Electronic Supplementary Information

Multifunctional PS@CS@Au-Fe_3O_4-FA Nanocomposites for CT, MR and Fluorescence Imaging Guided Targeted-Photothermal Therapy of Cancer Cells

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Calculation of the photothermal conversion efficiency

The photothermal conversion efficiency of the PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites and free ICG were measured according to the references.[1] The aqueous solution of the PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites (400 ppm) and free ICG underwent continuous irradiation of 808 nm laser (1.0 W/cm^2) for 300s, respectively. Then the laser was shut off, and the aqueous solution was naturally cooled to environment temperature. The temperature change of the aqueous solution was recorded (the first cycle of Fig.4b). The η value was calculated as follows:

$$\eta = \frac{hS(T_{Max} - T_{Surr}) - Q_{Dis}}{I(1-10^{-A_{808}})} \quad (1)$$

Where h is the heat transfer coefficient, S is the surface area of the centrifuge tube, and the value of hS is acquired from the Eq.4 and Fig.S4a. The maximum stable temperature (T_{max}) of the PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites was 69 °C and environmental temperature (T_{Surr}) was 28.3 °C. So, the temperature change (T_{Max}-T_{Surr}) of the PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites was 40.7 °C. The laser power I is 396 mW. The absorbance (A_{808}) of the PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites at 808 nm is 2.66. In order to obtain hS, a dimensionless parameter θ is introduced as followed:

$$\theta = \frac{T - T_{Surr}}{T_{Max} - T_{Surr}} \quad (2)$$

A sample system time constant τ_s can be calculated as Eq.3.

$$t = -\tau_s \ln(\theta) \quad (3)$$

According to Figure S4a, τ_s was determined to be 182.59s.

$$hs = \frac{m_D C_D}{\tau_s} \quad (4)$$

In addition, m is 0.2 g and C is 4.2 J/g·°C. Thus, according to Eq. 4, hS is calculated to be 4.60 mW/°C. Q_{Dis} represents heat dissipated from the light absorbed by the solvent and centrifuge tube itself, and it was calculated independently to be 14.0 mW using a centrifuge tube containing pure water.

Thus, entering according values of each parameters to Eq. 1, the 808 nm laser photothermal conversion efficiency (η) of the PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites can be deduced to be 43.8%. Similarly, the τ_s of the free ICG was determined to be 176.26 s (Fig.S4b), hS is calculated to be 4.76 mW/°C. The absorbance of the free ICG at 808 nm A_{808} is 1.83, then the 808 nm laser heat conversion efficiency (η) of the free ICG can be deduced to be 41.2%.

Supplementary Figures

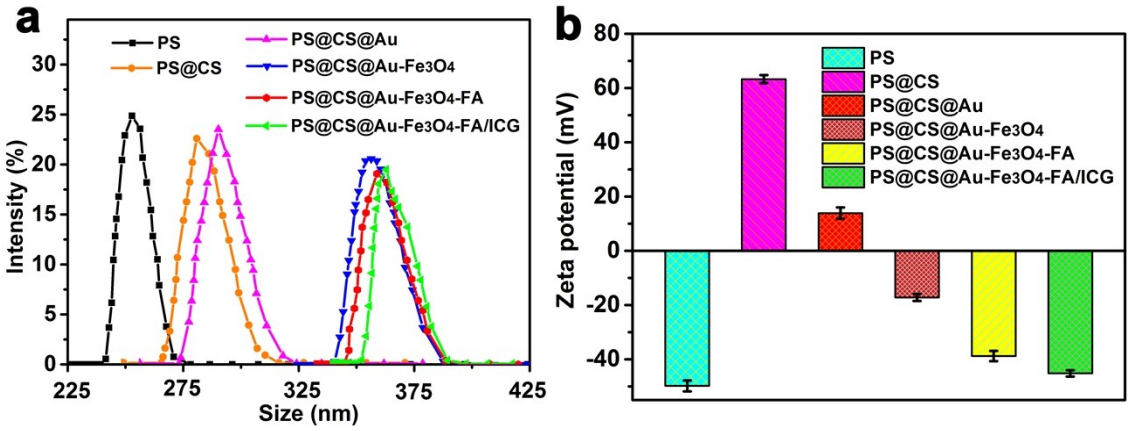

Fig. S1 (a) The size distribution and (b) the zeta potential of PS, PS@CS, PS@CS@Au, PS@CS@Au-Fe_3O_4, PS@CS@Au-Fe_3O_4-FA, PS@CS@Au-Fe_3O_4-FA/ICG

