Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supporting information

for

Quantum Dots Tethered Membrane type 3 matrix metalloproteinase-targeting Peptide for Tumor Optical Imaging

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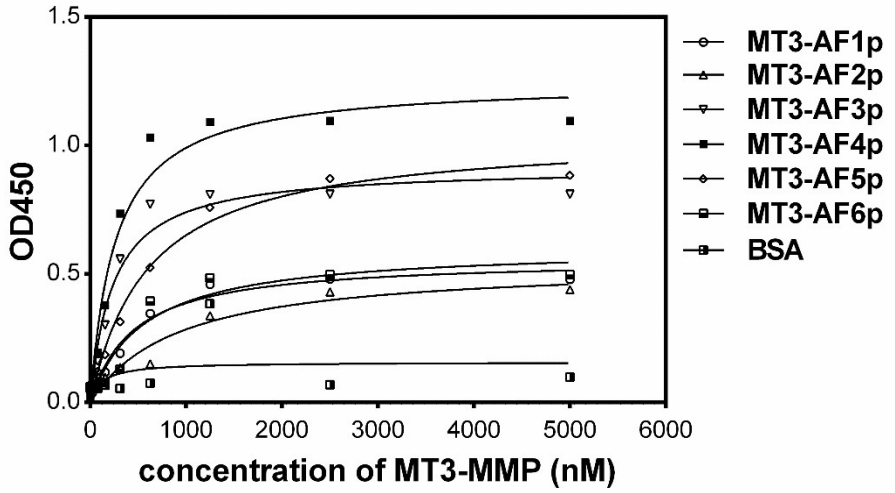

Figure S1. The MT3-MMP binding affinity was measured by ELISA and analyzed by GraphPad Prism 5.0 software (n=3).

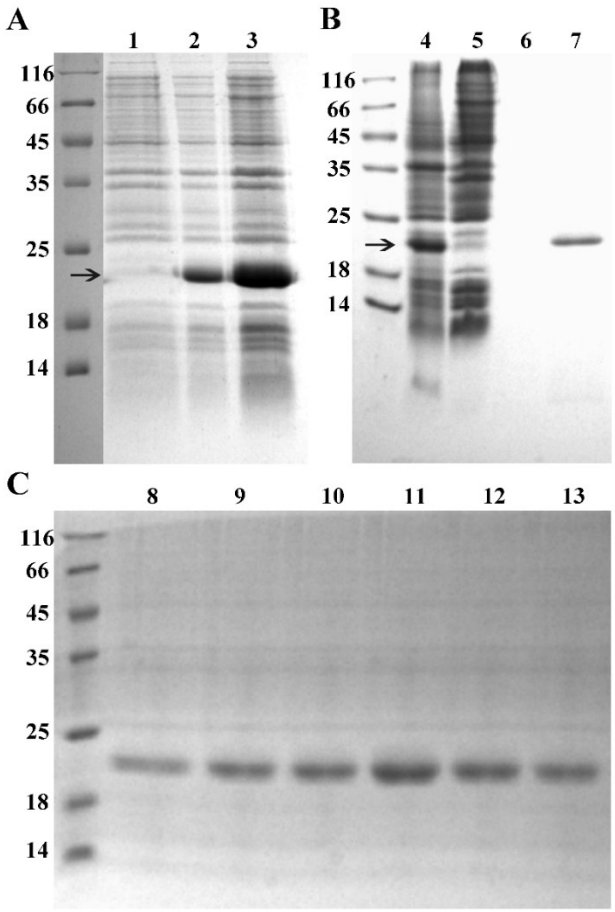

Figure S2. Validation of the expression, purification and renaturation of MT3-MMP by SDS-PAGE. Fig. S2A shows the inclusion bodies from the induced culture with IPTG for 0 h (1), 3 h (2) and 4 h (3). Fig.S2B shows the purification of inclusion body by His-tag affinity chromatography before (4) and after (5). The inclusion bodies were purified with 20 mM imidazole (6) and 100 mM (7) imidazole. Fig.S2C shows the MT3-MMP with catalytic activity after renaturation (8-13). Molecular weight (kDa) marker was labeled in numerals. Arrows indicate observed protein bands of interest.

