

Supporting Information

A small heterobifunctional ligand provides stable and water dispersible core-shell CdSe/ZnS quantum dots (QDs)

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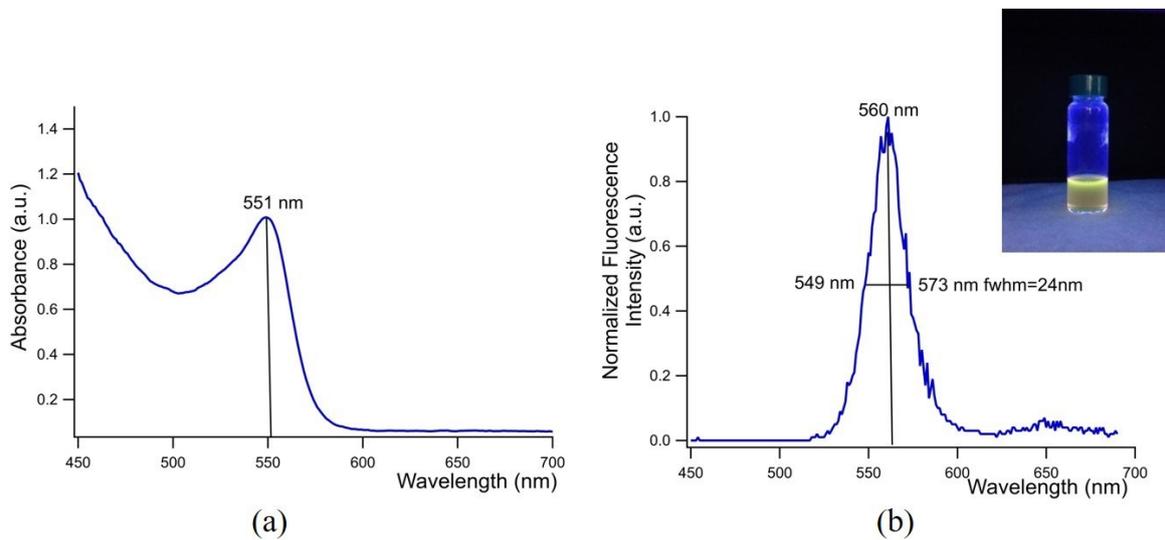


Figure S1. Absorbance (a) and fluorescence (b) spectra of CdSe QDs 3.

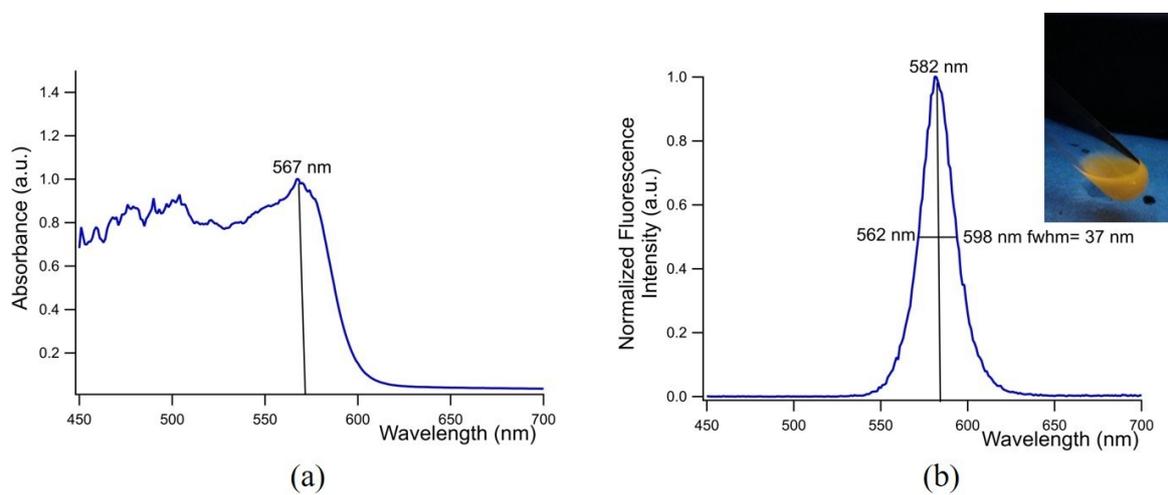


Figure S2. Absorbance (a) and fluorescence (b) spectra of core-shell CdSe/ZnS QDs 2.

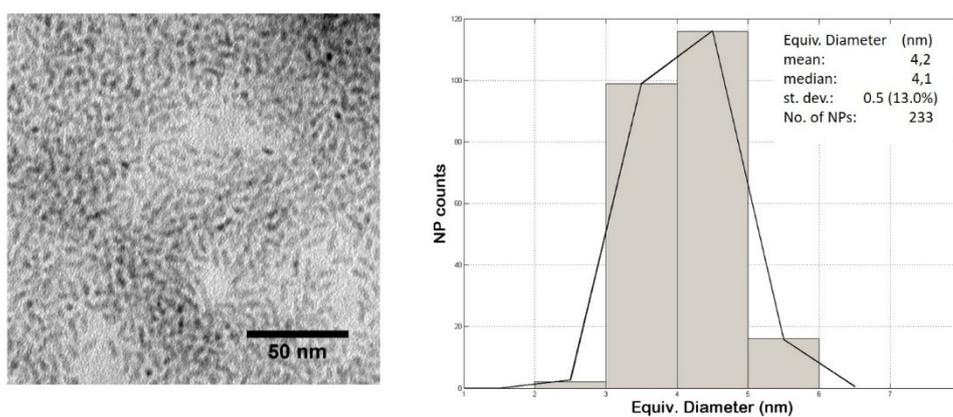


Figure S3. TEM images of CdSe/ZnS QDs 2.

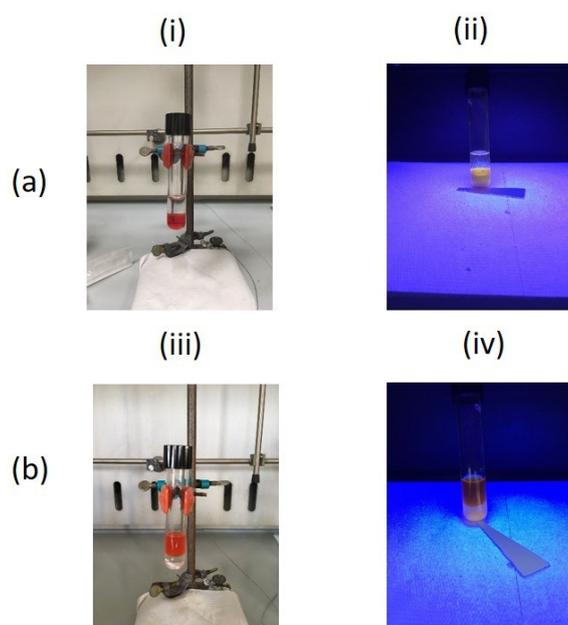


Figure S4. Pictures related to the phase transfer steps. (a) $t = 0$: (i) under white light, (ii) under UV light; (b) $t = 18$ h: (iii) under white light, (iv) under UV light.

