

## Supplementary information

Upconversion-magnetic carbon sphere for near infrared light-triggered bioimaging and photothermal therapy

Jiaxin Wang<sup>1,2</sup>, Chenjie Yao<sup>1</sup>, Bin Shen<sup>1</sup>, Xiaohui Zhu<sup>1</sup>, Yong Li<sup>1</sup>, Liyi Shi<sup>2</sup>, Yong

Zhang<sup>1</sup>, Jinliang Liu<sup>1,2</sup>, Yanli Wang<sup>1</sup>, Lining Sun<sup>2,3</sup>

1. School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, P. R. China
2. Research Center of Nano Science and Technology, Shanghai University, Shanghai, 200444, P. R. China
3. School of Material Science and Engineering, Shanghai University, Shanghai, 200444, P. R. China

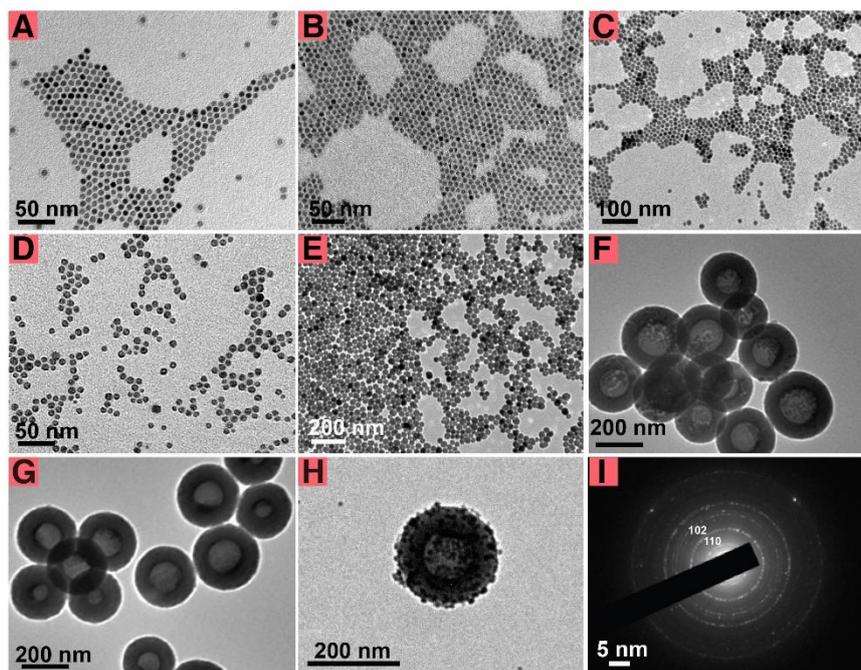
### **Corresponding authors**

Jinliang Liu, PhD, School of Environmental and Chemical Engineering, Research Center of Nano Science and Technology, Shanghai University, Shanghai, 200444, P. R. China. Email: [liujl@shu.edu.cn](mailto:liujl@shu.edu.cn). Yanli Wang, Professor, School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, P. R. China. Email: [wangyanli@staff.shu.edu.cn](mailto:wangyanli@staff.shu.edu.cn). Lining Sun, Professor, Research Center of Nano Science and Technology, and School of Material Science and Engineering, Shanghai University, Shanghai, 200444, P. R. China. Email: [lnsun@shu.edu.cn](mailto:lnsun@shu.edu.cn).

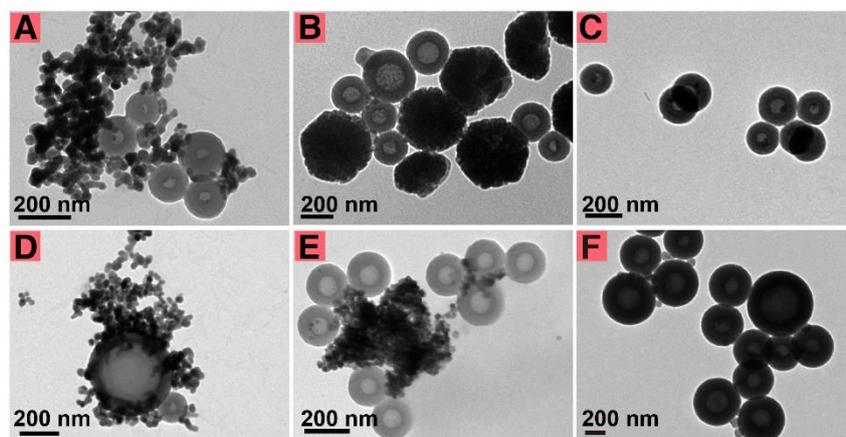
**Table S1.** Diameters of different samples.

