

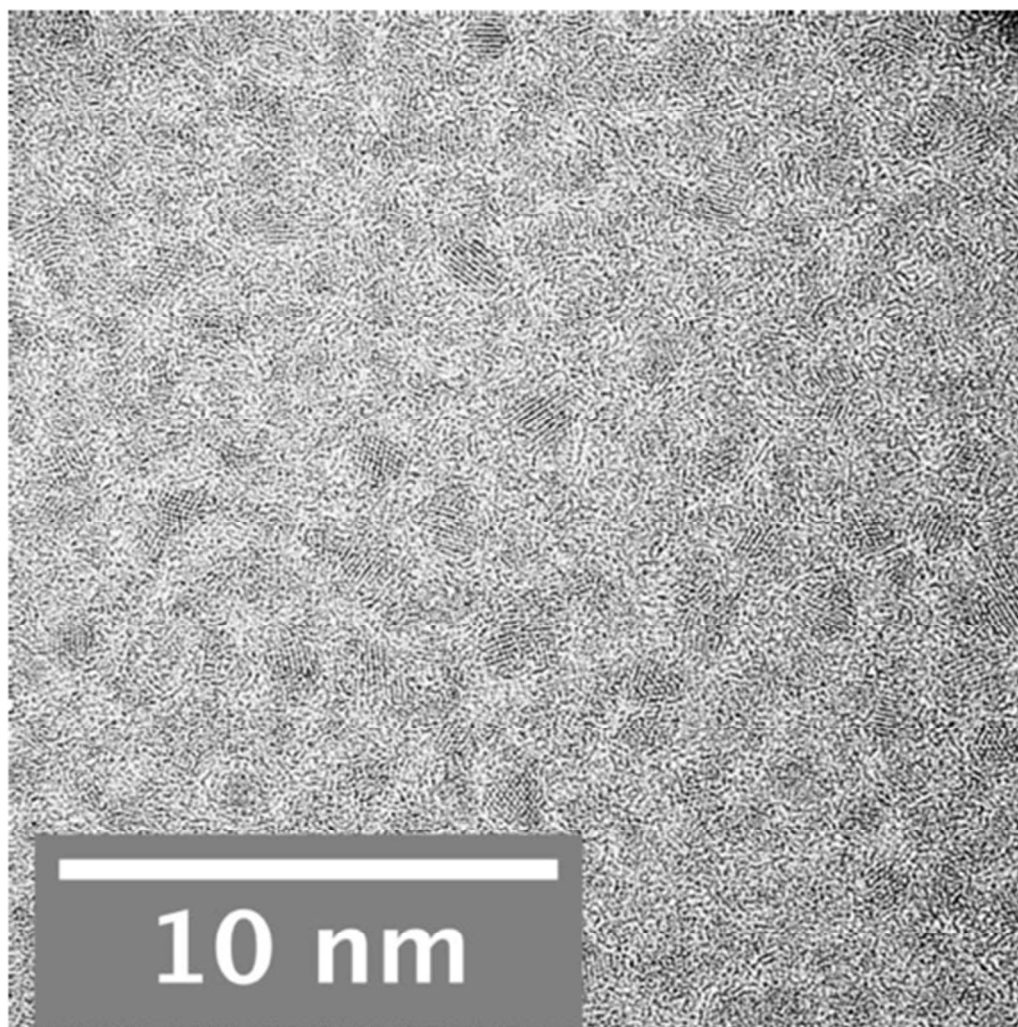
Supporting Information

Isolation of Bright Blue Light-Emitting CdSe Nanocrystals with 6.5 kDa Core in Gram Scale: High Photoluminescence Efficiency Controlled by Surface Ligand Chemistry

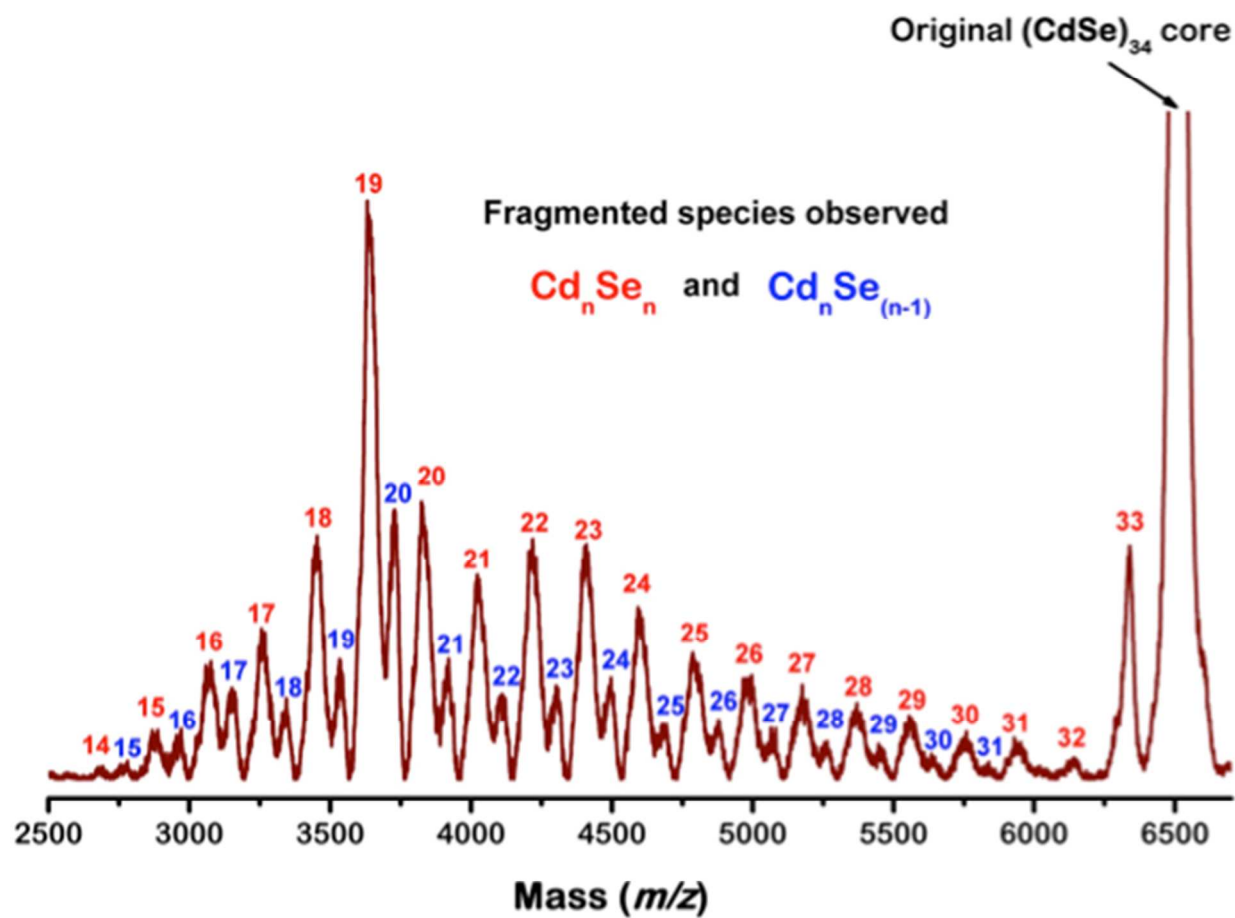
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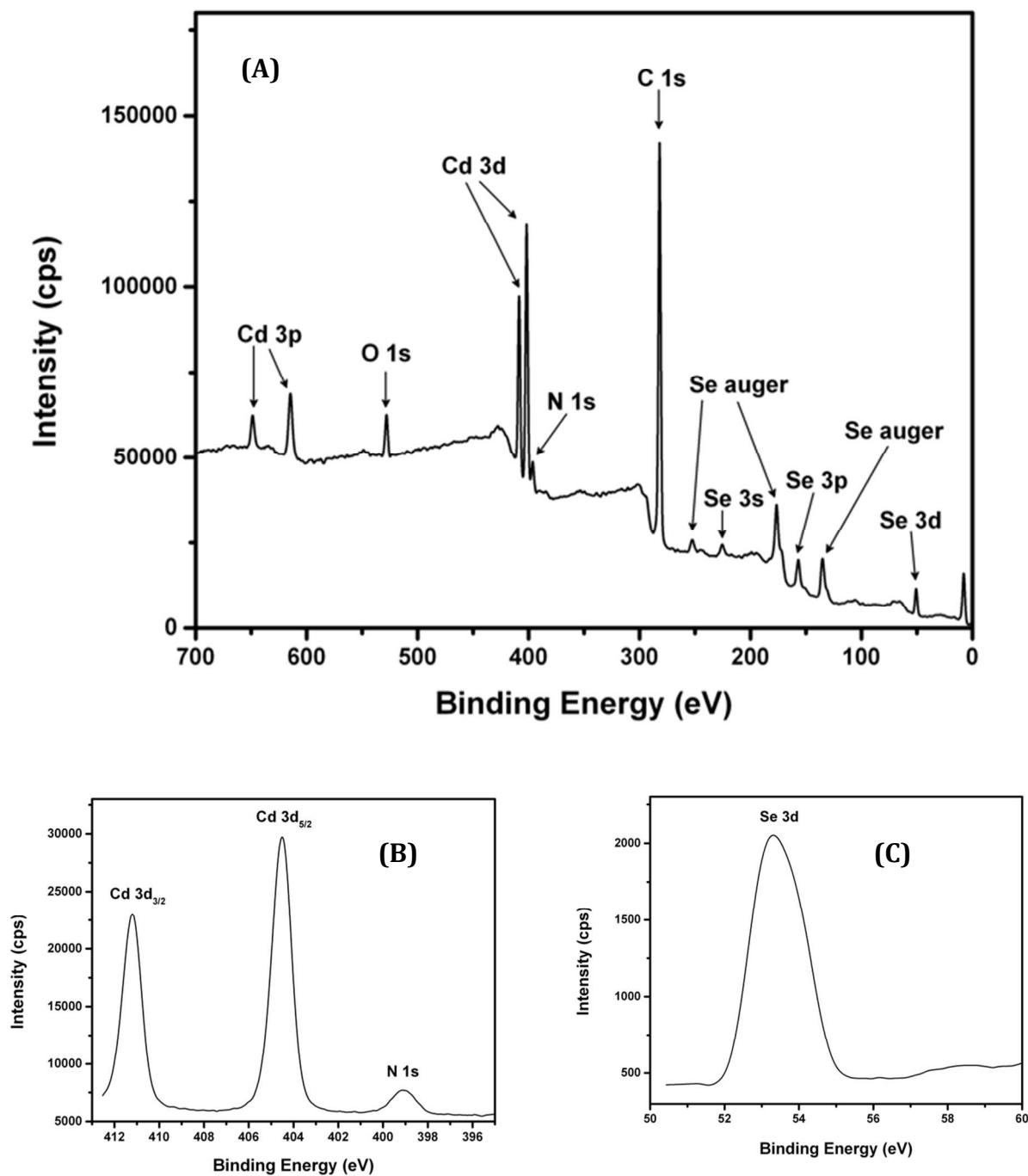
X-ray Photoelectron Spectroscopic (XPS) Analysis. All XPS spectra were collected on a Kratos Axis Ultra DLD system with an Mg anode at 1253.6 eV and X-ray power of 150 W. A charge neutralizer was used to prevent charging. The survey scans were collected from binding energies of 0-1000 eV with a 80 eV pass energy. For high resolution scans of Cd(3d), Se(3d), C(1s), and N(1s), a 20 eV pass energy was used. All data were collected so that the C 1s line was shifted to 284.6 eV. The measurements were conducted at a pressure $<5 \times 10^{-9}$ Torr. For XPS analysis, the samples were drop-casted on a piranha-cleaned silicon wafer inside a N₂ filled glove box and the solution was allowed to evaporate at room temperature. The piranha-cleaned silicon wafer was washed with copious amount of Nanopure water and ethanol, and then dried under high vacuum over night. The XPS analysis was performed for four different batches of CdSe nanocrystal and two different sample concentrations (3.0 and 6.0 mg/mL). (*Warning:* piranha solution is very corrosive and must be handled with extreme caution. It reacts violently with organic materials and may not be stored in tightly closed vessels).



