Supplementary Data

Confined Growth of Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres for Improved Computed Tomography Imaging and Photothermal Therapy

Limei Qin,[a] Dechao Niu,*[a] Yu Jiang,[a] Jianping He,[a] Xiaobo Jia,[a] Wenru Zhao,[a] Pei Li,[b] and Yongsheng Li*[a]

[a] Lab of Low-Dimensional Materials Chemistry, Key Laboratory for Ultrafine Materials of Ministry of Education, School of Materials Science and Engineering, East China University of Science and Technology, Shanghai 200237, China.

[b] Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China

E-mail: dcniu@ecust.edu.cn, ysli@ecust.edu.cn

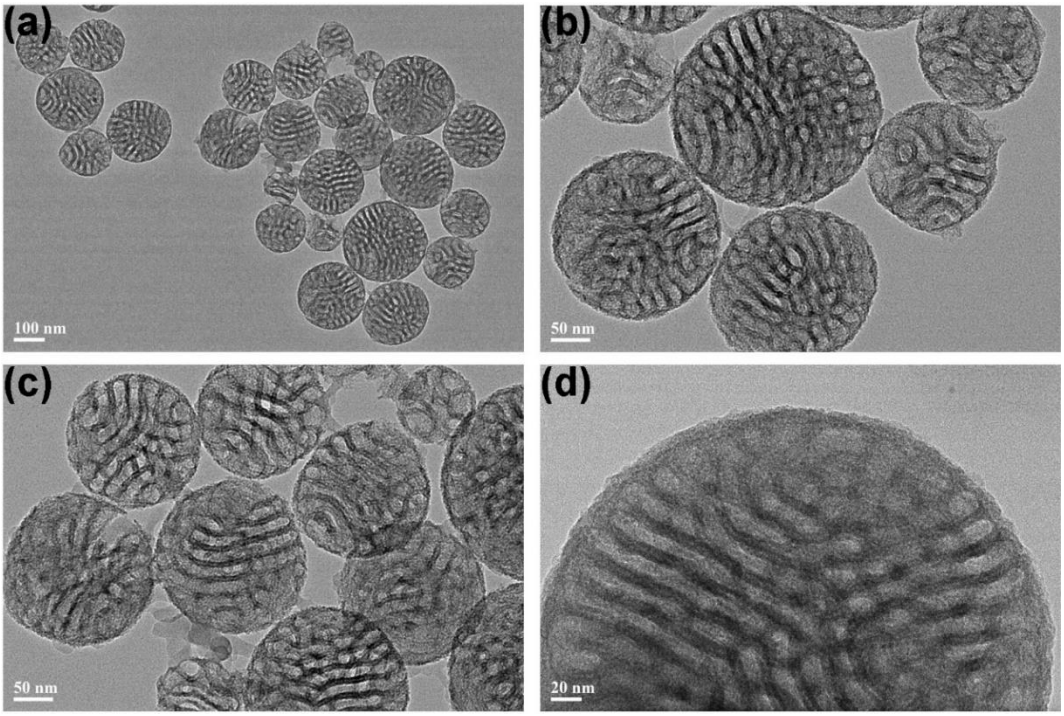

Fig. S1 TEM images (a-d) of DMSSs at different magnifications.

Abbreviations: TEM, transmission electron microscopy; DMSSs, Dual-Mesoporous Silica Nanospheres.

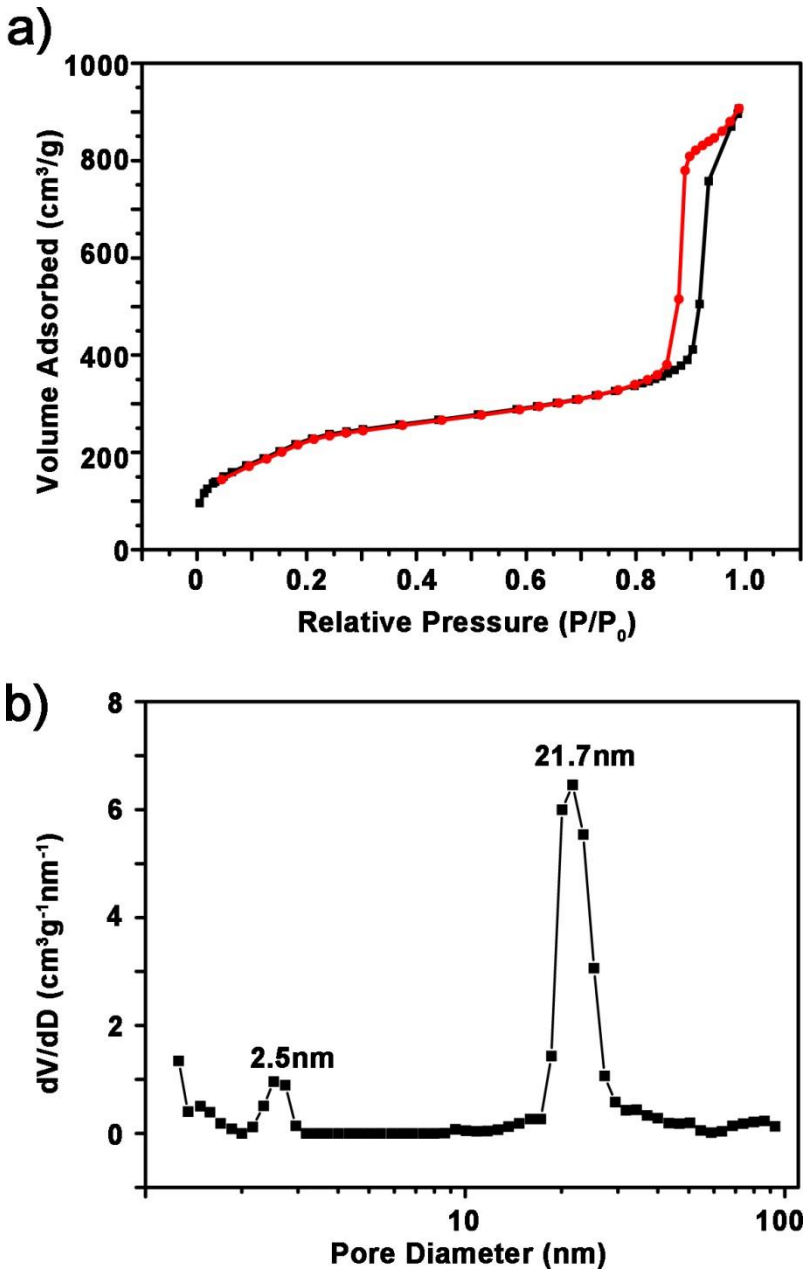

Fig. S2 (a) N_2 adsorption-desorption isotherm and (b) corresponding DFT pore-size distribution of DMSSs.

