

Supporting Information for A Toolkit for Bioimaging Using Near-Infrared AgInS₂/ZnS Quantum Dots

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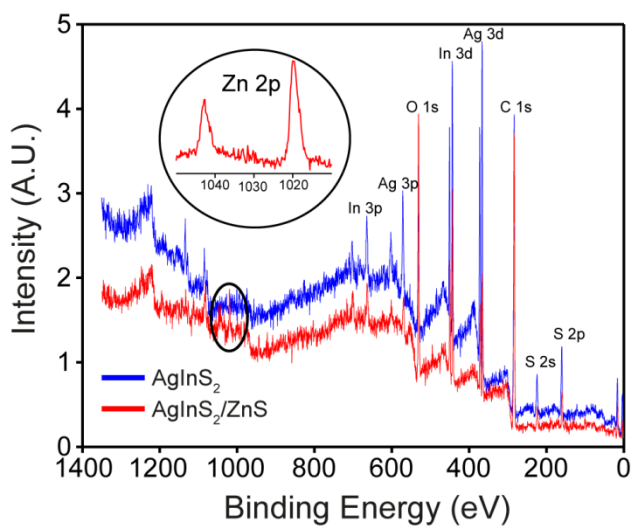


Fig. S1. XPS survey spectrum of core AgInS_2 and core/shell $\text{AgInS}_2/\text{ZnS}$ QDs.

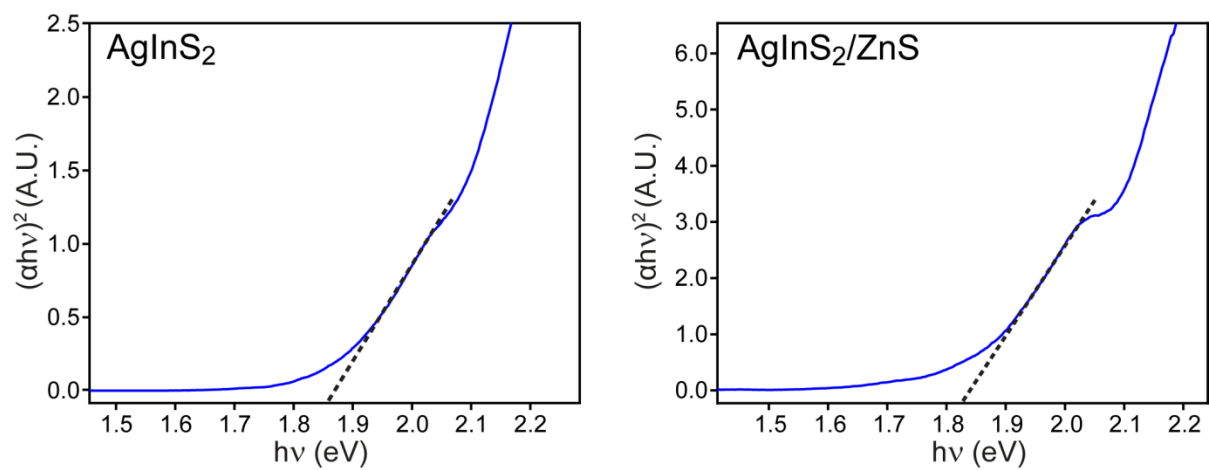


Fig. S2. Optical bandgaps of core AgInS_2 (left) and core/shell $\text{AgInS}_2/\text{ZnS}$ (right) QDs from extrapolating the linear portion of Tauc plots.