Material	Diameter (nm)	Cavity Diameter (nm)	Proportion <sup>a)</sup> (Fe <sub>3</sub> O <sub>4</sub> :NaOA:DA:HMT:UCNPs:water)	Concentration of NaOA (mg/mL)
FeCU-1	1638.10 ± 357.47	1133.60 ± 37.82	3:20:77.06:17.52:4.37:20	20
FeCU-2	254.10 ± 50.33	133.27 ± 36.62	3:2:15.42:3.5:4.37:9.7	10
FeCU-3	215.93 ± 28.07	111.11 ± 13.23	3:2:15.42:3.5:4.37:9.9	3.33

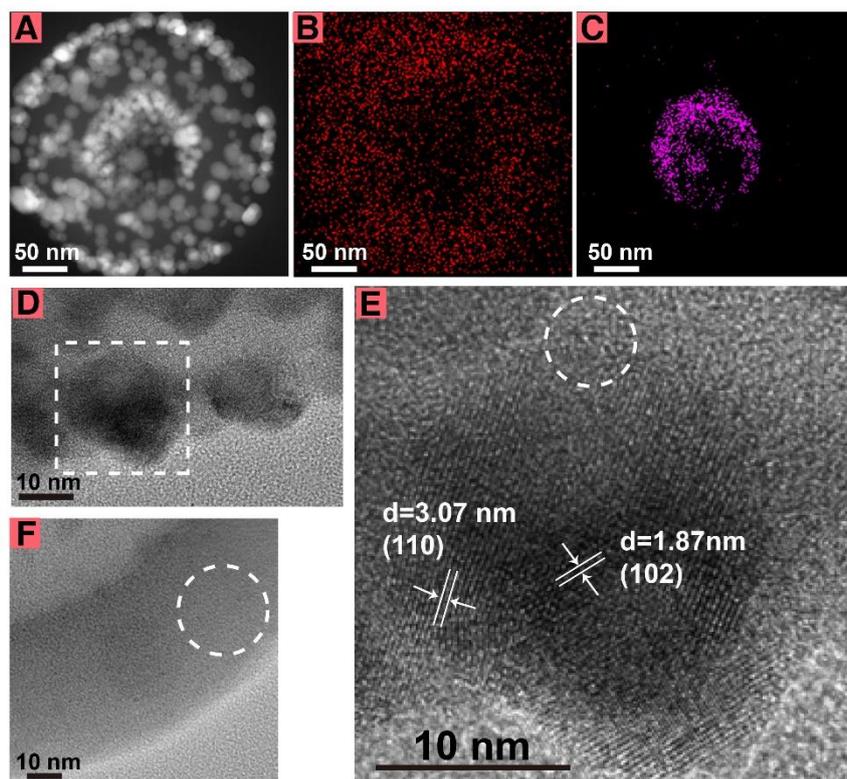
- a) The unit of water is mL and here it refers to total volume of water in the hydrothermal process, the unit of the rest composites is mg.



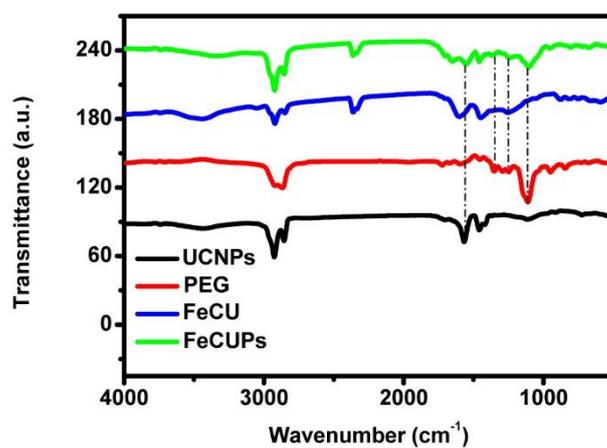
**Figure S1.** TEM images of  $\text{Fe}_3\text{O}_4$  (A),  $\text{NaGdF}_4:\text{Yb}^{3+},\text{Er}^{3+}$  (B),  $\text{NaGdF}_4:\text{Yb}^{3+},\text{Er}^{3+}@\text{NaGdF}_4$  (C),  $\text{NaGdF}_4:\text{Yb}^{3+},\text{Tm}^{3+}$  (D),  $\text{NaGdF}_4:\text{Yb}^{3+},\text{Tm}^{3+}@\text{NaGdF}_4$  (E), FeP (F), FeC (G), FeCU (H), and Selected area electron diffraction (SAED) of FeCU (I), UCNPs:  $\text{NaGdF}_4:\text{Yb}^{3+},\text{Tm}^{3+}@\text{NaGdF}_4$ .



