Supporting Information

Co-precipitation Synthesis of Near-infrared Iron Oxide Nanocrystals on Magnetically Targeted Imaging and Photothermal Cancer Therapy via Photoablative Protein Denature

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Figure S1. Absorption spectra of NIR-IO nanocrystals synthesized using different amounts of citrate.
Figure S2. HR-TEM image, and fast Fourier transform (FFT) pattern of a) low citrate weight (0.022 g) synthesis, and b) high citrate weight (0.11 g).

To calculate the photothermal conversion efficiency ($\eta$) of NIR-IO nanocrystals, the following equation was used:

$$\eta = \frac{h A \Delta T_{\text{max}} - Q_{\text{dis}}}{I (1 - 10^{-A_{\lambda}})} = \frac{m_D C_D}{\tau_s} \cdot \frac{A \Delta T_{\text{max}} - Q_{\text{dis}}}{I (1 - 10^{-A_{\lambda}})}$$

In this equation, $h$ is the heat transfer coefficient that can transfer to $m_D C_D (\tau_s)^{-1}$, $m_D$ (or $C_D$) is the mass (or heat capacity) of water, $A$ is the surface area of the container, $\Delta T_{\text{max}}$ is the temperature change of the sample at the maximum steady-state temperature, $Q_{\text{dis}}$ is the heat dissipation from the light absorbance of the solvent, $I$ is the laser power, and $A_{\lambda}$ is the sample absorbance at 808 nm. From this equation, the $\eta$ value and 90% highest temperature $\eta$ value of NIR-IO nanocrystals were calculated to be 21.2% and 41%, respectively.
Figure S3. Size distribution of NIR-IO in the water and PBS, 1-15 days, room temperature.
Figure S4. A) Hysteresis of NIR-IO nanocrystals synthesized using different amounts of citrate measured at room temperature and ranging from -10000 to 10000 G. B) $T_2$ relaxation rates as a function of the Fe concentration (mM) of Resovist® and NIR-IO nanocrystals in agar gel. C) $T_2$-weighted MR images of NIR-IO nanocrystals and Resovist®.
**Figure S5.** Dark-field reflectance images of HT-29 cancer cells treated with NIR-IO nanocrystals. The red arrows indicate nanocrystals that were internalized within the cell.
Figure S6. A) FTIR spectra of HT-29 cancer cells treated with PBS and NIR-IO nanocrystals collected by SR-IMS. The Fe concentration was 140 µg mL\(^{-1}\). In b-d, the FTIR spectra of the treated HT-29 cancer cells were magnified to show specific ranges at wavenumbers (cm\(^{-1}\)) of B) 3000-2800, C) 1700-1400 and D) 1300-900.
**Figure S7.** FTIR images of HT-29 cells incubated with PBS and NIR-IO nanocrystals. The Fe concentration was 140 µg mL\(^{-1}\).
**Figure S8.** A) Heating curves, B) thermographic images and C) H&E-stained images of mice bearing HT-29 tumors after intratumoral injection of Resovist® or NIR-IO nanocrystals (14 mg kg\(^{-1}\)) and 10-min exposure to 808-nm laser irradiation (1.5 W cm\(^{-2}\)).
**Figure S9.** MR images of mice before and after IT injection of NIR-IO nanocrystals. The gray arrow indicates the site of injection of NIR-IO nanocrystals.
Figure S10. Optical images showing the effects of treatment with PBS, NIR-IO nanocrystals, or NIR-IO nanocrystals + MF targeting via 808-nm laser irradiation.
Figure S11. MR images of mice before and after IV injection + MF targeting of NIR-IO nanocrystals. The red circles indicates the site of tumor and MF targeting position.
Figure S12. TEM images of NIR-IO nanocrystals synthesized with (A) 0.066 g of DPC or (B) 0.0099 g of DPC as a replacement for citrate.