# Supplementary Information for

## Cysteine-induced one-pot synthesis of Au nanoparticle chains with tuneable NIR absorption and application in photothermal-chemo cancer therapy

Pengcheng Gao, Yingying Wei, Qianrui Xu and Yong Jiang*

School of Chemistry and Chemical Engineering, Jiangsu Province Hi-Tech Key Laboratory for Biomedical Research, Southeast University, Nanjing 211189, P.R. China

* E-mail:yj@seu.edu.cn

### Materials

Chloroauric acid ($HAuCl_4 \cdot 4H_2O$), silver nitrate and L-cysteine (L-cys) were purchased from Aldrich. Sodium hydroxide (NaOH), TEOS, pyrogallol and sodium borohydride ($NaBH_4$) were purchased from Shanghai Chemical Reagent Corp. Doxorubicin hydrochloride (DOX) was purchased from Beyotime Biotechnology Co., Ltd. NH2-PEG-SH (Mw=500) was purchased from Yarebio (Shanghai, China). Phosphate buffer (PBS), Parenzyme and all the other biological reagents, including 1640 culture medium, fetal bovine serum (FBS) were purchased from Sangon Biotech.

MCF-7 cells were obtained from the Chinese Academy of Sciences Cells Bank. Water used in this experiment was purified by distillation of deionized water.

**The calculation of photothermal conversion efficiency**

According to previous literatures, the photothermal conversion efficiencies of AuNCs@mSiO$_2$ was calculated according to following equation

$$\eta = \frac{hs(T_{max} - T_{surr}) - Q_{dis}}{I(1 - 10^{-A_{808}})} \times 100\%$$

Where h is heat transfer coefficient, S is the surface area of the container. $T_{max}$ is the equilibrium temperature, $T_{surr}$ represent ambient temperature. These parameters can be calculated according to Fig. S5. The $Q_{dis}$ means the dissipated heat absorbed by the quaretz cell under laser irradiation and it was measured independently to be 0.086 W/°C using a quartz cuvette cell containing pure water. I is incident laser power (2 W cm$^{-2}$), $A_{808}$ is the absorbance of particles at 808 nm. The photothermal conversion efficiencies of AuNCs@mSiO$_2$ is 31.9%.

**Table. S1.** Details of Sample d-i including diameter, length, assembly number and wavenumber of LSPR.

| L-cys (μL) | Diameter (nm) | Length (nm) | Assembly Number | LSPR (nm) |
|---|---|---|---|---|
| 0 | 14.2±0.8 | 50.8±5 | 1 | 808 |
| 10 | 12.1±1.7 | 31.7±5.5 | 1 | 672 |
| 40 | 11.6±1.9 | 20.4±4.3 | 3±2 | 642 |
| 80 | 11.9±1.9 | 16.3±5.6 | 11±3 | 808 |
| 140 | 11.1±2.2 | 12.6±3.7 | 19±5 | 755 |
| 200 | 11.1±2.1 | 11.5±2.9 | — | 718 |