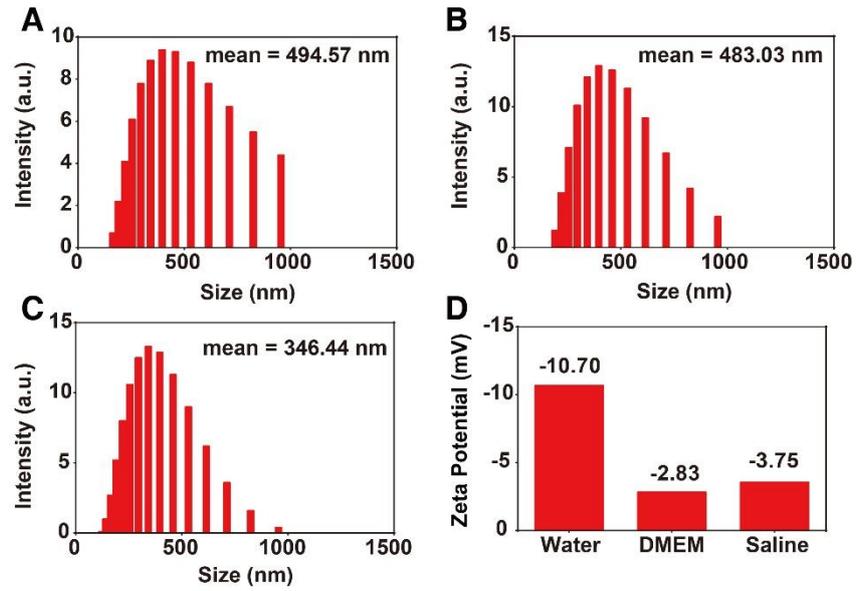
**Figure S2.** TEM images of unsuccessful loading of UCNPs on FeC. Impact of morphology (A), size (B) and surface status (C) of UCNPs, uneven size of FeC (D), water dispersion of FeC (E), chloroform dispersion of UCNPs (F) on the synthesis of FeCU.



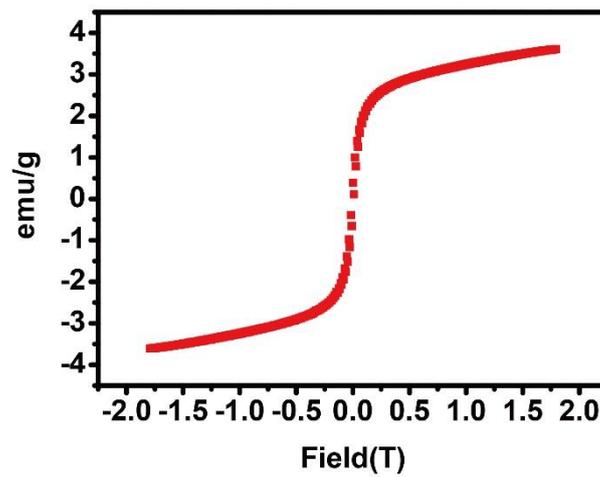
**Figure S3.** HADDF image of FeCU (A) and corresponding element mapping images of carbon (B) and Fe (C). HRTEM image of FeCU (D) and magnifying image of white square (E). HRTEM image of FeC (F).