Abbreviations: DFT, density functional theory; DMSSs, Dual-Mesoporous Silica Nanospheres.

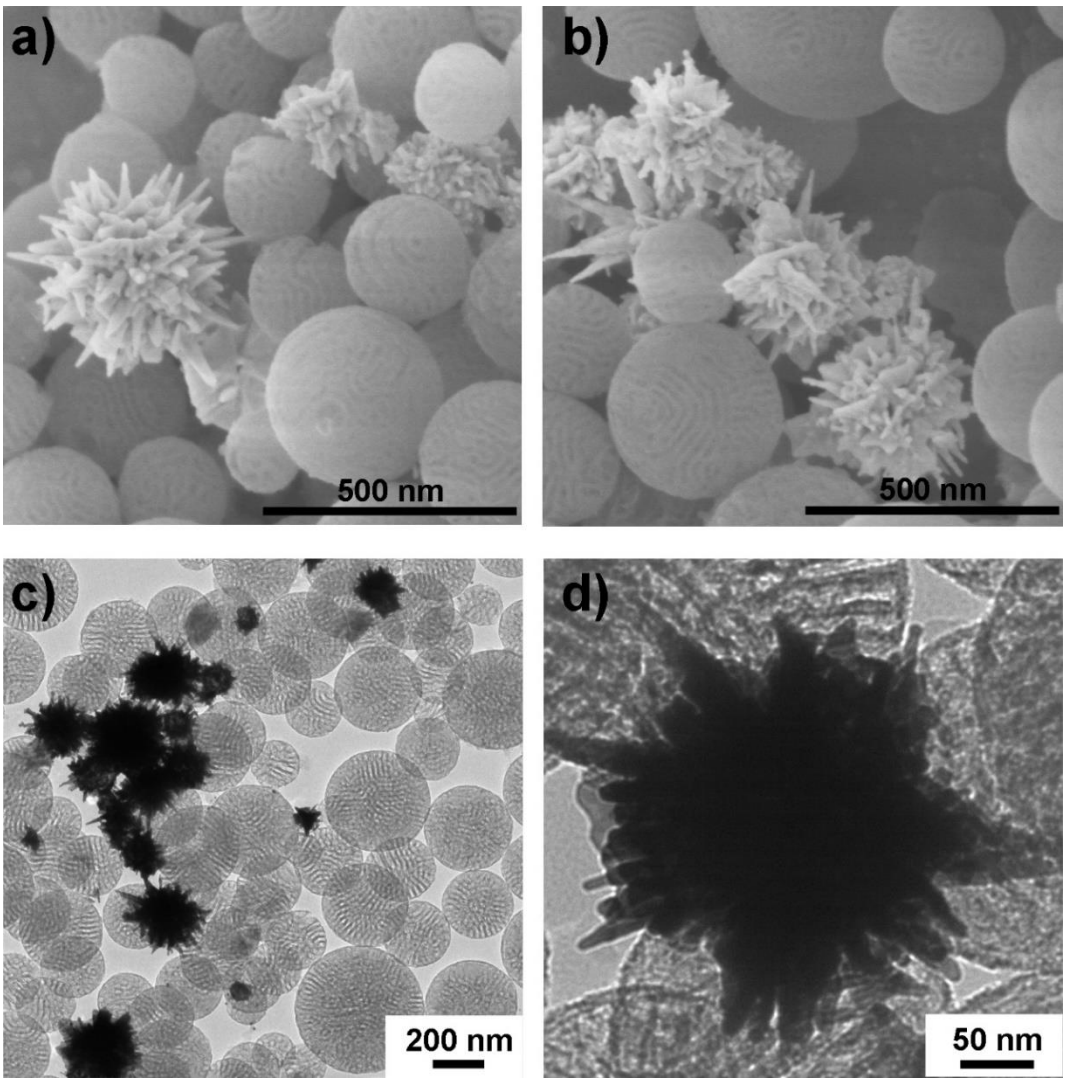

Fig. S3 SEM images (a, b) and TEM images (c, d) of as-prepared MGNRs@DMSSs without CTAB in Au seeds solution.

Abbreviations: SEM, scanning electron microscope; TEM, transmission electron microscopy; as-prepared MGNRs@DMSSs, as-prepared Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres; CTAB, N-Hexadecyltrimethylammonium Bromide; Au seeds, gold seeds.