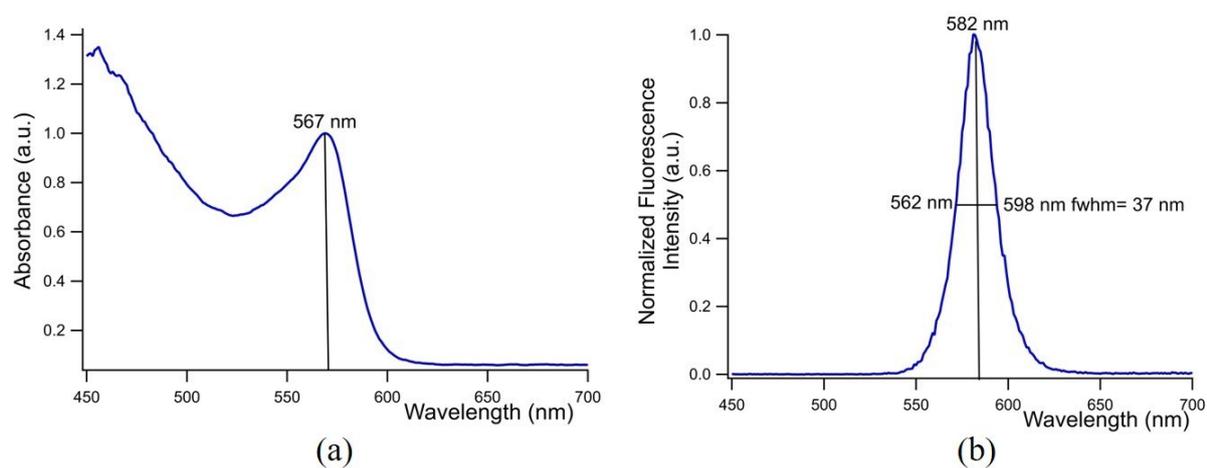


Figure S5. Absorbance (a) and fluorescence (b) spectra of DHLA-EDADA grafted CdSe/ZnS QDs **1**.

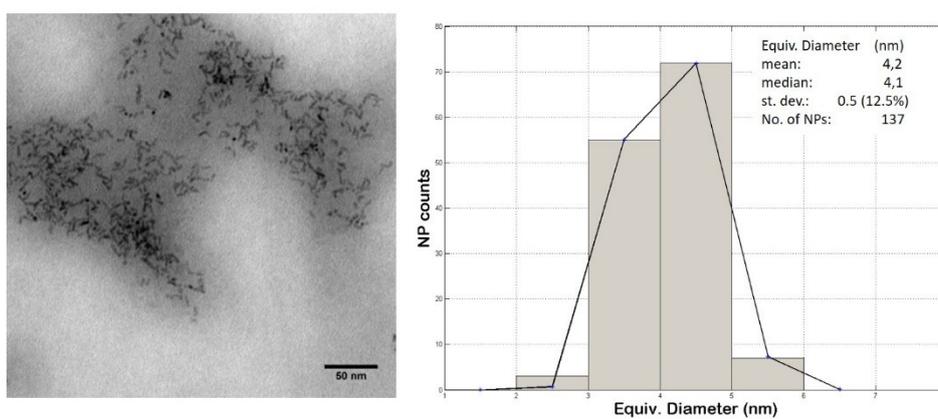


Figure S6. TEM images of DHLA-EDADA grafted CdSe/ZnS QDs **1**.

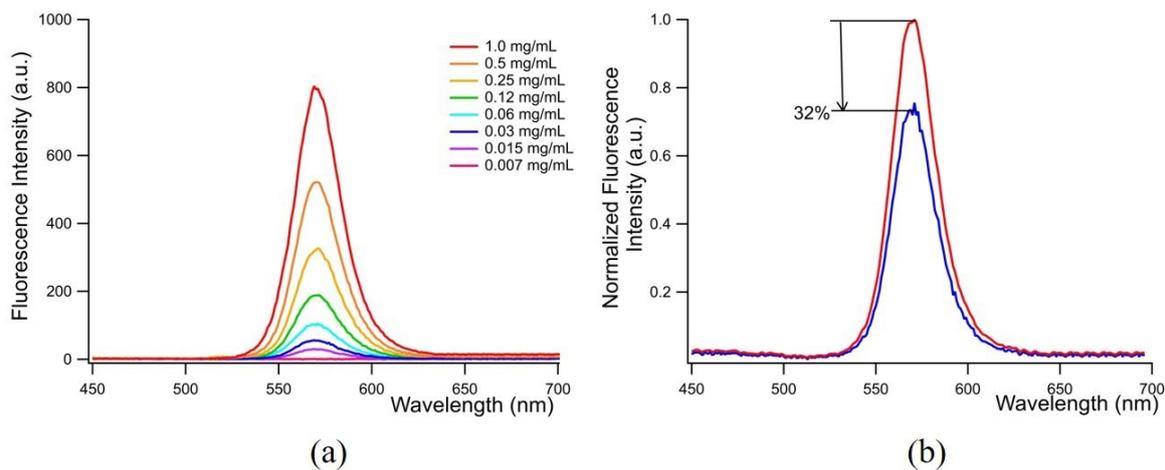


Figure S7. (a) Fluorescence spectra of DHLA-EDADA grafted CdSe/ZnS QDs **1** suspension in H₂O at different concentrations; (b) Fluorescence spectra of DHLA-EDADA grafted CdSe/ZnS QDs **1** (red line, H₂O) and TOPO grafted **2** (blue line, CHCl₃).

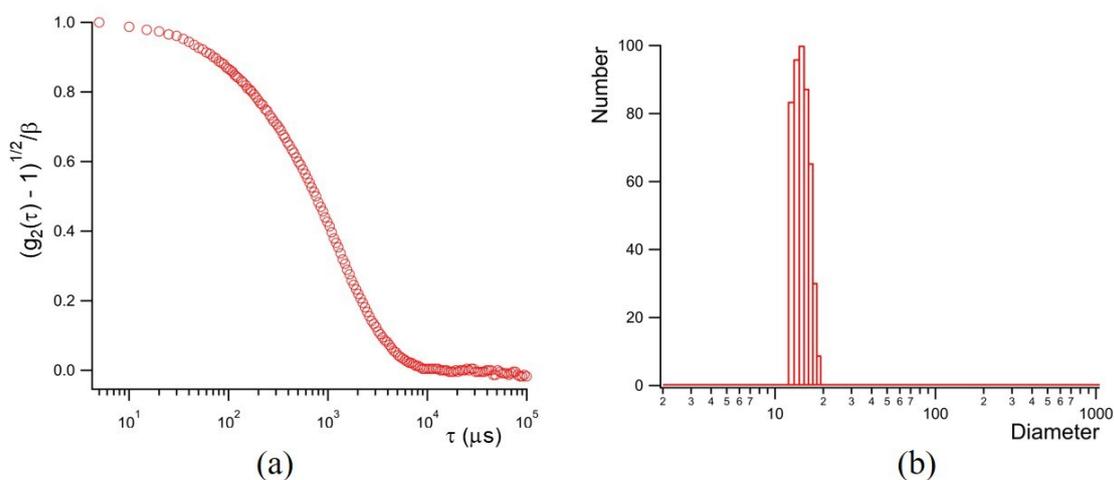


Figure S8. Dynamic Light Scattering of DHLA-EDADA grafted CdSe/ZnS QDs **1** in H₂O: (a) autocorrelation function; (b) size distribution.