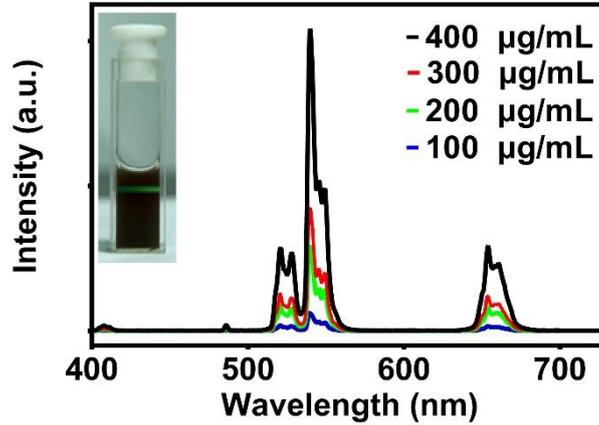
**Figure S4.** Fourier transform infrared spectroscopy (FTIR) spectra of UCNPs, PEG, FeCU, and FeCUPs. PEG: amphiphilic poly(ethylene glycol), UCNPs:  $\text{NaGdF}_4:\text{Yb}^{3+},\text{Tm}^{3+}@\text{NaGdF}_4$ .



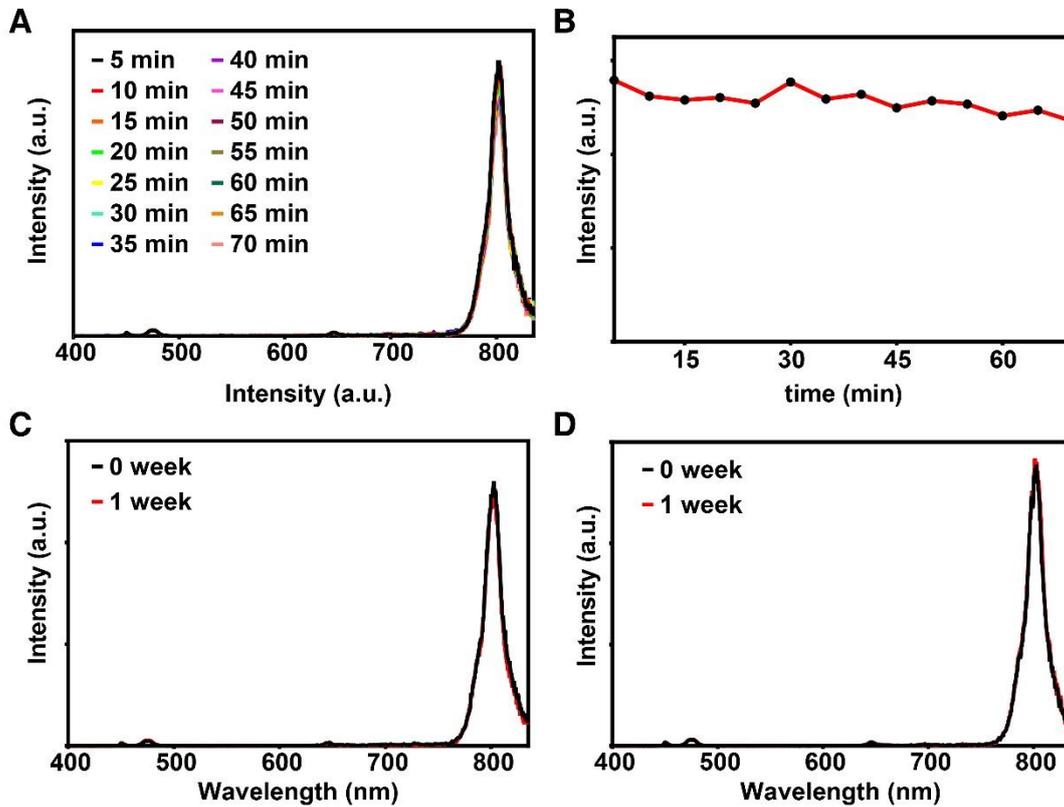
**Figure S5.** Dynamic light scattering (DLS) of FeCUPs in water (A), DMEM (B), saline (C) respectively, and the corresponding zeta-potential (D).



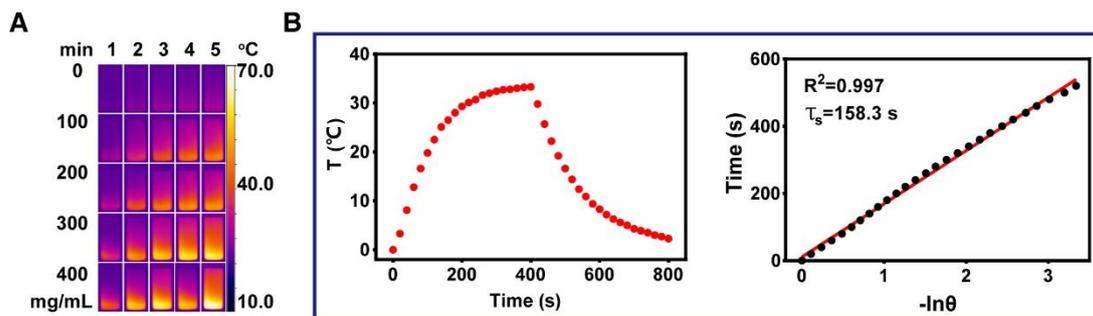
**Figure S6.** Hysteresis loops of FeCU.