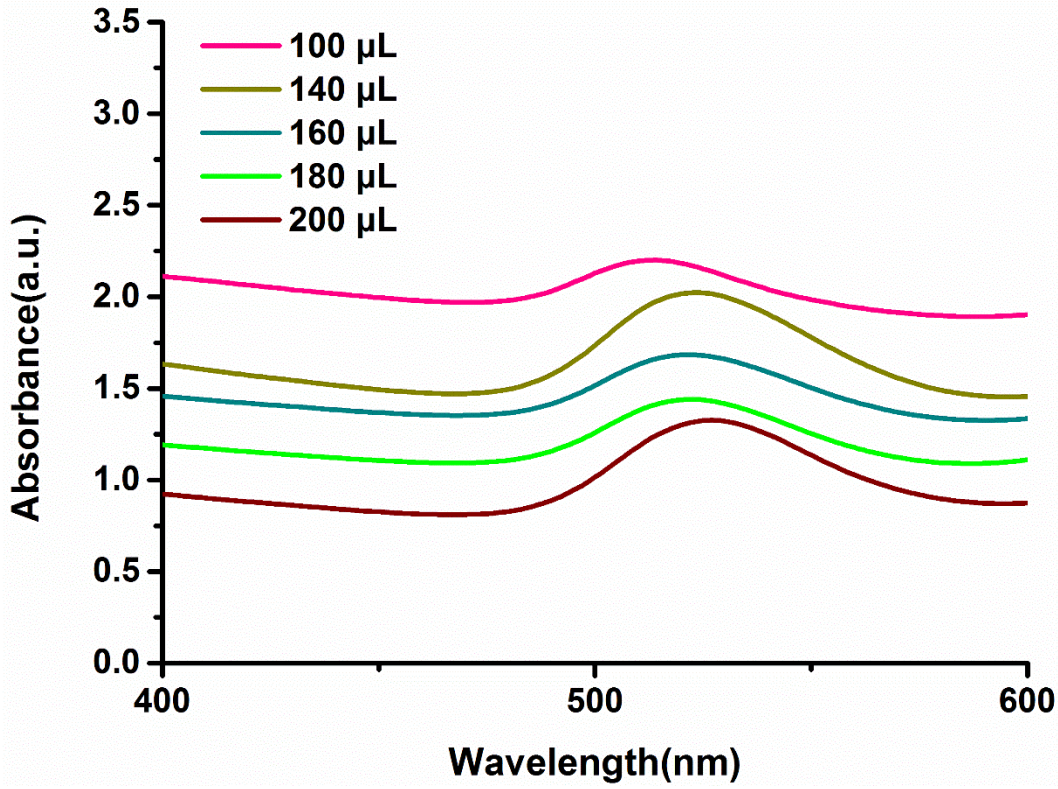


**Fig. S1.** UV spectrum of Fig. 1c with wavelength ranging from 400 to 600 nm.

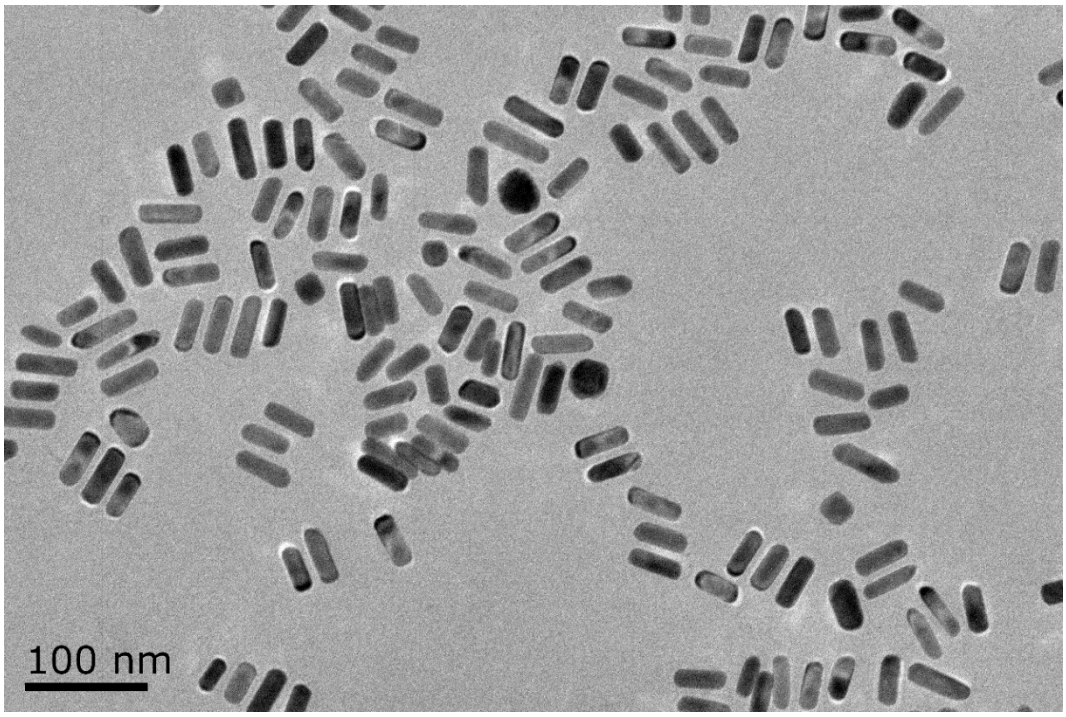


**Fig. S2.** TEM image of AuNPs with the addition Lysine (40 µL, 0.5 mM)

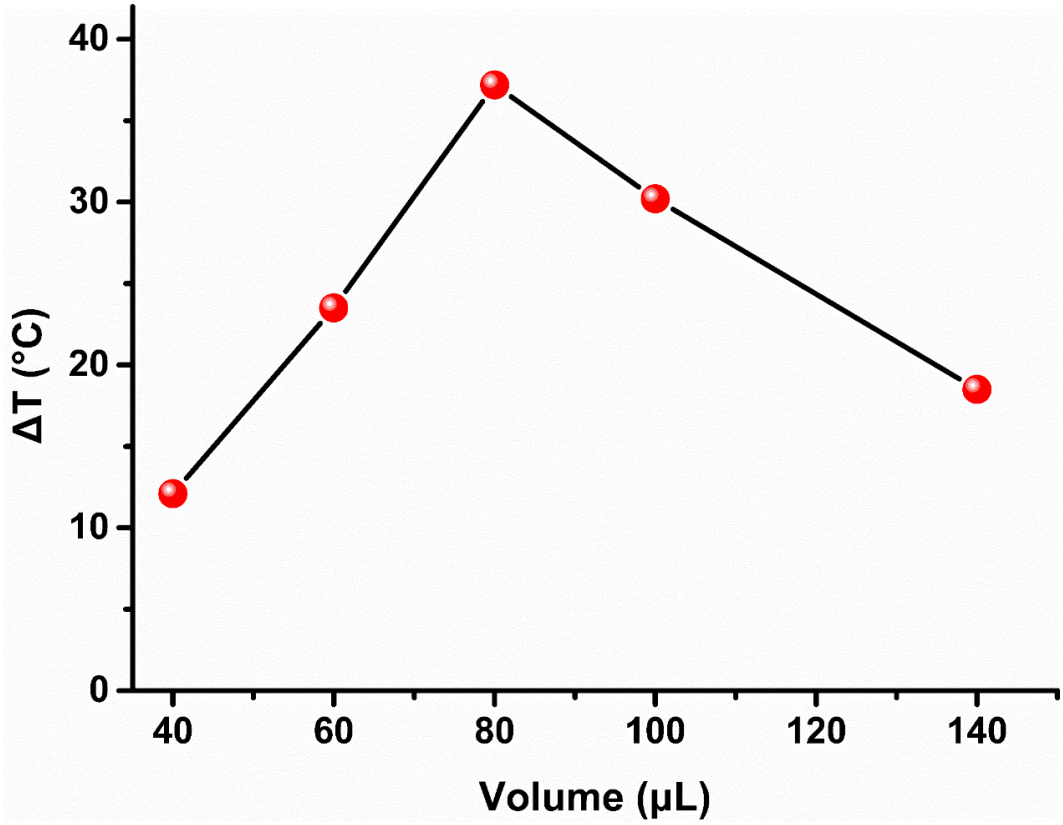


**Fig. S3.** The plot of temperature change (ΔT) of a fixed