Supporting information for

IR780-based light-responsive nanocomplexes combining phase

transition for enhancing multimodal imaging and photothermal

therapy

Mingzhu Liu[1], Ping Zhang[1,2],* Liming Deng[1], Dan Guo[1], Mixiao Tan[1], Ju Huang[1], Yuanli Luo[1], Yang Cao[1], Zhigang Wang*[1,2]

[1]Chongqing Key Laboratory of Ultrasound Molecular Imaging, [2]Department of Ultrasound, Institute of Ultrasound Imaging, The Second Affiliated Hospital of Chongqing Medical University, Chongqing 400010, China

*Corresponding authors: Prof. Zhigang Wang and Ping Zhang are co-corresponding authors. Tel: 86-023-63809616 E-MAIL: 303507@hospital.cqmu.edu.cn.

1. Calculation of the photothermal conversion efficiency is as follows:

The photothermal conversion efficiency (η) of cRGD-PLGA-IR780-PFP was calculated as follows.[1,2] 200 μl of the cRGD-PLGA-IR780-PFP aqueous solutions (5 mg/ml) were exposed to the 808 nm NIR laser (2 W/cm^2, 5 min), and then, the laser was turned off. The heating and cooling temperature patterns of samples were recorded an IR thermal camera and η was calculated according to Eq. (1):

$$\eta = \frac{hS\,(T_{Max} - T_{Surr}) - Q0}{I\,(1 - 10^{-A808})}$$

(1)

Where h and S are the heat transfer coefficient and the sample container surface area, respectively. Tmax is the steady state equilibrium temperature, Tsurr is ambient temperature of the surroundings. Q_0 is the baseline energy input by the solvent and sample container without cRGD-PLGA-IR780-PFP, I is the laser power, and the A808 is the absorbance (2.207) of cRGD-PLGA-IR780-PFP in 808 nm.

The hS can be measured by Eq. (2):

$$\tau_s = \frac{\Sigma_i\, m_i\, C_{p,i}}{hS} \tag{2}$$

Where m and C_p are the mass and heat capacity of water, repectively. The heat capacity (C_p) is about 4.2 J. g^{-1}. k^{-1} (heat capacity of water).

The Q_0 was measured by Eq. (3):

$$Q_0 = hS \, (T_{Max} - T_{Surr}) \tag{3}$$

The time constant was τs = 175.35 s based on the linear time data from cooling period after 300 s vs $-\text{Ln}\theta$. Therefore, the photothermal conversion efficiency calculated by the above Eqs was η =10.58%.
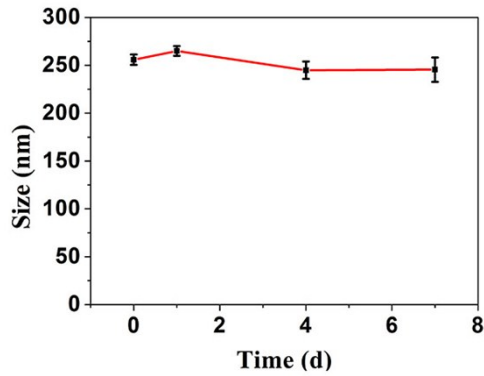
2. Supporting figures

Figure S1. The changes in mean size of cRGD-PLGA-IR780-PFP NPs during 7 days at room temperature measured by dynamic light scattering.
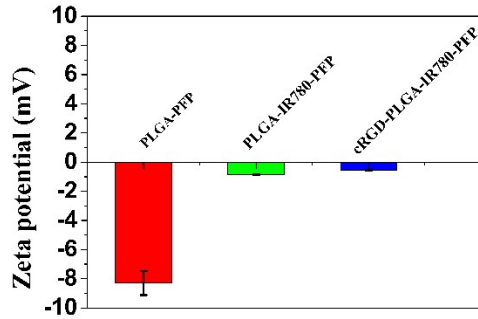