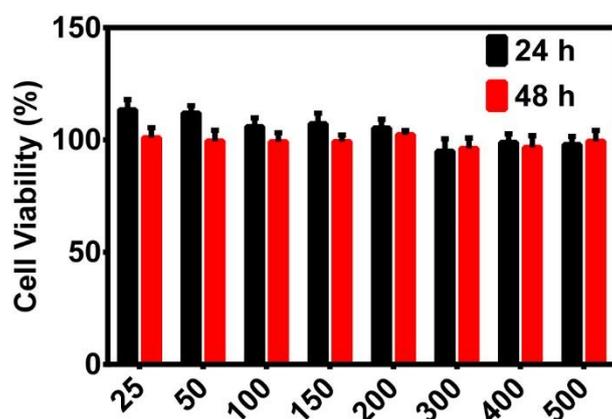
**Figure S7.** Upconversion emission spectra of FeCUPs (inset: photograph of FeCUPs illuminated with 980 nm laser irradiation at  $1.5\text{W}/\text{cm}^2$ , UCNPs:  $\text{NaGdF}_4:\text{Yb}^{3+},\text{Er}^{3+}@\text{NaGdF}_4$ ).



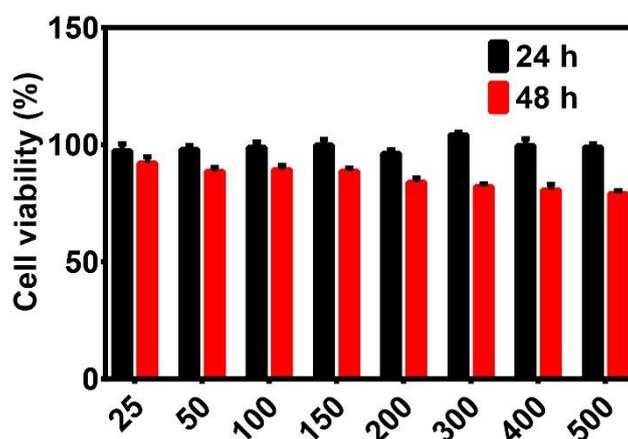
**Figure S8.** FeCUPs (400 μg/mL) in water under 980 nm NIR light: (A) Upconversion luminescence (UCL) spectra at different times (5–70 min); (B) Variation of UCL intensity at 800 nm in different times (5–70 min); (C) UCL spectrum change of FeCUPs (400 μg/mL, in water) in one week. (D) UCL spectrum change of FeCUPs (400 μg/mL, in saline) in one week.



