Electronic Supplementary Information

RGD-QD-MoS_2 nanosheets for targeted fluorescent imaging and photothermal therapy of cancer

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S1. Characterization

Morphology of the nanomaterials was characterized by transmission electron microscopy (TEM, Hitachi HT-7700, 120 kV) and high resolution TEM (HRTEM, Tecnai G2 F20 S-Twin electron microscope, 200 kV). Atomic force microscopy (AFM, BRUKER Dimension Icon with ScanAsyst) was used to characterize the thickness of MoS_2 NSs, BPM NSs and RGD-QD-MoS_2 NSs. Photoluminescence spectra of QDs and RGD-QD-MoS_2 NSs were recorded with a Shimadzu RF-5301 PC fluorescence spectrophotometer. UV-Vis-NIR absorption spectra was obtained from a Shimadzu UV-3600 spectrophotometer. Infrared spectra was recorded using a PerkinElmer FT-IR spectrometer. X-ray photoelectron spectroscopy (XPS) was performed on PHI 5000 VersaProbe with an Al Kα X-ray source. A ZetaPALS Potential Analyzer (Brookhaven) was used to determine the hydrodynamic size and Zeta potential of the nanosheets.

S2. Morphology of QDs, MoS_2 NSs, BPM NSs, and RGD-QD-MoS_2 NSs

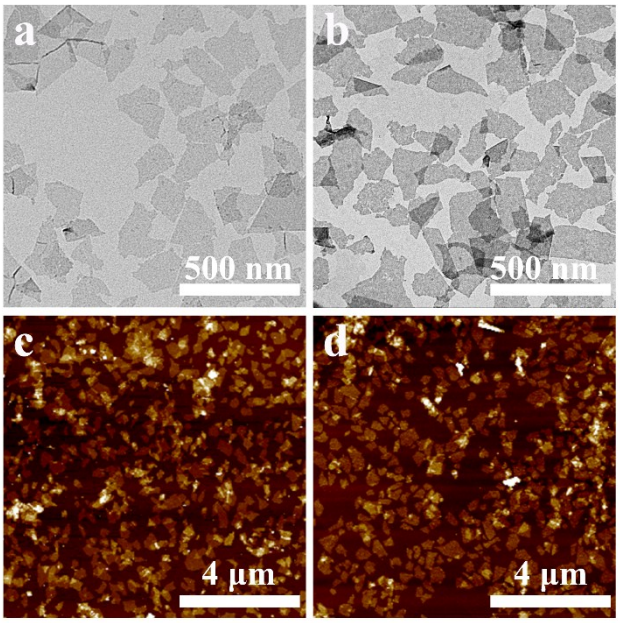

Fig. S1. Large area TEM images of (a) MoS_2 NSs and (b) BPM NSs; Large area AFM images of (c) MoS_2 NSs and (d) BPM NSs.

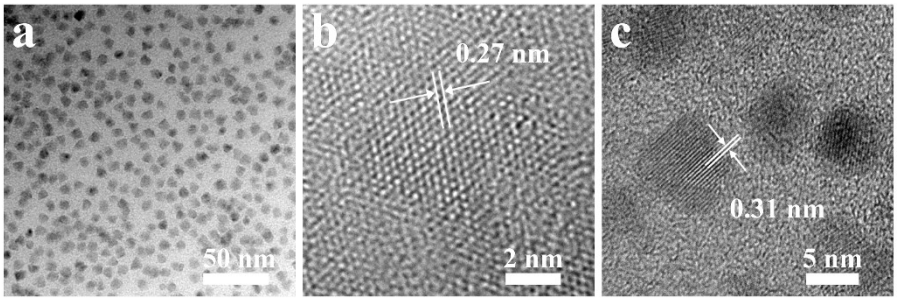

Fig. S2. (a) TEM image of QD580; (b) HRTEM image of MoS_2 NSs; (c) HRTEM image of RGD-QD580-MoS_2 NSs.