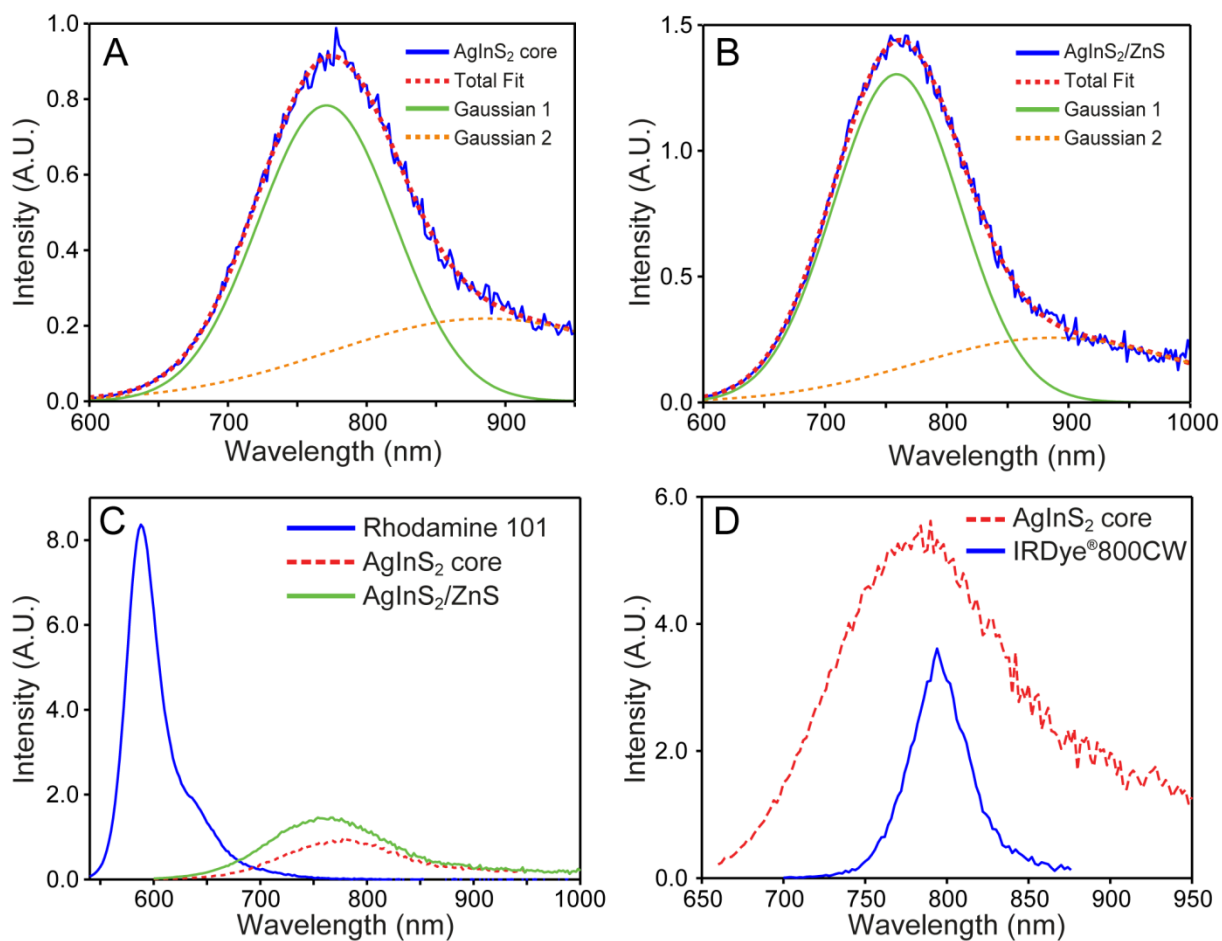


Fig. S3. a, b) Quantum yield measurements were calculated by Gaussian decomposition of the spectrum. The red tail of the emission was excluded when calculating the quantum yields. c) An example of the emission spectra of samples and Rhodamine 101 dye standard used to determine the quantum yields. d) An example of the emission spectra of AgInS₂ and IRDye[®] 800CW dye used to determine the quantum yield. This dye is not a good standard for AgInS₂/ZnS samples.

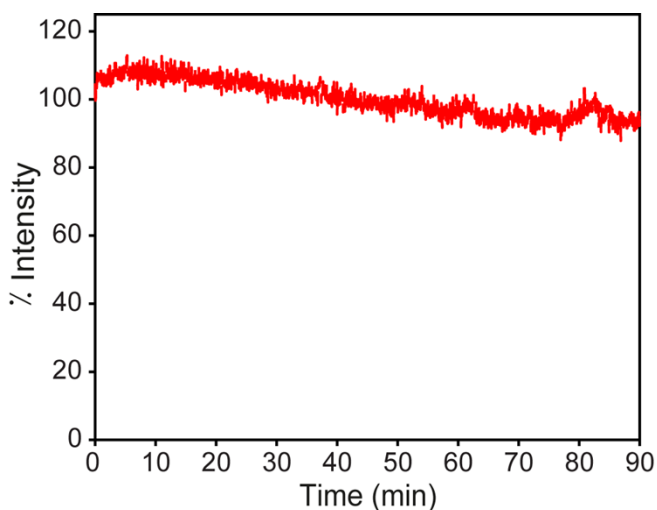


Fig. S4. Photostability of AgInS₂ quantum dots as measured by the emission intensity at 750 nm over the course of 1.5 hours of continuous illumination. Data on core/shell AgInS₂/ZnS dots are essentially identical.

