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Supplementary Information

Facile preparation of biocompatible Ti_2O_3 nanoparticles for second near-infrared window photothermal therapy

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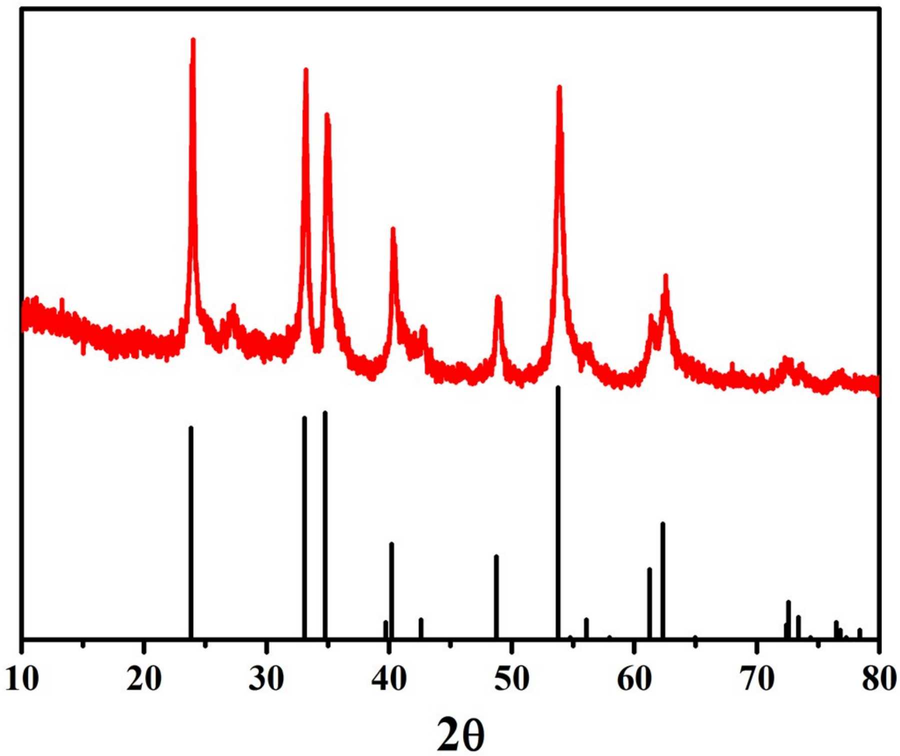

Fig. S1 Wide-angle X-ray diffraction pattern of Ti_2O_3 nanoparticles.

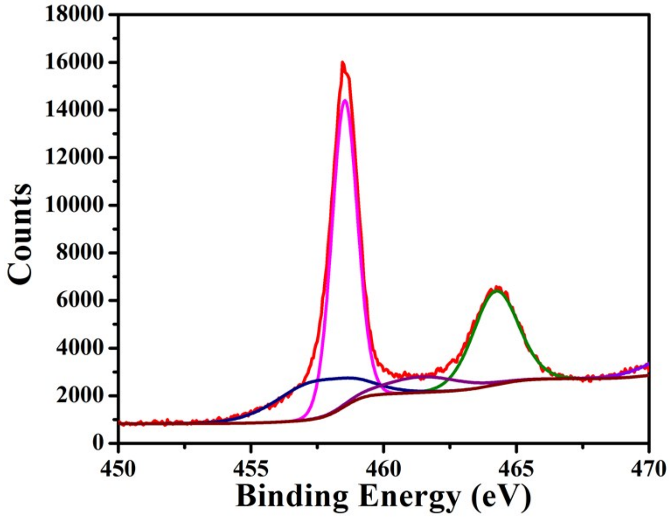

Fig. S2 XPS Ti2p orbits of Ti_2O_3 nanoparticles.

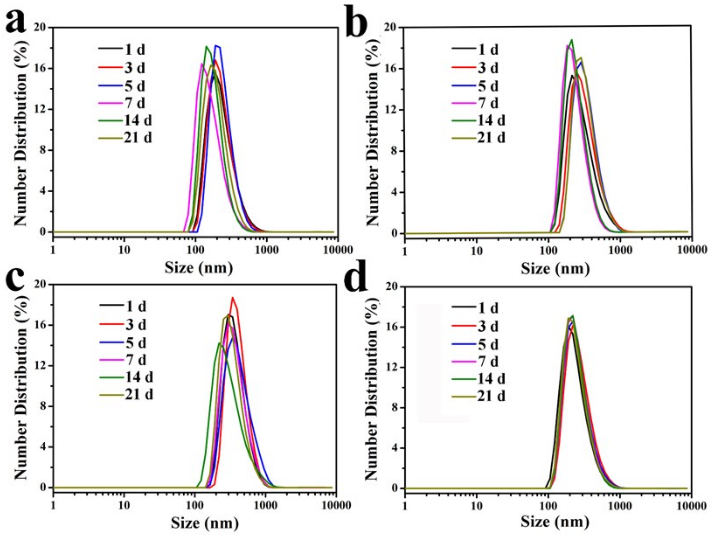

Fig. S3 Size distributions of Ti_2O_3@HA nanoparticles in (a) water, (b) PBS, (c) DMEM and (c) FBS measured by DLS.