concentration of AuNCs changed with the volume of L-cys.

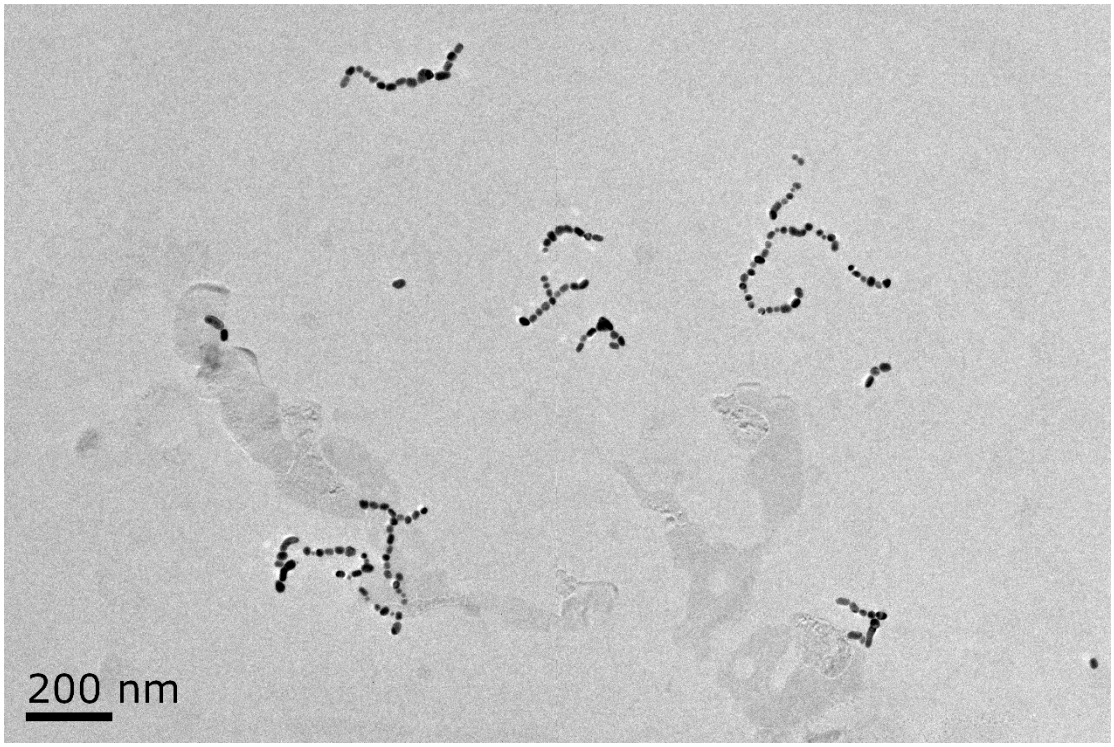


**Fig. S4.** TEM image of AuNCs after photothermal conversion experiment.

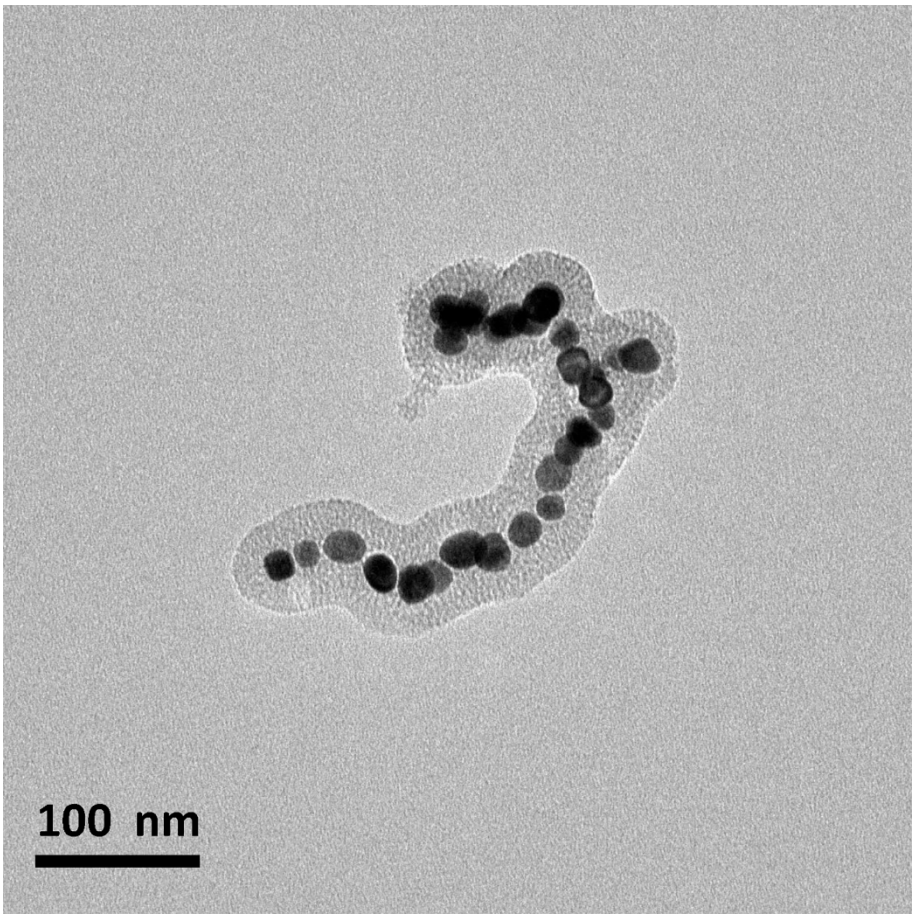


**Fig. S5.** Enlarged TEM image of a single AuNCs coated with Mesoporous $SiO_2$.

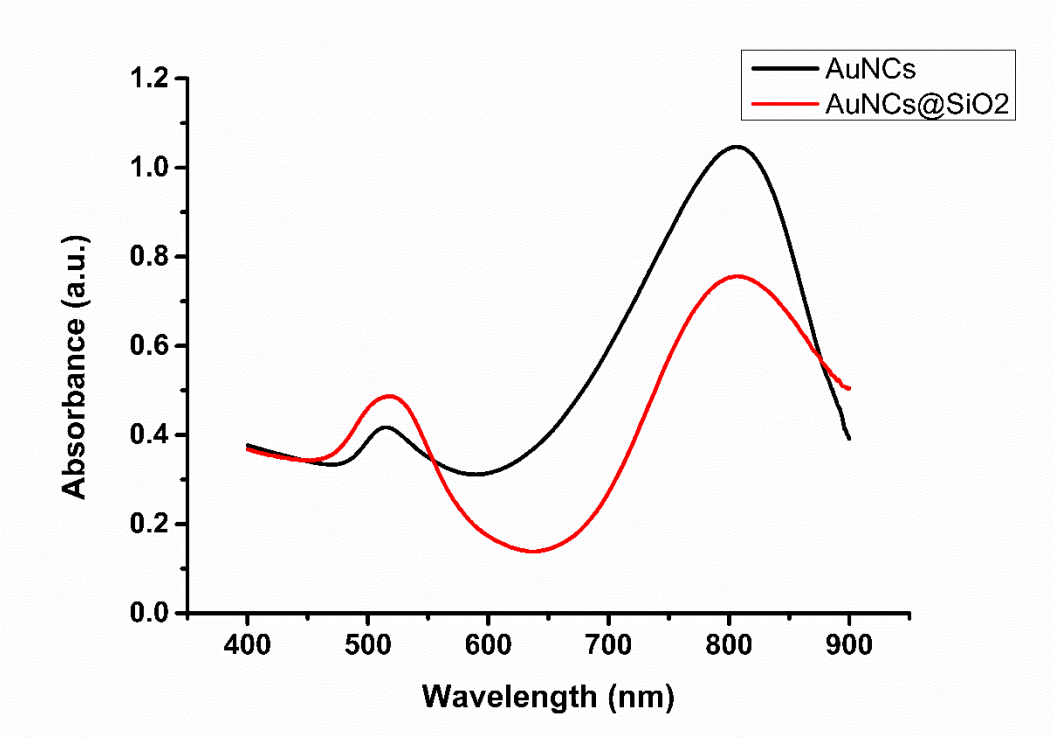