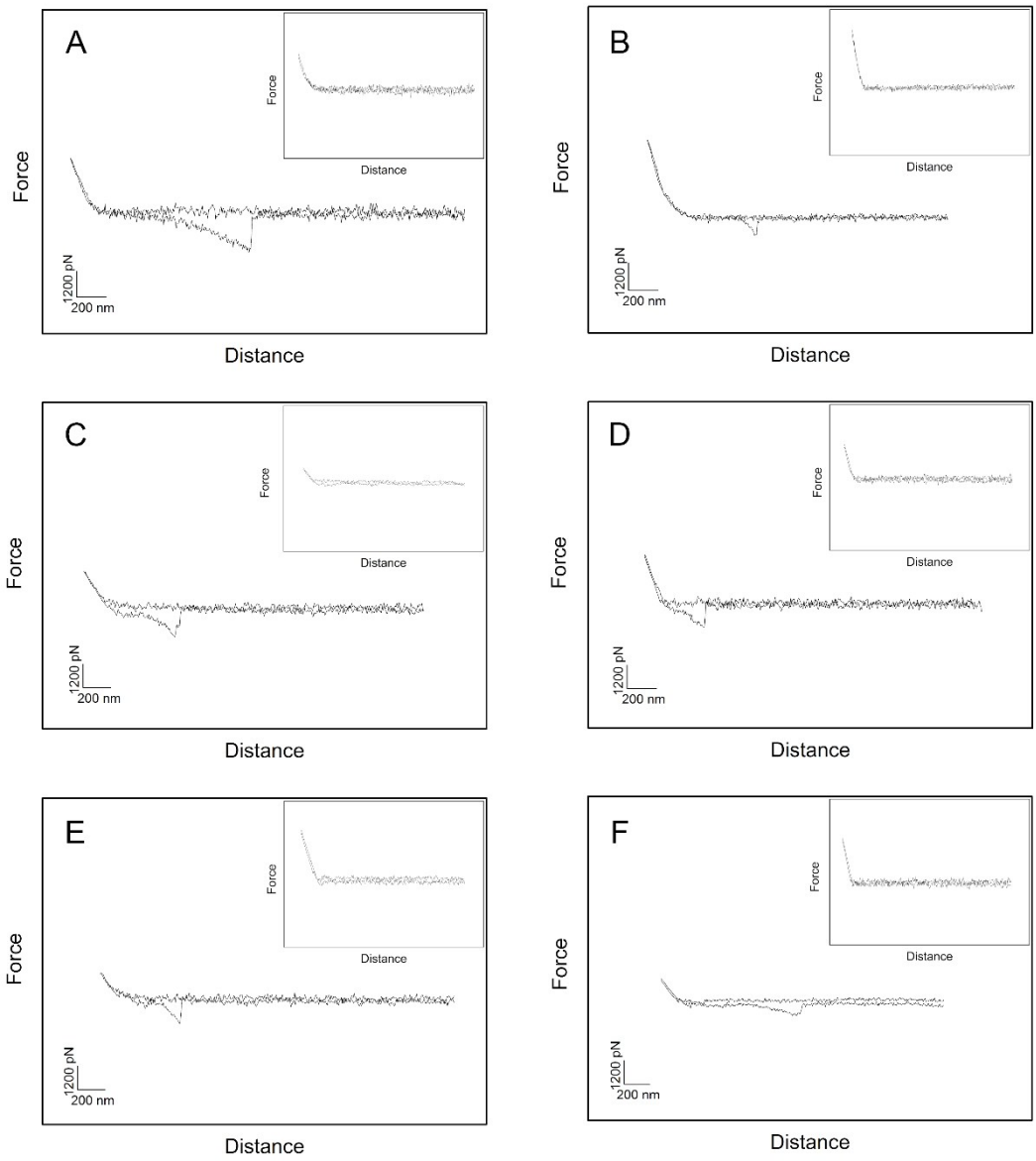

Figure S3. Force measurement of MT3-MMP and peptides. Force curves indicating the interactions between MT3-AF1p and MT3-MMP (A), MT3-AF2p and MT3-MMP (B), MT3-AF3p and MT3-MMP (C), MT3-AF4p and MT3-MMP (D), MT3-AF5p and MT3-MMP (E), as well as MT3-AF6p and MT3-MMP (F).