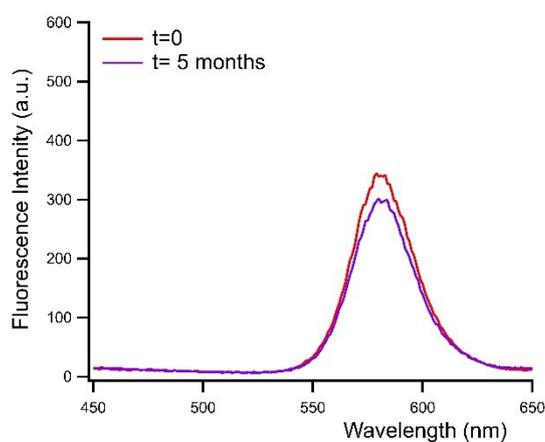


Figure S9. Fluorescence spectra of DHLA-EDADA grafted CdSe/ZnS QDs **1** in H₂O over five months.

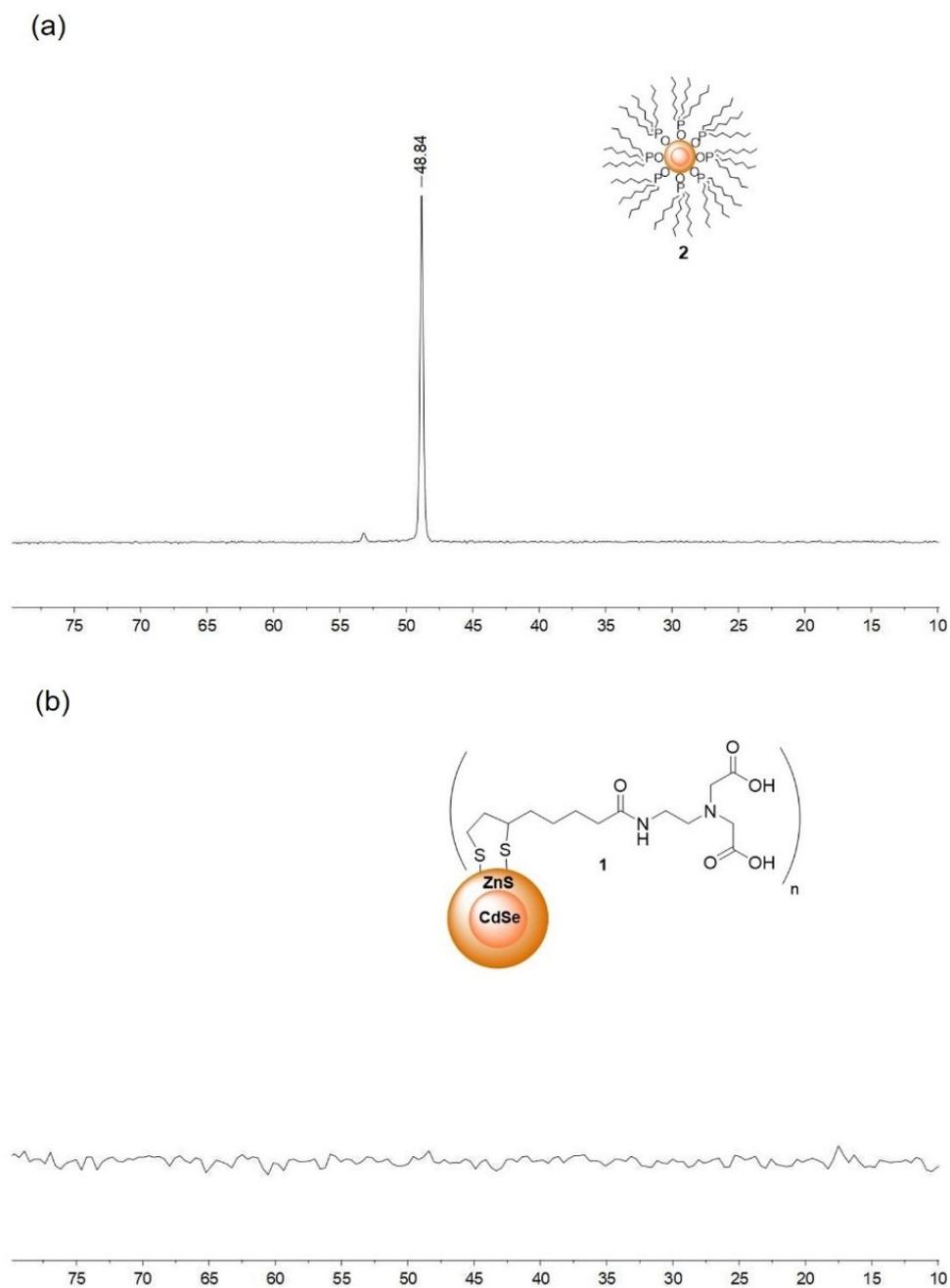


Figure S11. (a) ^{31}P NMR (400MHz) spectra of a) TOPO grafted CdSe/ZnS QDs **2** (5.0 mg/mL in CDCl_3); (b) DHLA-EDADA grafted CdSe/ZnS QDs **1** (5.0 mg/mL in D_2O).

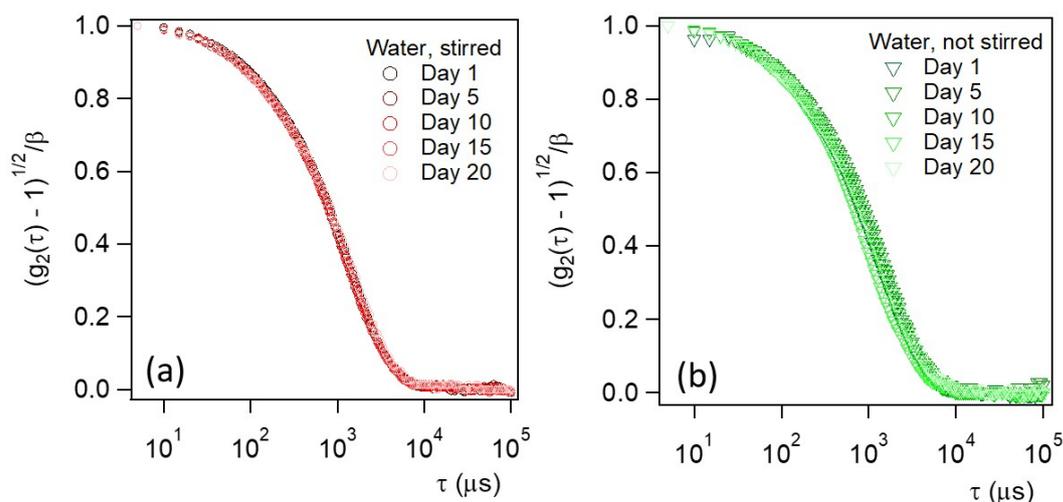


Figure S12. Normalized field autocorrelation functions for an aqueous dispersion of DHLA-EDADA-QDs **1** analyzed over time. (a) Samples stirred before each measurement; (b) samples not stirred before measurements.

