Theranostic Au Cubic Nano-aggregates as Potential Photoacoustic Contrast and Photothermal Therapeutic Agents

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Supporting Information

Calculation of the molar extinction coefficient of Au-80 CNAs:

We assumed the Au CNAs as hollow nanocubes.

The volume of the nanoparticles (NPs): $D^3 - d^3 = 1.69 \times 10^5\ nm^3$, where D represents the outer edge length and d represents the inner edge length.

The number of Au atoms per nanoparticle is: $\frac{\rho V}{M} \times N_A = 9.97 \times 10^6$, where ρ is the density of the Au, V is the volume of the NPs, M is the molar mass of Au, N_A is the Avogadro constant.

The mass of per particle: $9.97 \times 10^6 \times 197 = 1.97 \times 10^9$.

The concentration of Au atoms determined by ICP-AES: c_{atom}.

The concentration of nanoparticles: $c_{NPs} = \frac{c_{atom}}{\frac{\rho V}{M} \times N_A} = 3.82 \times 10^{-11}\ M$.

According to the Beer–Lambert law: A = εbc,

The extinction coefficient: $\varepsilon = \frac{A}{bc} = 2.19 \times 10^{10}\ M^{-1} \cdot cm^{-1}$.

Table S1. Different reaction conditions for synthesizing Cu_2O nanocubes with tunable sizes.

0.02 M $CuSO_4$ (mL)	0.05 M mPEG-NH_2 (μL)	molar ratio ($CuSO_4$:mPEG-NH_2)	0.1 M AA (mL)	0.5 M NaOH (mL)	Size (nm)
2	500	8:5	1	3	~700
2	300	8:3	1	3	~400
2	200	4:1	1	3	~300
2	100	8:1	1	3	~170
2	80	10:1	1	3	~120
2	50	16:1	1	3	~70

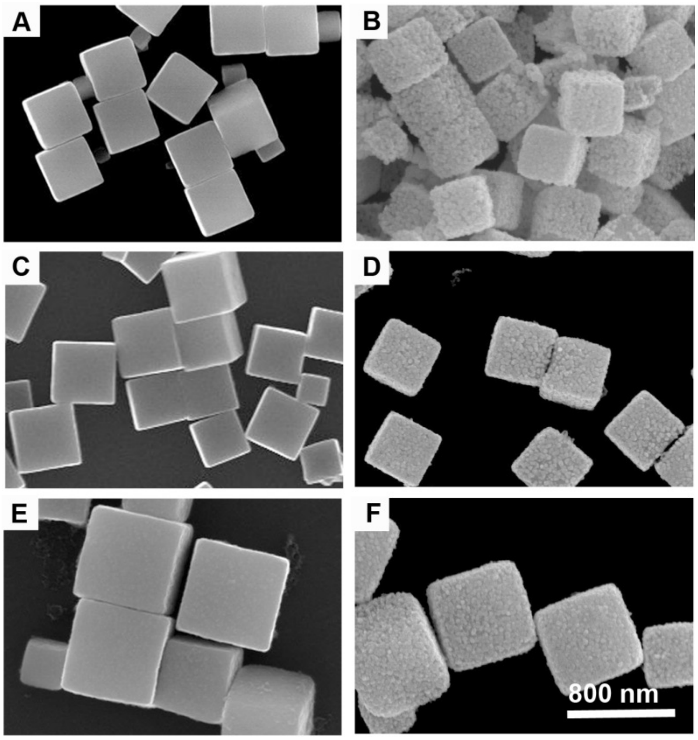

Figure S1. SEM images of Cu_2O-300 (A), Cu_2O-400 (C), Cu_2O-700 (E) and corresponding Au-330 CNAs (B), Au-435 CNAs (D), and Au-750 CNAs (F), respectively. All images share the same scar bar.