Sample	Radius (nm)	%Pd	MW-R (kDa)	% Intensity	% Mass
Silane: Peak 1	14.595	11.8	1783	3.4	48.0
Silane: Peak 2	82.535	8.8	102739	96.6	52.0
Polymer: Peak 1	6.142	7.2	235	8.6	97.1
Polymer: Peak 2	59.825	11.9	48387	91.4	2.9

Table S1. Hydrodynamic radius (Radius, nm), polydispersity (%Pd), apparent molecular weight (MW R kDa), scattering intensity (%Intensity), and mass weight (% Mass) of water-soluble AgInS₂/ZnS as a function of preparation method. Both samples showed ~10 nm sized materials and larger aggregates likely from side products or dust that was present as the samples were not filtered prior to measurement.

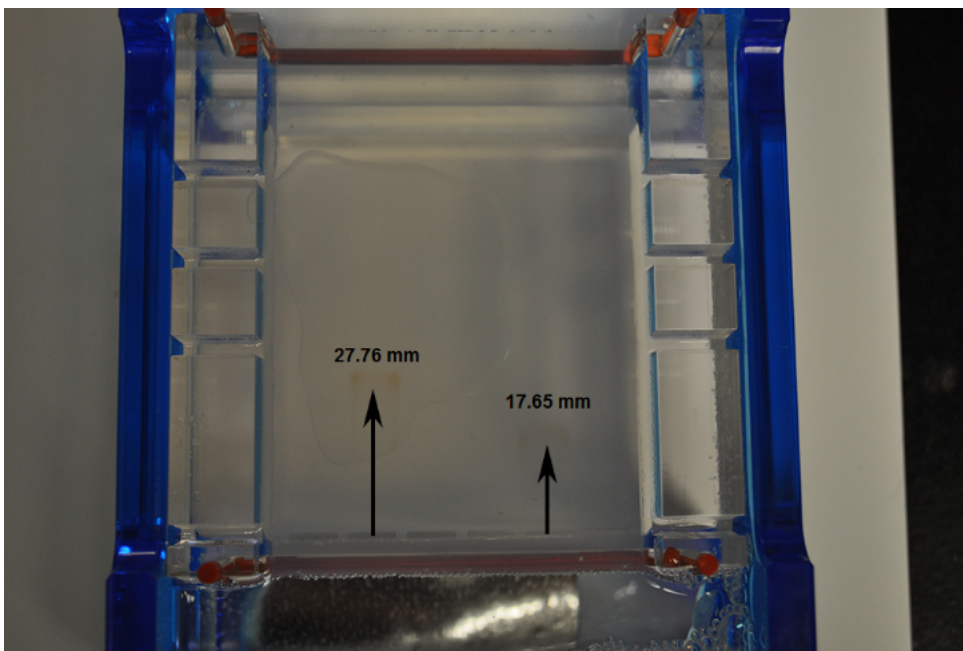


Fig. S5. Gel electrophoresis in 0.5% agar gel using pH 8 phosphate buffer at an applied voltage of 80 ± 2 volts across a gel distance of 10 cm for 45 min.

