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Electronic Supplementary Information

Organic-to-Aqueous Phase Transfer of Zn-Cu-In-Se/ZnS Quantum Dots with Multifunctional Multidentate Polymer Ligands for Biomedical Optical Imaging

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Fig. S1 The XPS survey spectra of (a) the Zn-Cu-In-Se (ZCISe) core QDs with different precursor feed ratios, and (b) the ZCISe (the feed molar ratio of Zn:Cu:In is 10:2:10) QDs before and after ZnS shell coating. The calculated molar ratio (cmr) of each QDs were shown below the corresponding spectrum.



Fig. S2 Evolution of both absorption and PL spectra of the as-prepared ZCISe core QDs (Zn:Cu=10:3) with reaction conditions: (a) the growth time, (b) the amount of DT and (c) the growth temperatures. According to the experiment results, our findings can be summarized as follows: (1) Fig. S2a shows that there is an optimal growth time for achieving highly fluorescent ZCISe QDs. For the QDs with Zn/Cu ratio of core is 10/3, the fluorescence increased gradually during the reaction time from 0 to 30 min. Further extending the growth time, the fluorescence no longer increased. However, the optimal growth time of near-infrared QDs is less than 30 min. Due to the copper salts, which near-infrared quantum dots need more, have higher reactivity than zinc salts. A long time heating is not necessarily beneficial to the growth of quantum dots. (2) The amount of DT has a vital influence to PL of QDs. Fig. S2b shows that with the increase of DT, the PL intensity enhanced. But the PL intensity diminished when the amount more than 0.7 mL (0.5 mL+ 0.2 mL). (3) The reaction temperature mainly determines the PL peak position and intensity. By increasing the temperature from 100 °C to 200 °C, the PL peak red-shifted gradually from 581 nm to 647 nm. The optimal temperature is 175 °C under our reaction conditions (Fig. S2c).



Fig. S3 FTIR spectra of PAA and PAA-MEA-EDA. The characteristic peak of -NH-CO- in 1656 cm^{-1} combining with the detection results of active amino and thiol indicated the successful syntheses of the multifunctional multidentate polymer ligands.



Fig. S4 (a) Absorption and (b) PL spectra of the initial oil-soluble and the resultant water-soluble NIR ZCISe/ZnS QDs. The insets of panel b show the digital photographs and pseudo-colored images of the as-prepared QDs before and after phase transfer under room light and NIR laser light (λ_{ex} =660 nm).



Fig. S5 Cell viability of L02 cells after incubating with cRGD-PME-QDs and the CdTe QDs as a comparision.