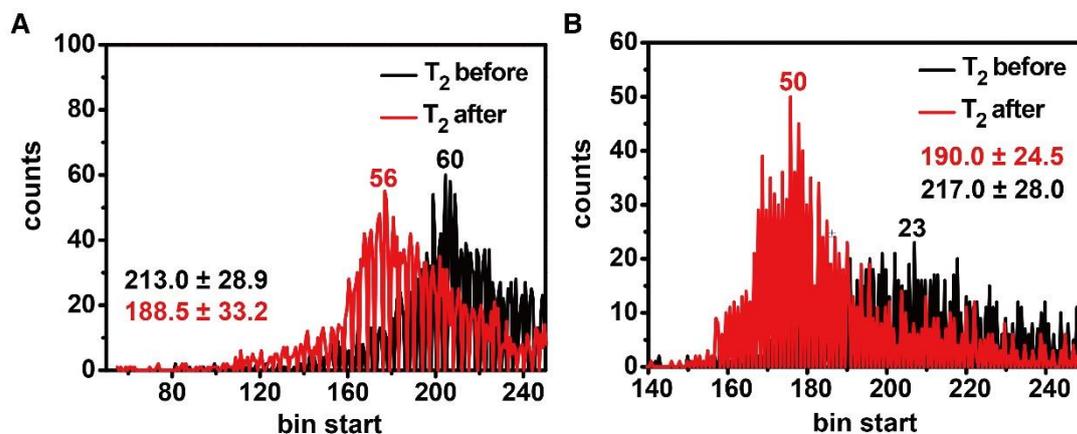
**Figure S9.** (A) Infrared thermal images at the time points of 0, 1, 2, 3, 4, and 5 min of the different concentrations of FeCUPs (808 nm, 1.5 W/cm<sup>2</sup>). (B left) The monitored temperature of FeCUPs (400 μg mL<sup>-1</sup>) under 808 nm laser irradiation (808 nm, 1.5 W/cm<sup>2</sup>) for 400 sec, and another 400 sec for cooling. (B right) Linear fitting of cooling time and  $-\ln\theta$ ,  $\theta=(T-T_{surr})/(T_{max}-T_{surr})$ ,  $\tau_s=\sum_i m_i C_{p,i}/(hs)$ ,  $T$  is the solution temperature,  $T_{surr}$  is the ambient temperature of surrounding environment,  $T_{max}$  is maximum temperature of solution,  $\tau_s$  is system time constant,  $i$  terms of  $m_i C_{p,i}$  are mass of the solvent (water) and heat capacity of solvent,  $h$  is heat transfer coefficient,  $s$  is the surface area of the container [1].



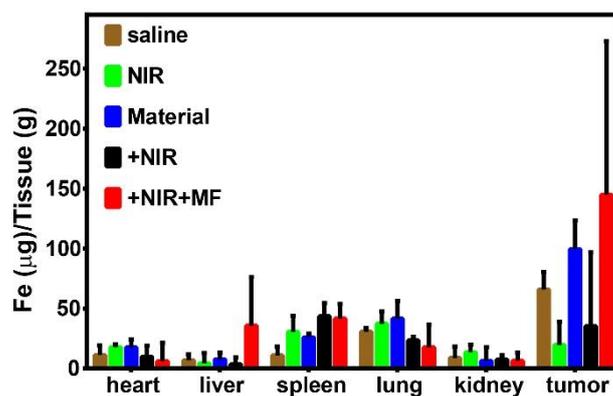
**Figure S10.** Cell viabilities of HeLa cells incubated with FeCUPs of gradient concentrations for 24/48 h.



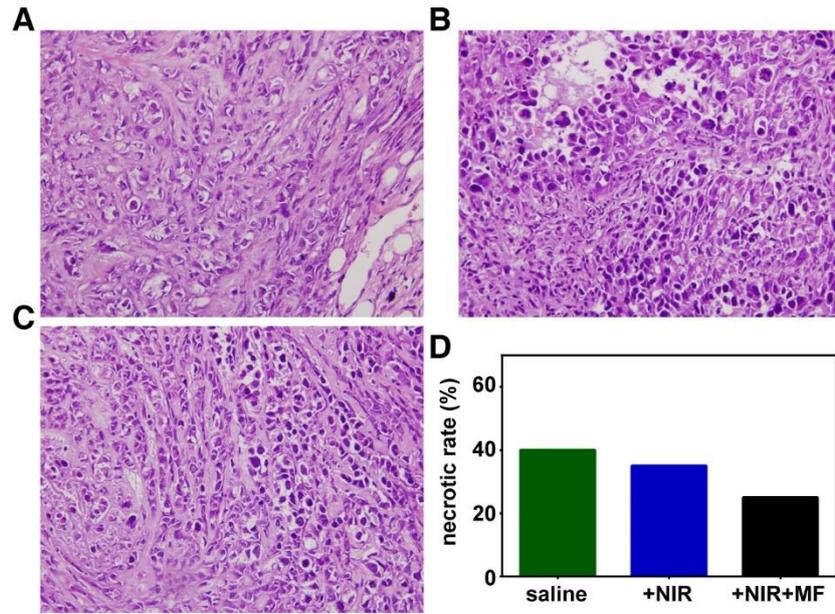
**Figure S11.** Cell viabilities of GES-1 cells incubated with FeCUPs of gradient concentrations for 24/48 h.