**Fig. S6.** UV-Vis spectra of AuNCs and AuNCs@mSiO2.

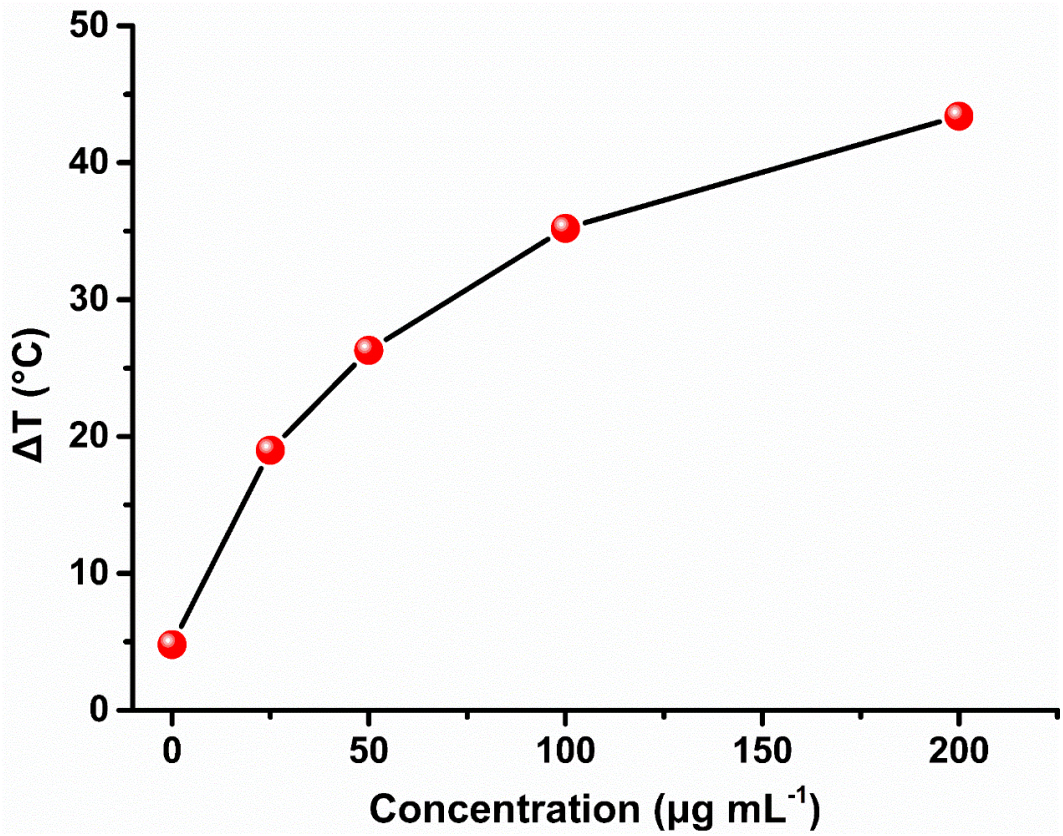


**Fig. S7.** The plot of temperature change (ΔT) of different concentration of AuNCs@mSiO$_2$.

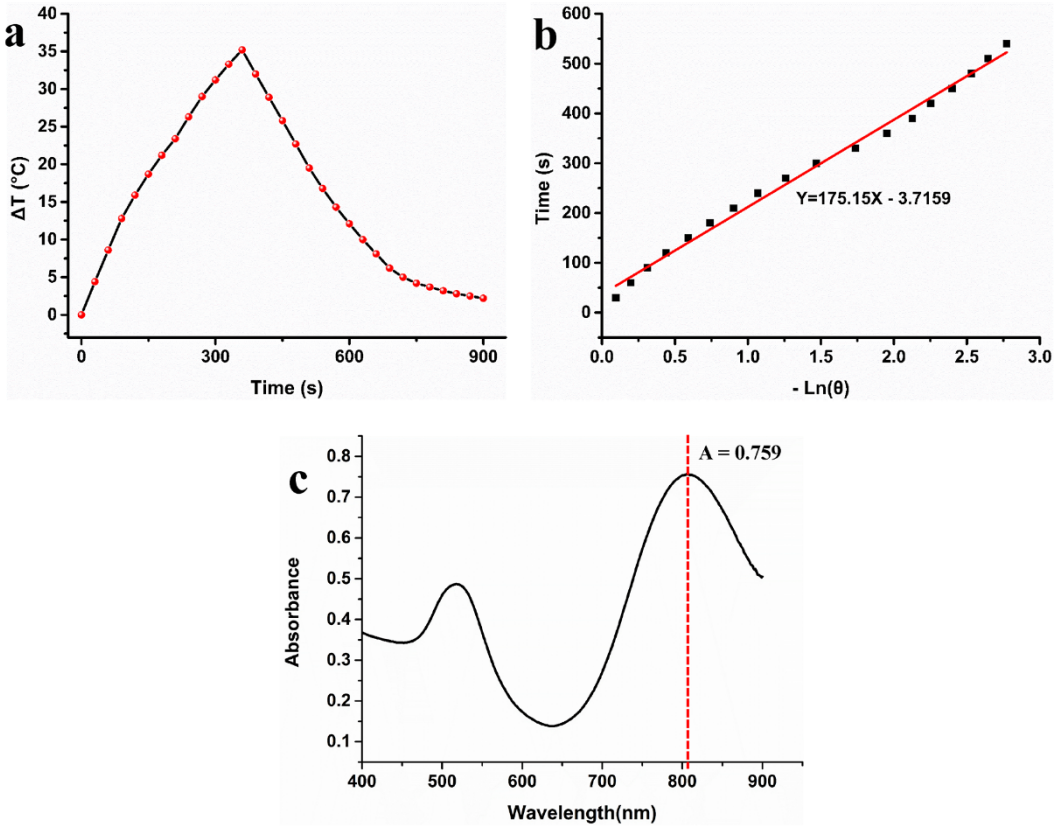


**Fig. S8.** (a) Photothermal curves of AuNCs@mSiO$_2$ aqueous solution (100 μg mL$^{-1}$, Au) under 808 nm laser irradiation (2 W cm$^{-2}$, 6 min) and a subsequent cooling process. (b) Time constant for heat transfer from the system is determined to be $\tau_s$= 175.15 by applying the linear time data from the cooling period versus negative natural logarithm of driving force temperature. (c)Absorption spectrum of AuNCs@mSiO$_2$ aqueous solution (100 μg mL$^{-1}$).