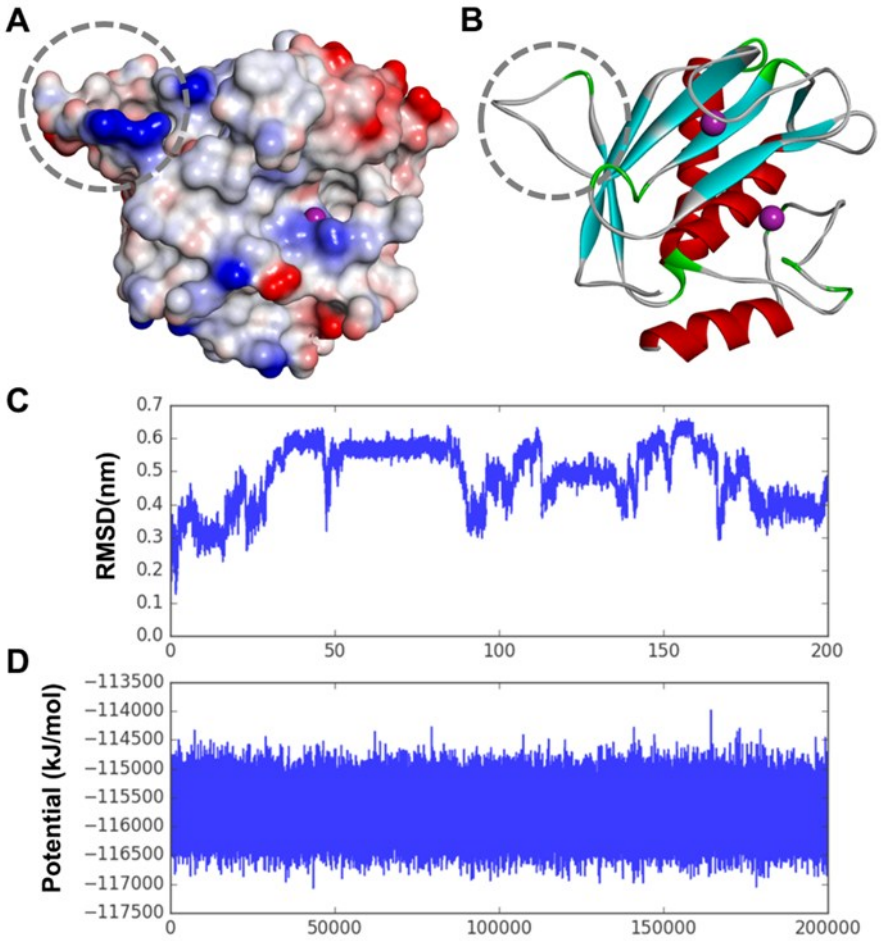

Figure S4. Preparation of protein. (A) Conformation of MT3-MMP; (B) Secondary structure of MT3-MMP. The MT-Loop region is shown by the dotted grey circle. (C) and (D) shows the results of MT3-AF4p during 0.1 μs MD simulation. (C) RMSD plot. (D) Potential energy.