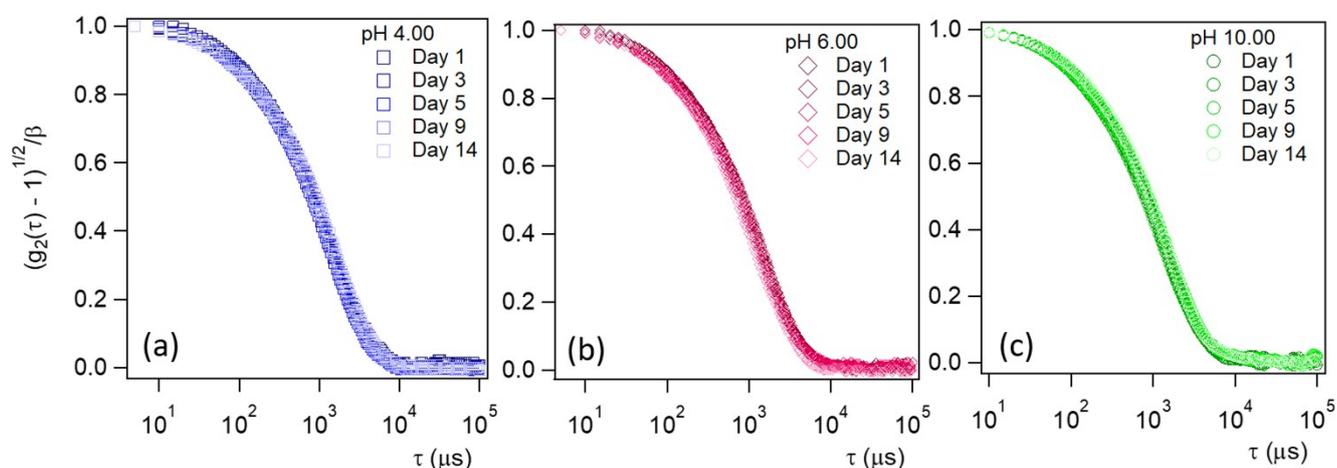


Figure S13. Normalized field autocorrelation functions for aqueous dispersions of DHLA-EDADA-QDs **1** at different pH values, analyzed over time. (a) pH 4.00; (b) pH 6.00; (c) pH 10.00.

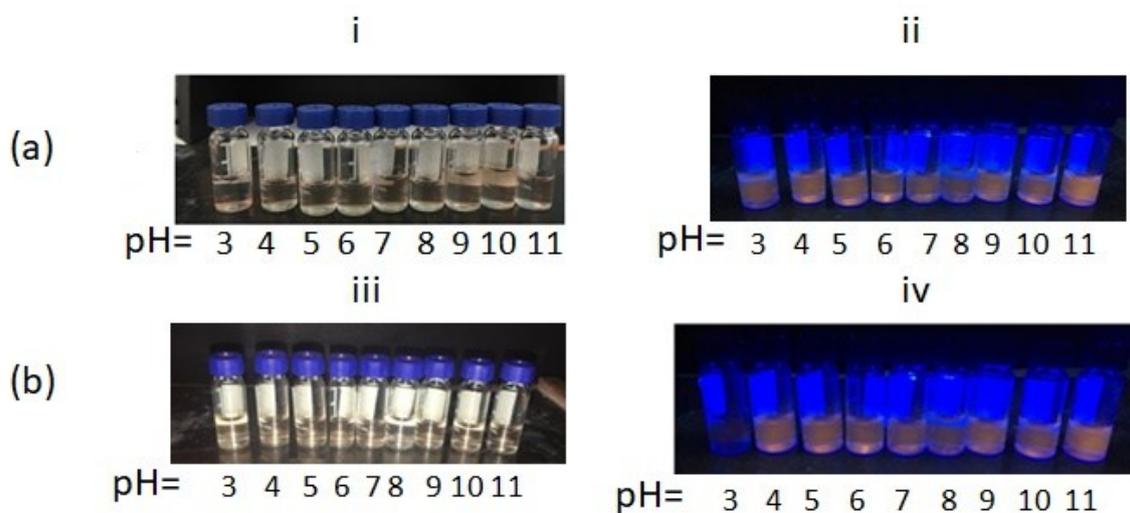


Figure S14. Pictures related to water solutions of DHLA-EDADA grafted CdSe/ZnS QDs **1** at different pH values (from pH 3.00 up to pH 11.00): (a) $t = 0$: (i) under white light, (ii) under UV light; (b) $t = 72\text{h}$: (i) under white light, (ii) under UV light.

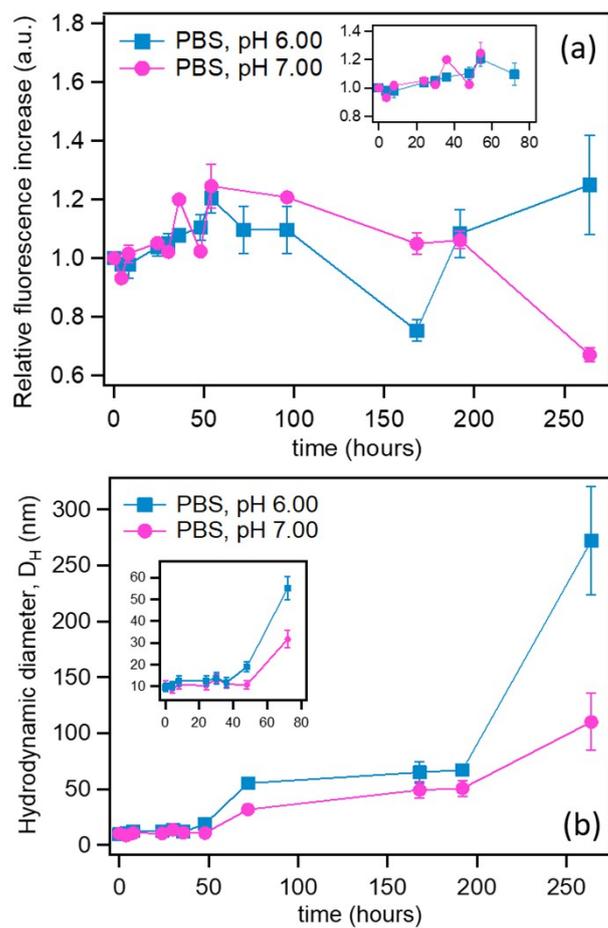


Figure S15. (a) Relative photoluminescence of DHLA-EDADA coated CdSe/ZnS QDs **1** in PBS buffer (100 mM, pH = 6.00 and 7.00); (b) Trend of hydrodynamic diameter for DHLA-EDADA-QDs **1** dispersed in PBS buffer (100 mM, pH = 6.00 and 7.00).