S3. XPS Spectra of RGD-QD-MoS_2 NSs

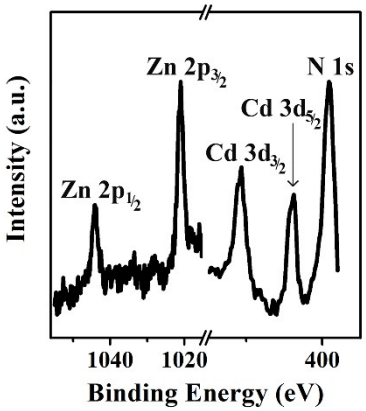

Fig. S3. XPS spectra of RGD-QD-MoS_2 NSs.

S4. Hydrodynamic Sizes and Zeta Potentials of MoS_2 NS, BPM NSs, and RGD-QD-MoS_2 NSs

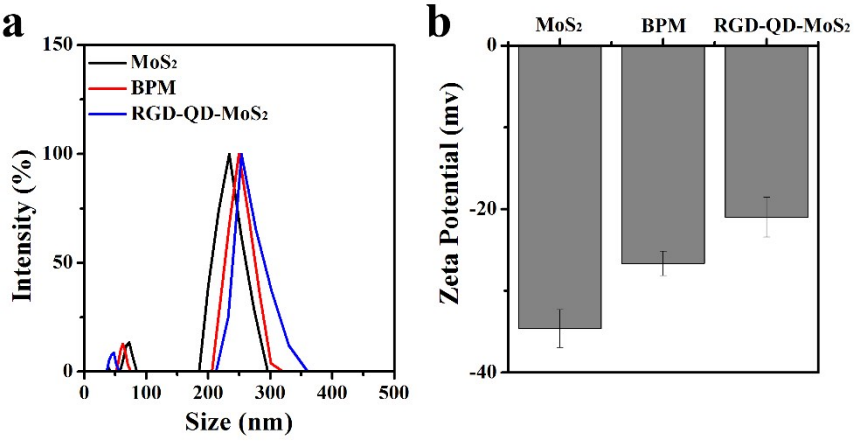

Fig. S4. (a) Hydrodynamic sizes determined by dynamic light scattering (DLS) and (b) Zeta potentials of MoS_2 NSs, BPM NSs, and RGD-QD-MoS_2 NSs.

S5. The Loading Efficiency of QDs on BPM NSs

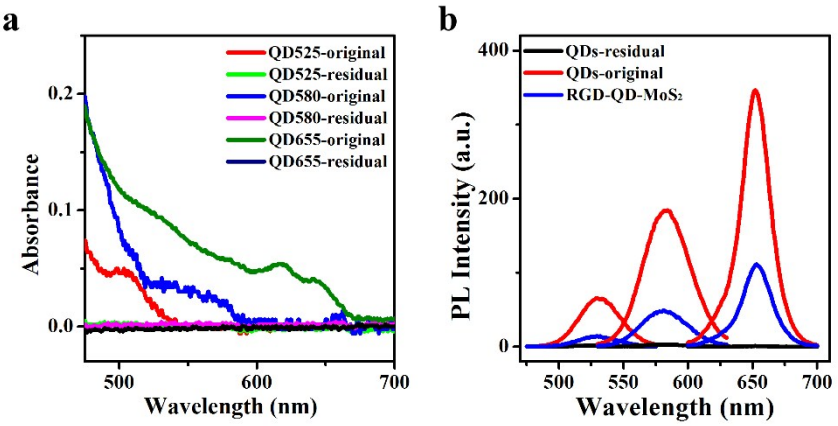

Fig. S5. (a) UV-Vis-NIR absorption spectra of different QDs in aqueous solutions before conjugation with BPM NSs, and the residual QDs in supernatant after the coupling reaction and centrifugation; (b) PL spectra of QDs, the corresponding residual QDs after the coupling reaction in supernatant, and RGD-QD-MoS_2 NSs.

S6. The Photoluminescence Quantum Yield (PLQY) of QDs and RGD-QD-MoS_2 NSs

Table S1. The PLQY of different QDs and RGD-QD-MoS_2 NSs.

