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Supporting Information

Molecular engineering of diketopyrrolopyrrole conjugated polymer nanoparticles by chalcogenide variation for photoacoustic imaging-guided photothermal therapy

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Photothermal conversion efficiencies of DPP-SO, DPP-SS and DPP-SSe NPs

To calculate the photothermal conversion efficiency (η), NPs aqueous solution (20 μg mL^{-1}) was irradiated at 808 nm for 10 min, the temperature was monitored by photothermal camera every 30 s in the irradiation. After the laser exposure, the temperature was continuously monitored every 30 s for 10 min when finally cooling to room temperature. The photothermal conversion efficiencies were calculated as follows: η was determined according to equation (1):

$$\eta = \frac{hS\Delta T_{max} - Q_{Dis}}{I(1 - 10^{-A808})} \qquad (1)$$

where η indicates the heat transfer coefficient, h and S are parameters related to solvent and container, h means heat transfer coefficient and S stands for surface area of the container. ΔT_{max} is the maximum temperature change of solvent. I stands the laser power used for irradiation, A808 means the absorbance of the nanoparticle aqueous solution at 808 nm. Q_{Dis} stands for the heat input due to light absorption by the solvent and container, and the Q_{Dis} was evaluated as 14 mW independently using pure water. hS can be determined by measuring the rate of temperature decrease after removing the light source according to equation (2):

$$\tau_s = \frac{m_D - C_D}{hS} \qquad (2)$$

Where, m_D and c_D indicate the mass (1.0 g) and heat capacity (4.2 J g $^{-1}$) of the waser in the solvent. τ_s is the time constant for heat transfer of the system, which can be calculated according to equation (3):

$$t = -\tau_s \ln(\theta) = -\tau_s ln\frac{T_t - T_{Surr}}{T_{Max} - T_{Surr}} \qquad (3)$$

where θ indicates the ratio of ΔT and ΔT_{Max}. t is the cooling time points when turn off the laser for 10 min. T_t is the corresponding temperature of PNPs during the cooling stage. T_{Max} means the maximum of the PNPs aqueous solution. T_{surr} stands for the temperature of the surrounding environment. From a plot of time against temperature during the cooling period, τ_s is calculated.