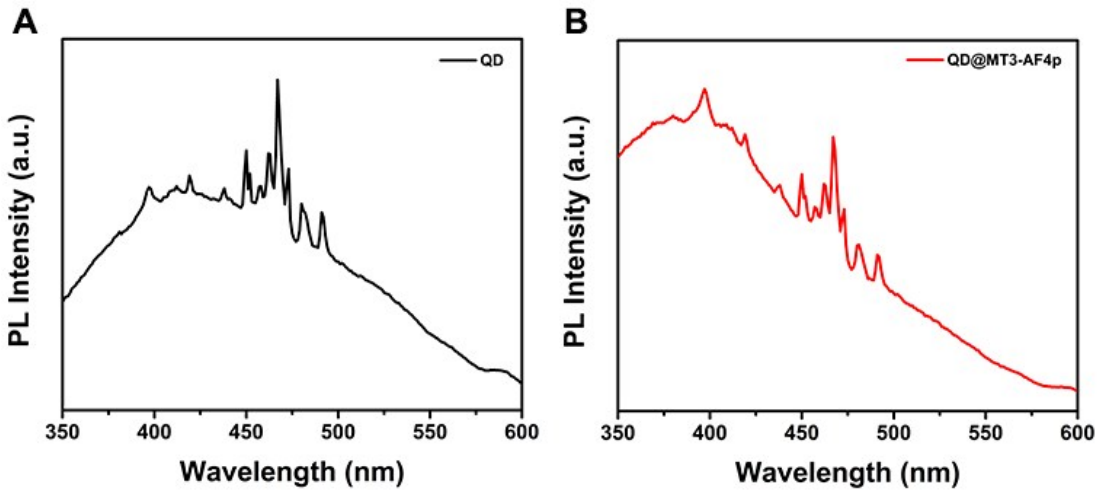

Figure S5. The excitation spectra of QD and QD@MT3-AF4p.

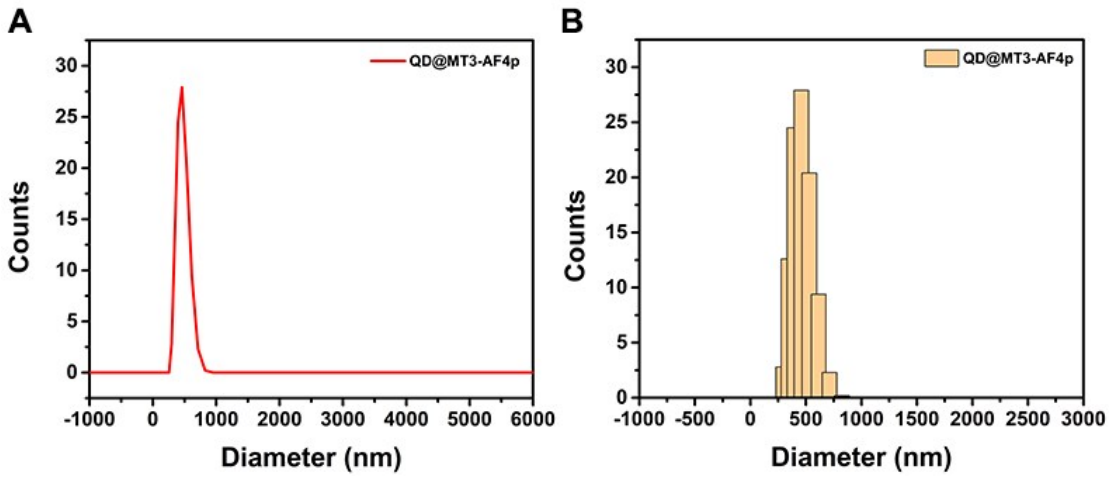

Figure S6. DLS characterization of QD@MT3-AF4p nanoparticles. The size distribution were shown in statistics graph (A, B).