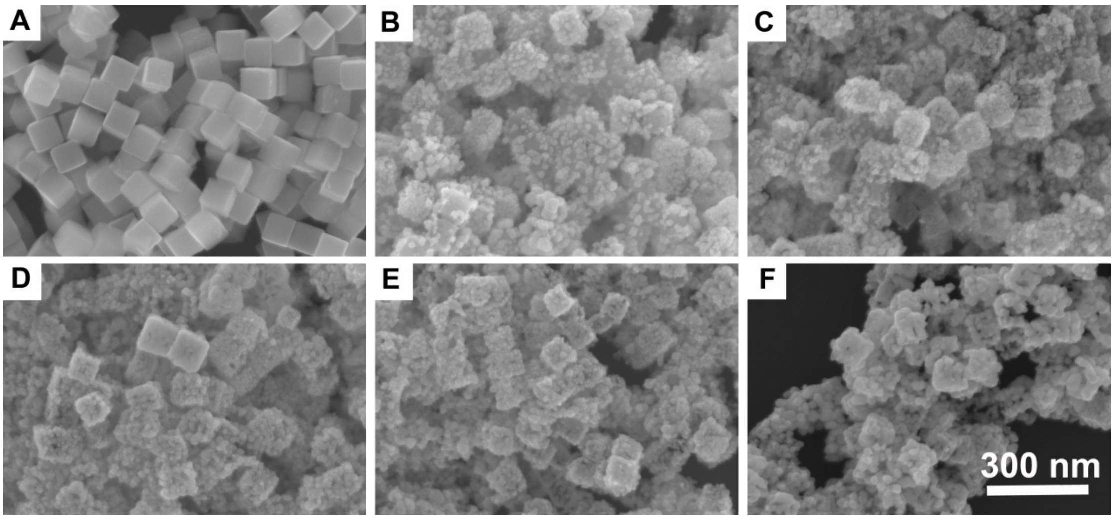

Figure S2. The SEM image of Cu_2O-70 nanocubes (A) and Au CNAs (B-F) by varying the molar ratio of $HAuCl_4$ to Cu_2O nanocubes. All images share the same scar bar.

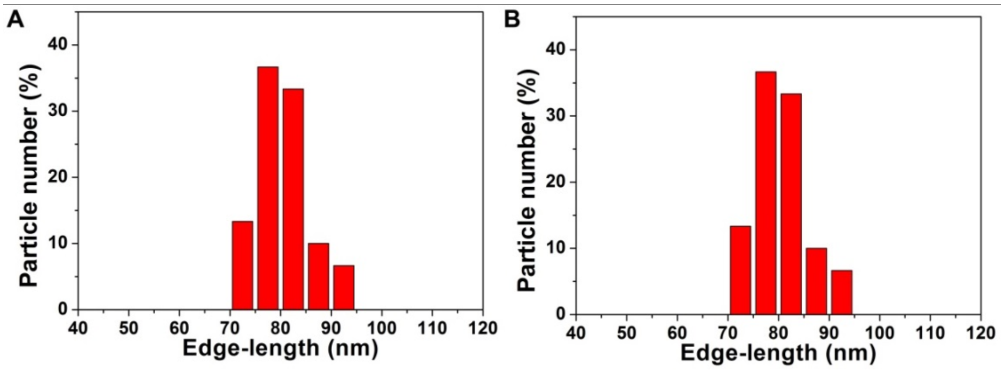

Figure S3. Size distributions of Cu_2O-70 nanocubes (A) with 70.03 ± 4.09 nm and Au-80 CNAs (B) with 80.90 ± 5.04 nm in diameter, respectively.