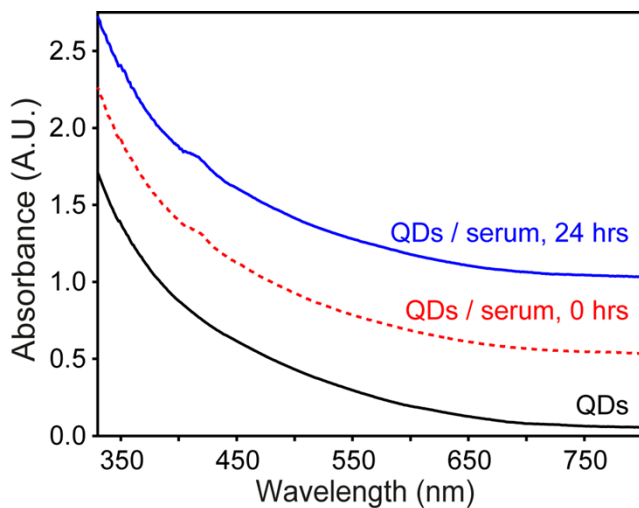


Figure S6. Absorption spectra of PEGylated AgInS₂/ZnS QDs in deionized water (bottom, solid black), after dilution by $\sim 75\%$ in adult bovine serum (middle, red dash), and after 24 hours incubation at 35 °C (top, blue solid). The QD spectra in serum have the serum component removed for clarity. The sample was centrifuged after 24 hours incubation which resulted in a 7% decrease in intensity in the absorption spectrum, which has been corrected for here. This demonstrates that the QDs are $\sim 93\%$ stable under physiological conditions.

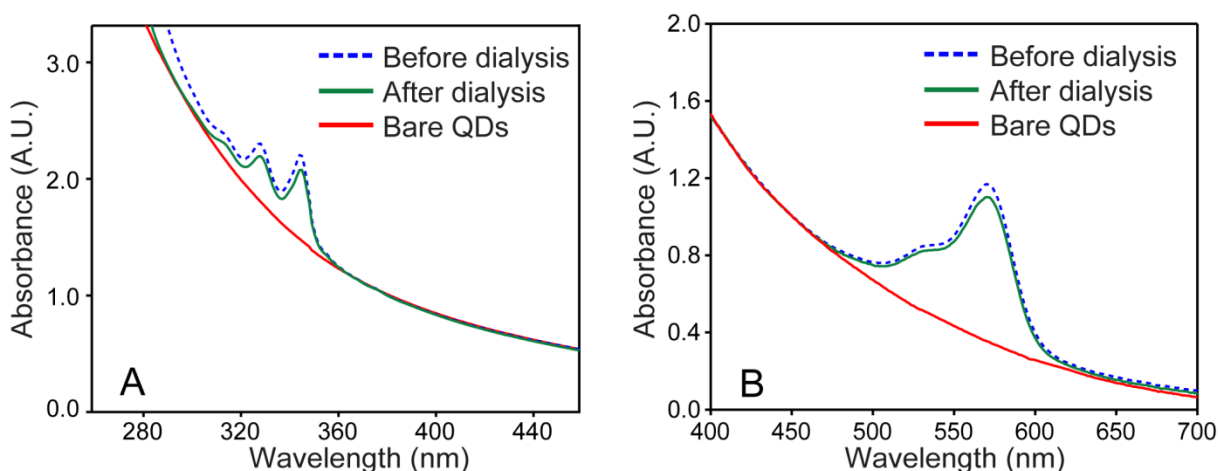


Fig. S7. Dye conjugation yield calculation based on absorbance spectra before and after dialysis. a) Pyrene-PEG-amine conjugated to polymer encapsulated QDs. b) Rhodamine B piperazine conjugated to silane coated QDs.