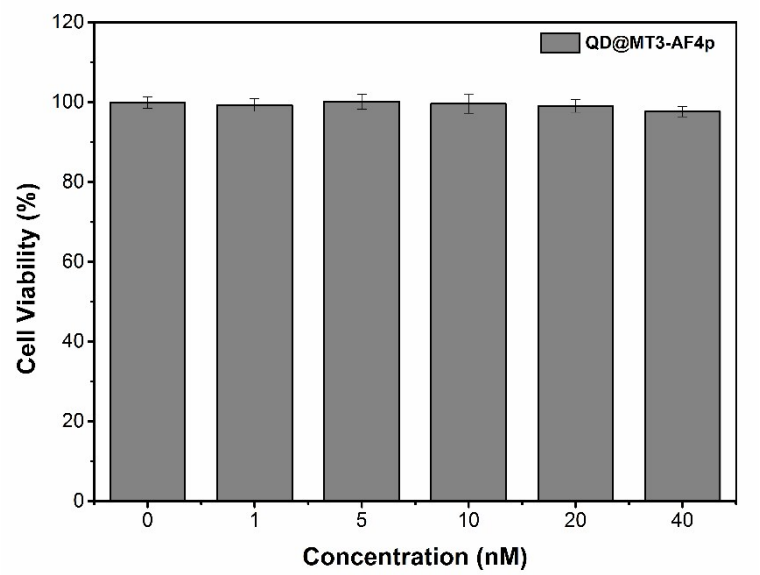

Figure S7. The normal cell line (HEK293) is treated with QD@MT3-AF4p, and the MTT assay is used for the assessment of cell viability (n=2).

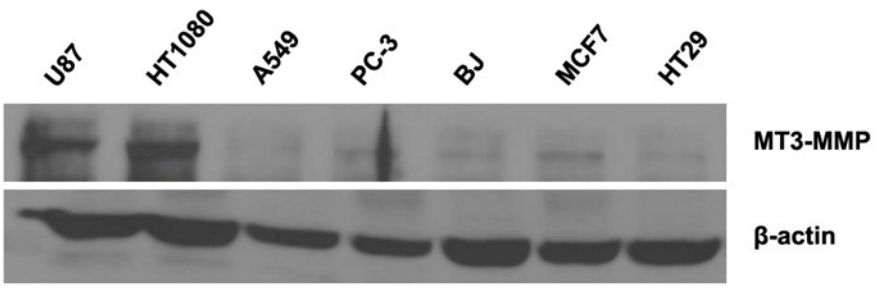

Figure S8. Analysis of the expression level of MT3-MMP in U87, HT1080, A549, PC-3, BJ, MCF7 and HT29 tumor cell lines. 40 µg of protein samples were loaded and performed to Western blot (n=2).

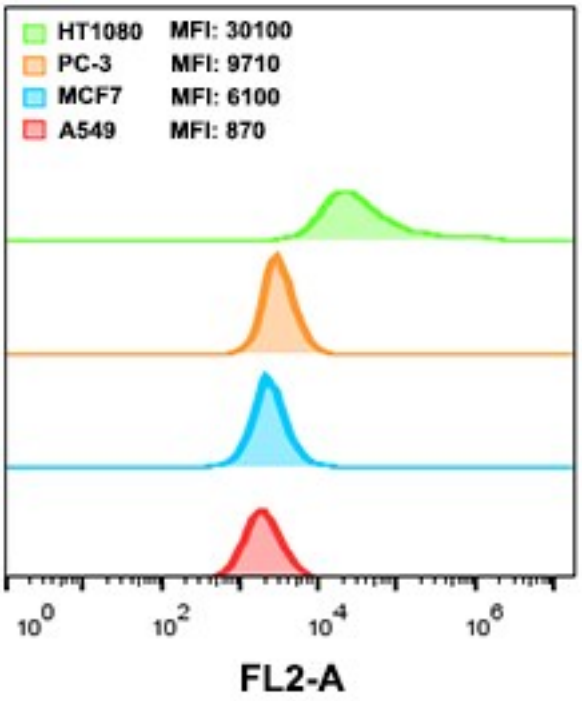

Figure S9. Flow cytometry analysis of HT1080, PC-3, MCF7 and A549. Tumor cell lines were incubated with QD@MT3-AF4p for 4 hours at a concentration of 20 nM. MFI: the mean fluorescence emission intensity.

