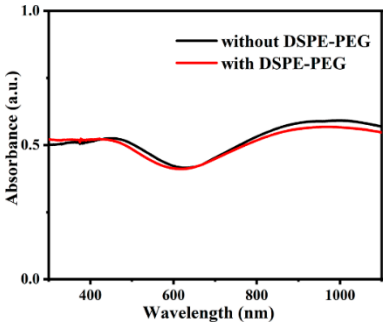

Figure S8. UV-Vis-NIR absorption spectra of PPy NSs with and without DSPE-PEG.

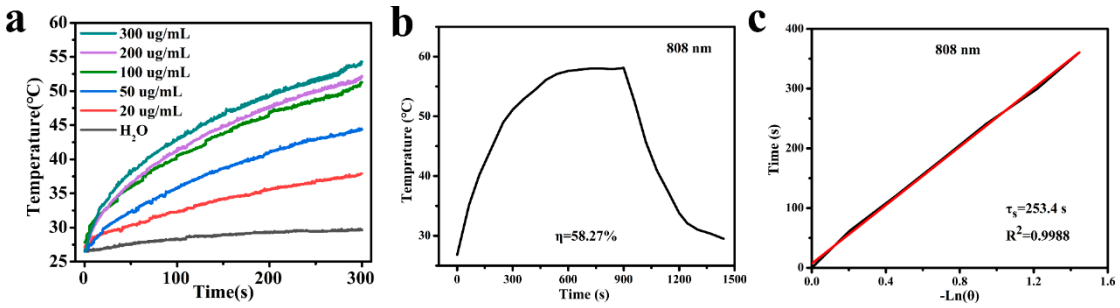

Figure S9. (**a**) Photothermal heating curves of PPy@DSPE-PEG NSs with different concentrations under 808 nm laser irradiation (1 W/cm², 5 min). (**b**) Photothermal heating and cooling curves of PPy@DSPE-PEG NSs (100 μg/mL) under 808 nm and (**c**) the time constant for heat transfer from the system using a linear regression of the cooling profile.

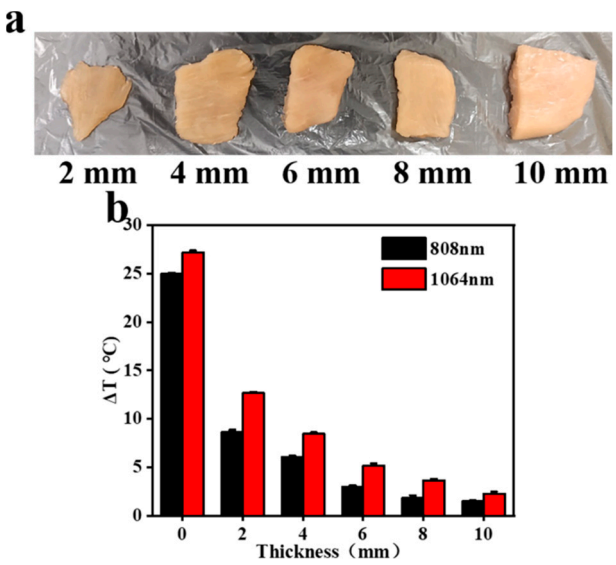

Figure S10. (**a**) Different thickness chicken breast pictures. (**b**) The temperature change values of PPy@DSPE-PEG NSs (100 μg/mL) irradiated with 808 nm/1064 nm laser irradiation (1 W/cm², 5 min) under different thickness of covered skin.

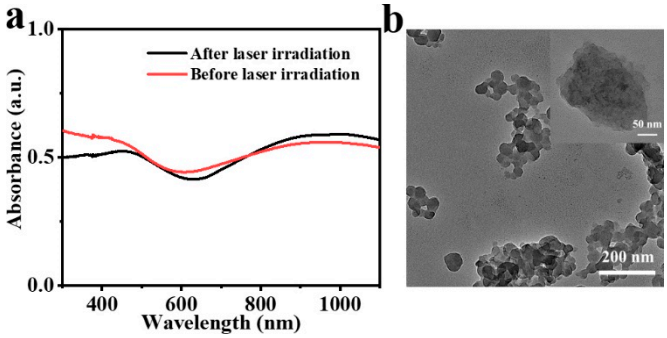

Figure S11. (**a**) UV-Vis-NIR absorption spectra of PPy@DSPE-PEG NSs before and after laser irradiation. (**b**) TEM image of PPy NSs after after 5-cycles laser irradiation.