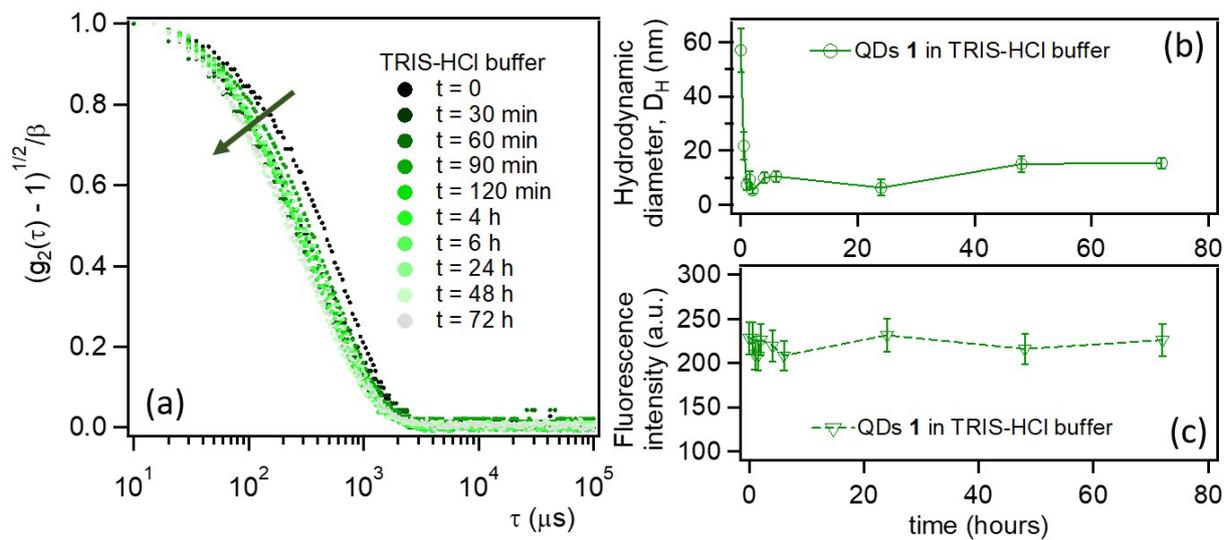


Figure S16. (a) Autocorrelation functions of DHLA-EDADA-QDs **1** in TRIS-HCl buffer suspension collected over time; (b) Trend of hydrodynamic diameters of DHLA-EDADA QDs **1** in TRIS-HCl buffer suspension collected over time; (c) Photoluminescence of DHLA-EDADA grafted CdSe/ZnS QDs **1** in TRIS-HCl buffer collected over time.

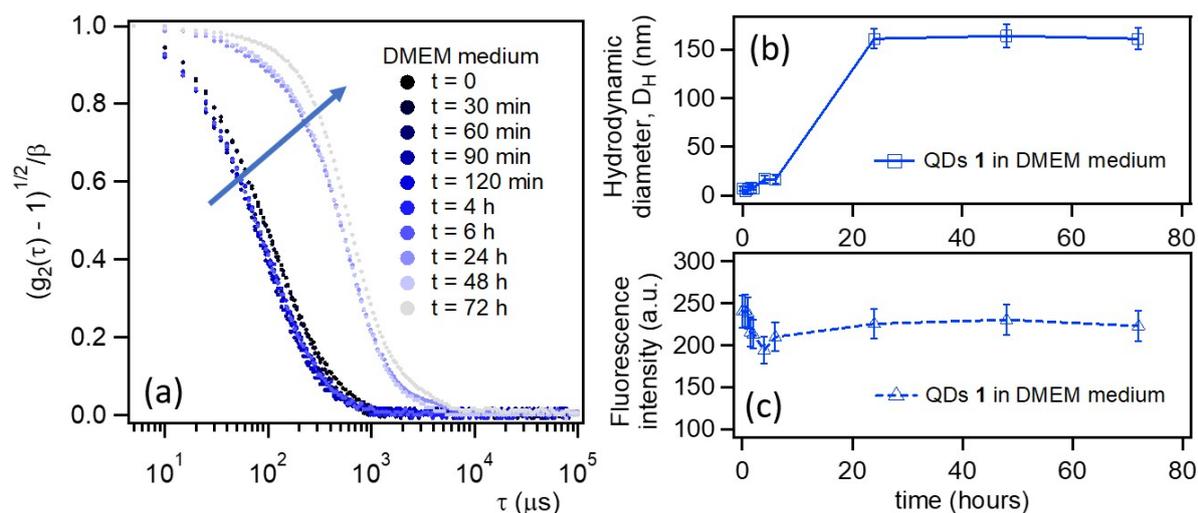
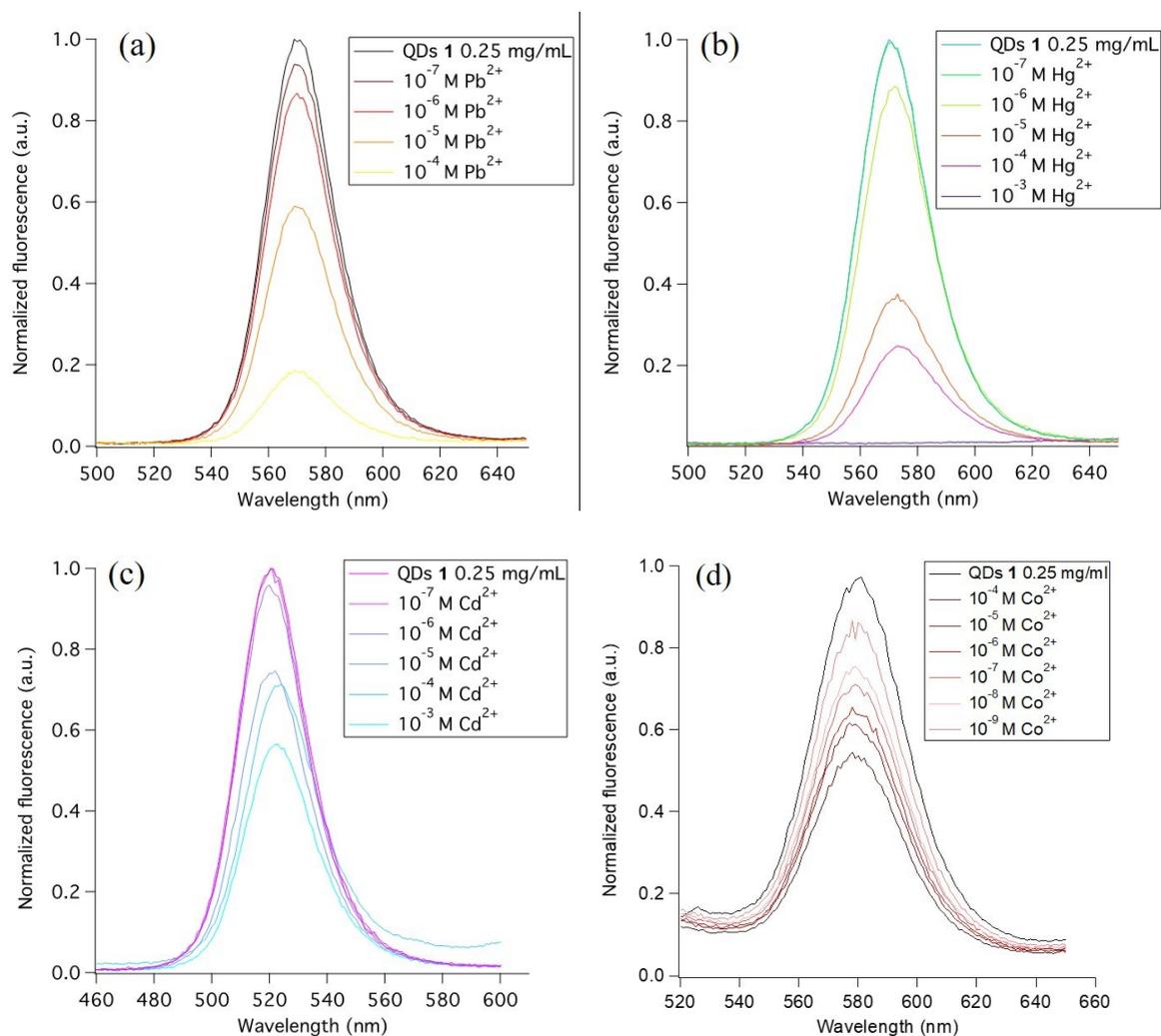