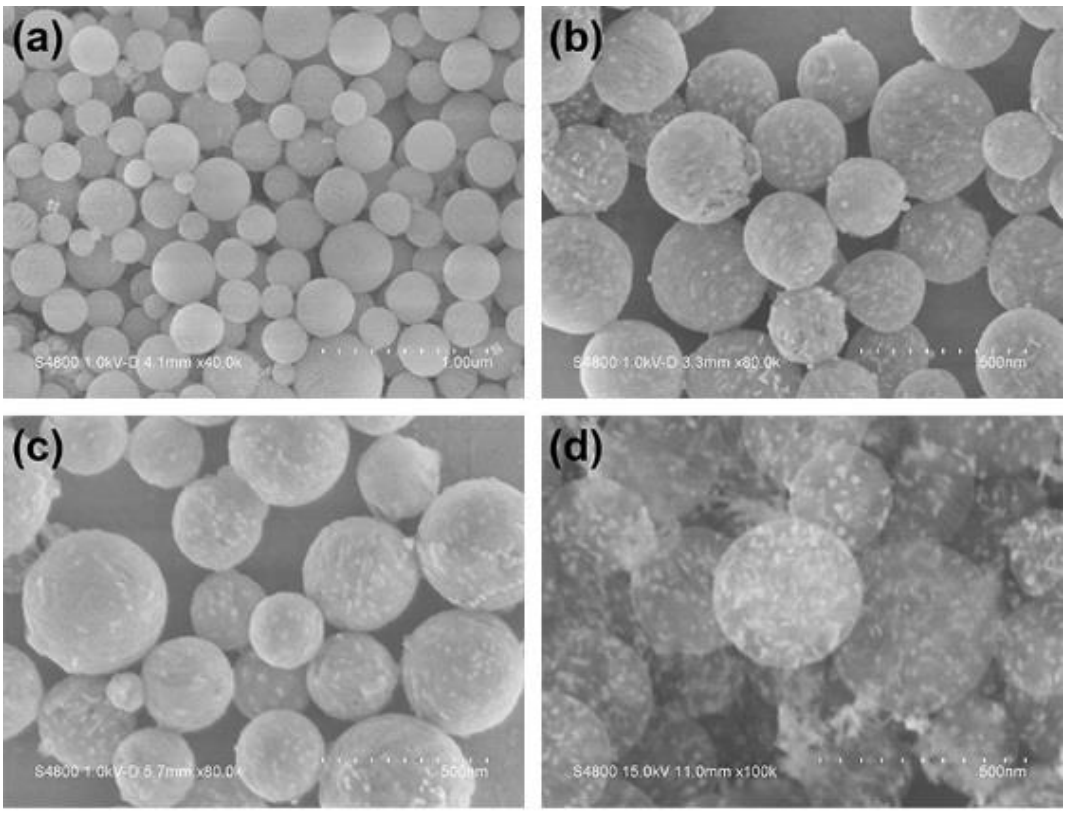

Fig. S4 SEM images of Au seeds@DMSSs (a) and MGNRs@DMSSs (b-d) at different magnifications and different detector voltages.

Abbreviations: SEM, scanning electron microscope; Au seeds@DMSSs, gold seeds encapsulated Dual-Mesoporous Silica Nanospheres; MGNRs@DMSSs, extracted Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres.

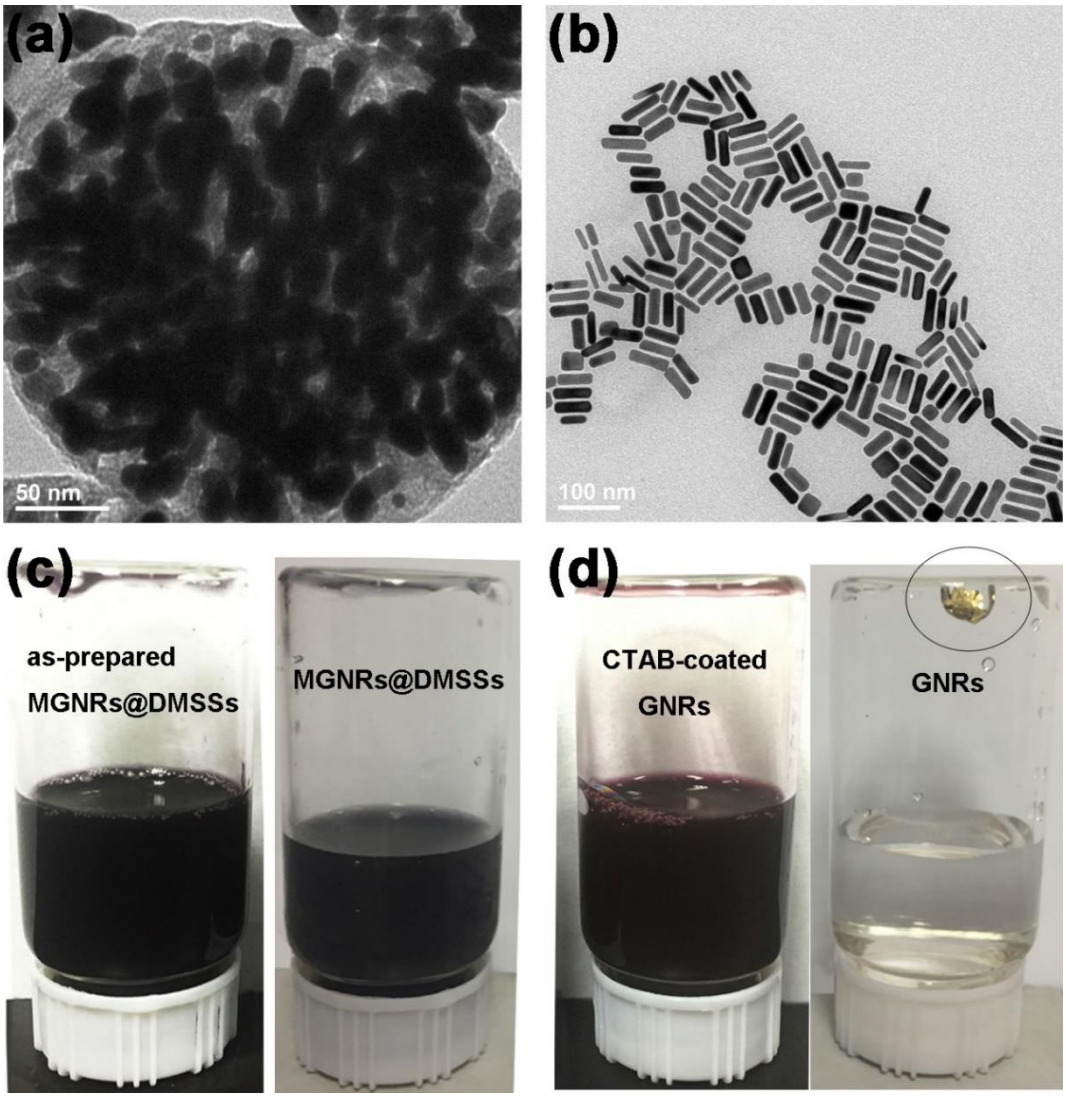

Fig. S5 TEM images of as-prepared MGNRs@DMSSs (a) and CTAB coated-gold nanorods (b) with the same growth solution and corresponding digital photos, dispersed in water (c) before and (d) after the extraction process.

Abbreviations: TEM, transmission electron microscopy; as-prepared MGNRs@DMSSs, as-prepared Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres; CTAB, N-Hexadecyltrimethylammonium Bromide.