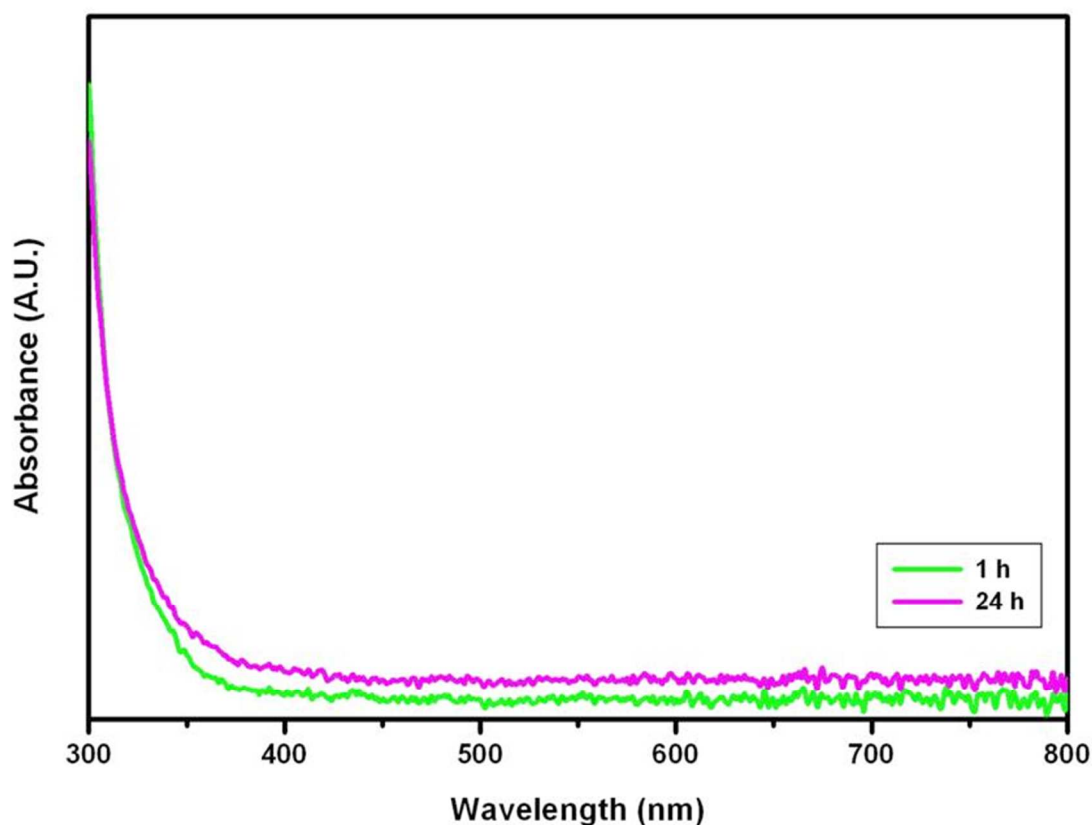
SI-Figure 1. High-resolution TEM image of OA-capped $(\text{CdSe})_{34}$ nanocrystals.



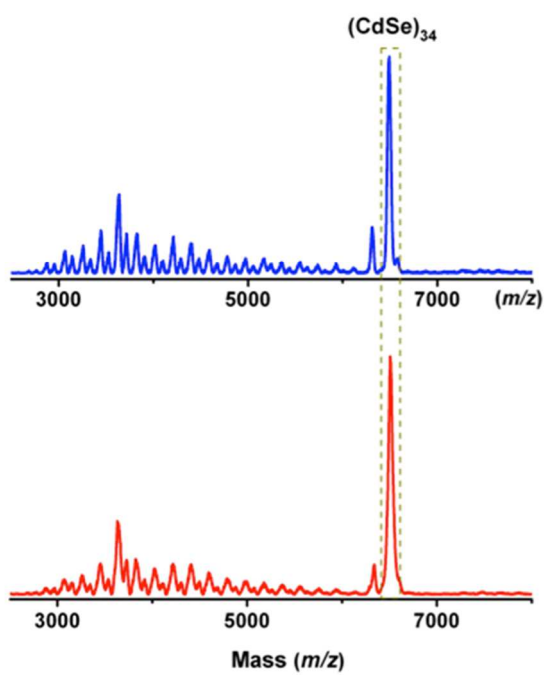
SI-Figure 2. Expanded and enlarged positive mode LDI-MS spectrum of OA-coated (CdSe)₃₄ nanocrystals at 60% laser power as demonstrated in manuscript figure 2. The spectrum was expanded to demonstrate the fragmented species Cd_nSe_n and $\text{Cd}_n\text{Se}_{(n-1)}$.