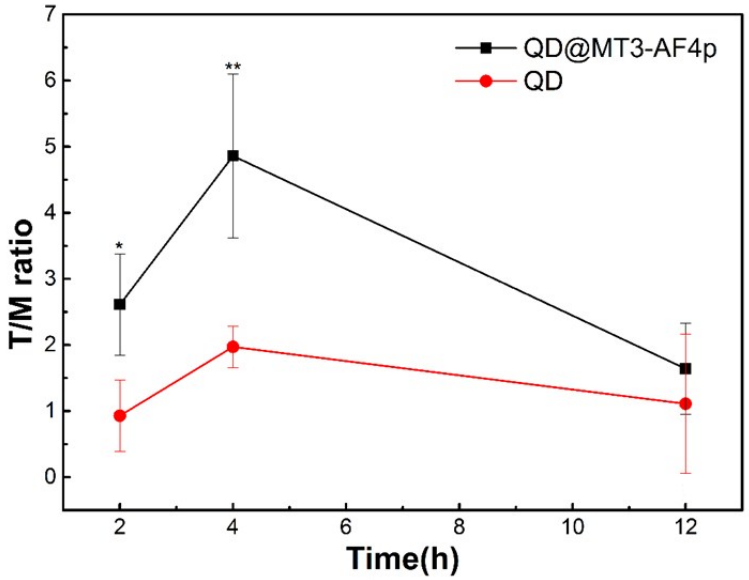

Figure S10. Tumor/muscle ratio revealed that the accumulating effects of QD@MT3-AF4p on HT1080 tumor bearing mice (n=3). * represents p-value ≤ 0.05, ** represents p-value ≤ 0.01.