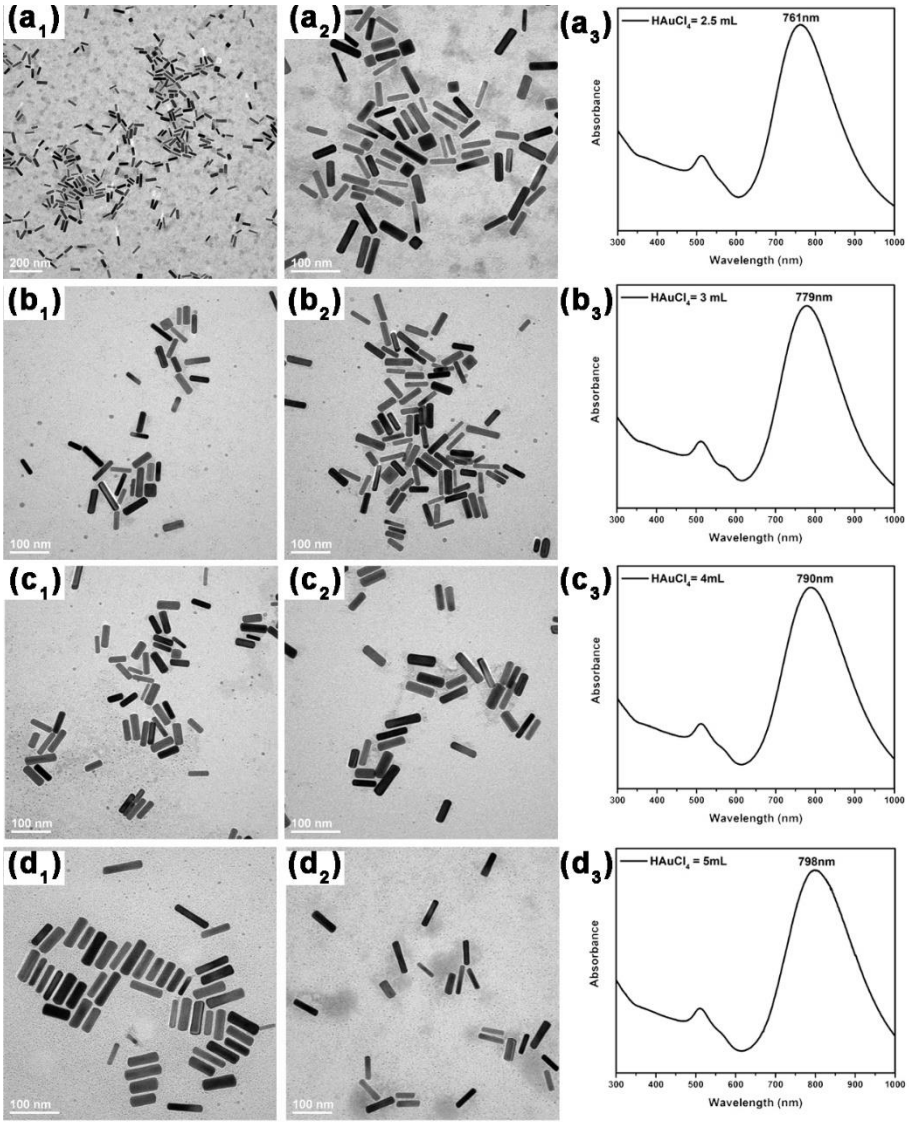

Figure S6. TEM images of GNRs and corresponding UV-vis-NIR spectra prepared using different growth solution with varied volumes $HAuCl_4$: (a_1-a_3) 2.5 ml, (b_1-b_3) 3 ml, (c_1-c_3) 4 ml and (d_1-d_3) 5 ml, respectively.

