

## Supporting Information

### ***In situ* aqueous synthesis of genetically engineered polypeptide - capped Ag<sub>2</sub>S quantum dots for second near-infrared fluorescence/photoacoustic imaging and photothermal therapy**

*Dong-Hui Zhao,<sup>‡a</sup> Xiao-Quan Yang,<sup>‡a,b</sup> Xiao-Lin Hou,<sup>a</sup> Yang Xuan,<sup>a</sup> Xian-Lin Song,<sup>b</sup> Yuan-Di Zhao,<sup>a</sup> Wei Chen,<sup>a</sup> Qiong Wang,<sup>\*c</sup> and Bo Liu<sup>\*a,b</sup>*

<sup>a</sup>Britton Chance Center for Biomedical Photonics at Wuhan National Laboratory for Optoelectronics - Hubei Bioinformatics & Molecular Imaging Key Laboratory, Collaborative Innovation Center for Biomedical Engineering, College of Life Science and Technology, Huazhong University of Science and Technology, Wuhan 430074, Hubei, P. R. China

<sup>b</sup>Key Laboratory of Biomedical Photonics (HUST), Ministry of Education, Huazhong University of Science and Technology, Wuhan 430074, Hubei, P. R. China

<sup>c</sup>Cancer center, Union Hospital, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430022, Hubei, P. R. China.

Fax: (+) 86 27-8779-2202

E-mail: [wdyxywq@163.com](mailto:wdyxywq@163.com) (Q. Wang) [lbyang@mail.hust.edu.cn](mailto:lbyang@mail.hust.edu.cn) (B. Liu)

Amino acid sequence of RGDPC<sub>10</sub>Acys and cysRGDPC<sub>10</sub>Acyscys:

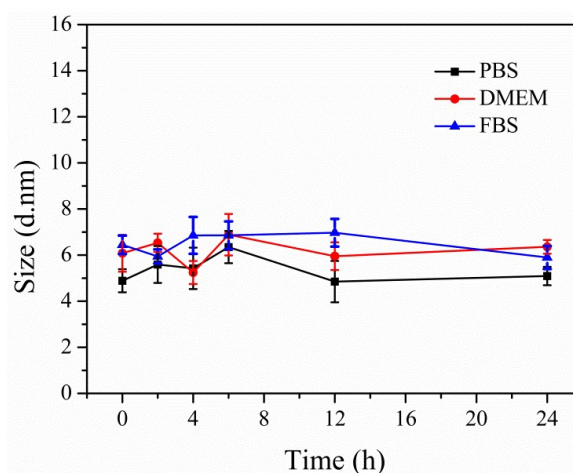
RGDPC<sub>10</sub>Acys: MRGS[6H]GSDDDDK WASYAVTGRGDSPASSTS[P]TSYRGPMG[C<sub>10</sub>]  
 ARMPT[A]IGDHVAPRDTSMGGC

cysRGDPC<sub>10</sub>Acyscys: MRGS[6H]GSDDDDK WASSGSGCSGSGT SYAVTGRGDSPASSTS[P]  
 TSYRDPMG[C<sub>10</sub>]ARMPT[A]IGDHVAPRDTSSGSGCSGSGTSMGGC

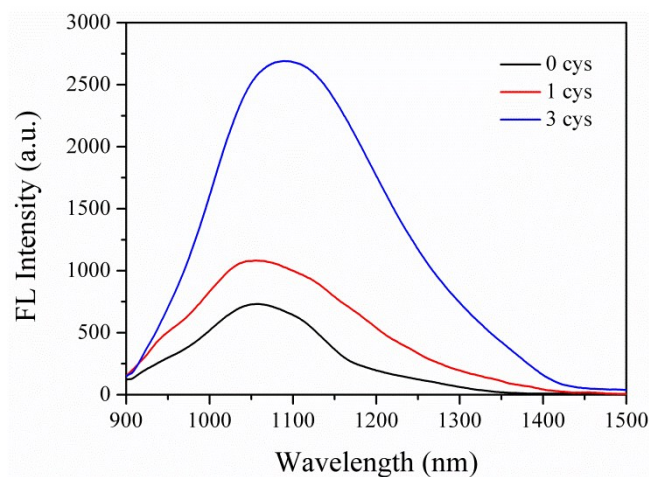
Abbreviations for polypeptide domains:

[6H]: HHHHHH  
 [P]: APQMLRELQETNAALQDVRELLRQQVKEITFLKNTVMESDAS  
 [A]: SGDLENEVAQLEREVRSLEDEAAELEQKVSRLKNEIEDLKA  
 [C<sub>10</sub>]: [AGAGAGPEG]<sub>10</sub>

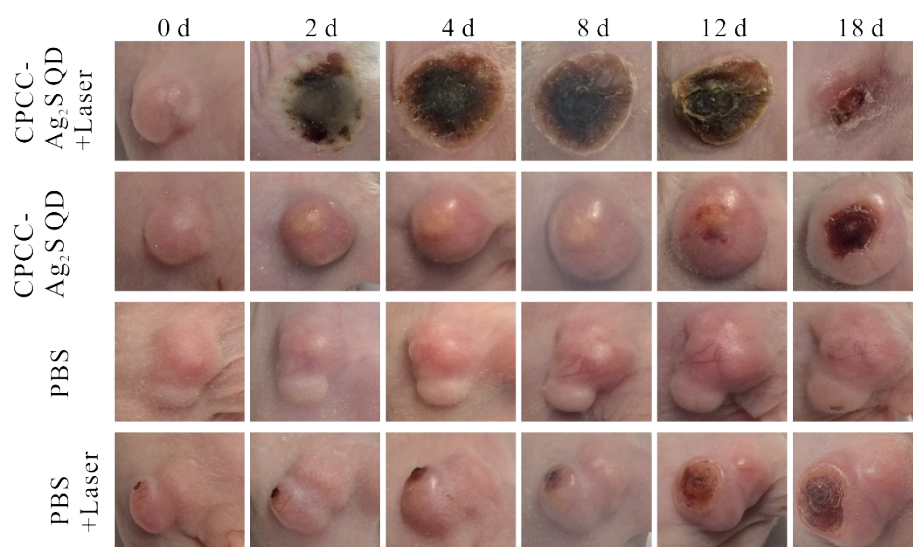
**Fig. S1** The sequences of the polypeptides used in the study.



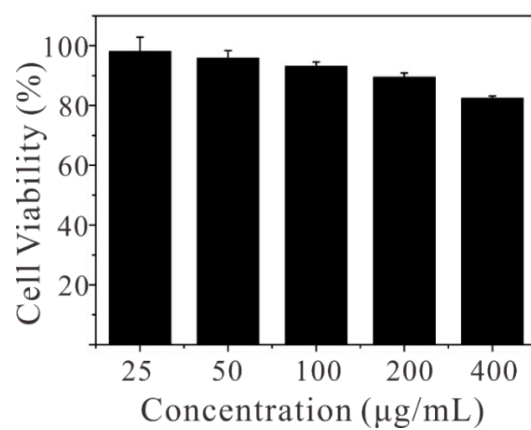
**Fig. S2** The colloidal stability of CPCC-Ag<sub>2</sub>S QDs. The CPCC-Ag<sub>2</sub>S QDs were dispersed in PBS, fetal bovine serum (FBS), and cell culture media (DMEM), and the hydrodynamic diameter of samples were measured at different time using a Malvern Zetasizer Nano ZS90 (Malvern Instruments Ltd., Malvern, UK).



**Fig. S3** The effect of the cysteine number of polypeptide on the QY of Ag<sub>2</sub>S QDs.



**Fig. S4** The photothermal therapy effect of CPCC-Ag<sub>2</sub>S QD *in vivo*.



**Fig. S5** The cell viability of HeLa cells incubation with different concentration of CPCC-Ag<sub>2</sub>S QD.