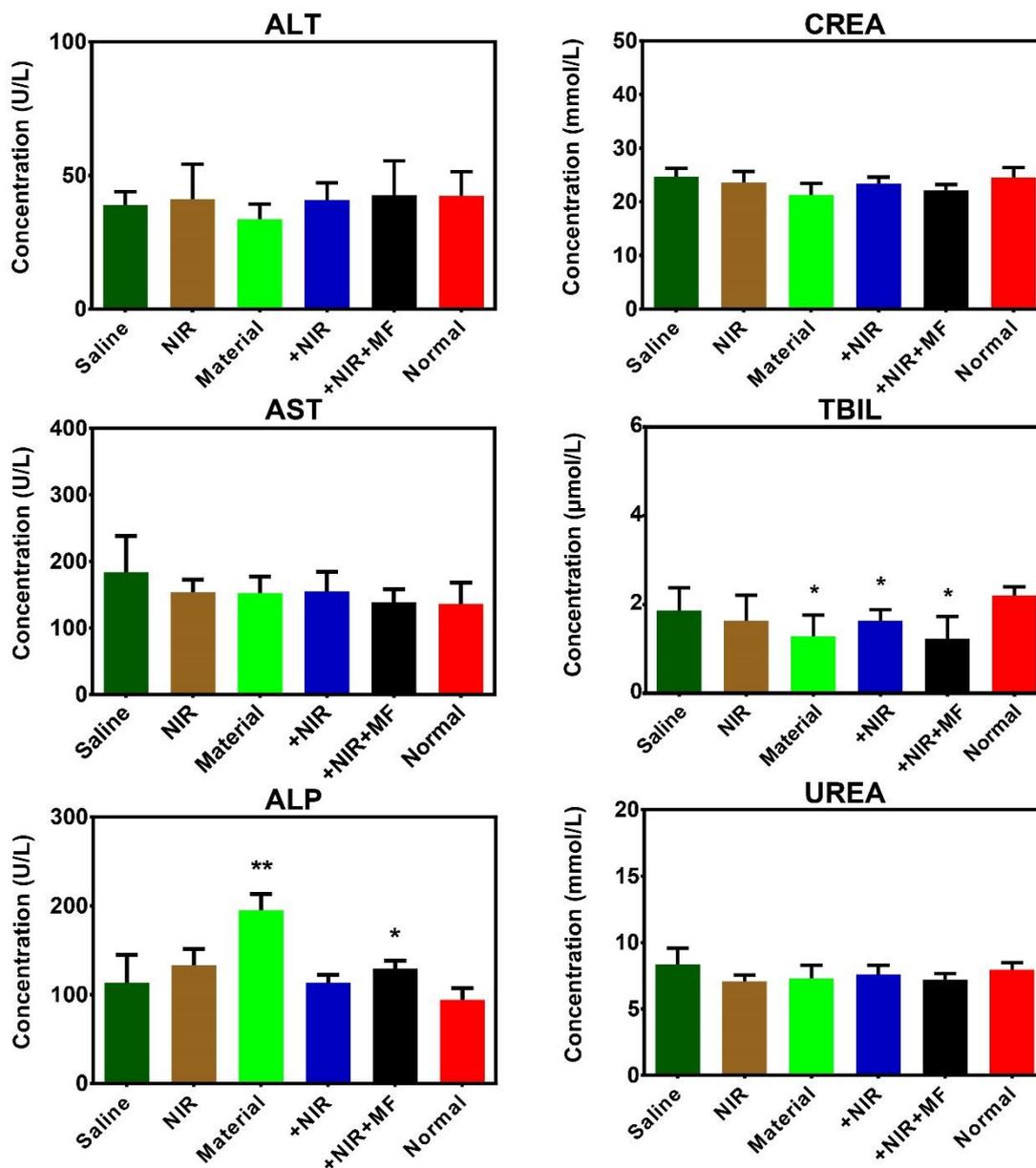
**Figure S12.** *T*<sub>2</sub>-weighted magnetic resonance signal intensity *in vivo* at selected region without magnet group (A) and with magnet group (B).