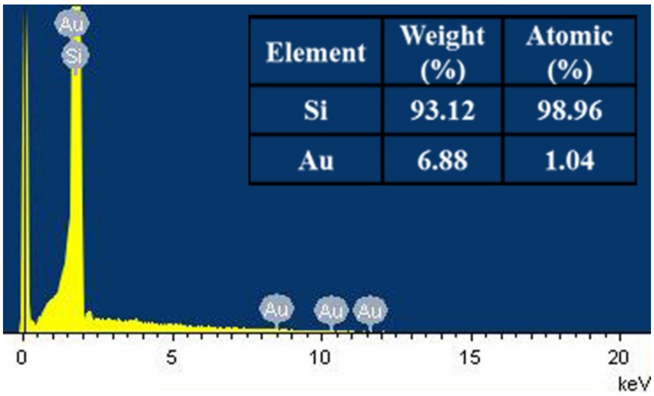

Figure S4. Elemental analysis of Au-80 CNAs on silicon wafer using energy dispersive X-ray spectrometry (EDS).

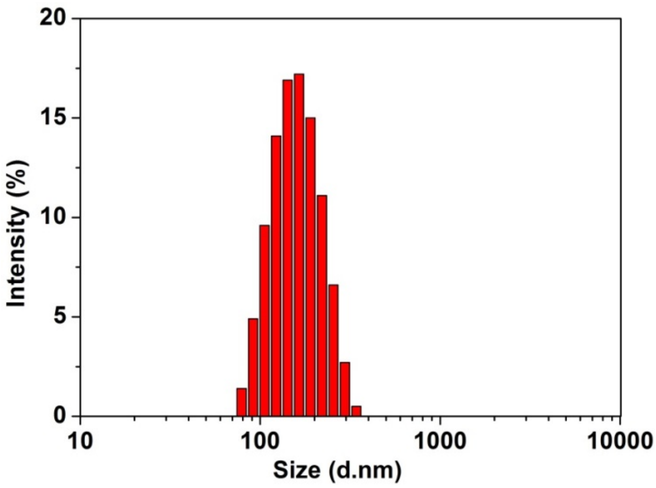

Figure S5. DLS shows hydrodynamic diameter of Au-80 CNAs.

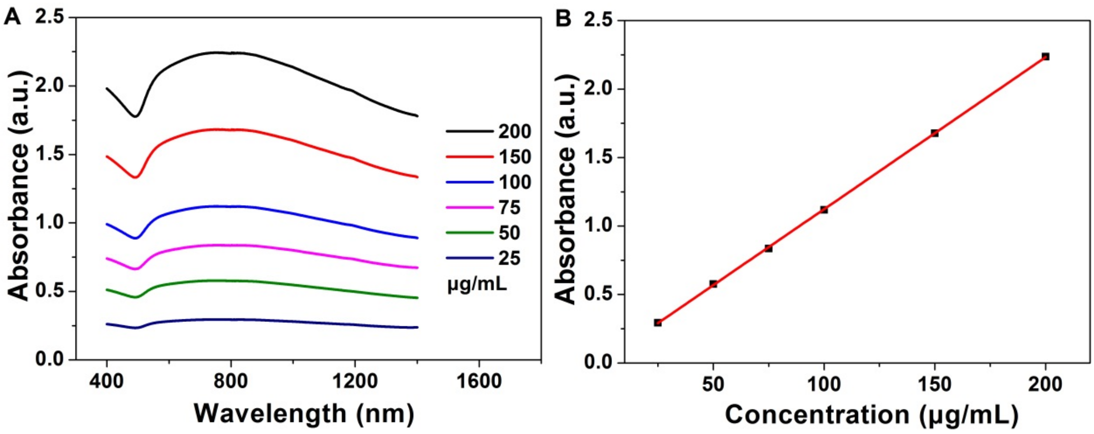

Figure S6. (A) Absorption spectra of Au-80 CNAs aqueous solutions with different concentrations. (B) A linear relationship for the absorbance at the wavelength of 808 nm as a function of the concentration.