Figure S17. (a) Autocorrelation functions of DHLA-EDADA-QDs **1** in DMEM buffer suspension collected over time; (b) Trend of hydrodynamic diameters of DHLA-EDADA QDs **1** in DMEM cell culture medium collected over time; (c) Photoluminescence of DHLA-EDADA grafted CdSe/ZnS QDs **1** in DMEM buffer over time.



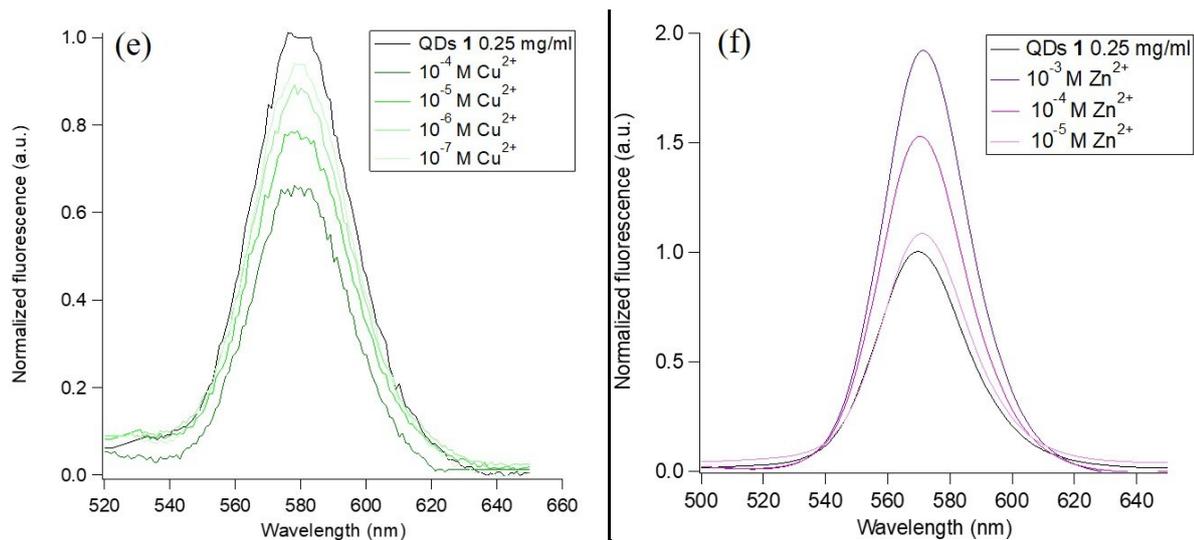


Figure S18. Fluorescence spectra of DHLA-EDADA grafted CdSe/ZnS QDs **1** titrated with: [Pb²⁺] 4.5 × 10⁻⁴ M - 1.0 × 10⁻⁷ M (a); [Hg²⁺] 4.5 × 10⁻³ M - 1.0 × 10⁻⁷ M (b); [Cd²⁺] 4.5 × 10⁻³ M - 1.0 × 10⁻⁷ M (c); [Co²⁺] 4.5 × 10⁻⁴ M - 1.0 × 10⁻⁹ M (d); [Cu²⁺] 4.5 × 10⁻⁴ M - 1.0 × 10⁻⁷ M (e); [Zn²⁺] 4.5 × 10⁻³ M - 1.0 × 10⁻⁵ M (f).

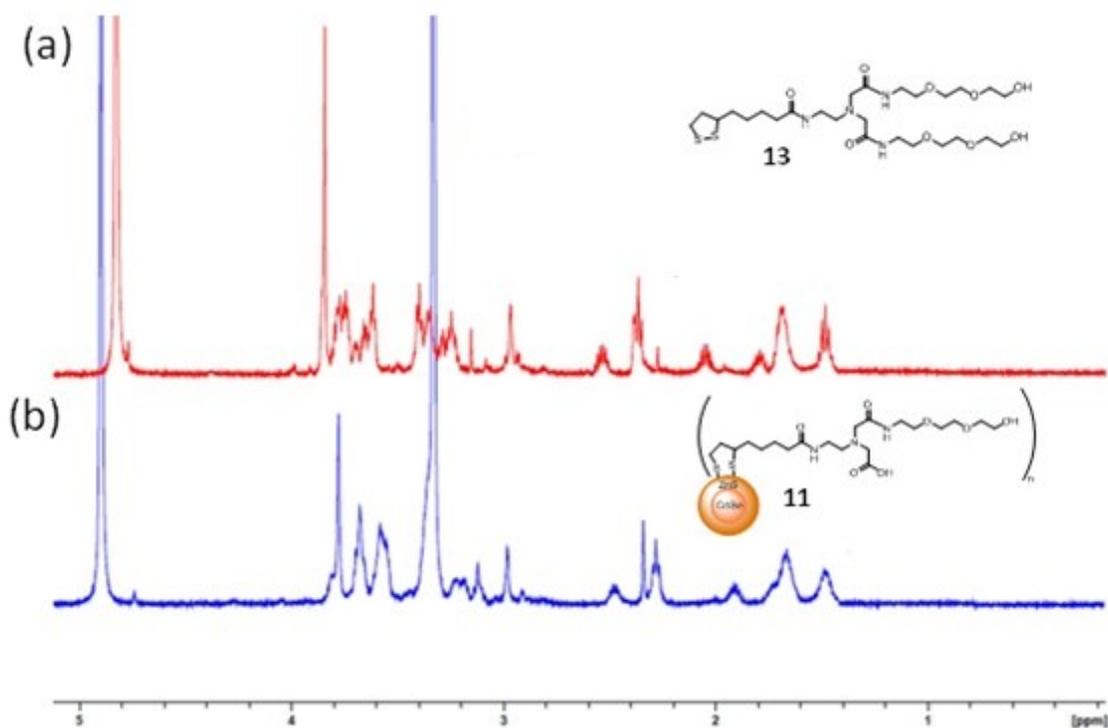


Figure S19. (a) ¹H-NMR spectrum (500 MHz, D₂O) of compound **13**; (b) ¹H-NMR spectrum (500 MHz, D₂O) of conjugated QDs **11**.