Abbreviations: TEM, transmission electron microscopy; GNRs: gold nanorods

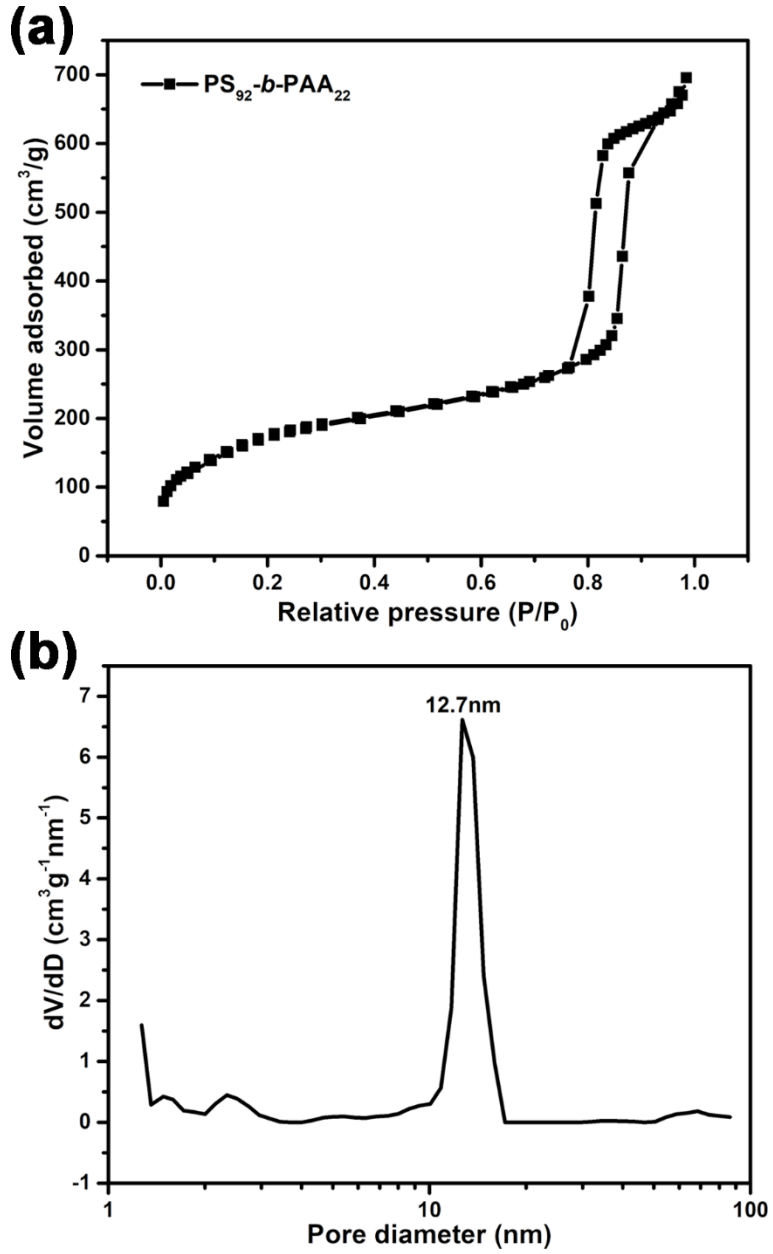

Figure S7. (a) N_2 adsorption-desorption isotherm and (b) corresponding DFT pore-size distribution of DMSSs-PS_{92} prepared by PS_{92}-*b*-PAA_{22} as template.

Abbreviations: DFT, density functional theory; DMSSs-PS_{92}, Dual-Mesoporous Silica Nanospheres prepared by using PS_{92}-*b*-PAA_{22} as template.

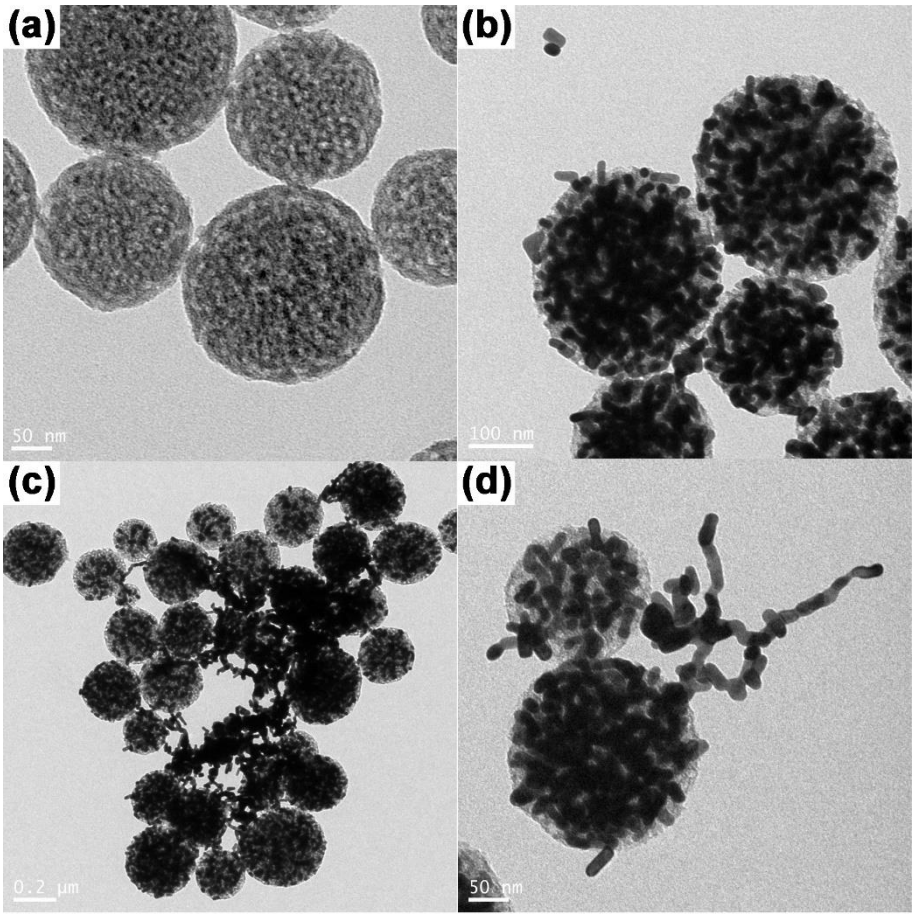

Figure S8. TEM images of (a) DMSSs-PS_{92} and (b, c, d) PEGylated MGNRs@DMSSs-PS_{92} at different magnifications.

Abbreviations: TEM, transmission electron microscopy; DMSSs-PS_{92}, Dual-Mesoporous Silica Nanospheres prepared by using PS_{92}-*b*-PAA_{22} as template. PEGylated MGNRs@DMSSs-PS_{92}: PEG modified Dual-Mesoporous Silica Nanospheres prepared by using PS_{92}-b-PAA_{22} as template.