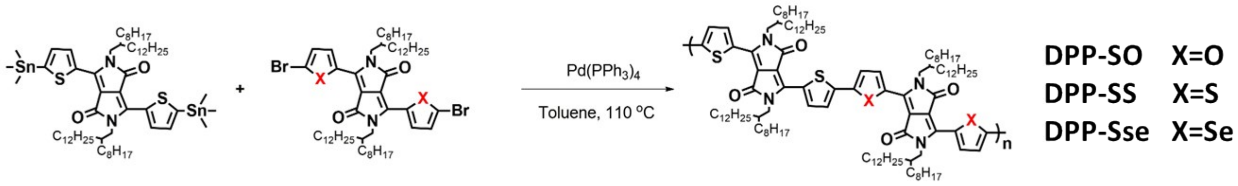

Fig. S1. Synthetic route of DPP-SO, DPP-SS and DPP-SSe

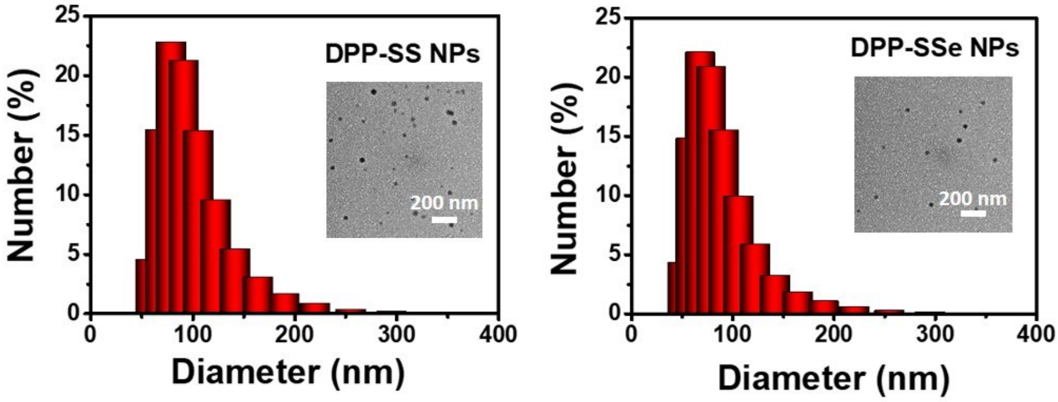

Fig. S2. DLS and TEM imaging of DPP-SS and DPP-SSe NPs aqueous solution

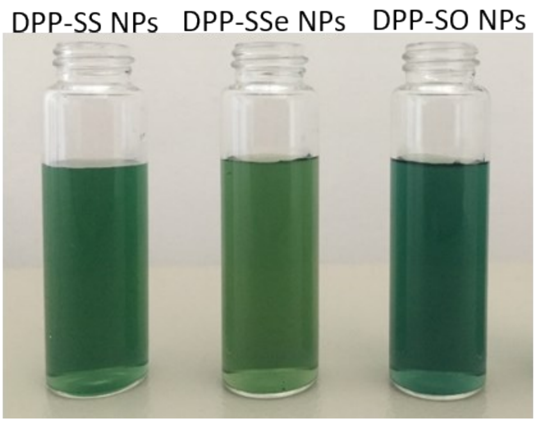

Fig. S3. The dispersibility of DPP NPs in PBS solution in 4 °C refrigerator for one month

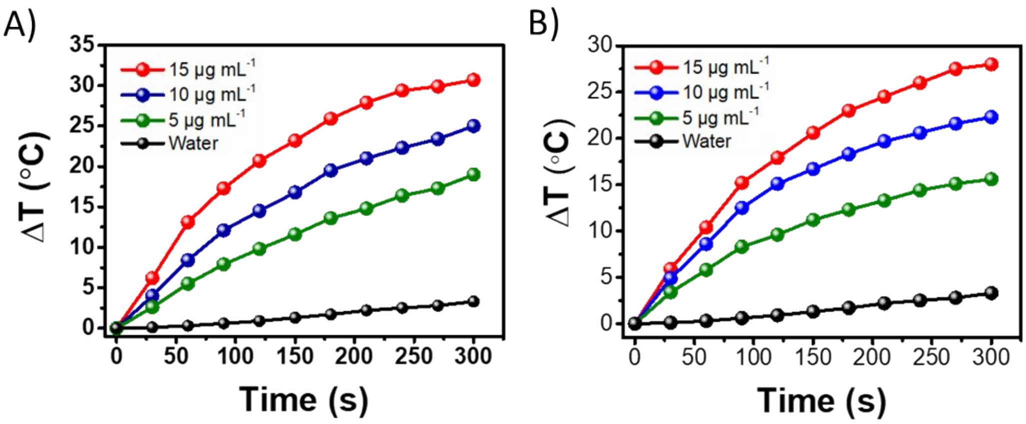

Fig. S4. Temperature elevation of (A) DPP-SS and (B) DPP-SSe NPs of various concentration

