Electronic Supplementary Information (ESI)

One-pot Synthesis of Near-Infrared Type II Quantum Dots and Their in vivo Applications

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A. One pot synthesis of near-infrared CdTe/CdS QDs

An oleylamine-sulfur solution was prepared by dissolving 0.1603 g of sulfur (1 M) in 5 mL of oleylamine. Separately, 4 mmol of cadmium oxide was dissolved in 4 g of myristic acid. The mixture was heated at ~200^{o}C for 40 minutes under argon flow, then 1 mL TBP: Te solution was injected under vigorous stirring into the hot reaction mixture. After the injection, the reaction temperature was decreased to 100 – 110^{o}C and stirred for ~15-20 minutes, then 1 mL of oleylamine-sulfur solution was slowly added into the hot reaction solution by syringe over the course of few minutes. The final mixture was left in the reaction pot at 100 - 110^{o}C for two to three hours. The NCs were separated from the surfactant solution by addition of ethanol and centrifugation. The NC precipitate could be redispersed in various organic solvents including hexane, toluene, and chloroform. Prior surface modification, the dispersion of QD chloroform solution was filtered using a syringe filter with a nominal pore diameter of 0.2 μm to remove dust particles.

B. Preparation of phopholipid-micelle coated QDs

The as-prepared organic-dispersible QDs were separated from by addition of ethanol (volume ratio of QDs to ethanol 1:3) and centrifugation (12000 rpm for 20 min). The precipitation was collected and dried in vacuum and re-dispersed in chloroform. Next, QD stock chloroform solution (~2 mg/mL) and DSPE-mPEG (1,2-Diacyl-sn-Glycero-3-Phosphoethanolamine-N-[Methoxy(Polyethylene glycol)]) chloroform solution (~10 mg/mL) were mixed together at a weight ratio of 1:4. The PEGylated phospholipids were purchased from Avanti polar lipids, Inc. and Laysan Bio Inc. Each mixture was gently stirred for 5 to 40 minutes. A Labconco rotory evaporator with a water bath of 25^{o}C was used to evaporate the organic solvent. The lipidic film, deposited on the reaction vial, was hydrated with 3 to 5 mL of HPLC water and subjected to ultrasonication for 10 to 20 minutes using a bath sonicator. The resulting dispersion was filtered through a 0.2 μm membrane filter and kept at room temperature for further use. To remove the

excess phospholipids from the QD dispersion, the micelle-encapsulated QDs were further purified using centrifugation at 10000 rpm for 15 minutes. The QDs precipitate was re-dispersed in 1 to 2 mL of HPLC water.

C. Characterization methods

Transmission Electron Microscopy (TEM) images were obtained using a JEOL model JEM-100CX microscope with an acceleration voltage of 100 kV. The specimens were prepared by drop-coating the sample dispersion onto a carbon coated 300 mesh copper grid, which was placed on a filter paper to absorb the excess solvent. Emission quantum yields (QYs) of the QDs chloroform dispersion were determined by comparing the integrated emission from the QDs to NIR dye solutions of matched absorbance. Samples were diluted so that they were optically thin. The effective size distribution of the QD suspensions was estimated using a dynamic light scattering particle size analyzer. The QDs were dispersed in 1x PBS at a concentration of 1 mg/mL for the measurement. These solutions were filtered through a 0.45 μm syringe filter membrane to remove the dust impurities and then analyzed directly.

D. Xenograph tumor model

5-6 week old female athymic nude mice (Hsd:Athymic Nude-*Foxn1*^{nu}) were obtained from Harlan Laboratories, Inc., and allowed an acclimation period of 1 week. The nude mice were housed in sterile M.I.C.E caging (Animal Care Systems, Centennial CO.) that contained sterile bedding, food and water. Animal care was set up in accordance with the guidelines of the Intuitional Animal Care and Use Committee (IACUC) established at the University of Buffalo.

Human pancreatic tumor models were created in the athymic mice by injecting PANC-1 (ATCC, CRL-1469) cells at a concentration of 2-3 x 10^6 cells in a 100 uL suspension of Matrigel (BD Biosciences) and medium mixture (1:1) maintained at 4^{o}C. This mixture was then injected subcutaneously in one scapular region of the mice using a 1mL Monoject tuberculin syringe with a 25g x 5/8" detachable needle. Tumor growth was monitored every 24-48 hours until a tumor size of approximately 5 mm^2 was obtained 10-14 days post transplantation of cells. Once tumors reached the appropriate size, the mice were injected with various functionalized QDs formulation by tail vein injection at a volume of 150μL containing 1mg of QD per injection. After injection, mice were anesthetized with Aerrane: isoflurane, USP (Baxter Healthcare Corporation, Deerfield,IL.) at an induction concentration of 5% isoflurane/1L O_2. Anesthesia maintenance concentrations were 2-3% isoflurane/1L O_2. Once proper plane of anesthesia was reached, the mice were imaged using the Maestro in-vivo optical imaging system (CRI, Inc., Woburn, MA.).