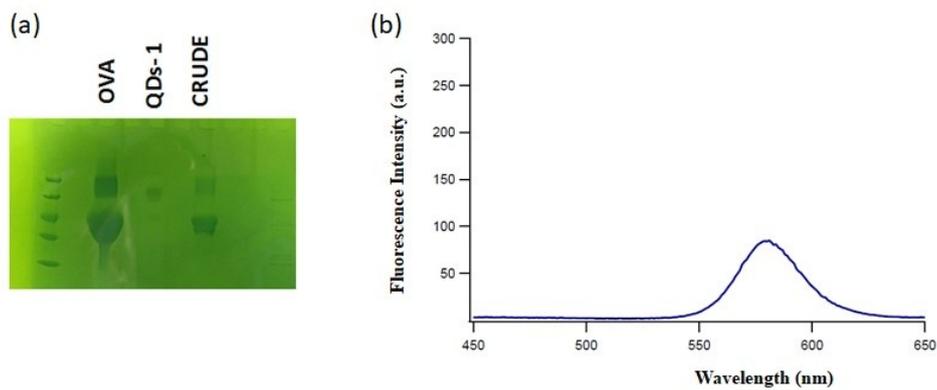


Figure S20. (a) Electrophoresis analysis of the conjugation reaction with OVA protein; (b) Fluorescence spectrum of QDs 1-OVA conjugate.

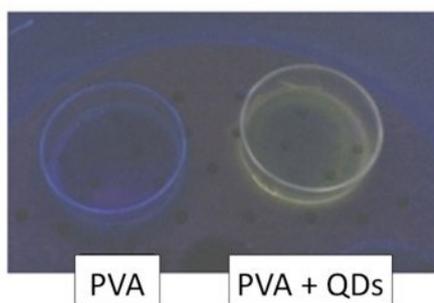


Figure S21. Picture of PVA film (left) and PVA-QDs 1 composite (right).

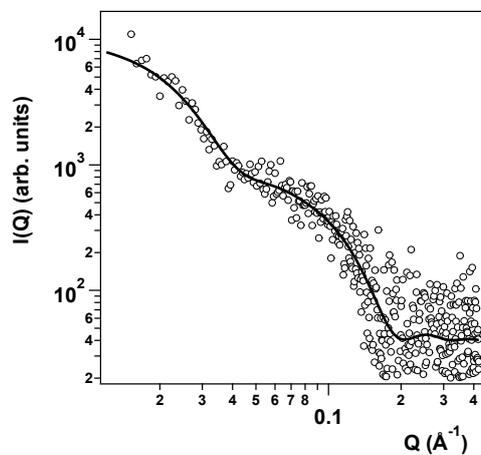
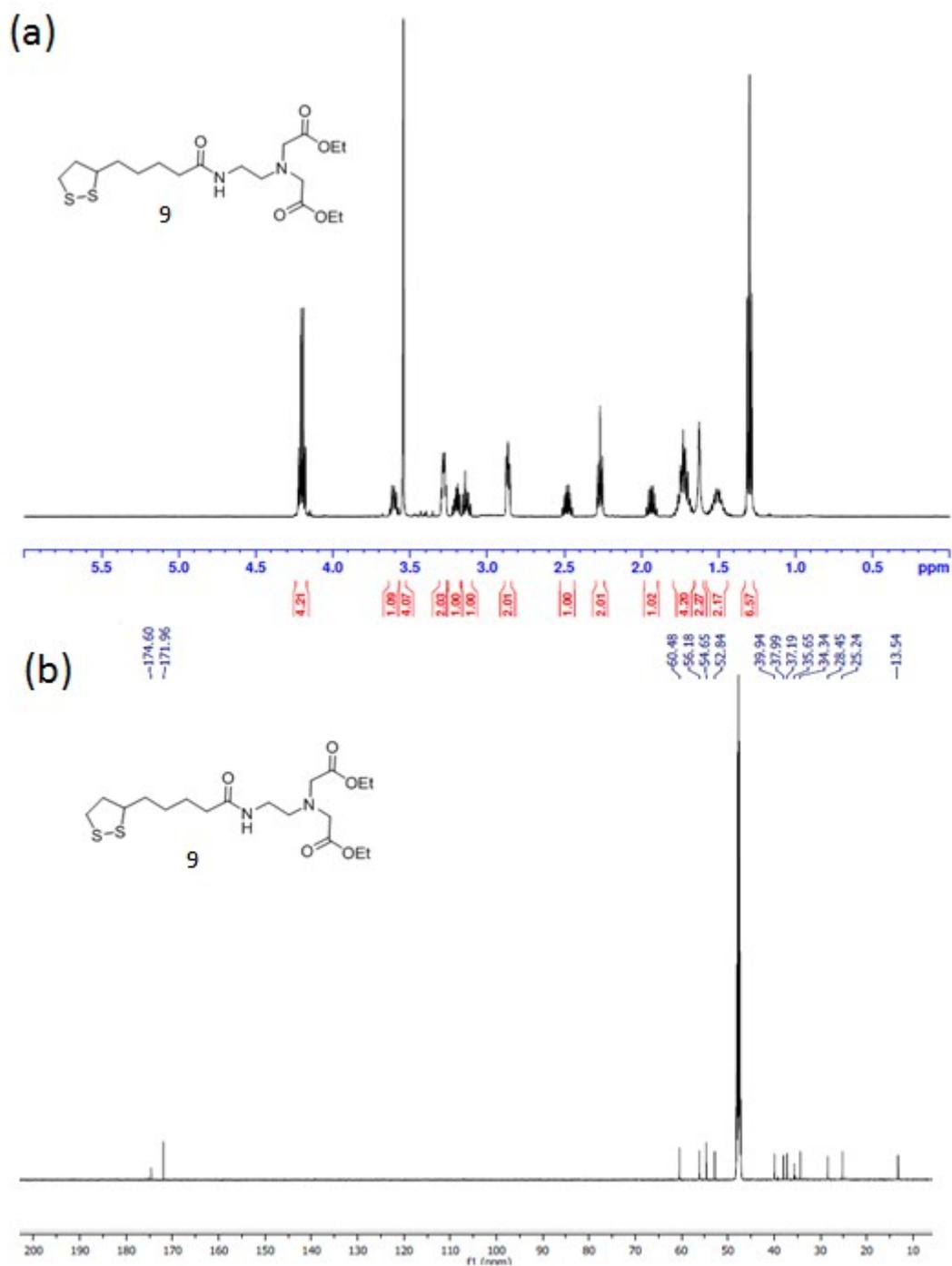


Figure S22. SAXS pattern obtained for the PVA-QDs 1 composite. Blue markers represent the experimental data while the black solid line is the curve fitting (see main text for details).



