Supporting Information for

# A Comparison Study of Gold Nanohexapods, Nanorods, and Nanocages for Photothermal Cancer Treatment

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**Calculation of volume and mass of an individual Au nanohexapod**

The volume of the octahedral core is:

$\frac{\sqrt{2}}{3} \times a^3 = \frac{\sqrt{2}}{3} \times 25.3^3 = 7.6 \times 10^3$ nm$^2$, where $a$ represents the edge length of the octahedron.

Under the assumption that each arm can be characterized as an ellipsoid with a circular cross section, the total volume of the six arms is:

$6 \times \frac{4}{3} \times \pi \times ab^2 = 6 \times \frac{4}{3} \times \pi \times 8.2 \times 6.8^2 = 9.5 \times 10^3$ nm$^3$, where $a$ and $b$ represent the large and small diameters of the ellipsoid, respectively.

Therefore, the volume of an individual Au nanohexapod is $7.6 \times 10^3 + 9.5 \times 10^3 = 1.7 \times 10^4$ nm$^3$. Based on the face-centered cubic (*fcc*) structure of solid Au, the atomic density of the Au nanohexapod is 59 atoms/nm$^3$ and the number of Au atoms per particle is: $59 \times 1.7 \times 10^4$ nm$^3$ = $1.0 \times 10^6$. The mass of an individual Au nanohexapod is: $1.0 \times 10^6 \times 197 = 2.0 \times 10^8$.

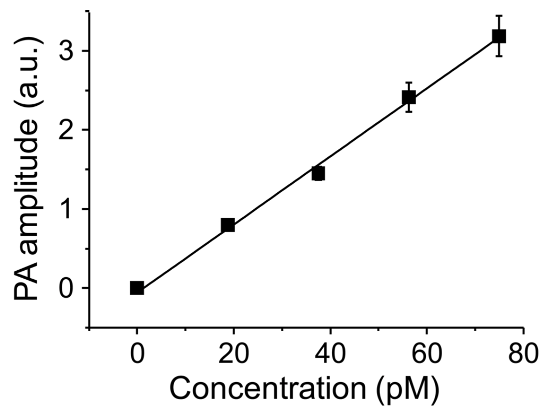


**Figure S1.** A plot of PA signal amplitude versus particle concentration for aqueous suspensions of Au nanohexapods.

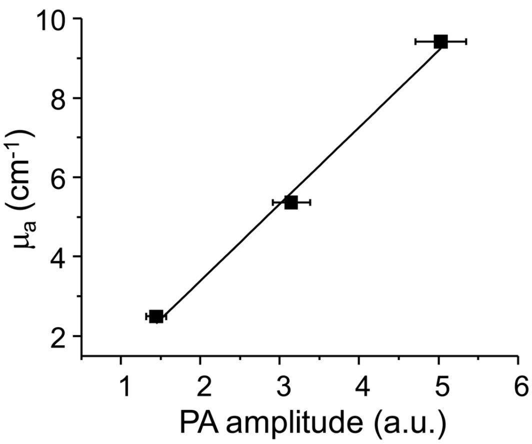


**Figure S2.** The linear relationship between the optical absorption coefficient ($\mu_a$) and PA signal amplitude for aqueous solutions of indocyanine green (ICG).

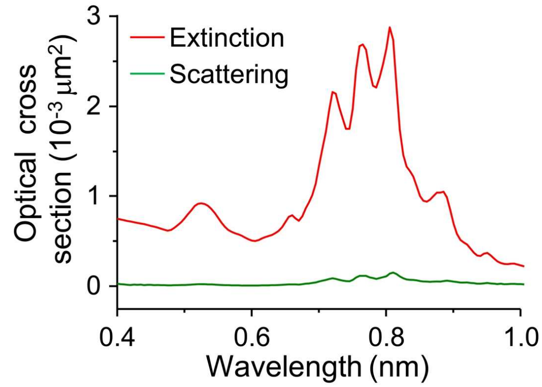


**Figure S3.** Extinction and scattering spectra calculated for a Au nanohexapod using the discrete dipole approximation (DDA) method.

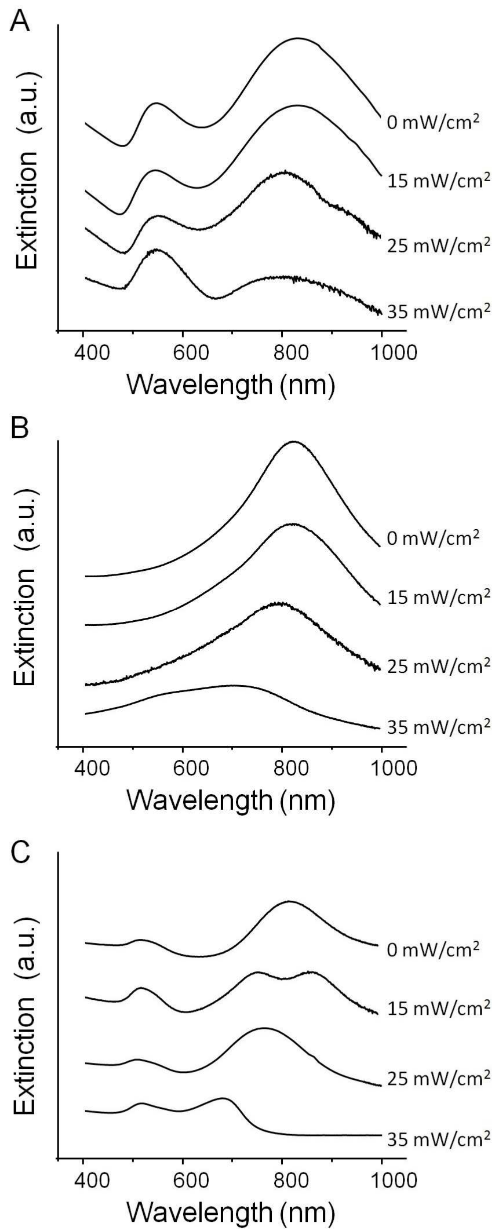


**Figure S4.** Photothermal stability of aqueous suspensions of Au nanostructures under irradiation by a pulsed laser: A) nanohexapods, B) nanocages, and C) nanorods.