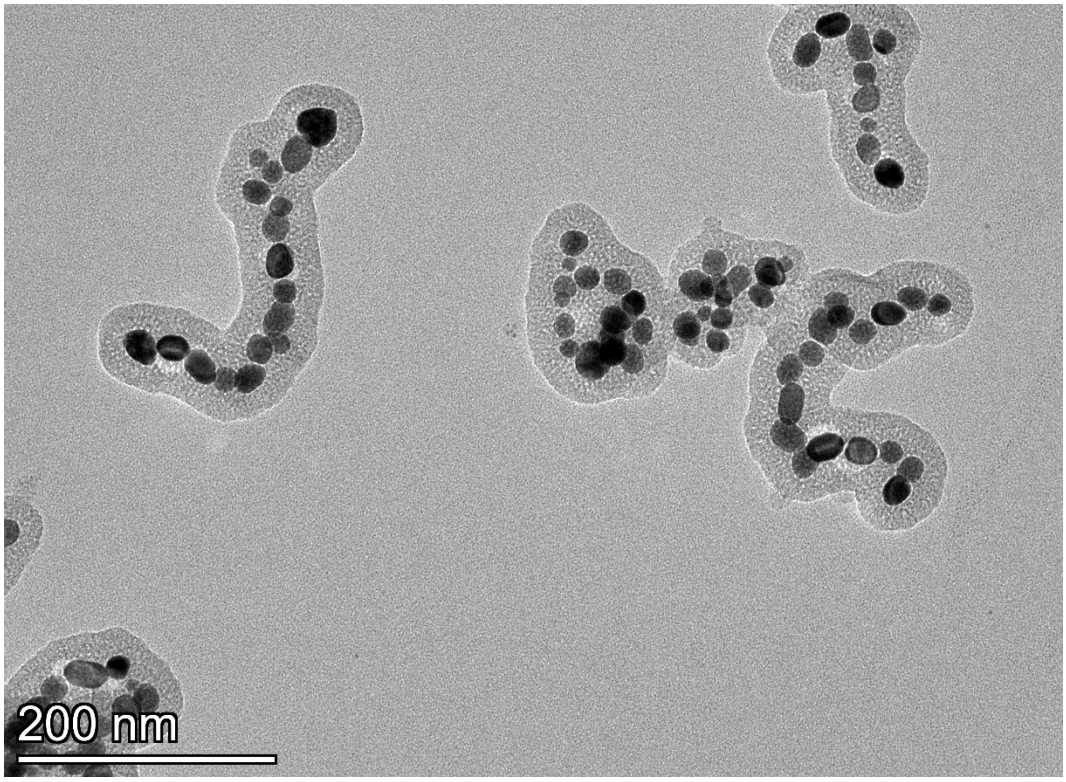


**Fig. S9.** TEM image of AuNCs@mSiO$_2$ after 5 heating-cooling cycles.

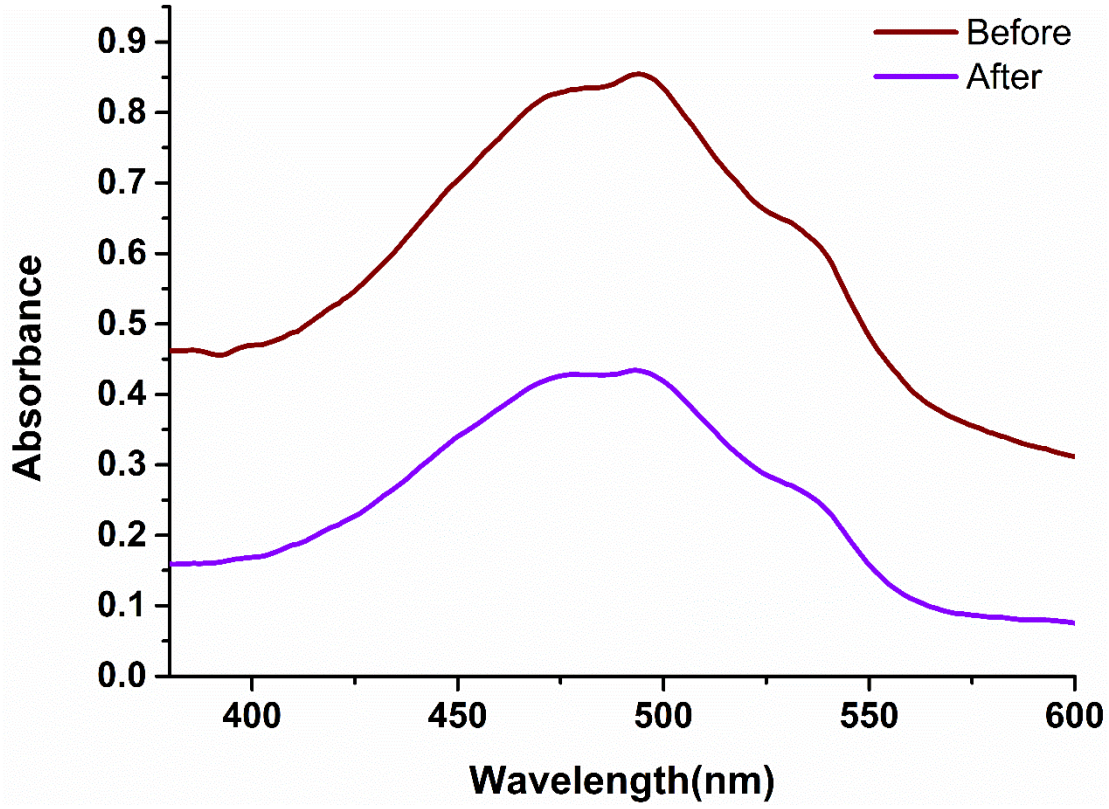


**Fig. S10.** UV-Vis spectra of DOX before and after interaction with the AuNCs@mSiO$_2$

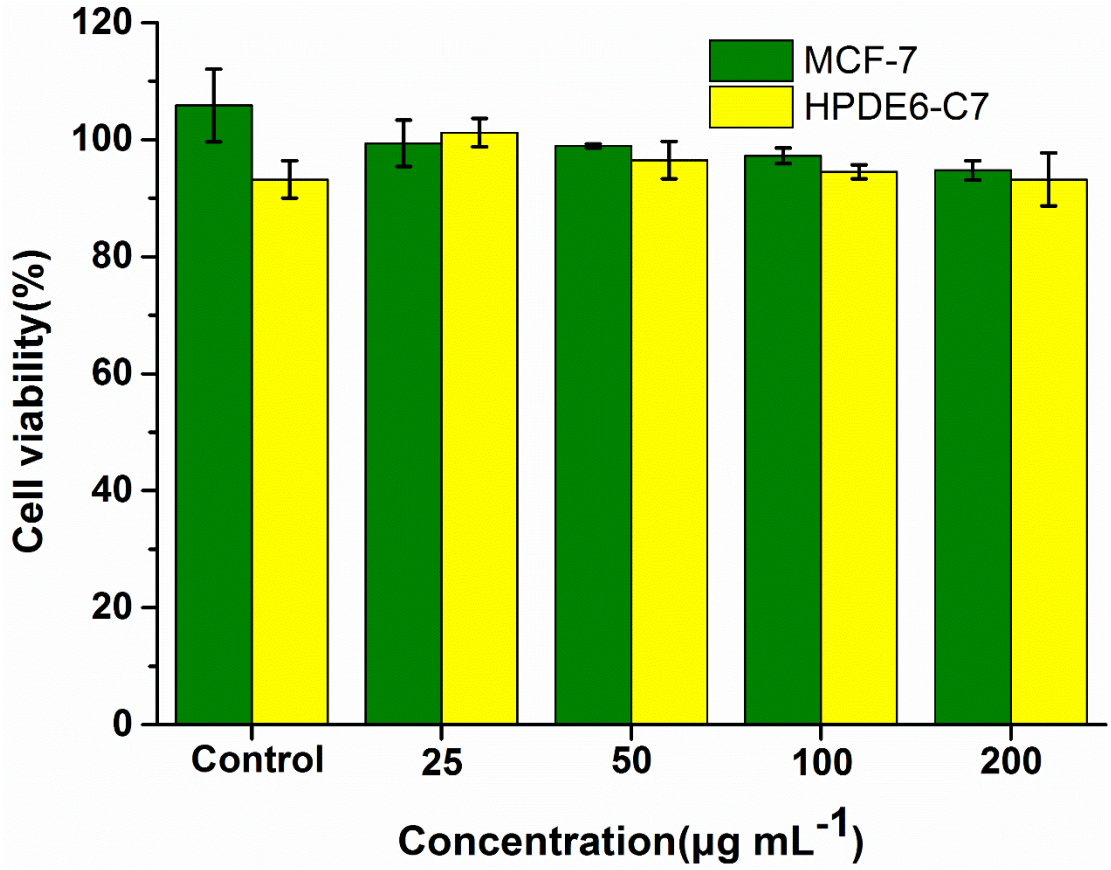


