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Supporting Information

Concurrent photothermal therapy and photodynamic therapy for cutaneous squamous cell carcinoma by gold nanoclusters under a single NIR laser irradiation

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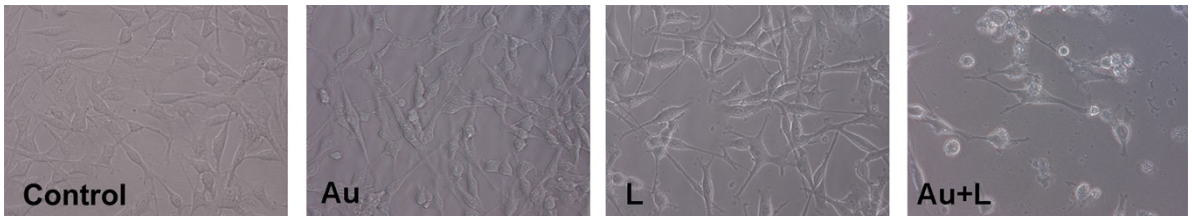

Fig. S1 Changes in cell morphology after diverse treatments: control, $Au_{25}(Capt)_{18}$, laser, $Au_{25}(Capt)_{18}$+laser (Au: 80 μg/mL, laser: 0.6 W/cm^2, 5 min).

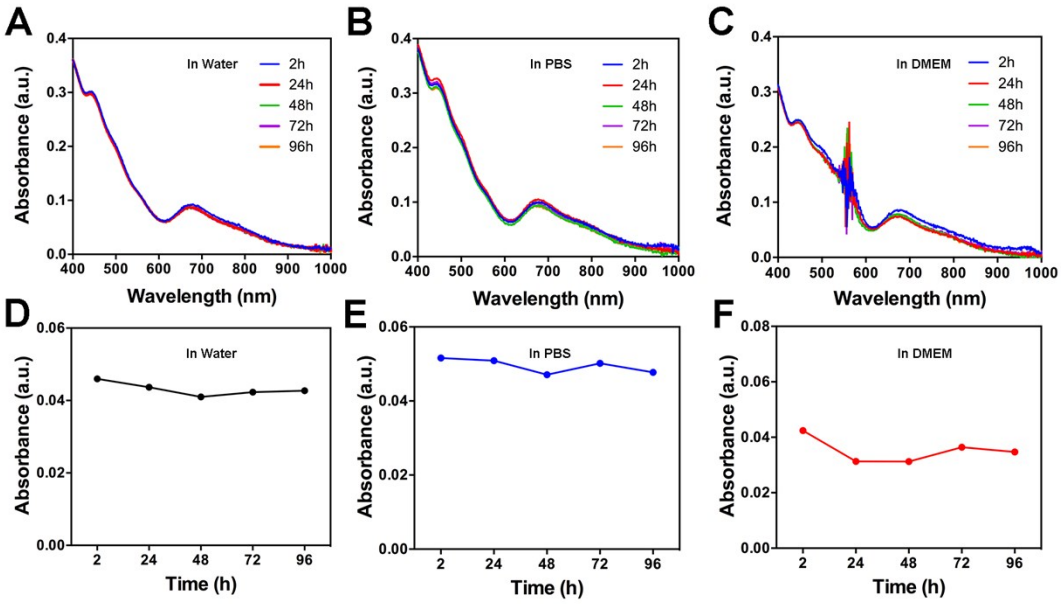

Fig. S2 Stability analysis. (A-C) The UV−vis absorption spectra of $Au_{25}(Capt)_{18}$ in different solution over 2, 24, 48, 72, and 96 h (A: in water, B: in PBS, C: in DMEM). (D-F) The variation of absorption value at 808 nm of $Au_{25}(Capt)_{18}$ in different solution over 2, 24, 48, 72, and 96 h (D: in water, E: in PBS, F: in DMEM).