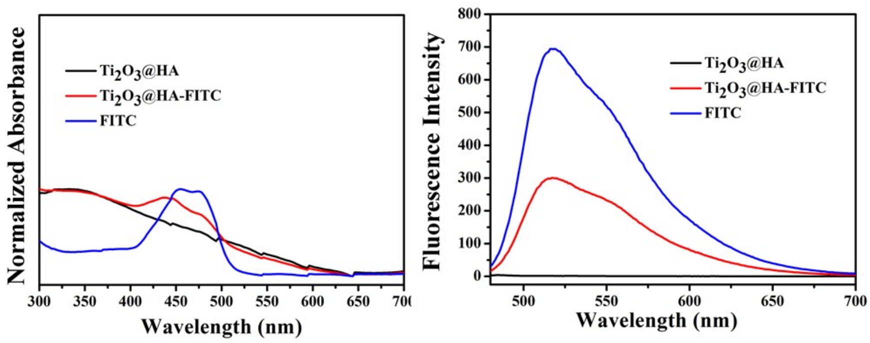

Fig. S4 The absorption spectra (a) and fluorescence spectra (b) of Ti_2O_3@HA-FITC.

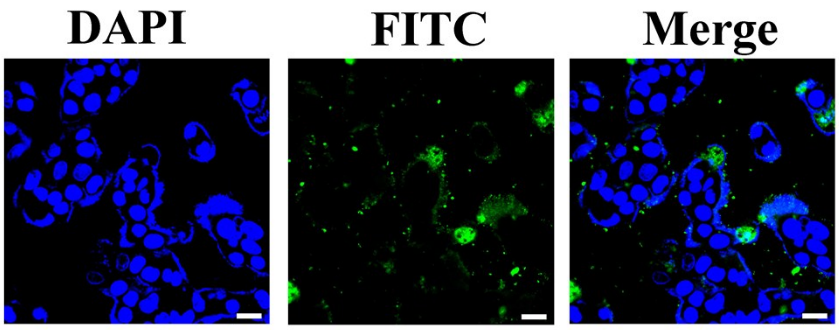

Fig. S5 CLSM images of NIH3T3 cells incubated with Ti_2O_3@HA for 6 h.

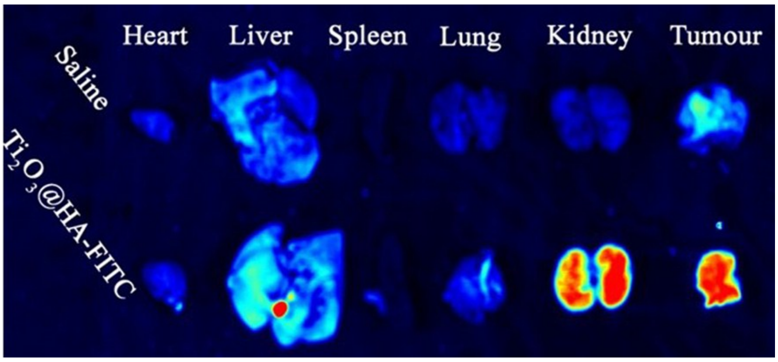

Fig. S6 *Ex vivo* fluorescence images of major organs obtained from mice with indicated treated after 12 h of Ti_2O_3@HA-FITC injection.

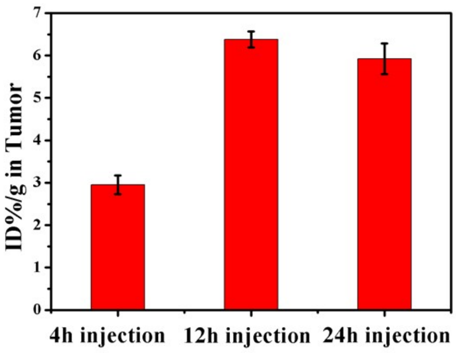

Fig. S7 Concentration of Ti_2O_3@HA nanoparticles at tumor sites after 4h, 12h and 24h of inejction.