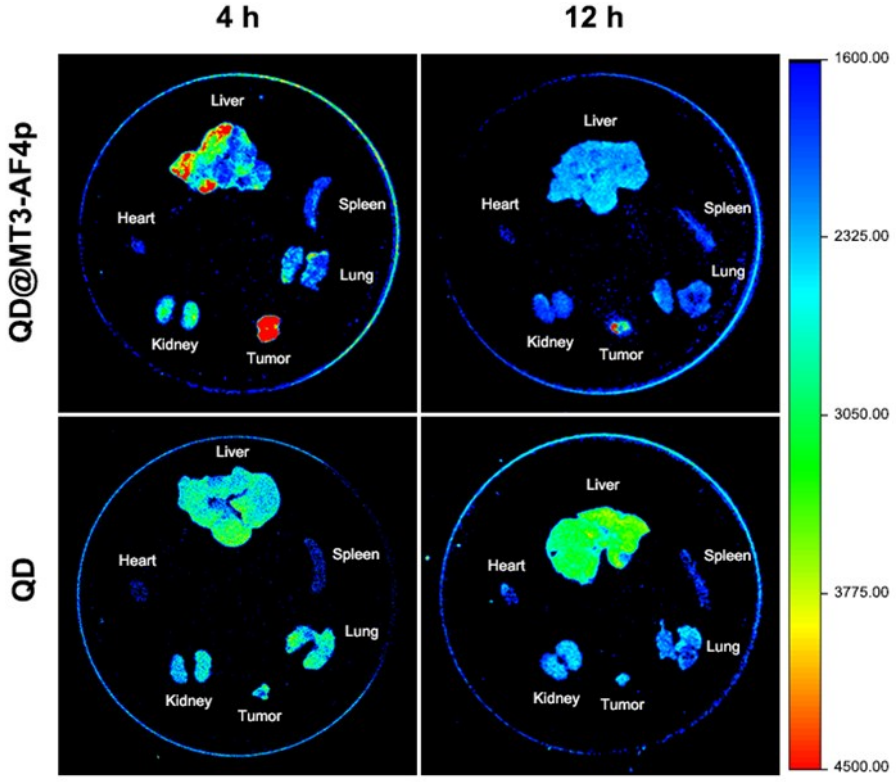

Figure S11. *Ex vivo* images of dissected organs of mice bearing HT1080 tumor showed a significant accumulating effect in tumor. The mice were sacrificed after intravenous injection of QD@ MT3-AF4p or QDs for 4 h and 12 h (n=3).

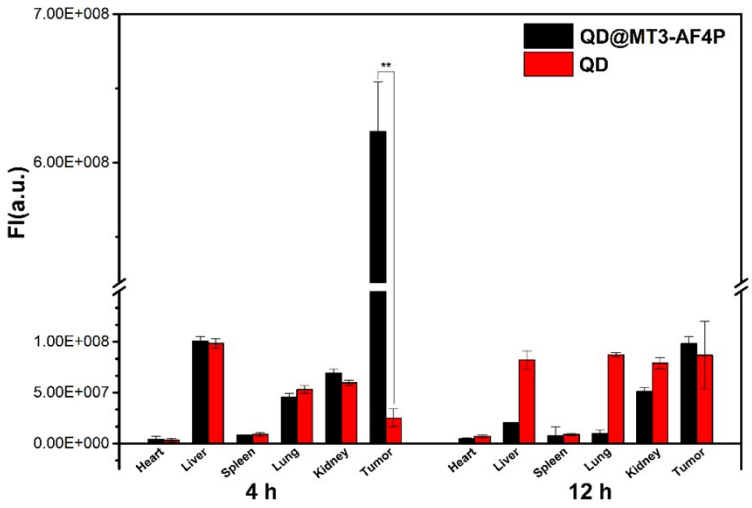

Figure S12. Analysis of the fluorescent intensity of QD@MT3-AF4p or QD in organs and tumor. Mice were sacrificed after injection of nanomaterials for 4 h and 12 h (n=3). ** represents p-value ≤ 0.01.

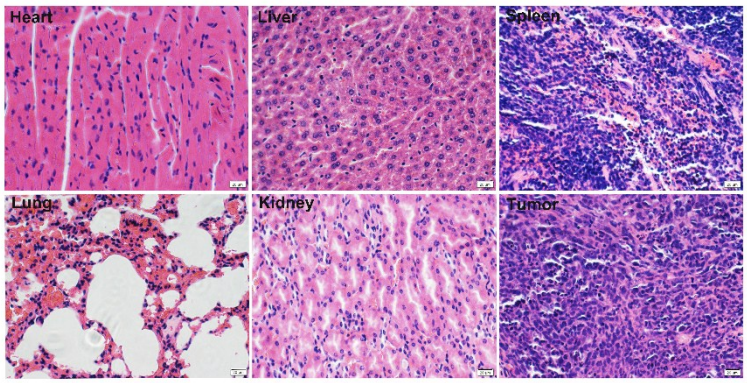

Figure S13. HE staining of main organs with 4 h post-injection of QD@MT3-AF4p. The scale bar is 20 nm.

Table S1. Zeta potentials showing MT3-AF4p is conjugated on nanomaterials successfully.

	zeta potential (mV)	
$QD@SiO_2$	14.0	14.1±0.1
	14.2	
	14.1	
$QD@SiO_2$-NH_2	14.9	14.8±0.1
	14.9	
	14.7	
$QD@SiO_2$-PAA	-30.7	-30.3±0.3
	-30.1	
	-30.2	
QD@MT3-AF4p	-25.6	-25.8±0.2
	-25.8	
	-26.0	