Electronic Supplementary Information (ESI)

# A Feasible Strategy for Self-Assembly of Gold Nanoparticles

## via Dithiol-PEG for Photothermal Therapy of Cancers

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## **General information**

All materials were obtained from commercial suppliers without further purification. Ultrapure water was used in all experiments. UV-vis spectra were recorded by Cary 60 UV-Vis, Agilent Tech. TEM photos were obtained from Tongji University (JEOL 1230, Japan). Colocalization was measured by confocal microscopy (LeicaTCS SP5). U87 cells were obtained from Shanghai East Hospital.

### Supporting experiments and figures

Thiol-PEG <sub>5000</sub> -thiol	GNPs	Thiol-PEG <sub>5000</sub> -thiol	MeO-PEG <sub>5000</sub> -thiol
percentage			
0	2×10⁻ <sup>8</sup> mol	0	50mg, 10 <sup>-6</sup> mol
10%	2×10 <sup>-8</sup> mol	5mg, 10 <sup>-7</sup> mol	45mg, 9×10 <sup>-7</sup> mol
25%	2×10 <sup>-8</sup> mol	12.5mg, 2.5×10 <sup>-7</sup> mol	37.5mg, 7.5×10 <sup>-7</sup> mol
50%	2×10 <sup>-8</sup> mol	25mg, 5×10 <sup>-7</sup> mol	25mg, 5×10 <sup>-7</sup> mol
66%	2×10 <sup>-8</sup> mol	33mg, 6.6×10 <sup>-7</sup> mol	17mg 3.4×10 <sup>-7</sup> mol
80%	2×10 <sup>-8</sup> mol	40mg, 8×10⁻ <sup>7</sup> mol	10mg, 2×10 <sup>-7</sup> mol
100%	2×10 <sup>-8</sup> mol	50mg, 10 <sup>-6</sup> mol	0

**Table S1.** Synthetic method of PEGylated GNPs with different composite ratio. GNPs were quantified via UV-Vis spectrum.



Figure S1.UV-Vis spectra of GNPs and SAGNPs of different sizes.



Figure S2. Size distribution analysis based on DLS.



**Figure S3.** TEM images of PEG mixture after 24 h reaction and negative staining. Percentage of dithiol-PEG: 10%, 50%, and 80%. (A) PEGs of different ratios mixed open to the air without GNPs. The scale bar is 1 $\mu$ m. (B) Oxygen-free reaction of PEG with different ratios after 48 h. (C) Oxygen-rich reaction of PEG with 0.1 mM of hydrogen peroxide. The scale bar is 0.5  $\mu$ m.



**Figure S4.** UV-Vis spectra of SAGNPs incubated with GSH at (A) 10 mM, (B) 1 mM, (C) 0.1 mM, (D) 0.01 mM, and (E) 0.001 mM. (F) UV-Vis spectra of SAGNPs reacted with Tris(2-carboxyethyl)phosphine (TCEP).



Figure S5. TEM images of mPEGs-GNPs reacted with 10 mM GSH.



**Figure S6**. The comparison of (A) UV-Vis spectra and (B) fluorescence spectra between SAGNPs and SAGNP-Cy5.5



**Figure S7**. (A) Cytotoxicity based on MTT assays of mPEG-GNPs and PEG. The amount of PEG was related to the molar ratio of SAGNPs by 500:1. (B) Cytotoxicity of SAGNPs on different cell lines.



Figure S8. Changes of cell state after irradiation.