E. Sentinel lymph node mapping

For lymph node mapping experiments, mice were anesthetized with Aerrane: isoflurane as mentioned above. Next, ~0.5mg of QDs in 0.1 mL of PBS buffer was injected subdermally into the mice paws. A few hours later, the mice were sacrificed, surgically opened, and observed with a Maestro imaging system.

F. Stability of As-synthesized CdTe core without CdS Shell

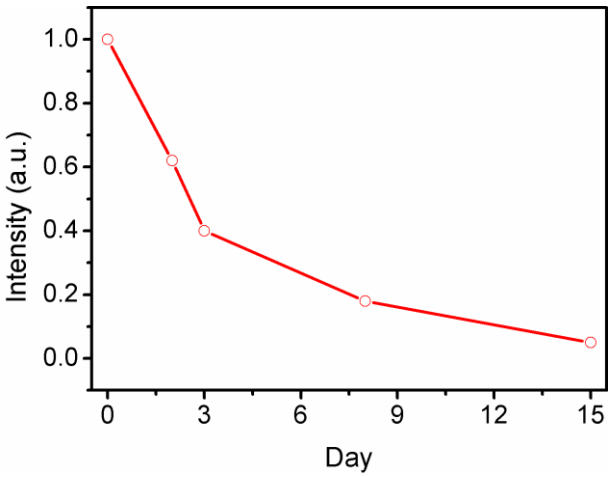

Figure S1. The intensity of as-synthesized CdTe core in chloroform against time.

G. Hydrodynamic diameter of phsopholipid micelle-encapsulated CdTe/CdS QDs

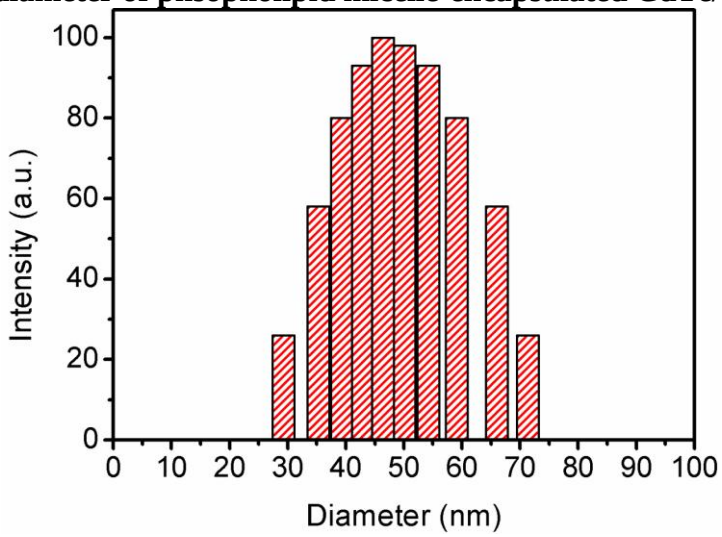

Figure S2. Hydrodynamic diameter of phsopholipid micelle-encapsulated CdTe/CdS QDs is ~48nm

H. Histological evaluation of major organs from a nude mouse injected with PBS.

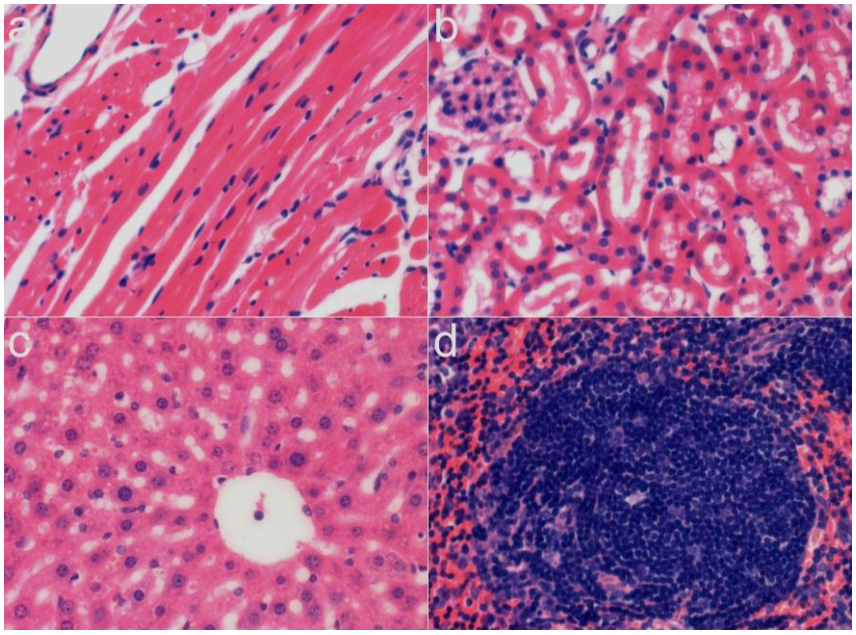

Figure S3. H&E-stained tissue sections from mice administered with PBS buffer saline as control. Tissues were harvested from (a) heart, (b) kidney, (c) liver, and (d) spleen, respectively.