Material	QD525	QD580	QD655
PLQY	19.9%	33.4%	65.9%
Material	RGD-QD525-MoS_2	RGD-QD580-MoS_2	RGD-QD655-MoS_2
PLQY	8.09%	13.5%	40.9%

S7. Cytotoxicity of MoS_2 NSs, BPM NSs, and QDs

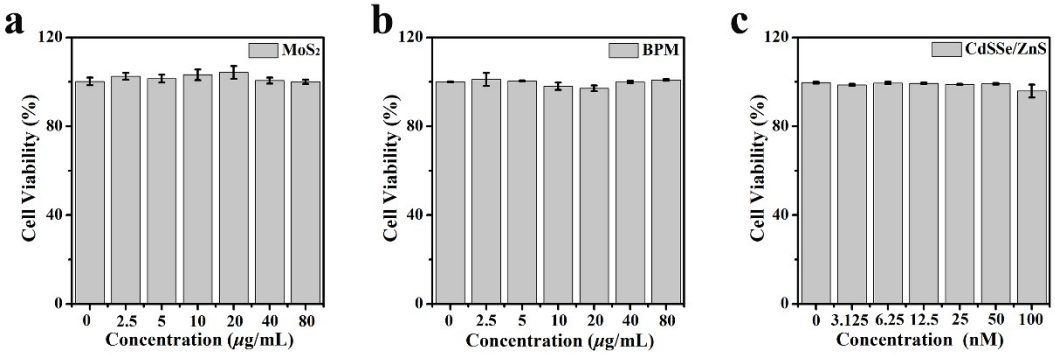

Fig. S6. Cell viabilities of HeLa cells after incubation with various concentrations of (a) MoS_2 NSs, (b) BPM NSs, and (c) CdSSe/ZnS QDs for 48 h. The cell viability was determined by the LDH-Cytotoxicity Colorimetric Assay Kit.

S8. *In Vitro* Fluorescent Imaging

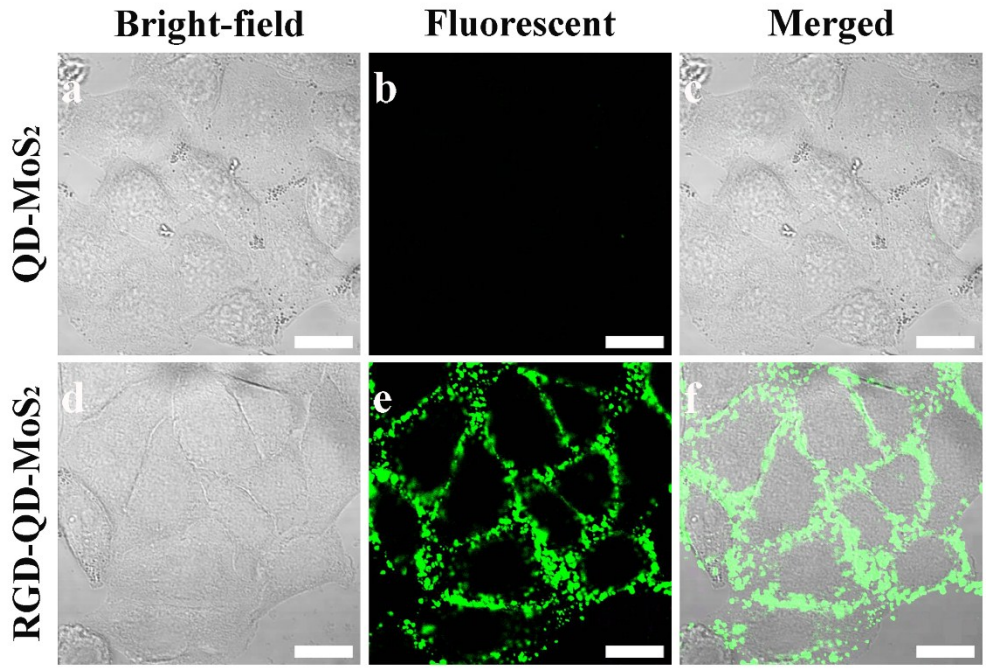

Fig. S7. Confocal fluorescence microscopy images of HeLa cells incubated with (a-c) QD-MoS_2 NSs without RGD, and (d-f) RGD-QD-MoS_2 NSs for 12 h. Both the nanosheets suspended in DMEM medium (no FBS) contain 40 μg/mL of MoS_2. All the cells were first fixed by formaldehyde and then blocked by BlockAid^{TM} Blocking Solution. The scale bar represents 20 μm.