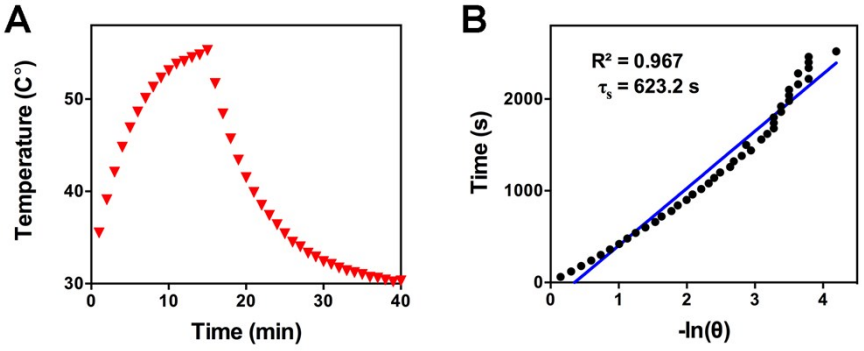

Fig. S3 Photothermal conversion efficiency of $Au_{25}(Capt)_{18}$. (A) The temperature change of $Au_{25}(Capt)_{18}$ aqueous solution under the irradiation of 808 nm laser (2 W/cm^2) for 15 min and the laser was removed immediately. (B) The time versus the negative natural logarithm of the temperature from the cooling period (after 15 min) in (A) and τ_s was calculated to be 623.2 s by applying

linear relationship.

The photothermal conversion efficiency (η) was calculated according to following equations:

$\theta = (T - T_{surr}) \div (T_{max} - T_{surr})$ (1)

$t = \tau_s \times (-\ln\theta)$ (2)

$\tau_s = 623.2$ s

$hS = (\sum m_i C_{p,i}) \div \tau_s$ (3)

$= [m(H_2O) \times c(H_2O) + m(quartz) \times c(quartz)] \div \tau_s$

$= (1 \times 4.2 + 5.76 \times 0.839) \div 623.2$

$= 14.49\ mW^oC^{-1}$

$Q_{Dis} = hS \times (T(H_2O)_{max} - T_{surr})$ (4)

$= 14.49 \times (35.3 - 28.8)$

$= 94.19$ mW

$\eta = [hS \times (T_{max} - T_{surr}) - Q_{Dis}] \div [I \times (1 - 10^{-A808})] \times 100\%$ (5)

$= [14.49 \times (55.3 - 28.8) - 94.19] \div [2000 \times (1 - 10^{-0.1889})] \times 100\%$

$= 41.1\%$

h (mW m^{-2} °C^{-1}): The heat transfer coefficient.

$\boldsymbol{T_{surr}}$ (°C): The ambient temperature of the surrounding environment (28.8 °C).

$\boldsymbol{T_{max}}$ (°C): The maximum equilibrium temperature (55.3 °C).

$\boldsymbol{Q_{Dis}}$ (mW): The heat absorbed by the solvent DI water and the quartz cell.

I : The 808 nm laser power density (2.0 W/cm^2).

$\boldsymbol{A_{808}}$: The absorbance of $Au_{25}(Capt)_{18}$ at 808 nm (0.1889).

$\boldsymbol{\tau_s}$: The time constant for heat transfer of the $Au_{25}(Capt)_{18}$ aqueous solution which was calculated by linear relationship of time versus -ln(θ) from **Fig. S3B** (623.2 s).

$\boldsymbol{m(H_2O)}$ and $\boldsymbol{c(H_2O)}$: The mass (1.0 g) and heat capacity (4.2 J/g) of the solvent DI water respectively.

m(quartz) and ***c(quartz)*** :The mass (5.76 g) and heat capacity (0.839 J/g) of the container quartz cell respectively.

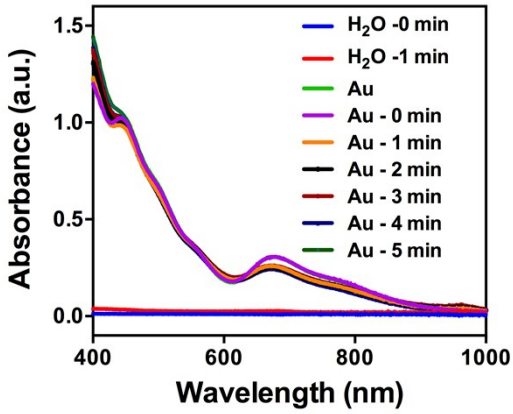

Fig. S4 •OH generation detection: Generation of •OH by $Au_{25}(Capt)_{18}$ (0.1 mg/mL) measured by the oxidation of TMB via recording fluorescence emission spectra at 654 nm subjected to laser irradiation at different time points (1 W/cm^2, 0 min~5 min), DI water with TMB irradiated by 808 nm laser (H_2O - 1 min) or not (H_2O - 0 min) , and pure $Au_{25}(Capt)_{18}$ solution (Au) were set as controls.