# Electronic Supplementary Information

## Tumor cell-targeted $Zn_3In_2S_6$ and Ag-Zn-In-S quantum dots for color adjustable luminophore

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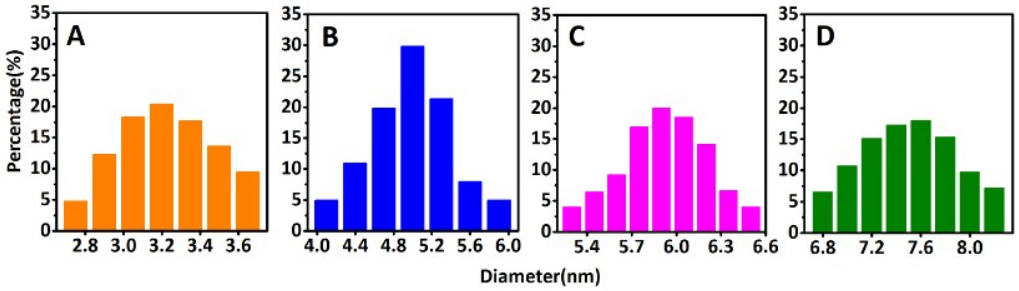


**Fig. S1.** Histograms of size distribution of sample ZIS1 (A), ZIS2 (B), ZIS3 (C) and ZIS4 (D) with the average sizes of 3.3 (PDI=0.048), 4.9 (PDI=0.052), 5.9 (PDI=0.059) and 7.5 nm (PDI=0.056), respectively. It can be seen from the PDI (polymer dispersity index) that all the samples demonstrate good dipersities with the PDI less than 0.06.

**Table S1.** ICP composition normalized with S and QYs of ZIS and AZIS QDs.

| sample | ICP composition of [Zn]:[In]:[S] | QY |
|---|---|---|
| ZIS2 | 2.89:2:6.21 | 7.6 |
| $AZIS_{0.025}$ | 2.91:2.02:6.21 | 3.2 |
| $AZIS_{0.05}$ | 2.73:1.99:6.21 | 6.8 |
| $AZIS_{0.1}$ | 2.66:1.97:6.21 | 27.6 |
| $AZIS_{0.2}$ | 2.39:1.98:6.21 | 21.9 |

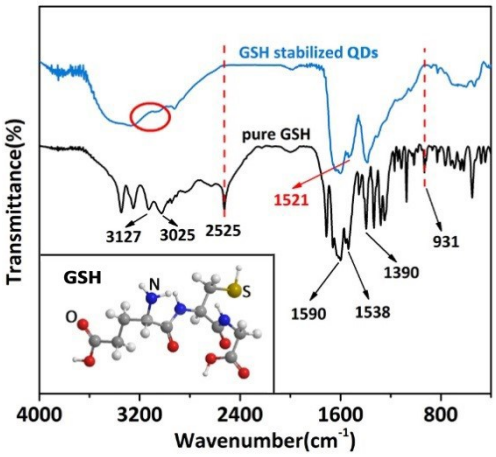


**Fig. S2.** FTIR spectra of pure GSH and GSH terminated nanocrystals (inset: 3D structure of a GSH molecule).

In order to certify the presence of GSH and clarify the coordination interaction between QDs and stabilizer, FTIR spectra were examined on the pure GSH and GSH stabilized ZIS QDs. As for pure GSH, the bands 3127 and 3025 $cm^{-1}$ shown in Fig. S2 originate from symmetric and asymmetric vibration of $–NH_2$. The S-H stretching and bend mode are around 2525 and 931 $cm^{-1}$. The bands 1590 and 1390 $cm^{-1}$ refer to the symmetric and asymmetric vibration bands of $COO^-$. The band at 1538 $cm^{-1}$ could be assigned to N-H bend mode. The most significant change of the spectrum obtained from GSH stabilized QDs is the disappearance of S-H stretching and bend mode, which are the result of

the coordination between thiol and QDs *via* the thiolate linkage. Other differences between the two spectra are the deformation of $–NH_2$ symmetric/asymmetric vibration and the small shift of N-H bend band (17 $cm^{-1}$, from 1538 $cm^{-1}$ for GSH to 1521 $cm^{-1}$ for QDs), which have rarely been reported. It has been verified the coordination interaction between amide and QDs.[1] As a consequence, we ascribe the changes of $–NH_2$ and N-H bands to the coordination interaction between amide and metal ions, and we can infer that the functional groups including the thoil and amide played important role in ensuring the stability and solubility of ZIS in water.