S9. Flow Cytometry Analysis

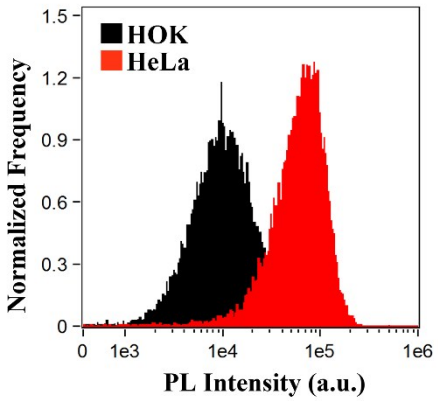

Fig. S8. The normalized frequency of HOK and HeLa cells with different PL intensity after incubation with RGD-QD-MoS_2 NSs.

S10. *In Vitro* Photothermal Therapy

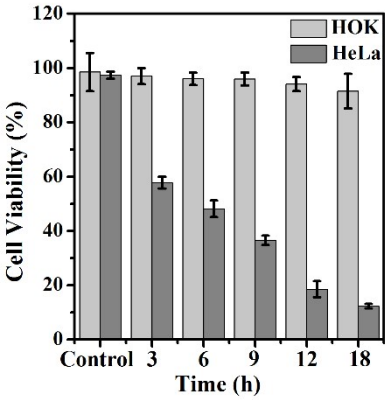

Fig. S9. Cell viability at different times after NIR laser irradiation. The cells were incubated with RGD-QD-MoS_2 NSs containing 40 μg/mL of MoS_2 for 12 h, and then irradiated by a 785 nm laser at 0.4 W/cm^2 for 5 min. Cells irradiated by NIR laser without RGD-QD-MoS_2 NSs incubation were used as control. Cell viability was detected with a LDH-Cytotoxicity Colorimetric Assay Kit.

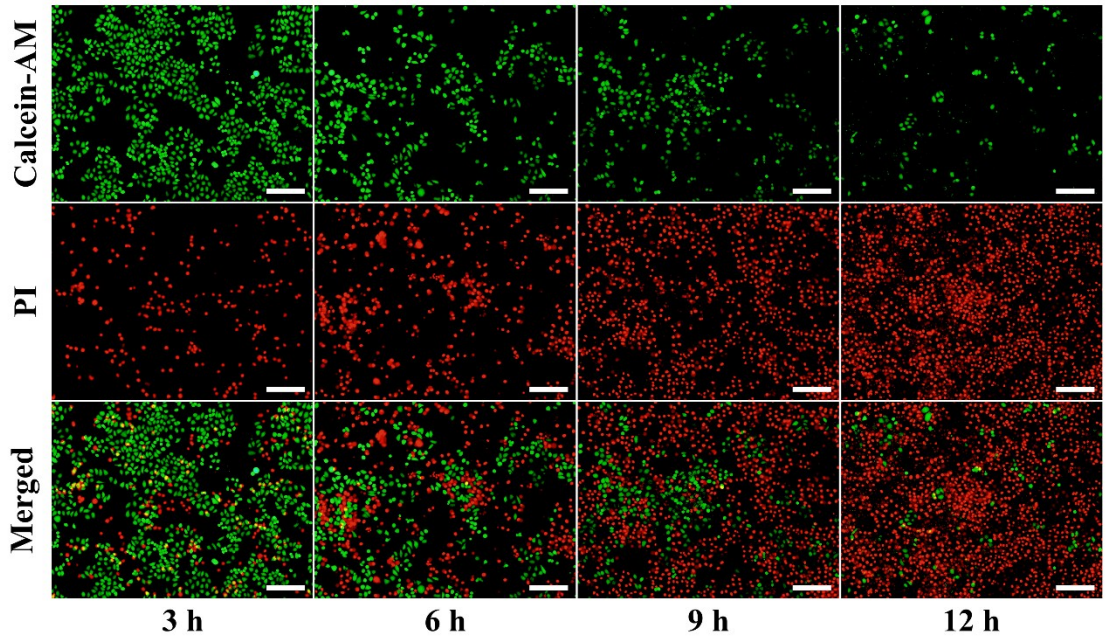

Fig. S10. Fluorescence microscopy images of HeLa cells co-stained with calcein-AM and PI at different times after 785 nm laser irradiation at the power density of 0.4 W/cm^2 for 5 min. Before the NIR laser irradiation, HeLa cells were incubated with RGD-QD-MoS_2 NSs (containing 40 μg/mL of MoS_2) for 12 h. Viable cells were stained green with calcein, and dead cells were stained red with PI.

