Supporting Information

A Multifunctional PB@mSiO$_2$-PEG/DOX Nanoplatform for Combined Photothermal-Chemotherapy of Tumor

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Materials and Methods

In vitro MR and PA imaging

The longitudinal relaxation time T1 (s) of PB@mSiO$_2$-PEG at different concentrations of 0, 62.5, 125, 250, 500, 1000, 2000 and 10000 μg mL^{-1} was measured in 1% agarose by a 3.0 Tesla scanner (TIM Trio, Siemens Medical Solutions, Erlangen, Germany) using the inversion-recovery pulse sequence method. T1 map imaging parameters: repetition time (TR) = 15 ms, echo time (TE) = 2 ms, field of view (FOV) = 160 × 160 mm^2, matrix size = 256 × 256, and slice thickness = 3 mm. T1 map and T1 color map images were processed. Then, the r1 relaxivities of PB (r1, μg ml^{-1} ms^{-1}) was calculated using T1 measurements of different concentrations of the NPs in 1% agarose using the following equation[1]: r1= (1/T1 – 1/T1(0))/[PB]

Where [PB] represents the concentration of PB@mSiO$_2$-PEG (μg mL^{-1}), 1/T1(0)(s^{-1}) is the relaxation rate without paramagnetic species, and 1/T1(ms^{-1}) is the relaxation rate with paramagnetic species.

To investigate the PA property of PB@mSiO$_2$-PEG nanocubes, PB@mSiO$_2$-PEG in PBS at the concentrations from 660 to 2000 μg mL^{-1} was detected by Innovative In vivo Photoacoustic 3-D Tomographic Imaging System (Endra Nexus 128, USA). And the excitation wavelength of the laser for PAI was chosen at 713 nm.

Results

PB compound have the ability to serve as a great T1-weighted MR contrast agent. We determined the longitudinal and transverse relativities (r1 values) of the PB@mSiO$_2$-PEG nanocubes at serial dilutions under a MR scanner (**Fig. S7**). The

concentration-normalized relaxivity values were measured to be r1 = 2.063 μg mL^{-1} ms^{-1} within concentration of 1000 μg mL^{-1}, while beyond the concentration, no distinctive linear relationship between concentration of PB@$mSiO_2$-PEG nanocubes and the relaxation rate (**Fig. S7**) were observed. The results were in excellent agreement with those reported in literature.[2-3] With a high r1 relaxivity, PB@$mSiO_2$-PEG nanocubes may serve as a great T1-weighted MR contrast agent. The PA intensities of all the samples of PB@$mSiO_2$-PEG nanocubes in aqueous solution increased linearly with increasing nanoparticles concentrations **(Fig. S7**), suggesting they are suitable for further *in vivo* PA imaging. With a good accumulation of the PB@$mSiO_2$-PEG/DOX nanoplatforms in cancer cells, PB@$mSiO_2$-PEG nanocubes have potential as an excellent MR and PA imaging probes to track its accumulation in tumor, so as to diagnose the tumor before treatments.

Figures and Figure legends

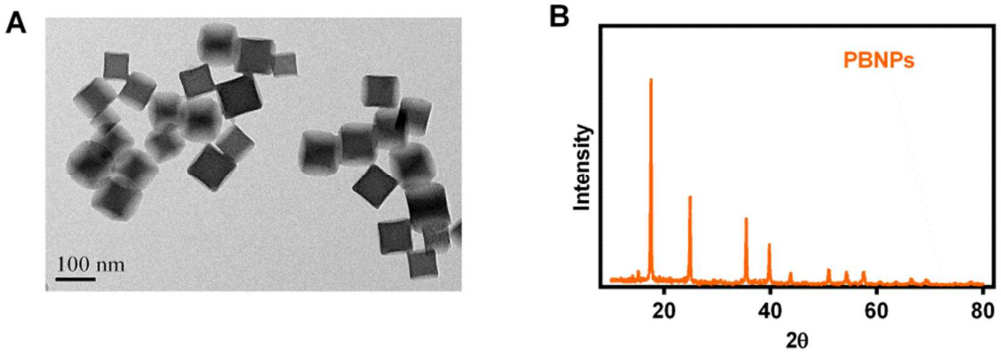

Fig. S1 characterization of PB nanocubes. (A) TEM image. (B) Powder X-ray diffraction pattern for PB nanocubes.