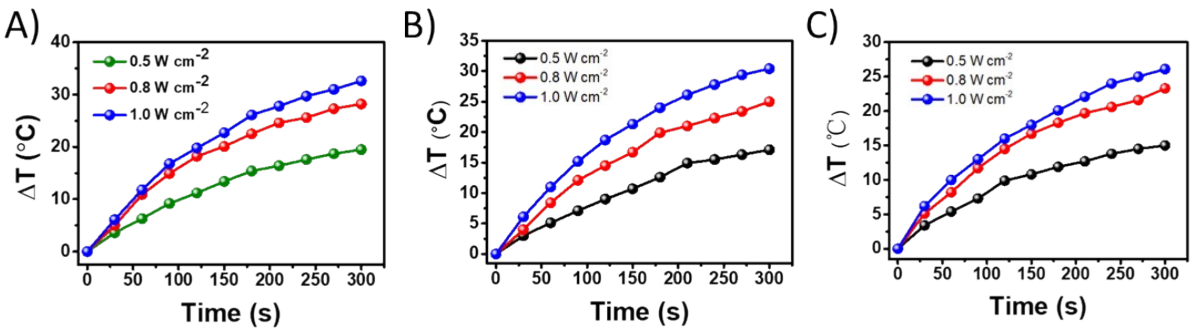

Fig. S5. Temperature profile of (A) DPP-SO, (B) DPP-SO and (C) DPP-SO NPs upon an irradiation 808 nm laser of different powers as a function of irradiation time

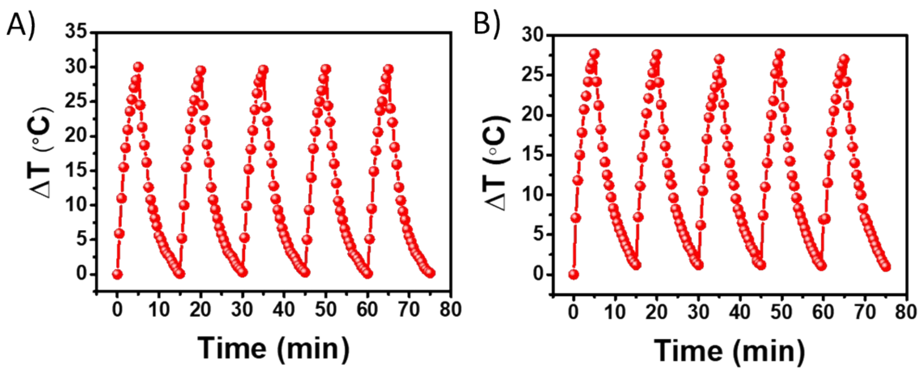

Fig. S6. Temperature elevation of (A) DPP-SS, (B) DPP-SSe NPs over five laser on/off cycles of 808 nm irradiation (0.8 W cm^{-2}, 10 min)

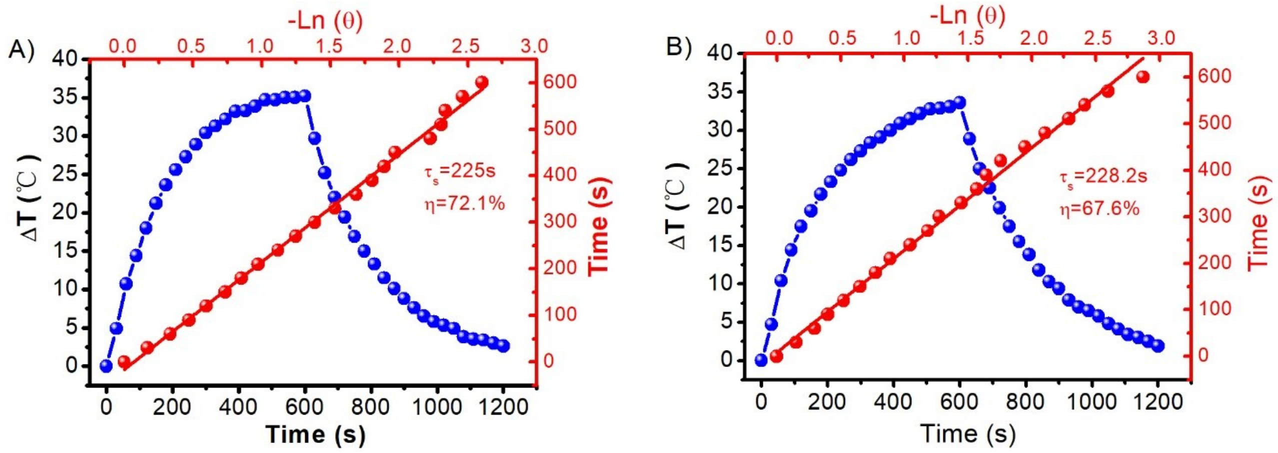

Fig. S7. Heating/cooling curves and linear analysis of (A) DPP-SS and (B) DPP-SSe NPs