**Fig. S11.** Cell viability of MCF-7 and HEPD6-C7 after incubation with different AuNCs@mSiO$_2$ concentration.

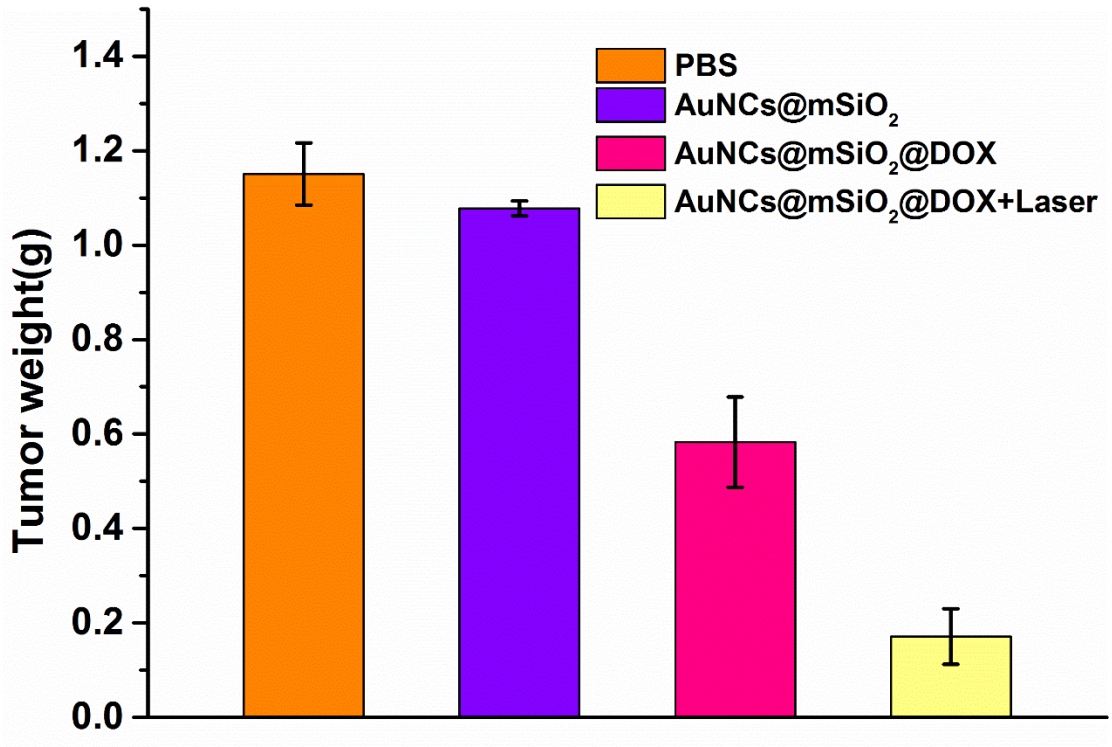


**Fig. S12.** Mean tumor weights of each group at the last day of experiment. Data are presented as means ± SD (n = 3).