S11. Serum Stability of RGD-QD-MoS_2 NSs

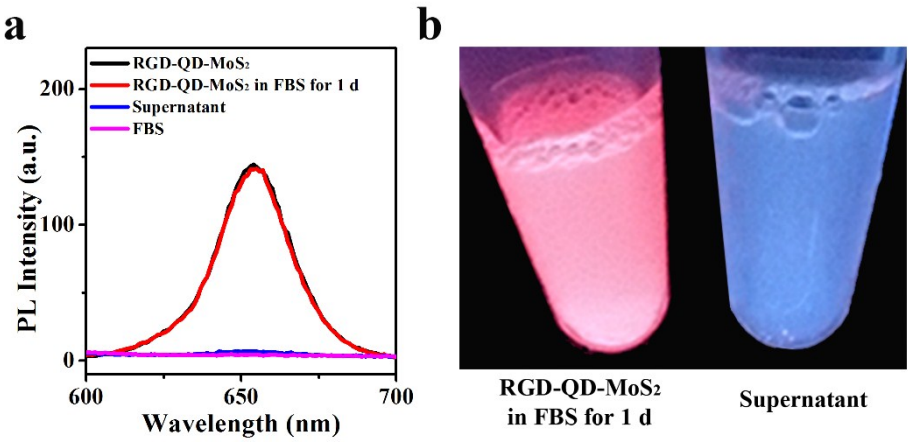

Fig. S11. (a) The photoluminescence spectra of RGD-QD-MoS_2 NSs suspended in FBS aqueous solution before and after centrifugation; (b) Photo of RGD-QD-MoS_2 NSs suspended in FBS aqueous solution and the supernatant of RGD-QD-MoS_2 NSs suspended in FBS after centrifugation under UV irradiation (365 nm).

S12. Biodistribution of RGD-QD-MoS_2 NSs and QD-MoS_2 NSs

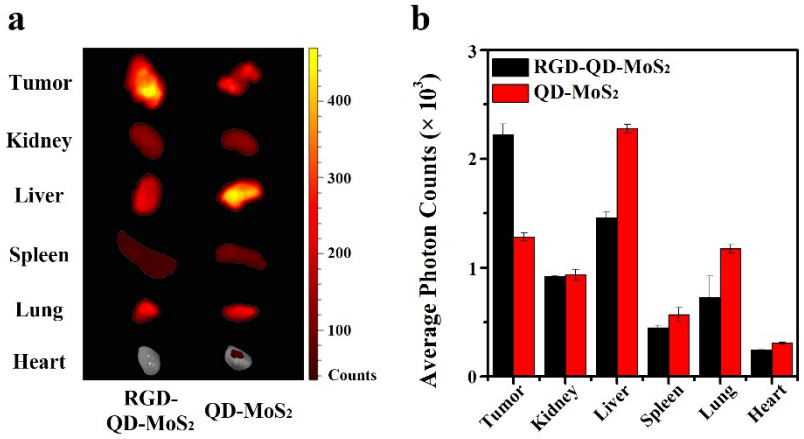

Fig. S12. (a) Fluorescence images and (b) Average photon counts of major organs and tumors of HeLa tumor-bearing Balb/c nude mice with i.v. injection of RGD-QD-MoS_2 NSs and QD-MoS_2 NSs.

S13. Tumor Temperature Evolution Curves

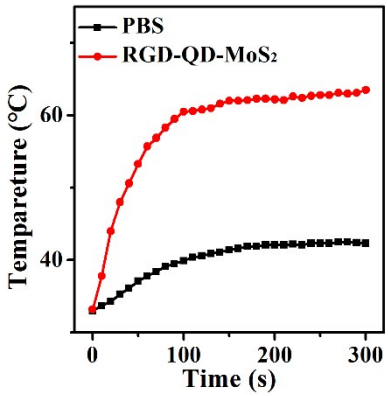

Fig. S13. Tumor temperature evolution curves of mice with i.v. injection of RGD-QD-MoS_2 NSs (containing 1.5 mg/mL of MoS_2, 200 μL) or PBS under 785 nm laser at 0.8 W/cm^2.