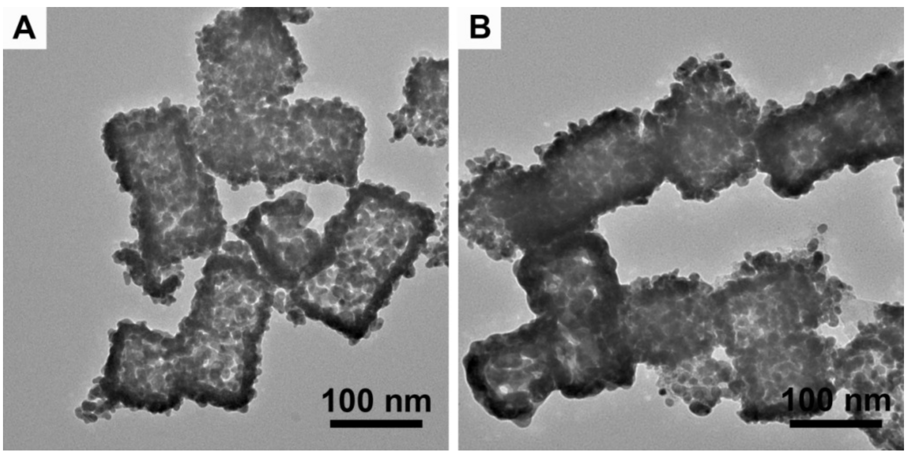

Figure S7. The TEM images of the Au CNAs in an aqueous solution before (A) and after (B) twice irradiation by the 808 nm laser at a power density of 2 W/cm^2 for 10 min.

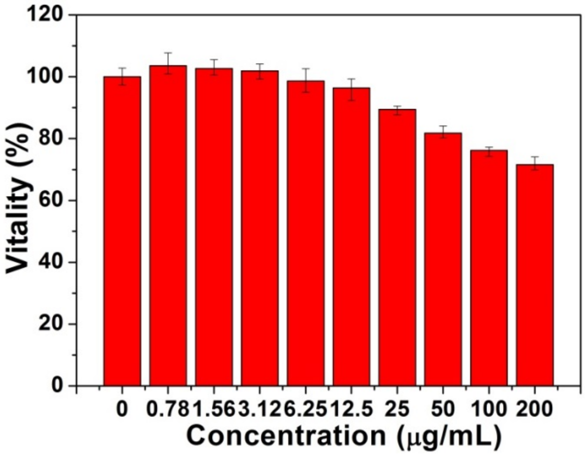

Figure S8. Cell vitality of Hep G2 cells after incubated with Au-80 CNAs nanoparticles with different Au concentrations at 37 °C for 24 h.

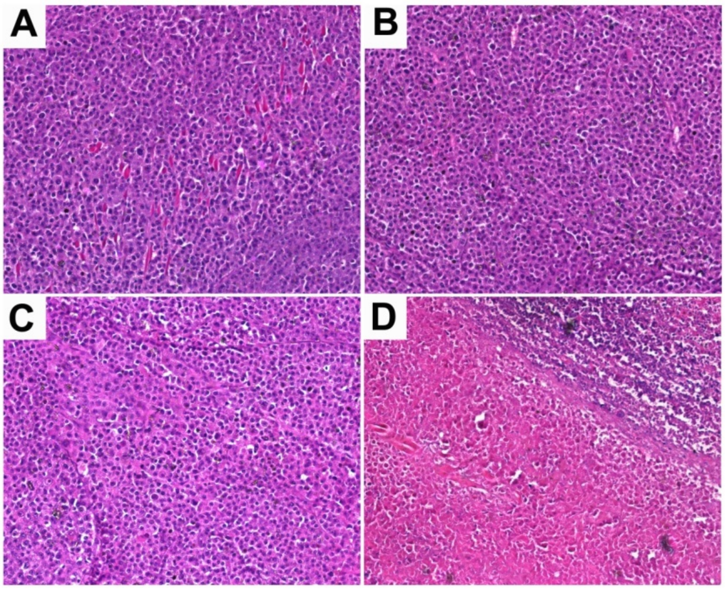

Figure S9. Representative Hematoxylin and eosin (H&E) staining histology images of tumor tissues from the mice after different treatments. (A) blank (no treatment); (B): laser only (exposed to 808 nm laser at 1 W/cm^2 for 5 min,); (C) Au-80 CNAs only (intratumorally injected with 120 μL of 200 μg/mL Au-80 CNAs); (D) Au-80 CNAs and laser co-treatment (intratumorally injected with 120 μL of 200 μg/mL Au-80 CNAs and then immediately exposed to 808 nm laser at 1 W/cm^2 for 5 min).

