Electronic supplementary information

Water-soluble Zn-Ag-In-Se quantum dots with bright and widely

tunable emission for biomedical optical imaging

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Fig. S1 UV-Vis absorption and PL spectra of the dispersions fabricated with different Zn/Ag/In/Se ratios. As shown, the absence of Zn from reaction system results in decreased PL intensity of QDs, while the absence of any of Ag, In and Se generates no PL emission. This indicates that the host QDs are the quaternary alloy of Zn, Ag, In and Se.



Fig. S2 The UV-Vis absorption and PL spectra of temporal evolution of ZAISe QDs ([Zn]/[Ag]/[In]/[Se]/[GSH] = 15/5/20/47.5/200, pH = 8.5). As shown, during the first 8 h of refluxing, the fluorescence intensity gradually increases and then tends to be stable. Meanwhile, slight red shift of PL peak from 650 to 662 nm is observed in the heating process.



Fig. S3 UV-Vis absorption and PL spectra of ZAISe QDs fabricated in different pH values of original solutions from 7 to 8.5 ([Zn]/[Ag]/[In]/[Se]/[GSH] = 15/5/20/47.5/200; the heating time was fixed at 8 h). As shown, 7.5 of pH value gave the optimal PL property of aqueous ZAISe QDs.



Fig. S4 UV-Vis absorption and PL spectra of ZAISe QDs obtained from different concentrations of GSH ([Zn]/[Ag]/[In]/[Se] = 15/5/20/47.5; pH = 7.5; the heating time was fixed at 8 h). With increasing the GSH concentration from 6 mM to 14 mM, the PL intensity of ZAISe QDs successively increases until it reaches a maximum at the GSH concentration of 12 mM.



Fig. S5 The XPS spectra of Zn 2p (a), Ag 3d (b), In 3d (c) and Se 3d (d) of the sample S5.



Fig. S6 In vitro cytotoxicity of the aqueous GSH-capped ZAISe QDs and N-acetyl-L-cysteinecapped CdTe QDs determined by MTT assay. Normal human liver cells (LO2) were cultured in a 96-well plate with medium containing different concentrations of aqueous QDs for 48 h. The concentration given in the figure was calculated according to the following formula: the mass of QDs/the sum of QDs solution volume and culture medium volume (the total volume).



Fig. S7 The mass spectra of RGD–succinic acid (a), TA–PEG₁₀₀₀–NH₂ (b, n = 20–25) and TA– PEG₁₀₀₀–Suc-RGD (c). The dispersion of the mass spectra line in (b) and (c) is caused by the Gaussian distribution of the molecular weight of NH₂–PEG₁₀₀₀–NH₂.



Fig. S8 The NIR fluorescence images of $\alpha_v\beta_3$ -positive U87MG tumor-bearing nude mouse before injection (background) and after intravenous injection with the 760-emitting QD-RGD probe acquired at various time points post-injection (P.I.) (λ ex = 660 nm).