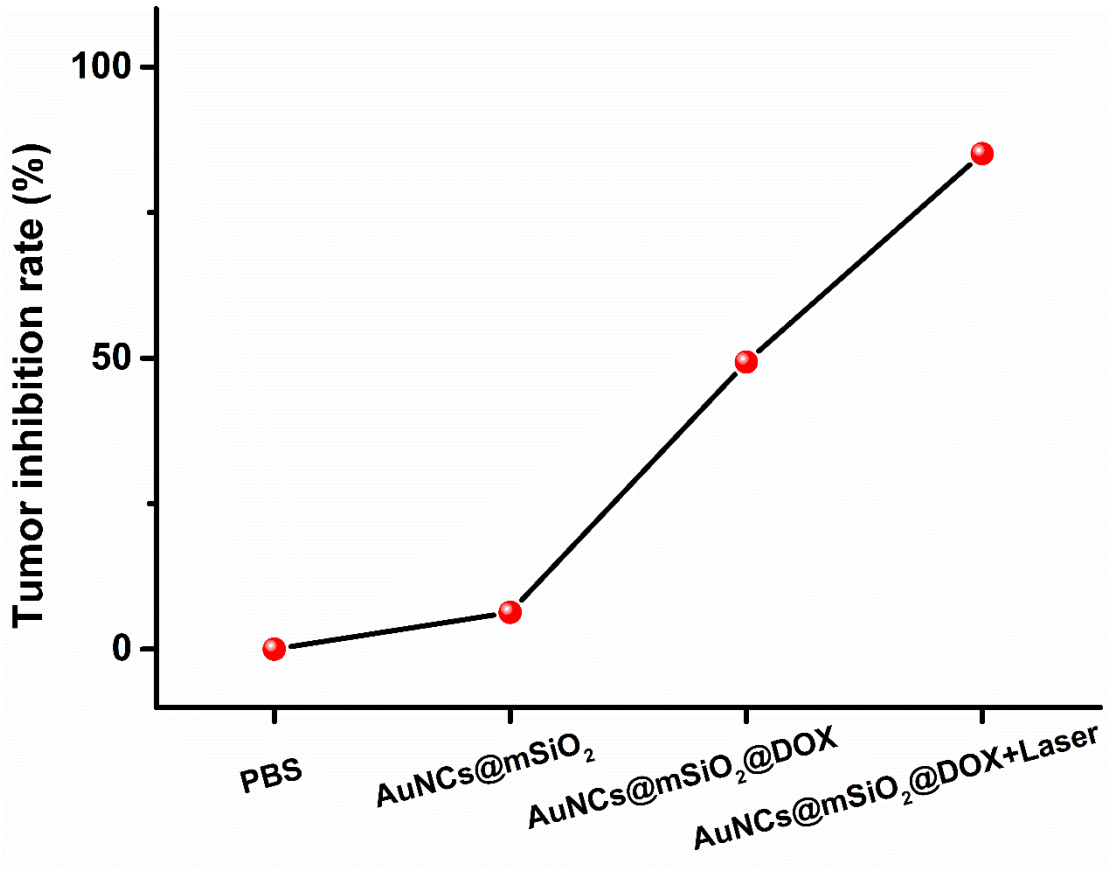


**Fig. S13.** Tumor inhibition rate of each group at the last day of experiment.

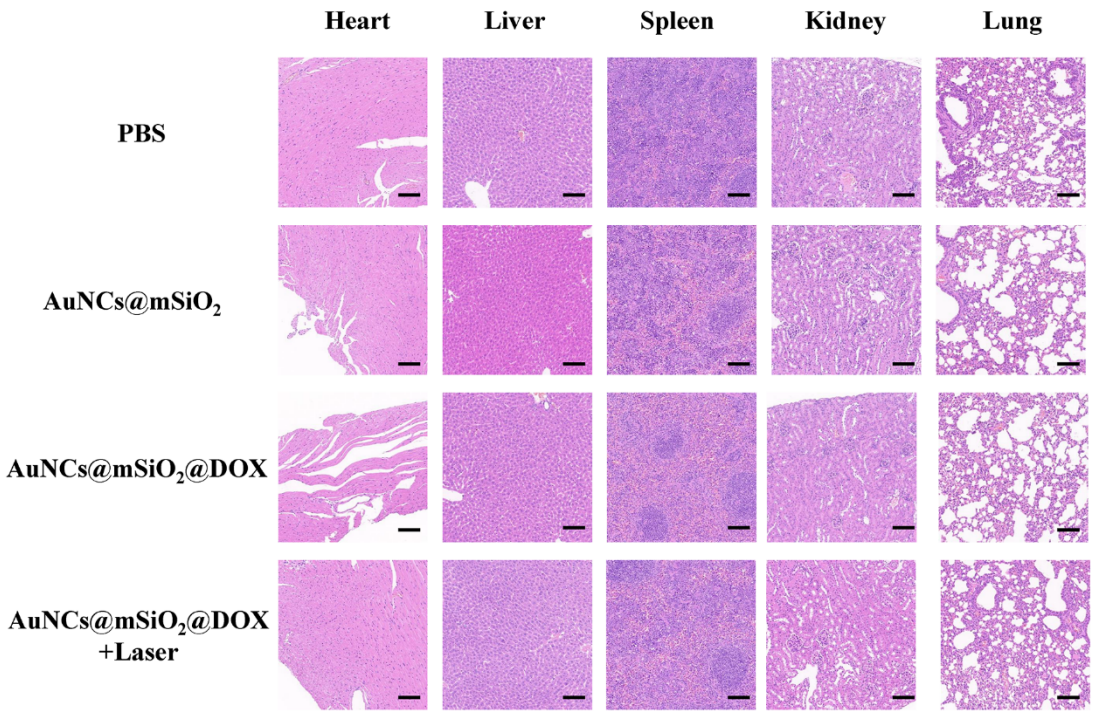


**Fig. S14.** H&E staining images of major organs with different treatment. Sacle bars is 100 μm.