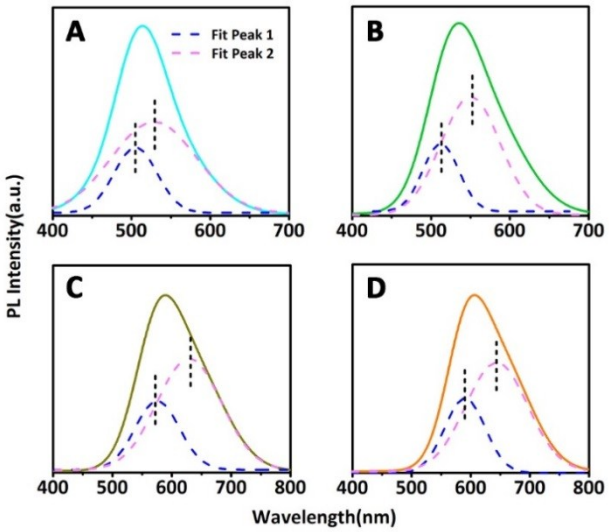


**Fig. S3.** Gaussian deconvolution PL spectra of $AZIS_{0.025}$ (A), $AZIS_{0.05}$ (B), $AZIS_{0.1}$ (C) and $AZIS_{0.2}$ (D), respectively.

Each of the PL spectrum could be well fitted by two Gaussian functions, noted as Peak 1 (decay faster, higher energy) and Peak 2 (decay slower, lower energy), respectively. According to the energy differences between the two peaks and the absorption band, coupled with the decay lifetime of each peak, Peak 1 and Peak 2 could be assigned to the surface trap states (shallow D-A pairs) and intrinsic trap states (deep D-A pairs) recombinations, respectively. Furthermore, the integral area of each peak represents the contribution to the entire spectrum. The deconvolution results show that the area of Peak 2 is much larger than that of Peak 1, suggesting that intrinsic states working as deep D-A pair transition dominate the main PL emission. This conclusion is also in good agreement with the results of PL lifetimes and decay dynamics.

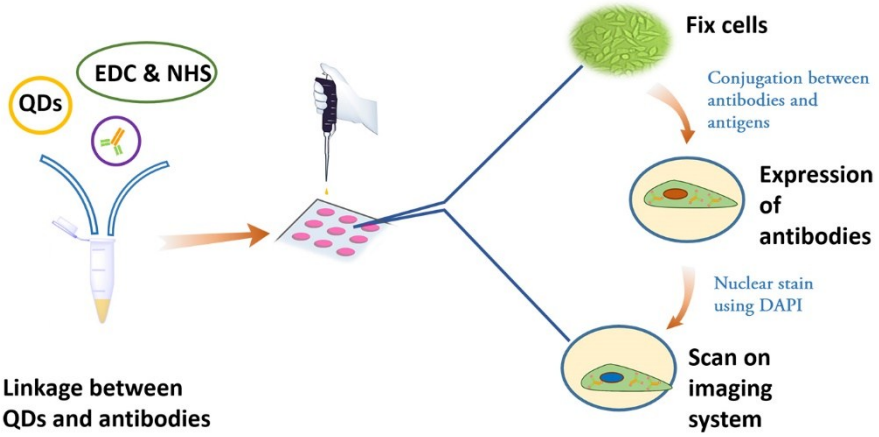


**Fig. S4.** Schematic diagram of the conjugation between AFP antibody and GSH stabilized QDs and delivery to Hep G2 cells.

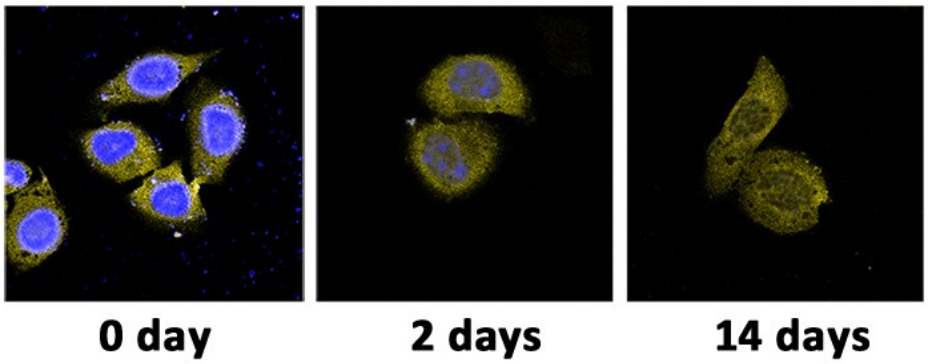


**Fig. S5.** Merged fluorescent pictures of DAPI and QDs labelled Hep G2 cells taken after incubation for different time.

## References

1. Hua-Yan, Y.; Yu-Wei, Z.; Zheng-Yong, Z.; Huan-Ming, X.; Shao-Ning, Y., *Nanotechnology* **2013,** *24* (5), 055706.