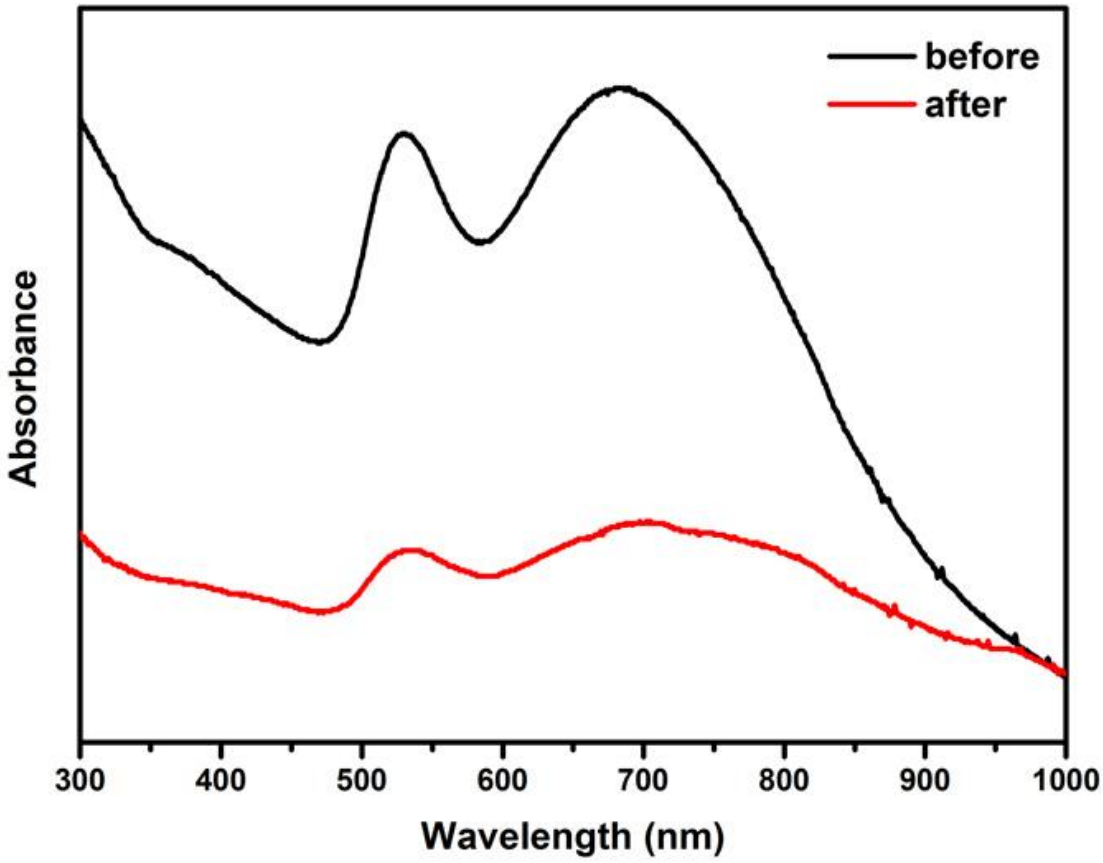

Fig. S9 UV-vis-NIR spectra of PEGylated MGNRs@DMSSs before and after 5 cycles of 808 nm laser irradiation.

Abbreviations: PEGylated MGNRs@DMSSs, PEG modified Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres.

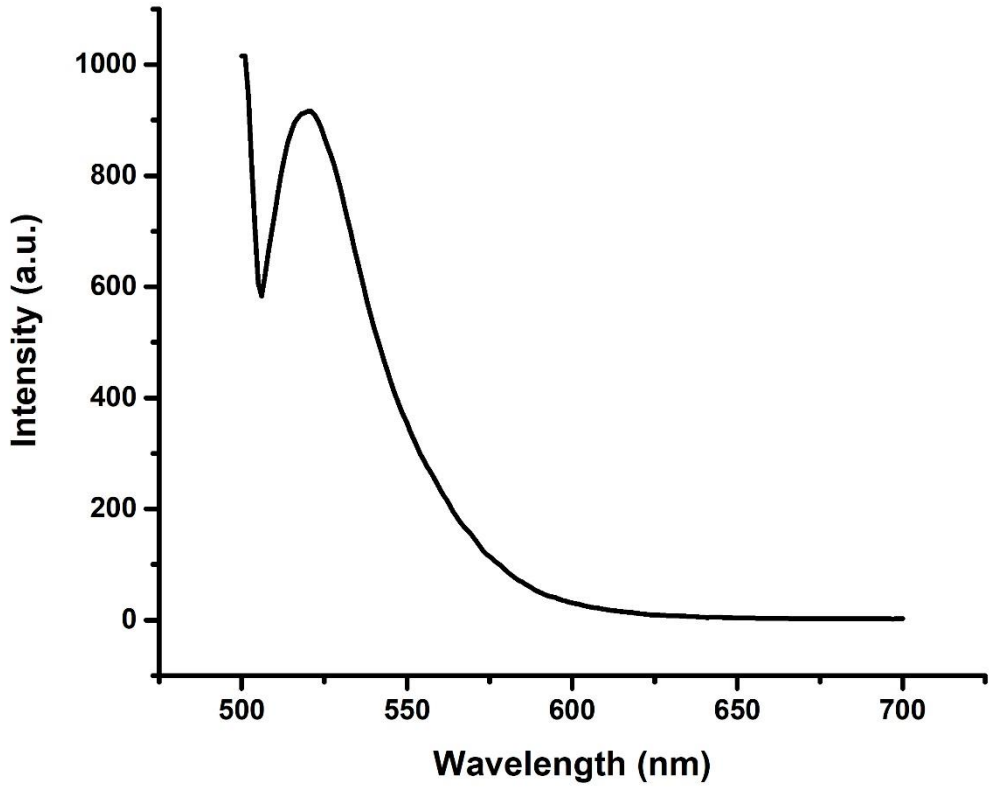

Fig. S10 Photoluminescence spectrum of FITC-labelled PEGylated MGNRs@DMSSs under the excitation wavelength of 488 nm.

Abbreviations: FITC, Fluorescein isthiocyanate; PEGylated MGNRs@DMSSs, PEG modified Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres.