S14. *In Vivo* Toxicity of RGD-QD-MoS_2 NSs

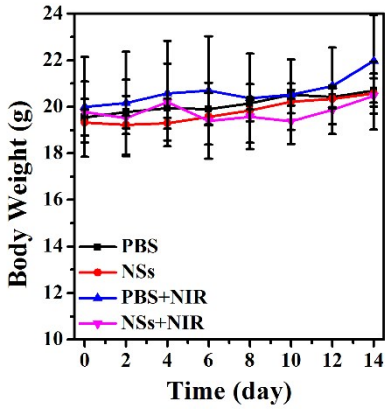

Fig. S14. Body weight of mice from all four groups: i.v. injection of PBS; i.v. injection of RGD-QD-MoS_2 NSs (dose = 15 mg/kg); i.v. injection of PBS plus NIR laser irradiation; and i.v. injection of RGD-QD-MoS_2 NSs plus NIR laser irradiation (dose = 15 mg/kg, 0.8 W/cm^2, 5 min).

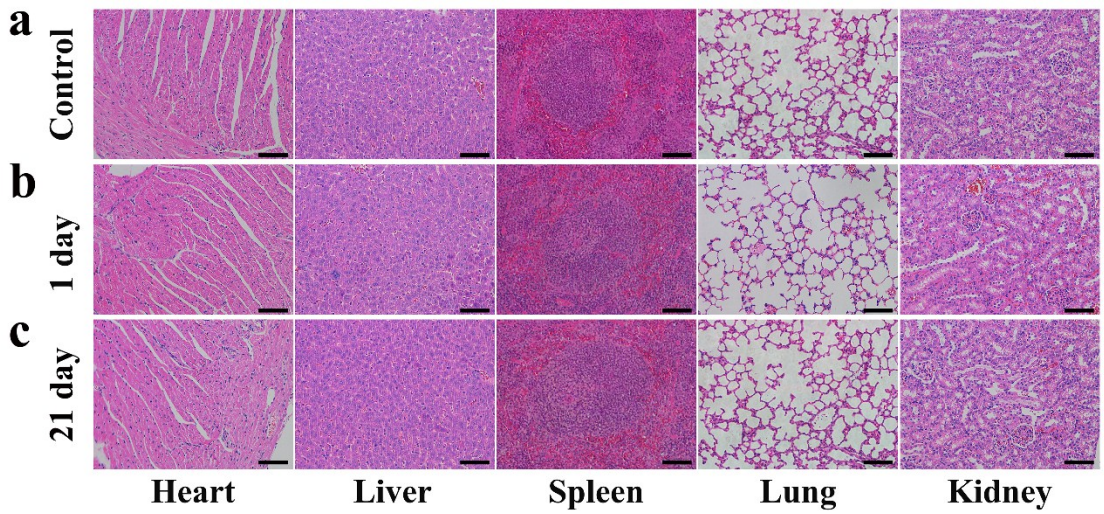

Fig. S15. H&E stained images of major organs of the Balb/c nude mice with different treatments. (a) Untreated healthy Balb/c nude mice were used as control; (b) Balb/c nude mice with i.v. injection of RGD-QD-MoS_2 NSs (dose = 15 mg/kg) for 1 day; (c) 21 day after the PTT treatment. Balb/c nude mice were i.v. injected of RGD-QD-MoS_2 NSs (dose = 15 mg/kg), and 785 nm laser irradiation was carried out at 24 h post-injection with a power density of 0.8 W/cm^2. The scale bar represents 100 μm.