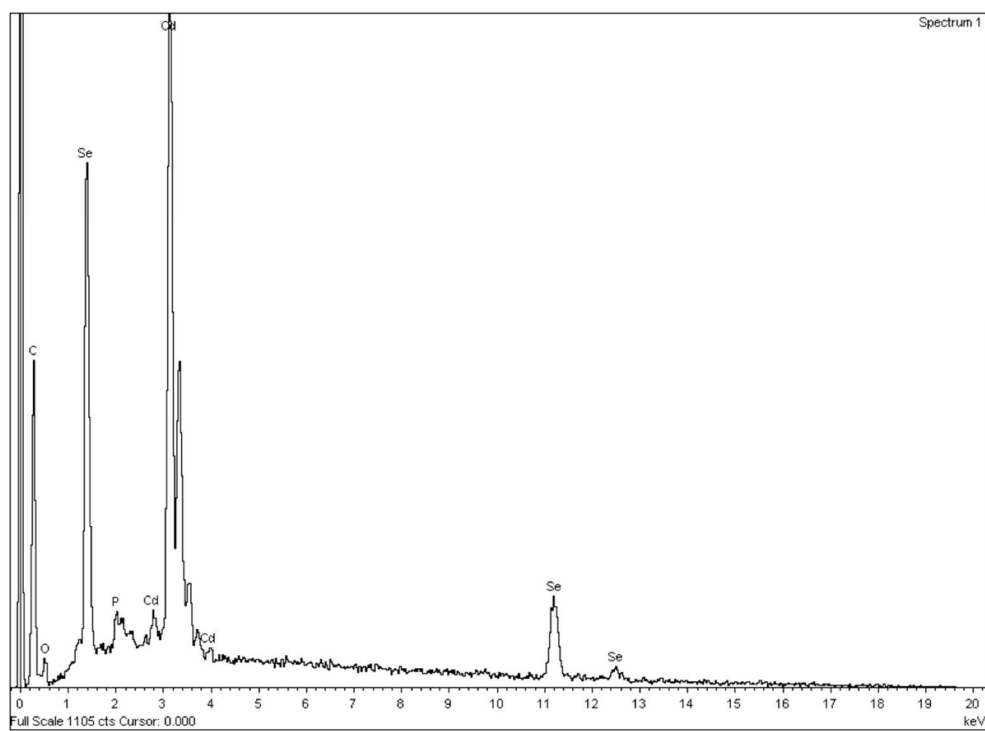
SI-Figure 3. (A) XPS survey spectrum of OA-coated (CdSe)₃₄ nanocrystals on silicon wafer. (Lower panel): High resolution XPS spectrum of Cd 3d (B) and Se 3d (C) core region for OA-coated (CdSe)₃₄ nanocrystals deposited on the silicon wafer.



