Electronic Supplementary Information

# Aqueous Synthesis of PEGylated Copper Sulfide Nanoparticles for Photoacoustic Imaging of Tumors

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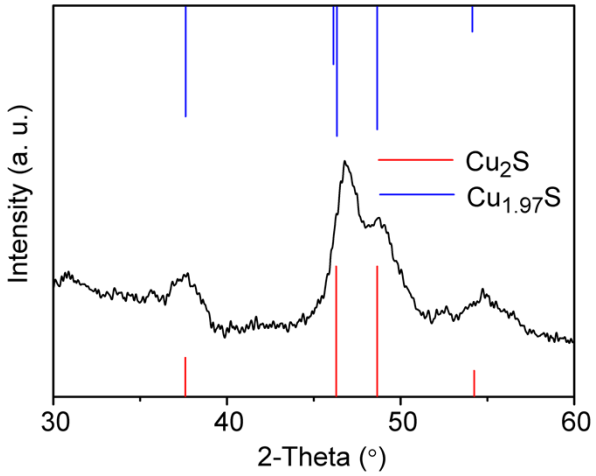


**Figure S1.** XRD patterns of PEGylated copper sulfide nanoparticles (NPs). The vertical solid line shown below the pattern is standard bulk XRD data for chalcocite ($Cu_2S$) (JCPDS No. 31-0482), above the pattern is djurleite ($Cu_{1.97}S$) (JCPDS No. 20-0365).

**Table S1**. The experimental and theoretically predicted hydrodynamic sizes of the differently sized PEGylated copper sulfide NPs.

| Sample | Experimental hydrodynamic size[a] (nm) | Theoretical hydrodynamic size[b] (nm) |
|---|---|---|
| CS-2.7 | 7.1 ± 0.1 | 8.1 |
| CS-4.8 | 10.7 ± 0.3 | 10.1 |
| CS-7.2 | 14.9 ± 0.4 | 12.6 |

[a] Average results of three measurements.

[b] The theoretical hydrodynamic sizes were obtained by assuming a simple addition of the core size and two times of the calculated hydrodynamic size of the PEG derivatives ($d_{PEG} = 0.03824 M_n^{0.559}$).[1]

**Synthesis of the TGA-capped copper sulfide NPs.**

In brief, 0.092 g (1 mmol) of thioglycolic acid (TGA) was dissolved in 50 mL of water, and then 0.05 g (0.5 mmol) of CuCl was then introduced while stirring. Nitrogen gas was introduced to purge the reaction solution for 1 h. The pH value of the reaction mixture was adjusted to 9.00 by dropwise addition of 0.5 M NaOH aqueous solution. After that, 0.0187 g (0.25 mmol) of TAA was then introduced while stirring. The resultant mixture was then heated to 90°C, and the reaction was allowed for 2 h under nitrogen protection. Then the solution was cooled to room temperature. And the hydrodynamic size of TGA-capped copper sulfide NPs dispersed in water was characterized by dynamic light scattering.

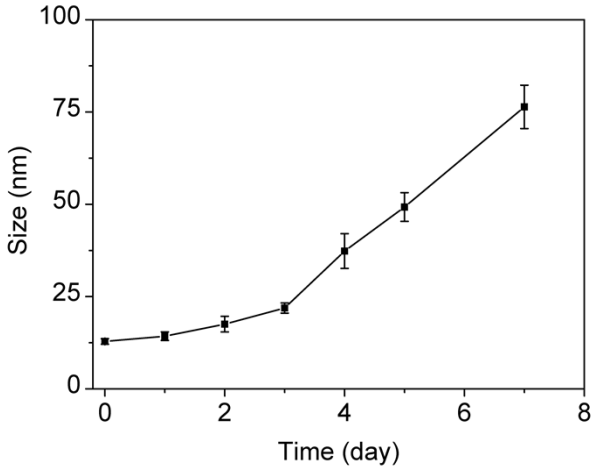


**Figure S2.** Temporal evolution of the hydrodynamic size of the as-prepared TGA-capped copper sulfide NPs in water.

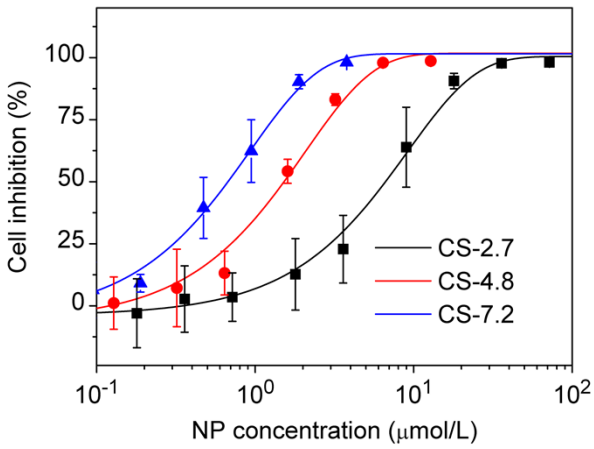


**Figure S3.** The concentration-dependent growth-inhibition of HeLa cells by copper sulfide NPs of 2.7 nm (black), 4.8 nm (red), and 7.2 nm (blue), respectively.

References

1 R. A. Sperling, T. Liedl, S. Duhr, S. Kudera, M. Zanella, C. A. J. Lin, W. H. Chang, D. Braun, W. J. Parak, *J. Phys. Chem. C*, 2007,**111**, 11552-11559.