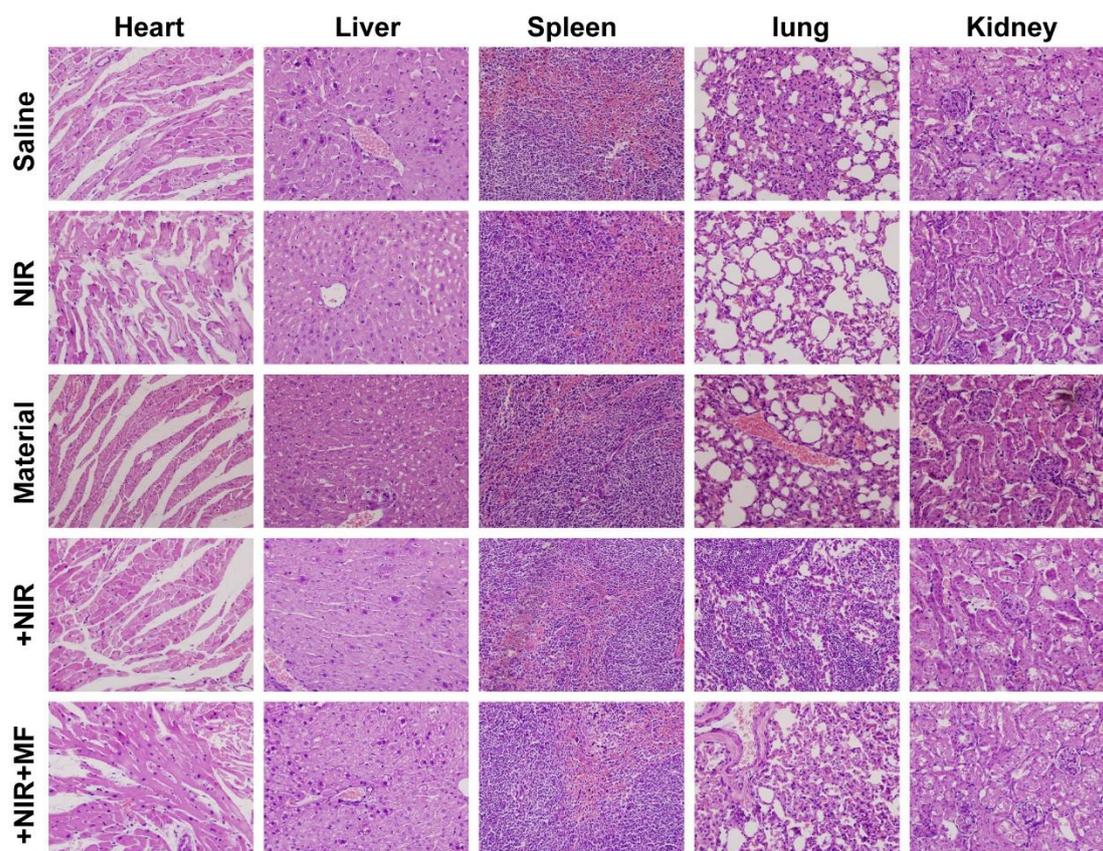
**Figure S13.** The distribution of Fe element in internal organs (heart, liver, spleen, lung, kidney, tumor).



**Figure S14.** H&E stained images of tumor in saline group (A), +NIR group (B), +NIR+MF group (C); and corresponding necrotic rate of each group (D).



**Figure S15.** Hepatic and renal function indicators from blood serum biochemistry results after 28 days (\* =  $p < 0.05$ ; \*\* =  $p < 0.01$ , compared with the normal group, one-way ANOVA). Normal (healthy mice, blank), Saline( dose = 100  $\mu$ L, control), NIR (dose = 100  $\mu$ L, 808 nm NIR, 10 min , control), +NIR (does = 2 mg/kg, 808 nm NIR, 10 min, test), +NIR+MF (does = 2 mg/kg, 808 nm NIR, magnet, 10 min, test), control groups were injected with saline, test groups were injected with saline solution of FeCUPs, n = 3.



**Figure S16.** H&E stained images of heart, liver, spleen, lung, and kidney of mice in different groups (saline, NIR, material, + NIR, + NIR + MF) at 28 days after injection. Normal (healthy mice, blank), Saline ( dose = 100  $\mu$ L, control), NIR (dose = 100  $\mu$ L, 808 nm NIR, 10 min , control), +NIR (does = 2 mg/kg, 808 nm NIR, 10 min, test), +NIR+MF (does = 2 mg/kg, 808 nm NIR, magnet, 10 min, test), control groups were injected with saline, test groups were injected with saline solution of FeCUPs, n=3.

#### References

- [1] D.K. Roper, W. Ahn, M. Hoepfner. Microscale heat transfer transduced by surface plasmon resonant gold nanoparticles. *J Phys Chem C*. 2007; 111: 3636-3641.