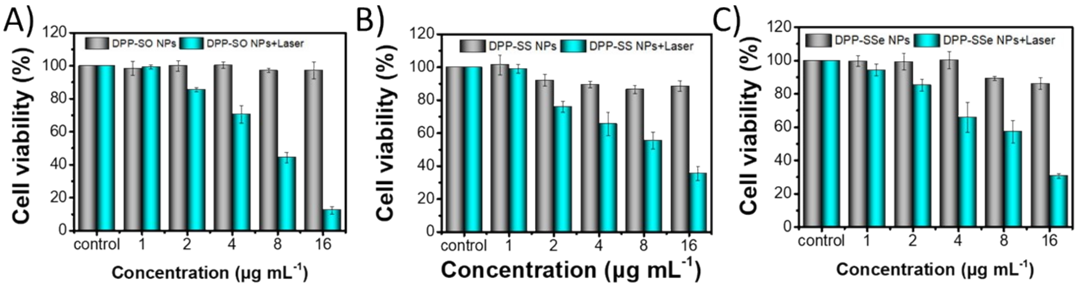

Fig. S8. (A) Viability of H446 cells after incubation with DPP-SO, DPP-SS and DPP-SSe NPs (internal concentrations of 0, 1, 2, 4, 8, 16 μg mL^{-1}) plus laser irradiation (808 nm, 0.8 Wcm^{-2}, 5 min) for 24 h.

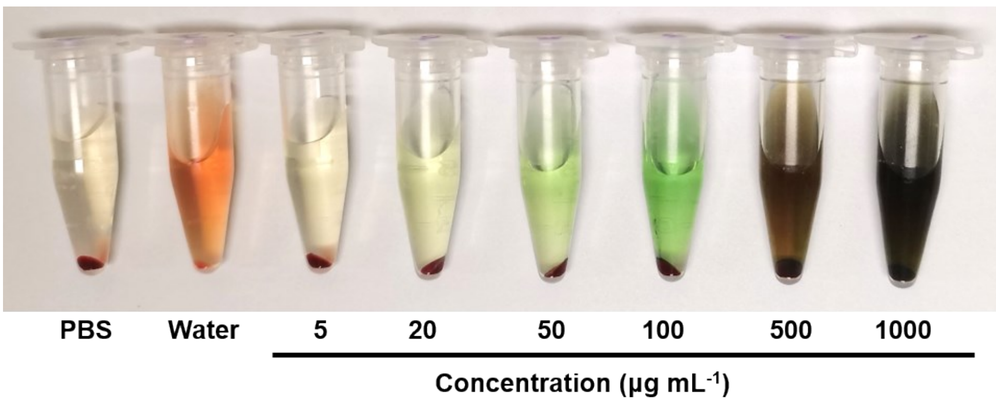

Fig.S9 Blood compatibility of DPP NPs (negative control: PBS; Positive control: pure water)

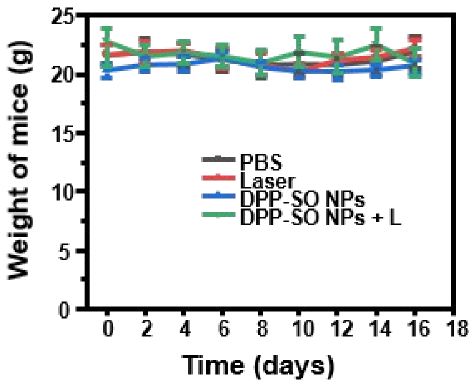

Fig. S10. Weight change of mice.