Figure S2. The mean zeta potential of various NPs (PLGA-PFP, PLGA-IR780-PFP

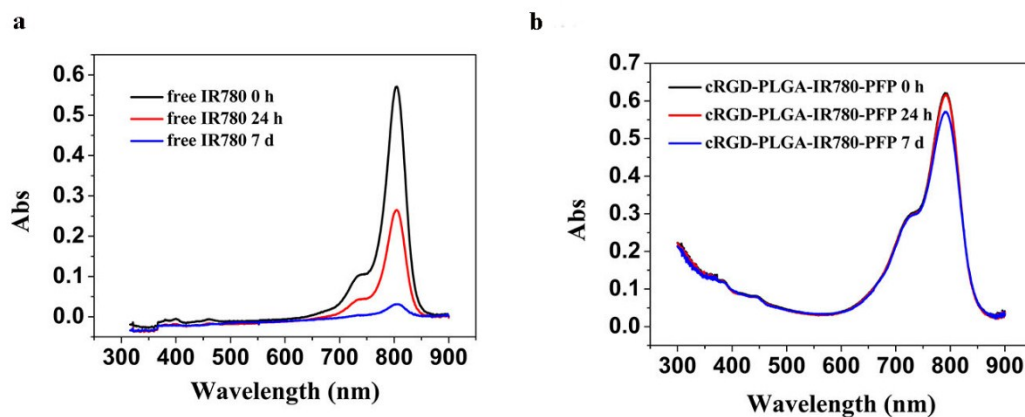and cRGD-PLGA-IR780-PFP) measured by dynamic light scattering.

Figure S3. (A, B) US-vis-NIR absorption spectrum of free IR780 and cRGD-PLGA-IR780-PFP storing in daylight over a period of 7 days.
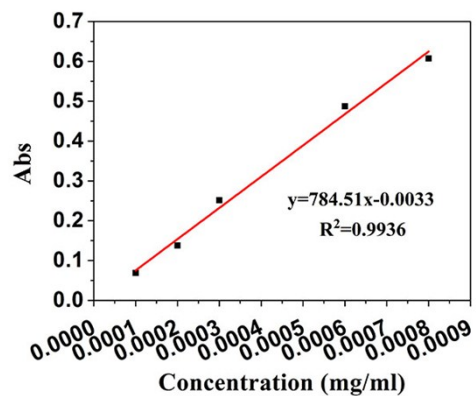

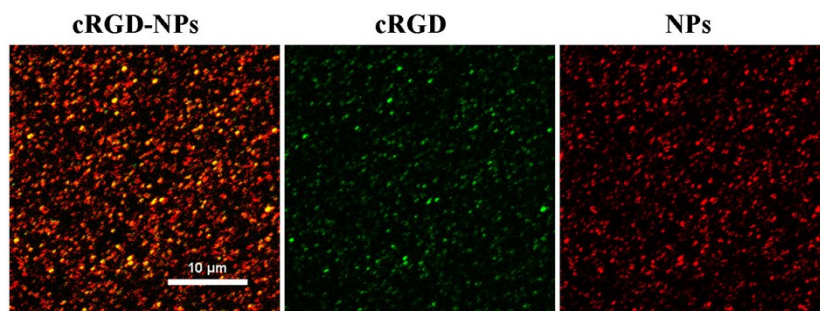Figure S4. The standard curve of IR780 measured by US-vis-NIR absorption spectrum.

Figure S5. Confocal microscope images of cRGD-NPs (cRGD-PLGA-IR780-PFP). The NPs shell was labelled with DiI, and the cRGD petide were marked with FITC.
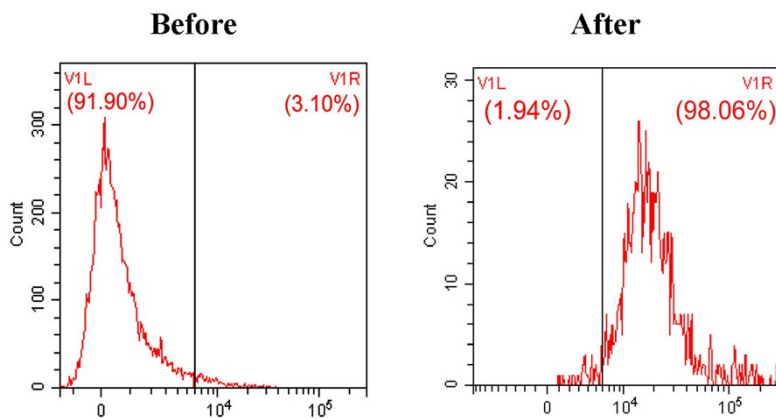