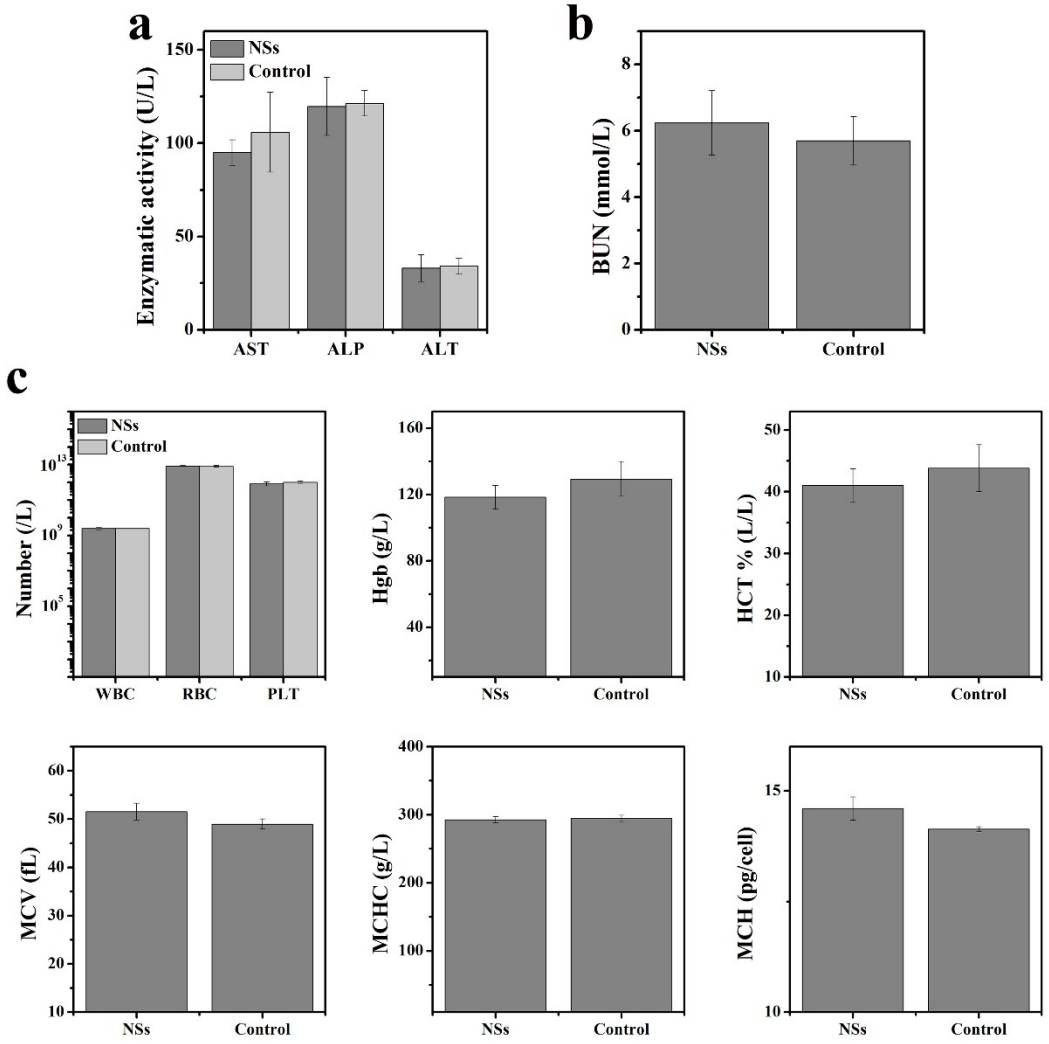

Fig. S16. Serum biochemistry assay and complete blood panel test. Healthy Balb/c mice with i.v. injection of RGD-QD-MoS_2 NSs (15 mg/kg) were sacrificed at 21 days post-injection for blood collection. Untreated healthy mice were used as control. (a) Liver function markers: alaninie aminotransferase (ALT), alkaline phosphatase (ALP), and aspartate aminotransferase (AST); (b) Blood urea nitrogen (BUN) levels; (c) Blood levels of white blood cells (WBC), red blood cells (RBC), platelets (PLT), hemoglobin (Hgb), hematocrit (HCT), mean corpuscular volume (MCV), mean corpuscular hemoglobin concentration (MCHC), and mean corpuscular hemoglobin (MCH) of RGD-QD-MoS_2 NSs treated mice (NSs) and untreated mice (Control). Statistic was based on triplicate samples.