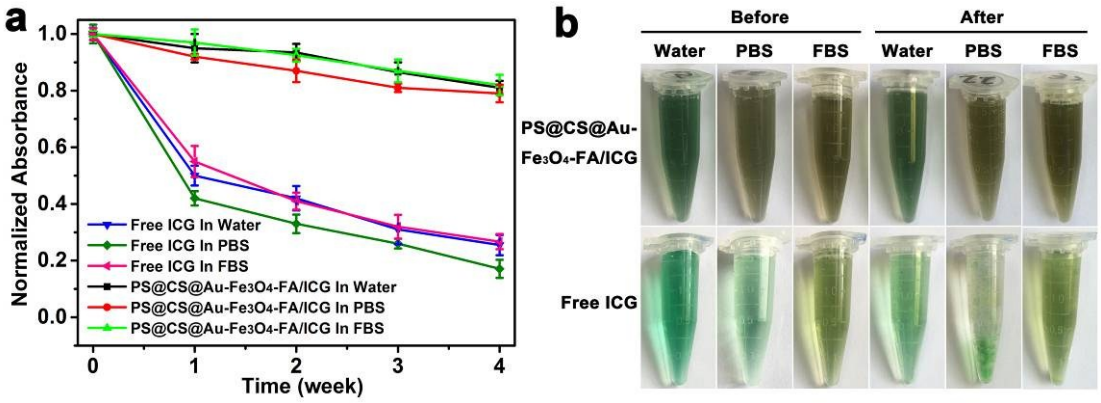

Fig. S2 (a) The normalized absorbance intensities and (b) photos of free ICG and PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites in the water, PBS solution and FBS solution over 4 weeks

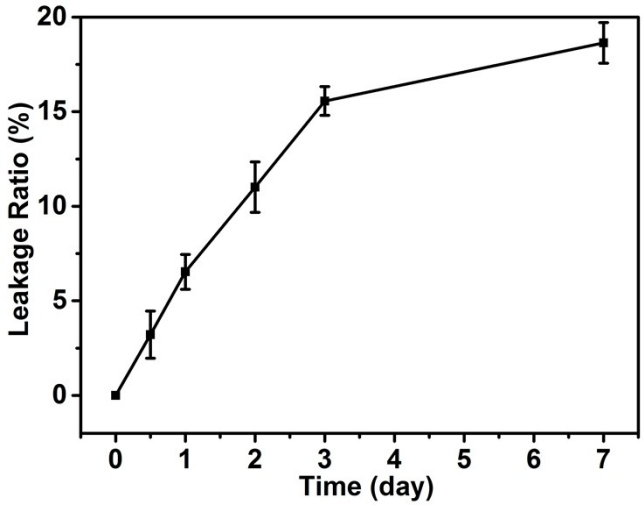

Fig. S3 The leakage ratio of the ICG from PS@CS@Au-Fe_3O_4-FA nanocomposites over a week

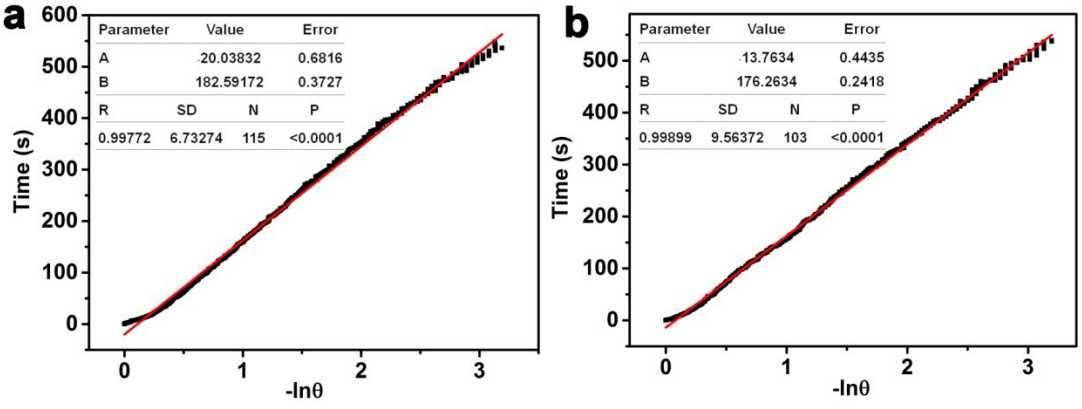

Fig. S4 (a) Linear time data versus -ln(θ) of the PS@CS@Au-Fe_3O_4-FA/ICG nanocomposites (400 ppm, ICG loading content was 9%). (b) Linear time data versus -ln(θ) of the free ICG (36 μg/mL).

Reference

1. X. Liu, B. Li, F. Fu, K. Xu, R. Zou, Q. Wang, B. Zhang, Z. Chen and J. Hu, *Dalton Trans.*, 2014, **43**, 11709-11715.