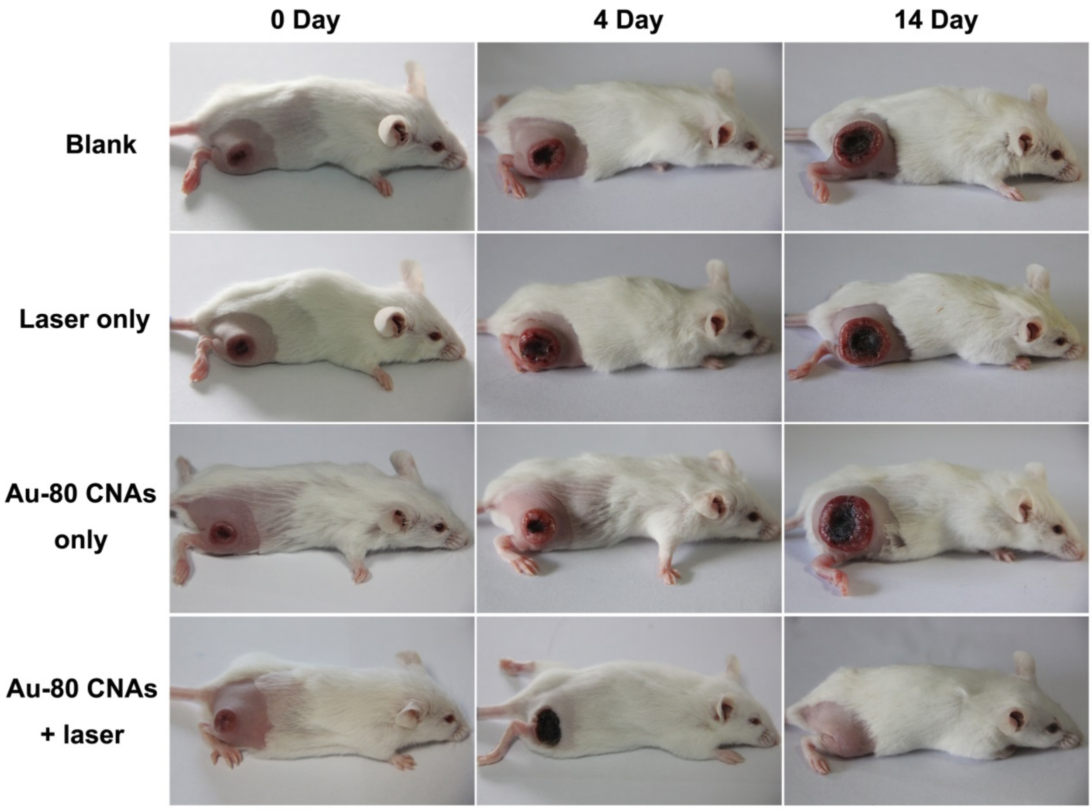

Figure S10. The digital photographs of S180 tumor-bearing mice taken at 0 day before treatments, 4 days and 14 days after treatments of different groups. Treatments: blank (no treatment); laser only (exposed to 808 nm laser at 1 W/cm^2 for 5 min,); Au-80 CNAs only (intratumorally injected with 120 μL of 200 μg/mL Au-80 CNAs); Au-80 CNAs + laser (intratumorally injected with 120 μL of 200 μg/mL Au-80 CNAs and then immediately exposed to 808 nm laser at 1 W/cm^2 for 5 min).