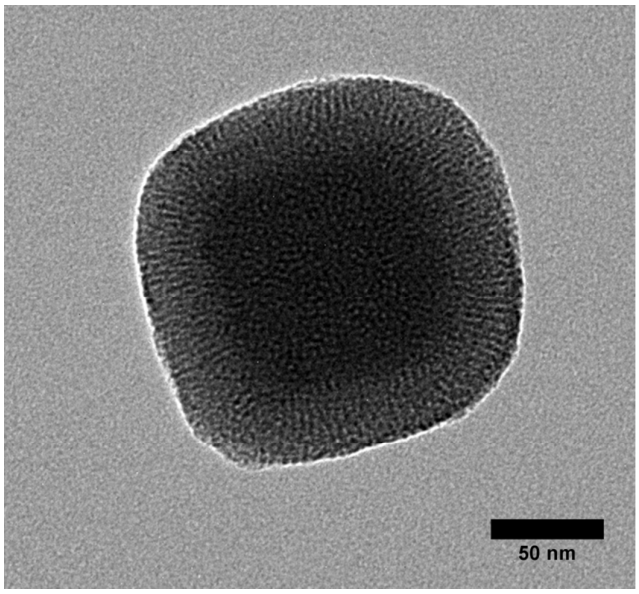

Fig. S2 HRTEM image of the PB@$mSiO_2$ nanocube.

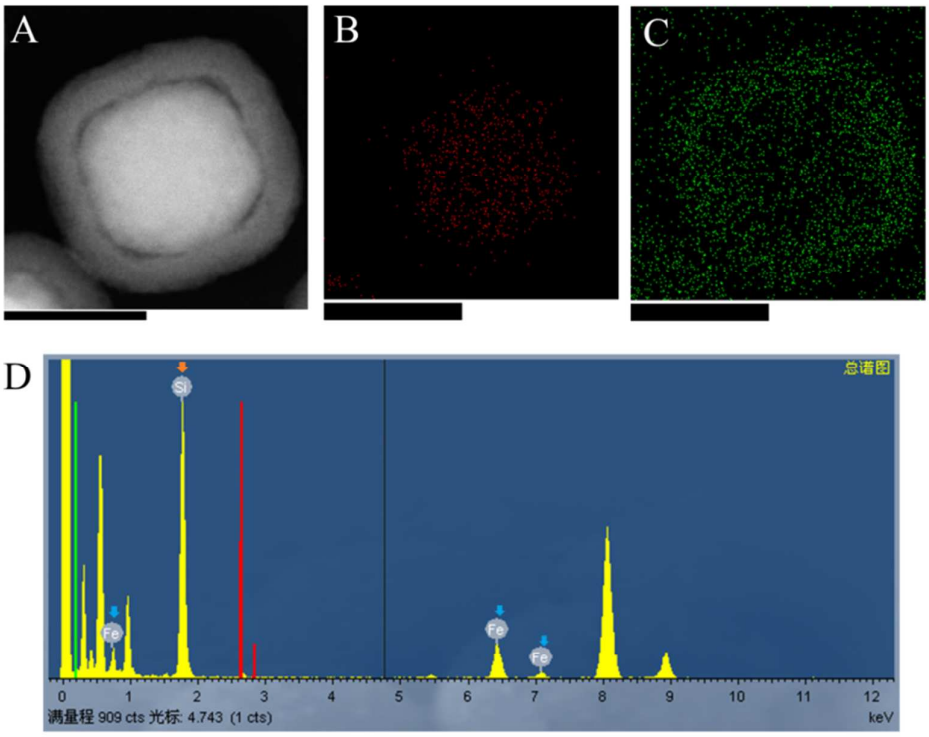

Fig. S3 (A)TEM image; (B and C) elemental mapping of Fe (red) and Si (green) atoms in the PB@$mSiO_2$; (D) EDX spectrum of Fe (orange arrow) and Si (blue arrows) atoms. Scale bar: 90 nm. Spectroscopy of PB@$mSiO_2$ analysis shows the ratio of