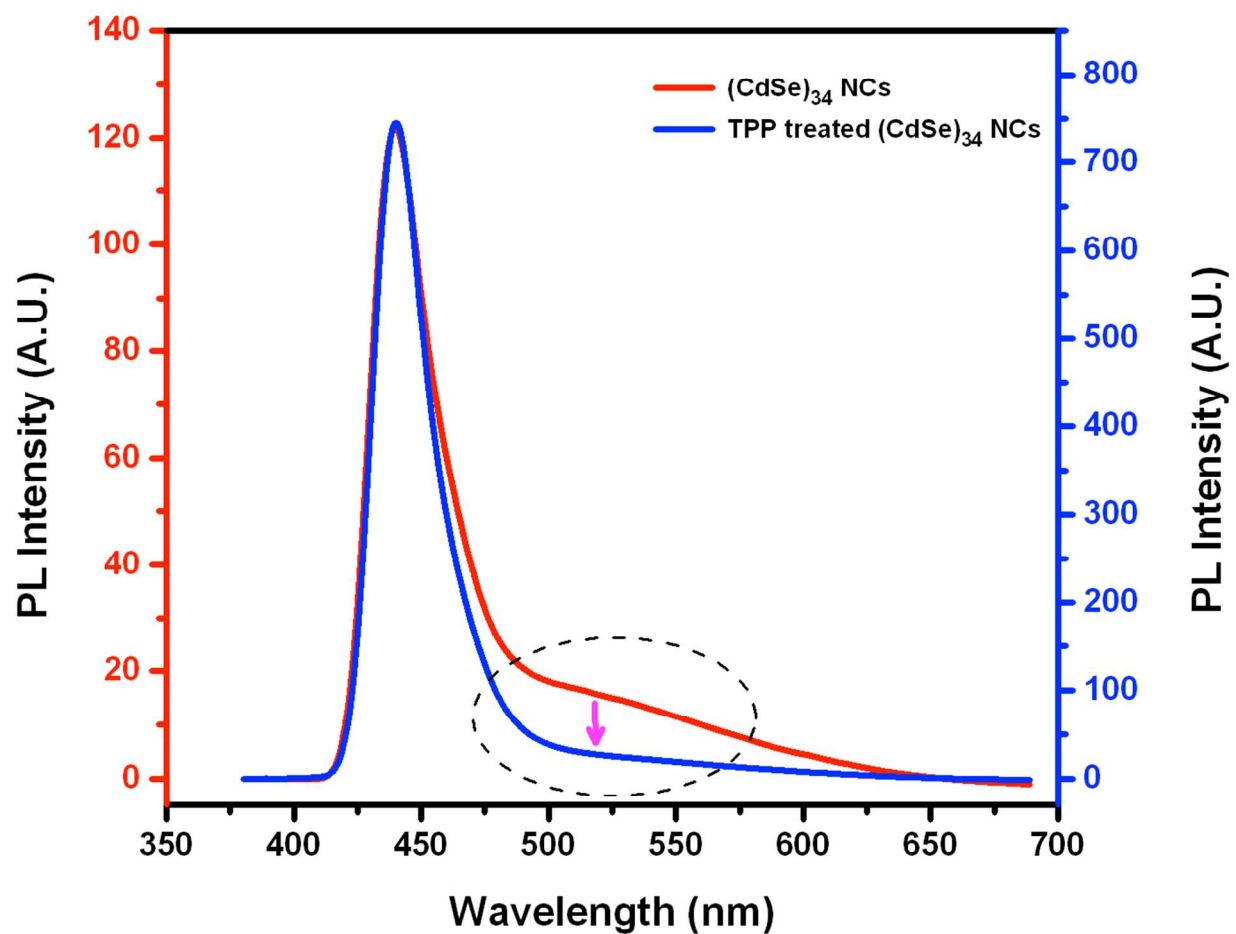
SI-Figure 4. Time dependent UV-visible absorption spectra of the Cd-octylamine (Cd-OA) precursor reacted with TOP-Se precursor at room temperature. The absence of peak in the 400 nm region implied absence of $(\text{CdSe})_{34}$ nanocrystals in the reaction mixture. The Cd-OA and TOP-Se precursors were prepared as follows: first a stock solution of TOP-Se was prepared by dissolving freshly ground Se powder (200 mg, 2.53 mmol) in 2.26 mL TOP (1.87 g, 5.06 mmol) at 100 °C for 2h under argon atmosphere and then, cooled down to room temperature. Separately, $\text{Cd}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (100 mg, 0.37 mmol) was dissolved in 3 mL octylamine (2.35 g, 18.2 mmol) at room temperature under argon atmosphere. Next, 680 μL of TOP-Se precursor was injected into the Cd-OA precursor and stirred at RT under Ar atmosphere. Progress of reaction was monitored via UV-visible absorption spectroscopy by diluting 10 μL of reaction mixture in 3-mL of toluene at different time intervals.



SI-Figure 5. Positive mode LDI-MS of OA-capped (red) and mixed TPP treated OA-capped (blue) $(\text{CdSe})_{34}$ nanocrystals.



SI-Figure 6. EDX spectrum of TPP treated OA-capped (CdSe)₃₄ nanocrystals.



SI-Figure 7. PL spectra of OA-coated (red) and OA-coated TPP treated (blue) $(\text{CdSe})_{34}$ nanocrystals with 380 nm excitation.