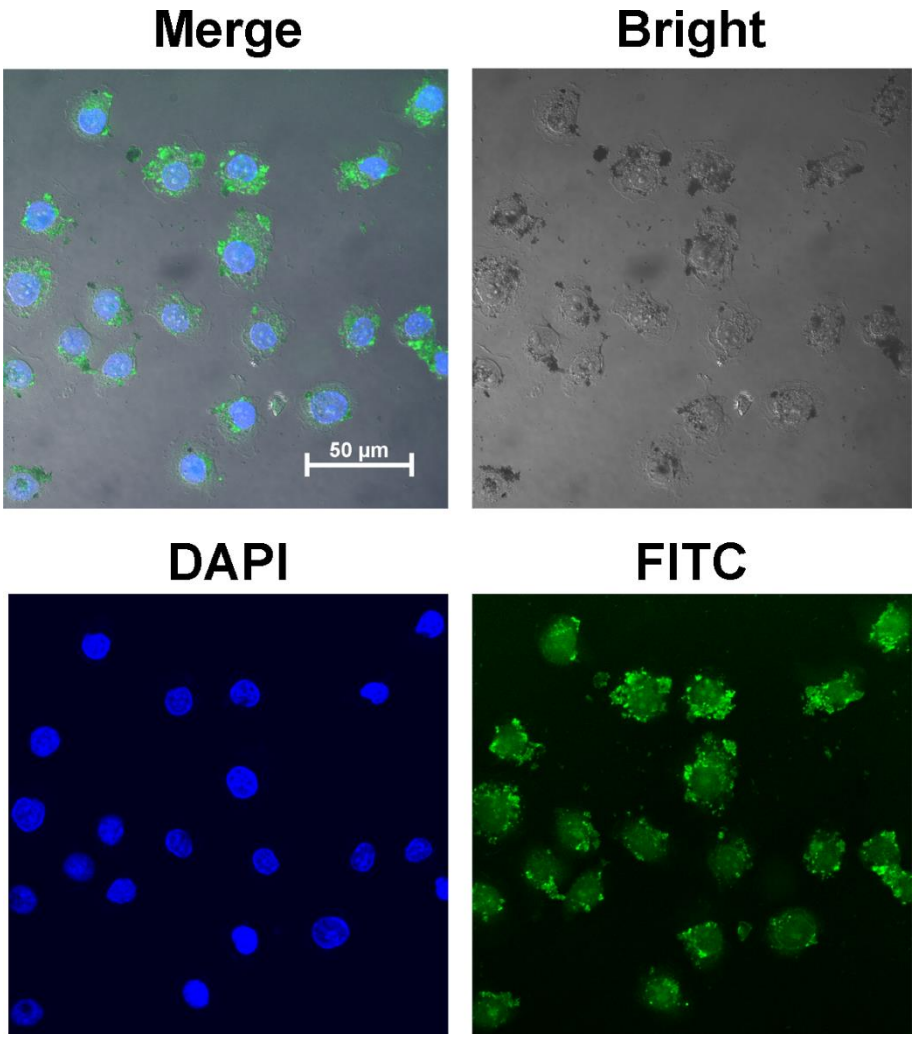

Fig. S11 Confocal laser scanning microscope (CLSM) images of SMMC-7721 cells after incubation with FITC-labelled PEGylated MGNRs@DMSSs for 4 h.

Abbreviations: FITC, Fluorescein isthiocyanate; PEGylated MGNRs@DMSSs, PEG modified Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres.

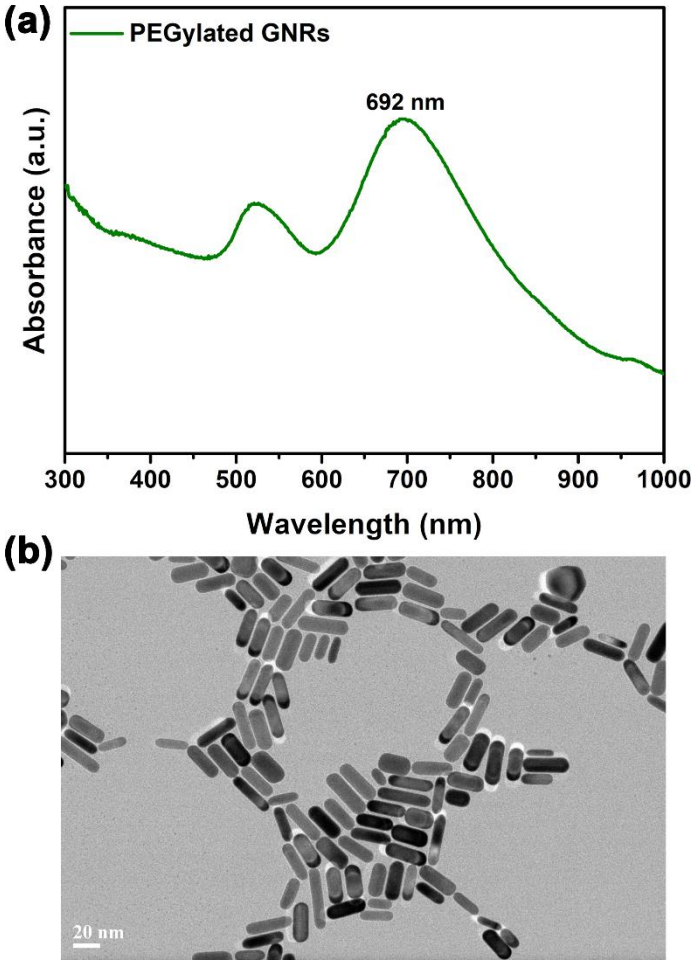

Fig. S12 (a) UV-vis-spectra and (b) TEM image of PEGylated GNRs with UV-vis absorption at 692 nm.

Abbreviations: PEGylated GNRs, PEG modified gold nanorods..

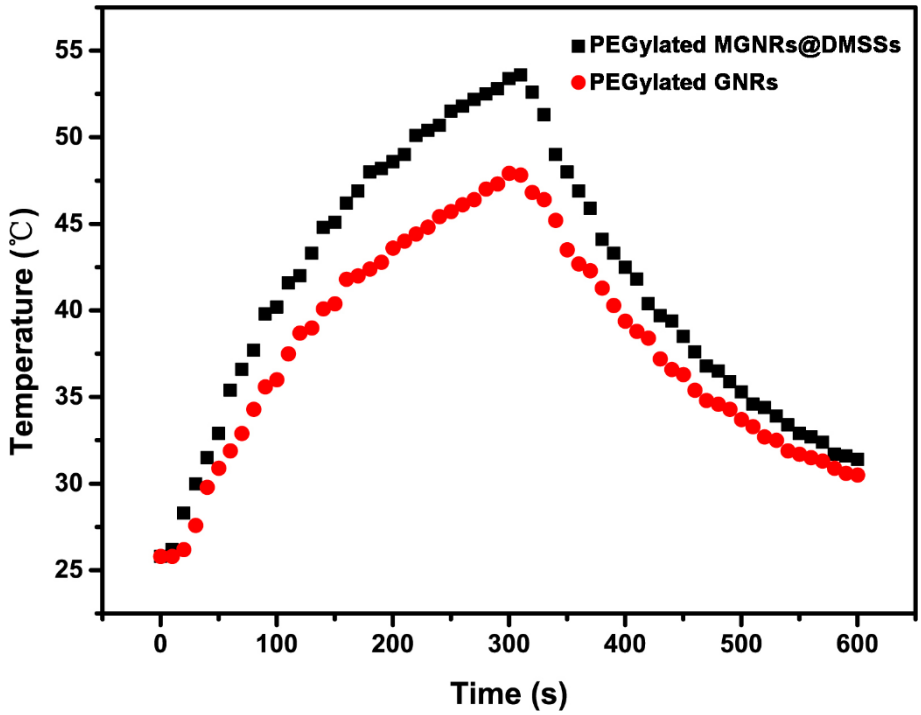

Fig.S13 Temperature curves of the aqueous dispersion of PEGylated GNRs and PEGylated MGNRs@DMSSs ([Au]=70 μg mL^{-1}, 1 mL) with the NIR laser (808 nm, 1.5 W cm^{-2}), in which the irradiation lasted for 5 min, and then the laser was turned off.

