## **Supporting Information**

## Albumin-Constrained Large-Scale Synthesis of Renal Clearable Ferrous Sulfide Quantum Dots for T<sub>1</sub>-Weighted MR Imaging and Phototheranostics of Tumors

Weitao Yang <sup>a, 1</sup>, Chenyang Xiang <sup>a, 1</sup>, Yan Xu <sup>a</sup>, Shizhen Chen <sup>b</sup>, Weiwei Zeng <sup>a</sup>, Kai Liu <sup>a</sup>, Xiao Jin <sup>a</sup>,

Xin Zhou <sup>b,\*</sup>, and Bingbo Zhang <sup>a,\*</sup>

a. Department of Medical Ultrasound, Shanghai Tenth People's Hospital, Tongji University Cancer Center, Tongji University School of Medicine, Shanghai 200072, China.

b. Key Laboratory of Magnetic Resonance in Biological Systems, State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, National Center for Magnetic Resonance in Wuhan,
Wuhan Institute of Physics and Mathematics, Innovation Academy of Precision Measurement
Science and Technology, Chinese Academy of Sciences, Wuhan, 430071, China.

<sup>1</sup> These authors contributed equally to this study.

Corresponding Authors:

\* Bingbo Zhang, Email: <u>bingbozhang@tongji.edu.cn</u>

\* Xin Zhou, Email: <u>xinzhou@wipm.ac.cn</u>



Fig. S1. Digital photograph of one-pot synthesized FeS@BSA QDs (10 L).



Fig. S2. Time-dependent absorbance spectra of FeS@BSA QDs synthesized at Fe/S ratios of (A) 2:1, (B) 1:1, (C) 1:4, (D) 1:8, and (E) 1:16. (F) The corresponding absorbance of different Fe/S ratios at 650 nm.



Fig. S3. Hydrodynamic sizes of FeS@BSA QDs synthesized at different temperature (37 °C, 65 °C, 90 °C).



Fig. S4. Hydrodynamic sizes of FeS@BSA QDs synthesized at different amounts of BSA (0 mg, 50 mg, 100 mg,

and 200 mg).



Fig. S5. XRD pattern of FeS@BSA QDs.



Fig. S6. Magnetization of FeS@BSA QDs and FeS aggregation.



Fig. S7. Time-dependent (A) UV-vis absorption spectrum and (B) longitudinal relaxation time of FeS@BSA QDs.



Fig. S8. Photothermal conversion efficiency of FeS@BSA QDs. (A) The temperature change of FeS@BSA QDs solution under the irradiation of laser for 5 min and the laser was removed immediately. (B) The time versus the negative natural logarithm of the temperature from the cooling period (after 5 min) in (A) and  $\tau_s$  was calculated to be 417.55 s by applying linear relationship.

The photothermal conversion efficiency  $(\eta)$  was calculated according to following equations:

 $\theta = (T - T_{surr}) \div (T_{max} - T_{surr}) \xrightarrow{f} \cdots \cdots$ Equation (1)

 $t = \tau_s \times (-\ln\theta)$ 

 $\tau_s = 417.55 \text{ sc}$ 

 $hS = (\sum m_i C_{p,i}) \div \tau_s$  .....Equation (3)

 $= [m(H_2O) \times c(H_2O) + m(quartz) \times c(quartz)] \div \tau_s$ 

 $=(1 \times 4.2 + 5.5 \times 0.839) \div 417.55$ 

 $= 21.11 \text{ mW/^{o}C}$ 

 $Q_{Dis} = hS \times (T(H_2O)_{max} - T_{surr})$  .....Equation (4)

 $= 21.11 \times (30.3 - 25)$ 

= 111.883 mW

= [21.11×(56.5-25)-111.883] ÷ [2000×(1-10<sup>-1.1</sup>)] ×100%

= 30.04%

*h* (mW m<sup>-2</sup> °C<sup>-1</sup>): The heat transfer coefficient;  $T_{max}$ (°C): The maximum equilibrium temperature (56.5 °C);  $T_{surr}$ (°C): The ambient temperature of the surrounding environment (25 °C);  $m(H_2O)$  and  $c(H_2O)$ : The mass (1.0 g) and heat capacity (4.2 J/g) of the solvent DI water respectively; m(quartz) and c(quartz): The mass (5.5 g) and heat capacity (0.839 J/g) of the container quartz cell respectively;  $Q_{Dis}$ (mW): The heat absorbed by the solvent DI water and the quartz cell; *I*: The laser power density (2.0 W/cm<sup>2</sup>);  $A\lambda$ : The absorbance of FeS@BSA QDs (1.1);  $\tau_s$ : The time constant for heat transfer of the FeS@BSA QDs solution which was calculated by linear relationship of time versus -ln( $\theta$ ) from Fig. S8.



Fig. S9. Fluorescence emission spectra of FeS@BSA:Sq QDs.



**Fig. S10.** The biodistribution of Fe in main organs and tumor at different time intervals (2, 6, and 24 h) postinjection of FeS@BSA QDs (n = 3, mean ± SD).



Fig. S11. The blood circulation of FeS@BSA QDs in mice after intravenous injection as determined by measuring

Fe element at different time intervals (n = 3, mean  $\pm$  SD).



Fig. S12. Histological analysis of tumor section stained with H&E from mice with different treatment groups (PBS,

Laser irradiation only, FeS@BSA injection only, and FeS@BSA injection plus laser irradiation).