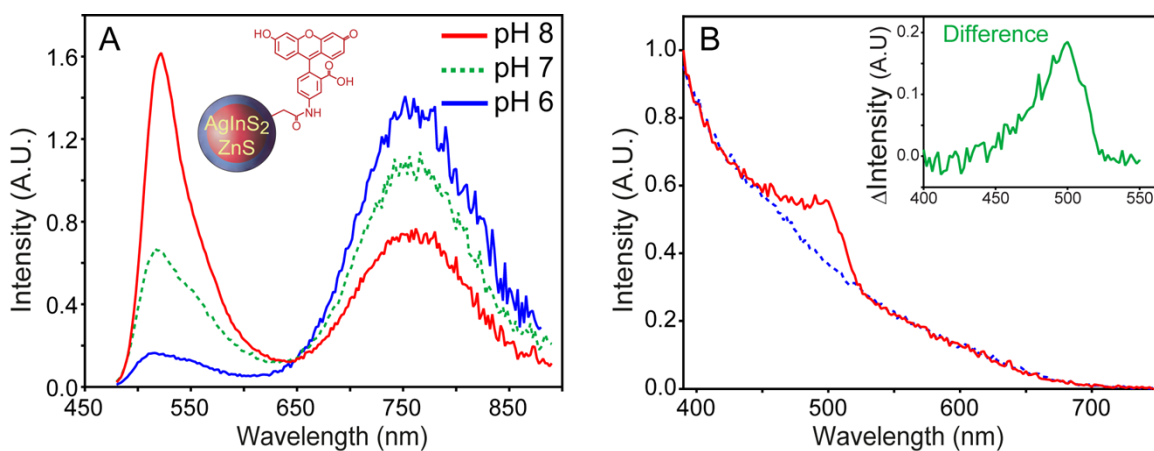


Fig. S8. a) Normalized emission of water-soluble AgInS₂/ZnS quantum dot-fluorescein dye conjugates as a function of pH demonstrate the ability to ratiometrically report the chemical environment of the buffer solution. b). Photoluminescence excitation spectra of water-soluble AgInS₂/ZnS dots and the same conjugated to fluorescein display fluorescein-like features (inset), which is indicative of energy transfer from the organic chromophore to the quantum dot.

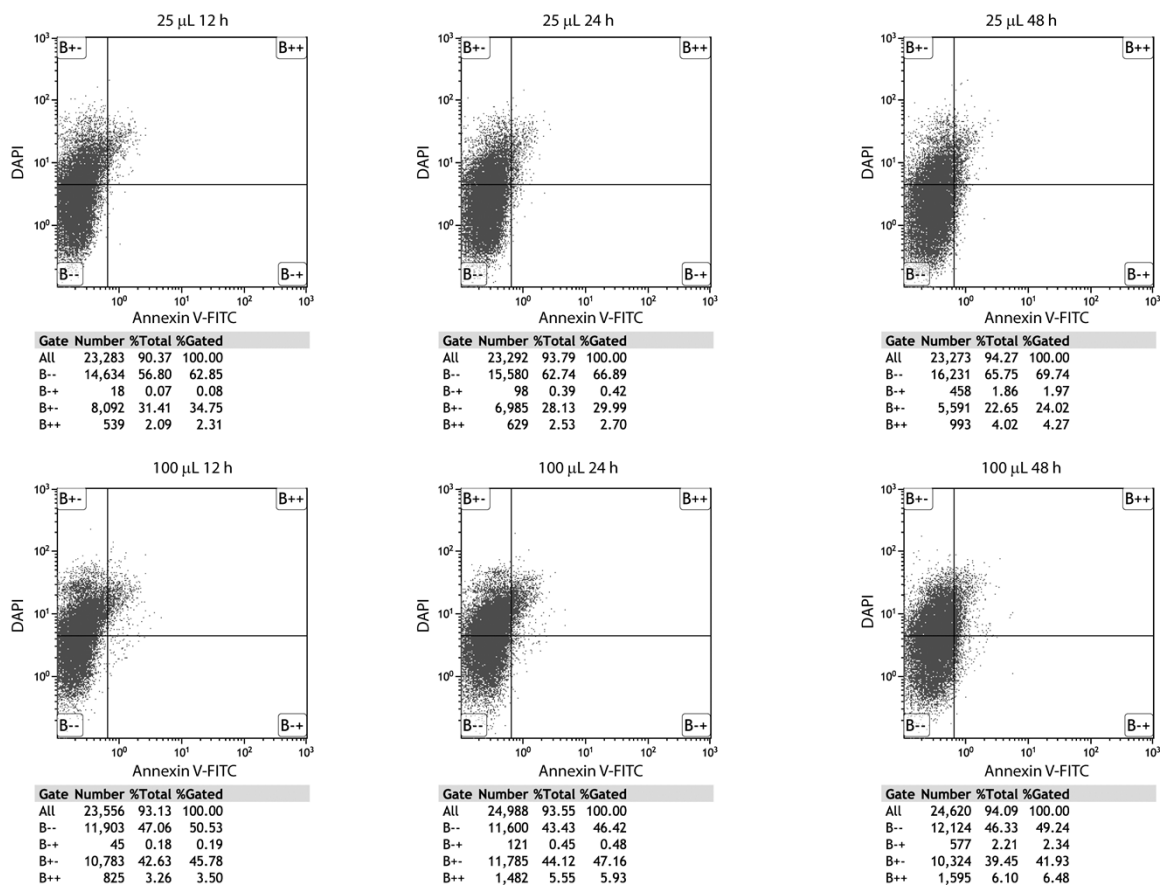


Fig. S9. Flow cytometry results of HeLa cells exposed to 25 µL and 100 µL of PEGylated AgInS₂/ZnS QDs after 12, 24, and 48 hours incubation.