Abbreviations: PEGylated GNRs, PEG modified gold nanorods; PEGylated MGNRs@DMSSs, PEG modified Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres.

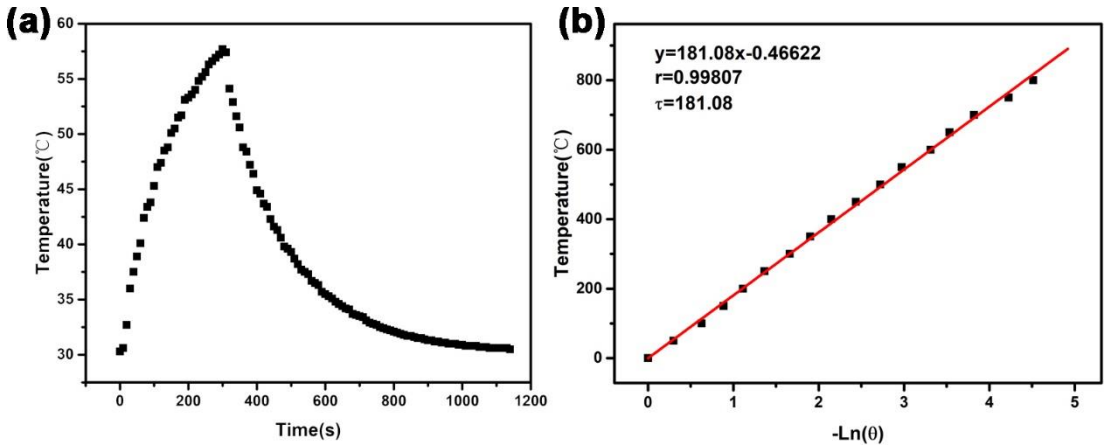

Fig. S14 Calculation of the photothermal-conversion efficiency of PEGylated MGNRs@DMSSs at 808 nm. (a) photothermal effect of an aqueous dispersion of PEGylated MGNRs@DMSSs under irradiation with a 808 nm NIR for certain periods, then the laser turned off; (b) Time constant (τ) from the system determined by applying the linear time data from the cooling period.

Abbreviations: PEGylated MGNRs@DMSSs, PEG modified Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres.

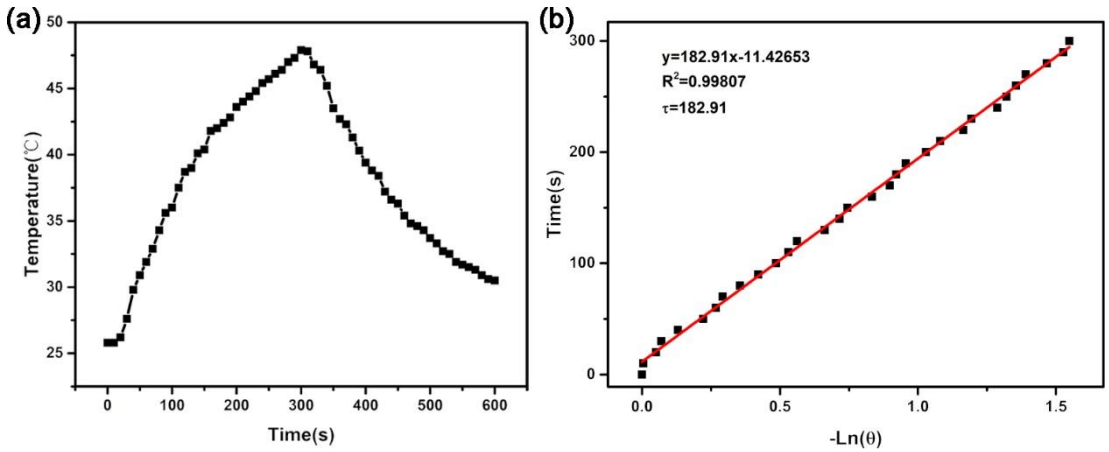

Fig. S15 Calculation of the photothermal-conversion efficiency of PEGylated GNRs at 808 nm. (a) photothermal effect of an aqueous dispersion of PEGylated GNRs under irradiation with a 808 nm NIR for certain periods, then the laser turned off; (b)Time constant (τ) from the system determined by applying the linear time data from the cooling period.

Abbreviations: PEGylated GNRs, PEG modified gold nanorod.

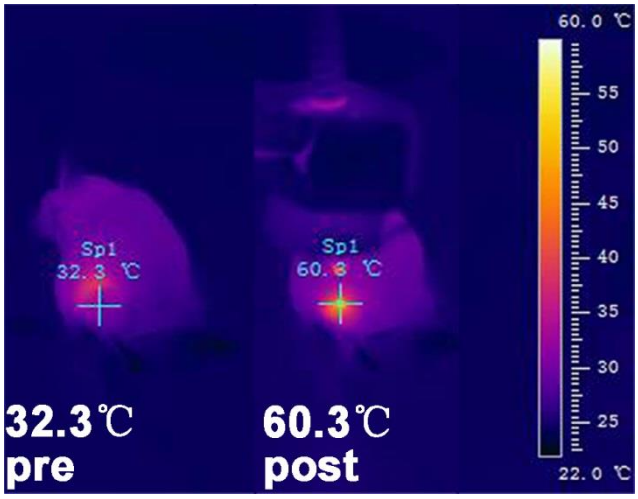

Fig. S16 Thermal images of tumor-bearing mice injected with PEGylated MGNRs@DMSSs ([Au] = 5.3 mg/mL, 50 μL), followed by irradiation with 808 nm laser (1.5 W cm^{-2}) pre and post injection.

Abbreviations: PEGylated MGNRs@DMSSs, PEG modified Multiple Gold-Nanorices in Dual-Mesoporous Silica Nanospheres.