Fe to Si elements is 11.43/88.57

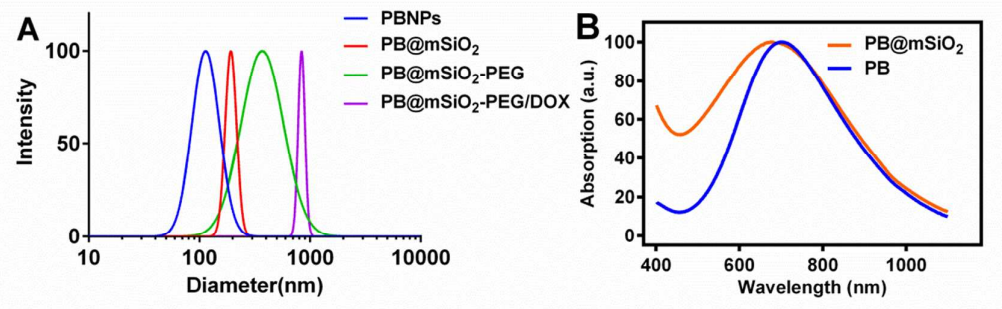

Fig. S4 (A) DLS of PB, PB@$mSiO_2$, PB@$mSiO_2$-PEG, PB@$mSiO_2$-PEG/DOX nanocubes; (B) UV-vis-NIR absorbance spectra of PB and PB@$mSiO_2$ nanocubes.

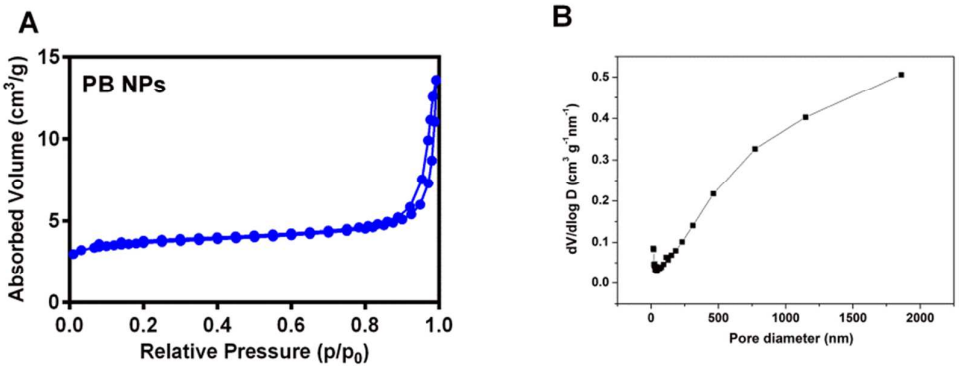

Fig. S5 (A) N_2 gas adsorption-desorption isotherms and (B) the corresponding pore size distribution for PB nanocubes.