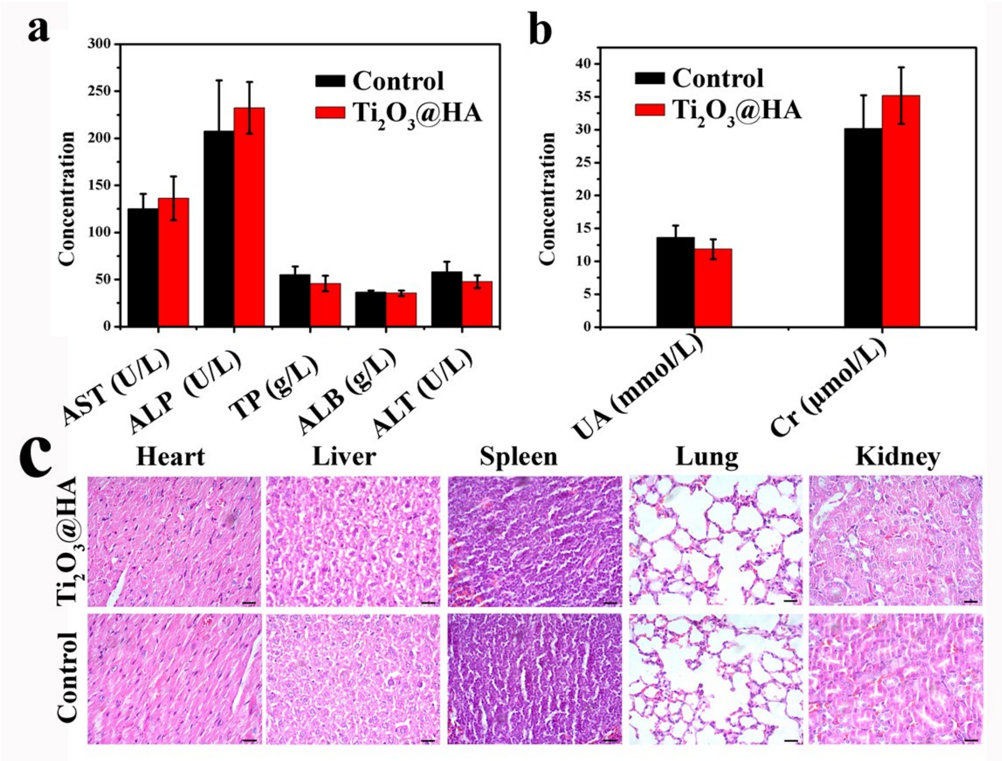

Fig. S8 Serum biological parameters obtained from mice at 7 days after injected with Ti_2O_3@HA (n=4), or PBS solution (n=4, control) (A); hematoxylin and eosin (H&E)-stained tissue sections from mice at 7 days after injected with Ti_2O_3@HA (n=4), or PBS solution (n=4, control).

Materials

The Titanium(III) oxide（99.9%, 100 mesh）was purchased from J&K Scientific Ltd. 3-aminopropyl-triethoxysilane was supplied by TCI. Hyaluronic acid (Mw = 61000) was purchased from Shandong Furuida Biological Biomedicine Co., Ltd. 4’, 6-diamidino-2-phenylindole (DAPI) and Cell Counting Kit-8 (CCK-8) were obtained from Dojindo Molecular Technologies. LIVE/DEAD Viability/Cytotoxicity Kit and Annexin V-Fluoroisothio cyanate (FITC)/propidium iodide (PI) apoptosis detection kit were provided by Invitrogen. All other chemicals, if not specified, were used as received without further purfification.

Calculation of the photothermal conversion efficiency

To evaluate the photothermal conversion efficiency, the temperature change of the aqueous dispersion (200 μg mL^{-1}) was recorded as a function of time under continuous irradiation of the 1064 nm laser with a power density of 1.4 W·cm^{-2} until the solution reached a steady-state temperature.

The photothermal conversion efficiency, η, was calculated using Equation 1 described by previous reports [1,2], where h is the heat transfer coefficient, A is the surface area of the container, Tmax is the equilibrium temperature, T_{Surr} is ambient temperature of the surroundings, $\Delta T_{max} = T_{max} - T_{Surr}$, I is incident laser power (1.4 W cm^{-2}), and A_λ is the absorbance of Ti_2O_3@HA at 1064 nm. Q_s is the heat associated with the light absorbance of the solvent, which is measured independently to be 25.2 mW using deionized water without nanoparticles.

$$\eta = \frac{hA\Delta T_{max} - Q_s}{I(1-10^{-A_\lambda})} \qquad (1)$$

The value of hA is derived according to Equation 2:

$$\tau_s = \frac{m_D C_D}{hA} \qquad (2)$$

Where τ_s is the time constant of sample system, m_D and C_D are the mass (1 g) and heat capacity (4.2 J g^{-1}) of deionized water used as the solvent, respectively.

In order to obtain the hA, herein introduce θ, which is defined as the ratio of ΔT to ΔT_{max}:

$$\theta = \frac{\Delta T}{\Delta T_{max}} \qquad (3)$$

hA can be determined by applying the linear time data from the cooling period versus –Lnθ (Fig. 2d,e). Substituting hA value into Equation 1, the photothermal conversion efficiency (η) of Ti_2O_3@HA can be calculated:

$hA = m_D C_D/\tau_s = 4.2$ J/260; $A\lambda = 0.834$; $\tau_s = 260$; $I = 1.4$ W cm^{-2}; $\Delta T_{max} = 33.9$ °C

$\eta = ((4.2/227.8)\times 33.9-0.0252)/(1.4\times(1-10^{-0.834})) = 50.19\%$

References

1. M. Wang, K. Deng, W. Lu, X. Deng, K. Li, Y. Shi, B. Ding, Z. Cheng, B. Xing, G. Han, Z. Hou and J. Lin, *Adv. Mater.*, 2018, **30**, 1706747- 1706755.
2. X. Yu, A. Li, C. Zhao, K. Yang, X. Chen and W. Li, *ACS Nano*, 2017, **11**, 3990-4001.