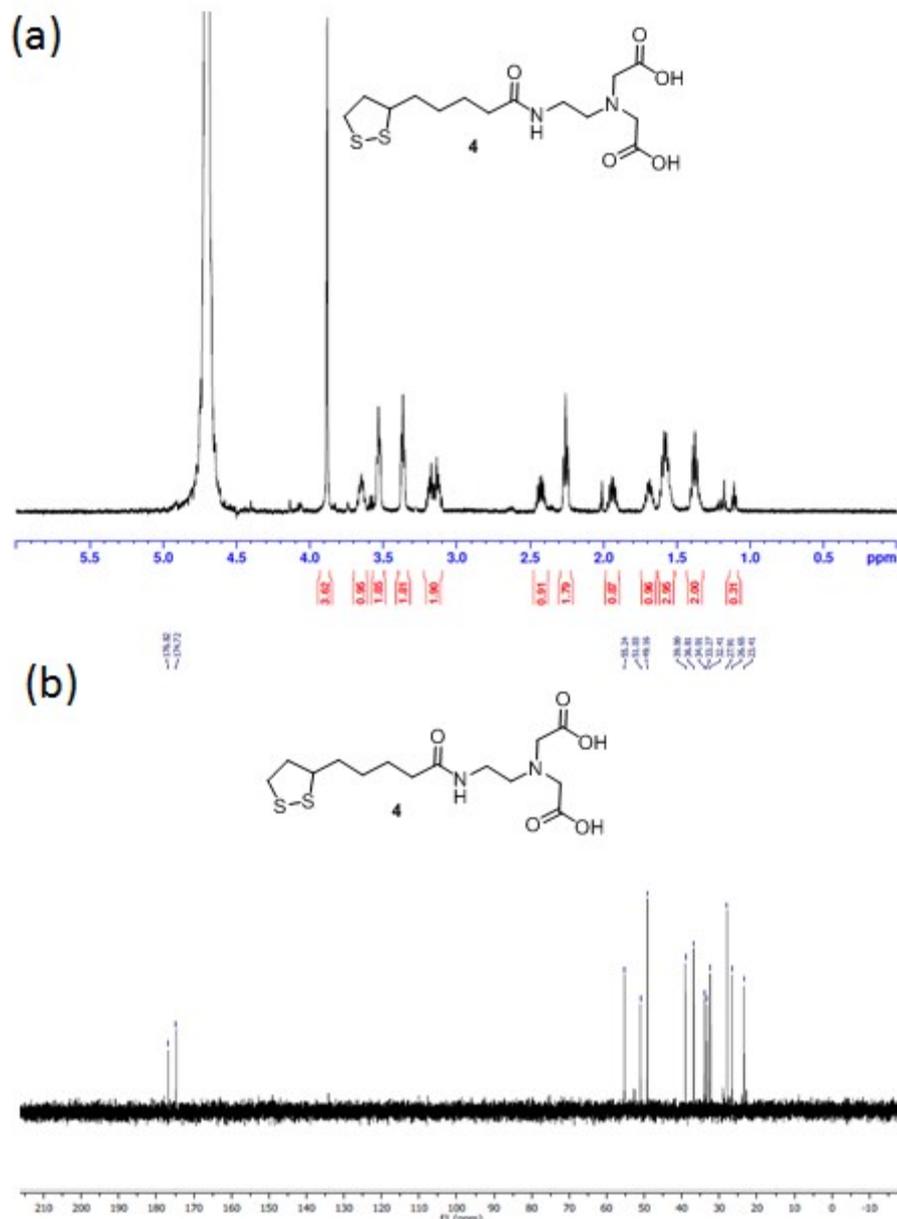
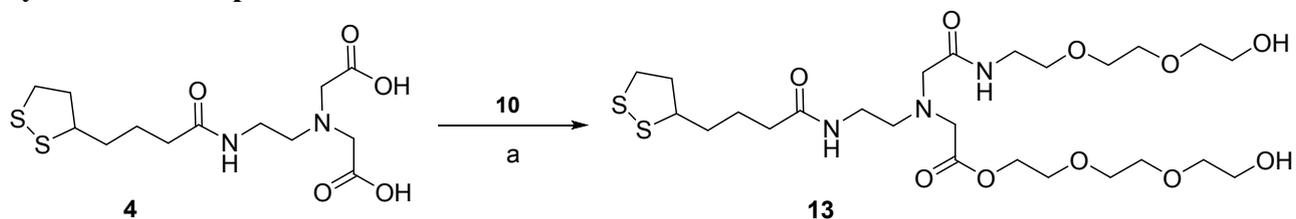


Figure S24. (a) $^1\text{H-NMR}$ (500 MHz, D_2O) spectrum of compound **4**. (b) $^{13}\text{C-NMR}$ (125 MHz, D_2O) spectrum of compound **4**.

Synthesis of compound **13**



To a solution of compound **4** (100 mg, 0.24 mmol) in DMF (0.5 mL), 1,1'-Carbonyldiimidazole (99 mg, 0.61 mmol) and Triethylamine (67 mg, 0.65 mmol) were added. The reaction mixture was stirred at r.t. for 30', then, a solution of **10** (160 mg, 0.61 mmol) in DMF (0.5 mL) was added. After 18 h at r.t., the reaction mixture was diluted with AcOEt (250 mL) and washed with

H₂O (3 x 15 mL) and BRINE (2 x 15 mL). Organic phase was dried over Na₂SO₄ filtered and reduced in vacuum. The crude was purified by flash column chromatography on silica gel (DCM:MeOH, 20:1) to give **13** as a yellow oil (82 mg, 56%). ¹H-NMR (500 MHz, D₂O): δ 3.89-3.75 (m, 9H), 3.43-3.28 (m, 9H), 2.51-2.45 (m, 1H), 2.25 (t, *J* = 5 Hz, 2H), 1.94-1.88 (m, 1H), 1.78-1.62 (m, 4H), 1.53-1.44 (m, 2H). ¹³C-NMR (125 MHz, D₂O) 177.5, 170.7, 70.4, 70.2, 61.3, 58.8, 55.6, 54.0, 41.3, 4.6, 38.7, 36.2, 30.9, 21.6. ESI-MS *m/z*: calcd for [M + H]⁺ 612.29. Found 613.37.

S-Video: Water dispersion of QDs **1** in NMR tube (3.0 mg/mL in D₂O) and lyophilization of QDs **1** is reported. Then the last section of the video shows QDs **1** as lyophilized powder and dispersion of QDs **1** (after 3 cycles of lyophilization) at the concentration of 13.0 mg/mL.