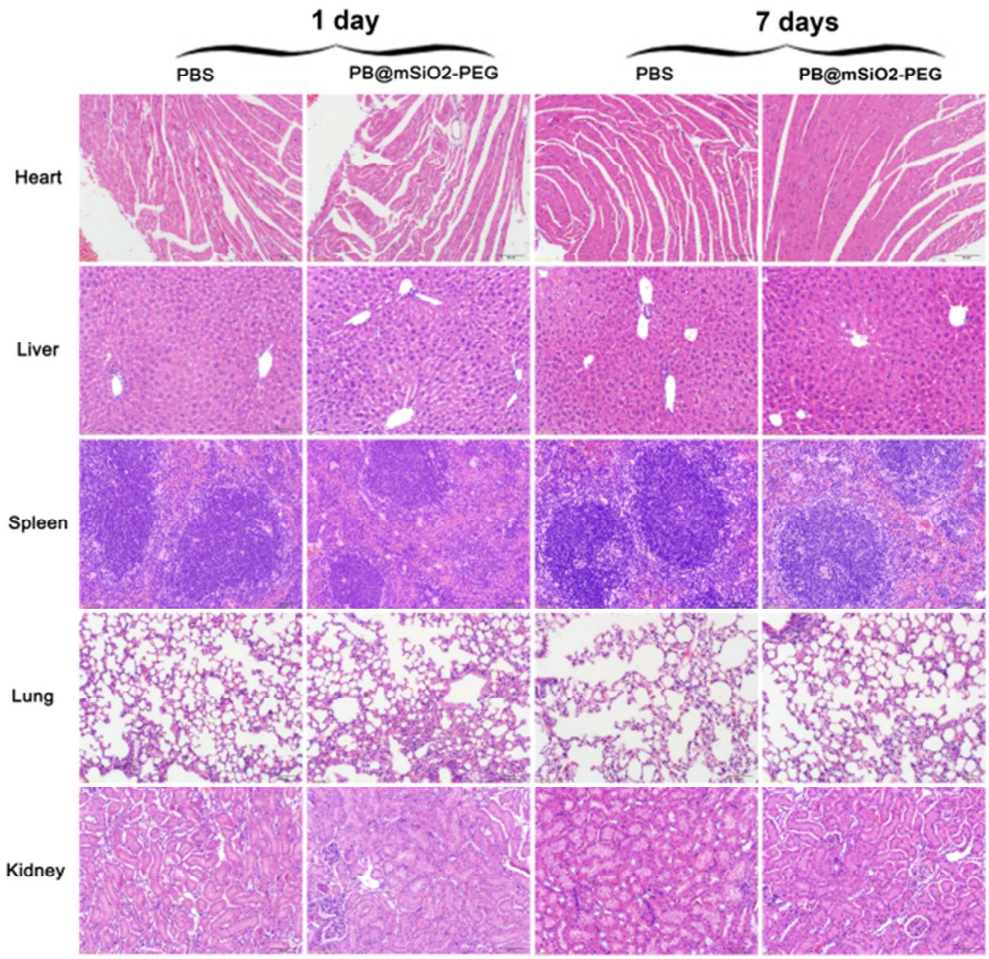

Fig. S6 Representative hematoxylin and eosin stained histological images from the major organs (heart, liver, spleen, lung, and kidneys) of mice. Scale bar: 50 μm

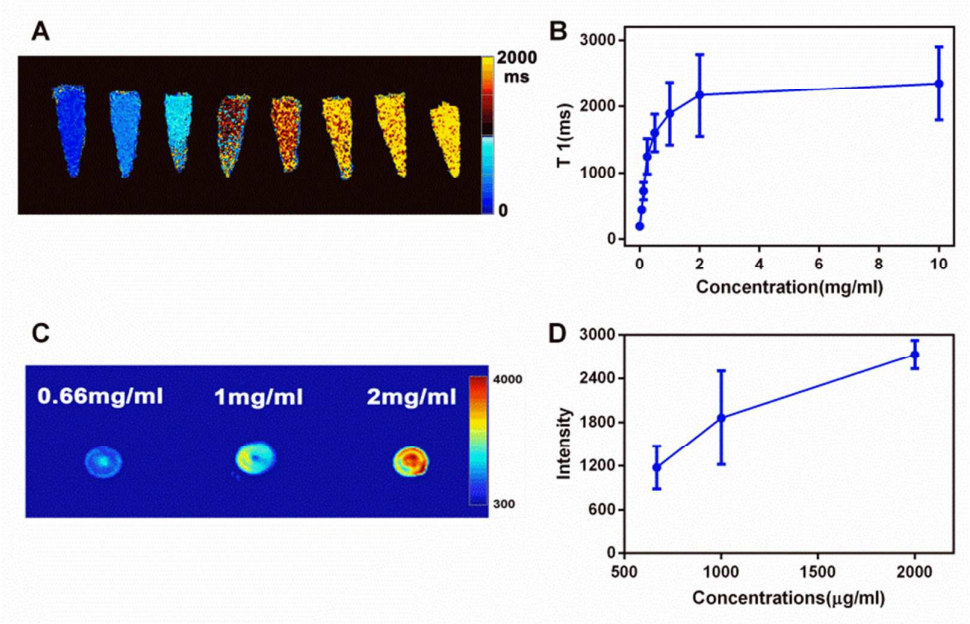

Fig. S7 *In vitro* MR and PA imaging. (A) and (B) T1 maps of different concentrations of PB@mSiO2-PEG nanocubes and their relative signals. (C) and (D) PA imaging and density of aqueous dispersions contained different concentrations of PB@mSiO$_2$-PEG nanocubes.

Reference

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