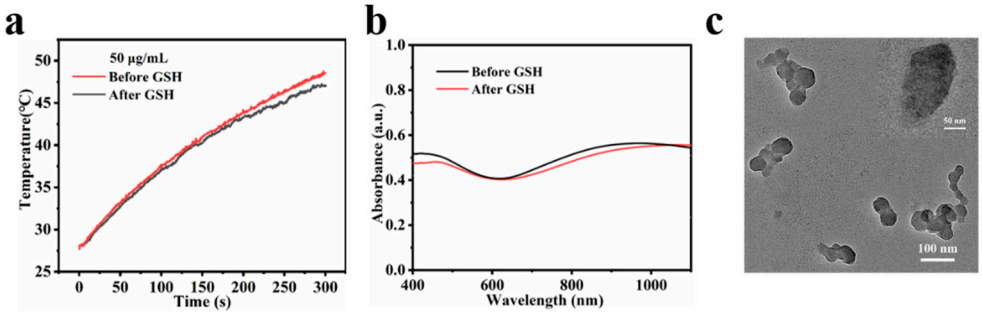

Figure S12. (**a**) Photothermal heating curves of PPy@DSPE-PEG NSs soaked and un-socked in the simulated solution of tumor environment (PBS with 5 mM GSH, pH = 5.0) under 1064 nm laser irradiation. (**b**) UV-Vis-NIR absorption spectra of PPy@DSPE-PEG NSs before and after soaked in tumor microenvironment simulation fluid. (**c**) TEM image of PPy NSs after soaked in the simulated solution of tumor environment.

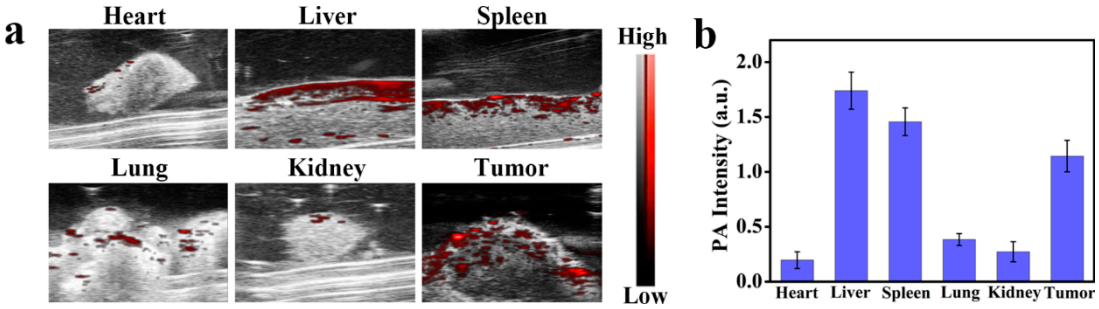

Figure S13. Pseudo-color pictures (**a**) and intensity (**b**) of photoacoustic signal intensity in major organs and tumor tissues after 24 h injection of PPy@DSPE-PEG NSs (4 mg/kg).

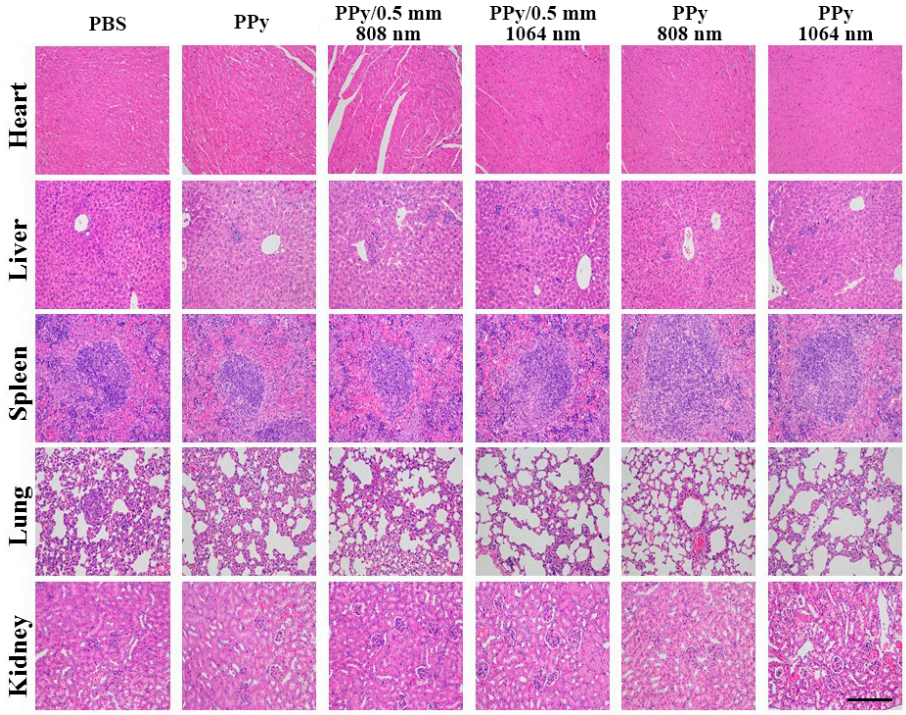

Figure S14. H&E staining images of heart, liver, spleen, lung and kidney at the end of the treatment cycle (14 day). (Scale bar = 200 μm).