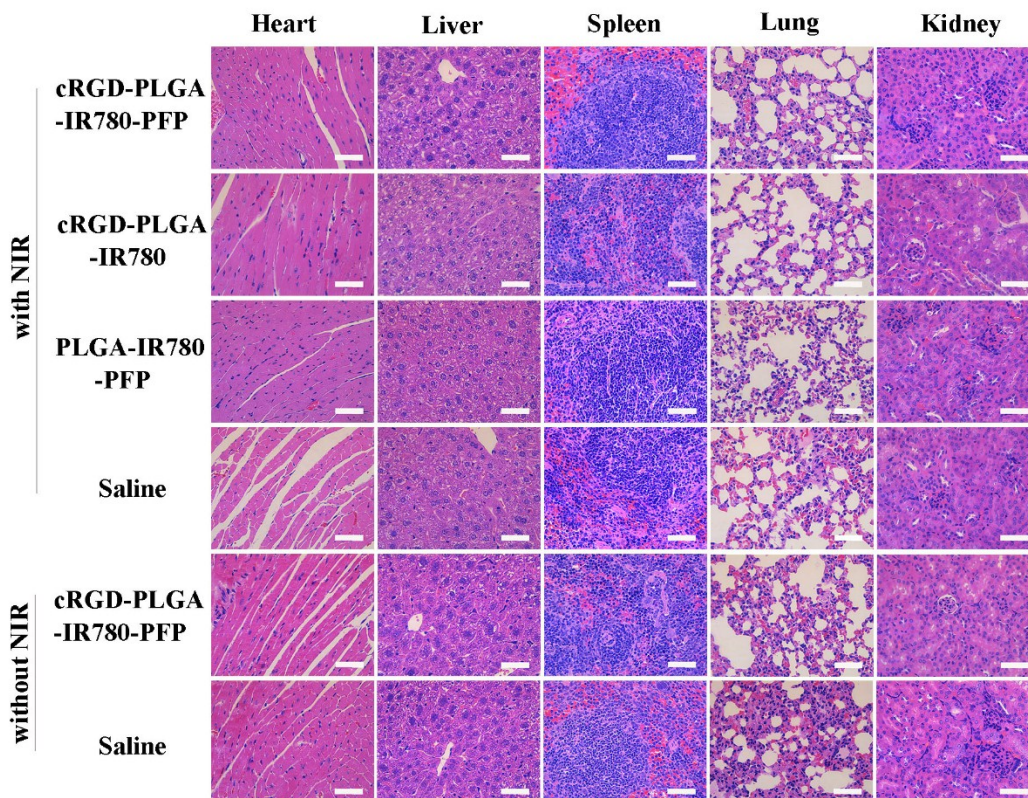Figure S6. Flow-cytometry results of nanoparticles before and after being conjugated with FITC labeled-cRGD peptide.

Figure S7. HE staining of major organs and tumors of different groups on the 2nd day after various treatments. (scale bar is 50 μm).

Reference

[1] X. Xu, X. Liu, L. Tan, Z. Cui, X. Yang, S. Zhu, Z. Li, X. Yuan, Y. Zheng, K.W.K. Yeung, P.K. Chu, S. Wu, Acta biomaterialia, 2018, **77**, 352-364.

[2] L. Deng, X. Cai, D. Sheng, Y. Yang, E.M. Strohm, Z. Wang, H. Ran, D. Wang, Y. Zheng, P. Li, T. Shang, Y. Ling, F. Wang, Y. Sun, Theranostics, 2017, **7**, 4410-4423.