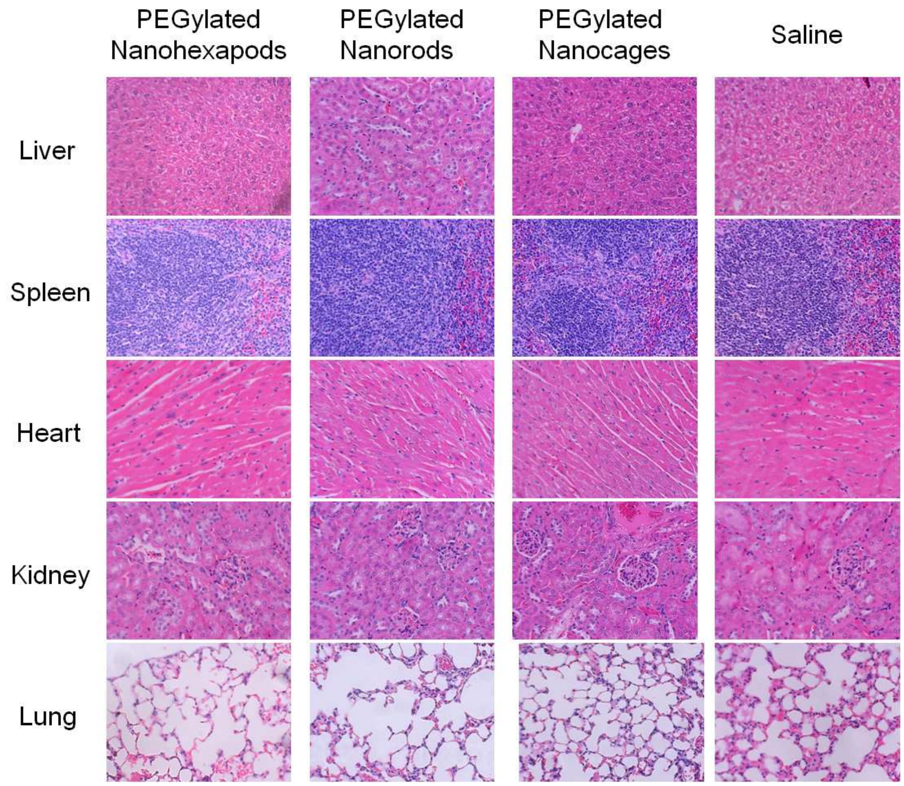


**Figure S5.** Representative histology images of major tissues from mice intravenously administrated with PEGylated Au nanostructures or saline at 7 days post injection.

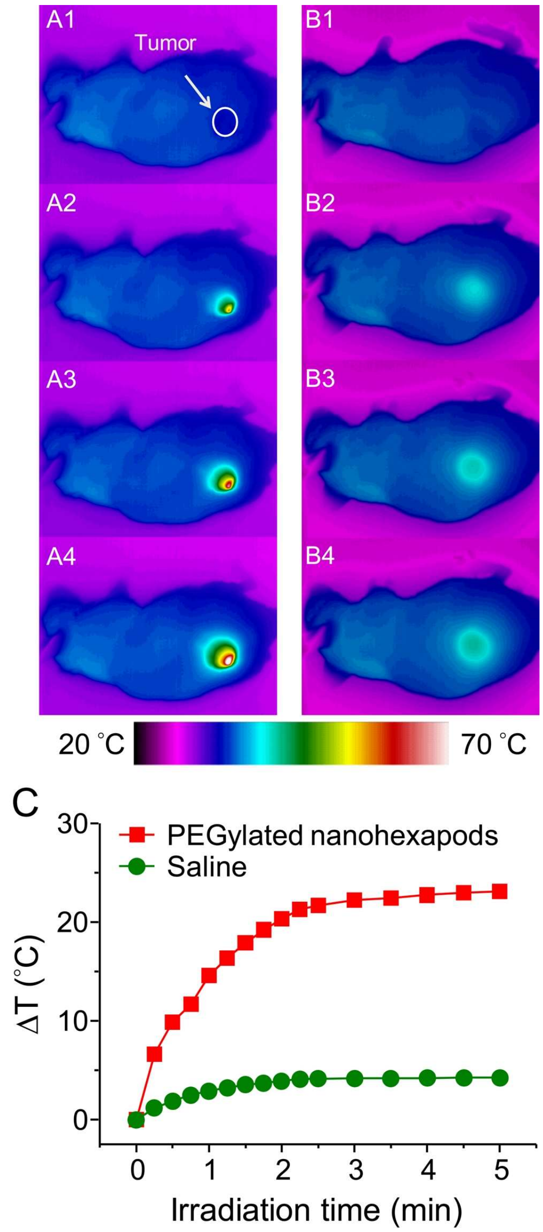


**Figure S6.** Thermographs of tumor-bearing mice receiving photothermal treatment for different periods of time: A1, B1) 0; A2, B2) 0.5; A3, B3) 2; and A4, B4) 5 min. The mice were injected intratumorally with either (A1-A4) aqueous suspensions of PEGylated nanohexapods and (B1-B4) saline, respectively. C) Plots of average temperature increase within the tumor region as a function of irradiation time (n = 1). The laser power density was 1.0 W/cm$^2$.