Supporting information

A New Green Titania with Enhanced NIR Absorption for Mitochondria-Targeted Cancer Therapy

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Supplementary figures

Figure S1. Nanocrystal size distribution histograms of $B$-TiO$_2$-$x$ (a) and $G$-TiO$_2$-$x$ (b).

Figure S2. Energy dispersive X-ray spectrum of the as-synthesized $B$-TiO$_2$-$x$ and $G$-TiO$_2$-$x$. 
Figure S3. Raman spectra of white TiO$_2$, as-synthesized $B$-TiO$_{2-x}$ and $G$-TiO$_{2-x}$.

Figure S4. X-ray Photoelectron Spectroscopy spectra of the G-TiO$_{2-x}$. The shoulder peaks (in blue) at ~457 eV in the Ti 2$p_{3/2}$ and at 463 eV in Ti 2$p_{1/2}$ XPS spectra are correlated with Ti$^{3+}$ while the main peak (in magenta) at 458.9 and 464.6 eV corresponding to Ti 2$p_{3/2}$ and Ti 2$p_{1/2}$ of Ti$^{4+}$, respectively.
Figure S5. UV-vis absorbance spectrum of aqueous solutions containing $G$-$\text{TiO}_2$-$x$ (Ti concentration: 50 ppm).

Figure S6. (a) Temperature elevation of the aqueous solution containing $G$-$\text{TiO}_2$-$x$ at determined Ti concentration (2 mL, 50 ppm) as a function of irradiation time and power densities (980 nm). (b) Photothermal stability investigation after laser irradiation for 10 cycles (980 nm, 0.72 W cm$^{-2}$, 5 min).

Figure S7. (a) UV-vis absorbance spectra of aqueous solutions containing $G$-$\text{TiO}_2$-$x$-TPP at varied concentrations and (b) the corresponding linear plot of absorbance vs concentrations at 920 nm.
Figure S8. Hydrodynamic diameter distribution (a) and Zeta potential (b) of the as-synthesized G-TiO$_{2-x}$ and after PEG, TPP modification.

Figure S9. FT-IR spectra of the G-TiO$_{2-x}$ and after PEG, TPP modification.

Figure S10. (a) Pharmacokinetic profile of G-TiO$_{2-x}$-TPP following intravenous administration. (b) Biodistribution of G-TiO$_{2-x}$-TPP at 24 h after intravenous injection in mice. Each experiment was repeated three times in triplicate. Data were shown as the means ± SD.
Figure S11. *In vitro* cell viabilities of three types of normal cells (BRL, NRK-52E, BCECs) and two types of brain-related cancer cells (U87MG and PC12) incubated with $G$-TiO$_2$-TPP at different concentrations for 24 h, evaluated by a standared MTT assay. Corresponding optical microscopic images of the *in vitro* cell morphology of five types of cells incubated without (c1-g1) or with $G$-TiO$_2$-TPP (c2-g2) (Ti concentration:100 ppm) for 24 h. Each experiment was repeated three times in triplicate. Data were shown as the means ± SD. All the scale bars in (c-g) are 100 $\mu$m.
Figure S12. The variations of blood indexes of Kunming mice after intravenous injection of physiological saline (control) or G-TiO$_2$-TPP (8 mg Ti/kg) at different time points (i.e., 0, 3, 15, 30 days). Each experiment was repeated three times in triplicate. Data were shown as the means ± SD.

Figure S13. Time courses of histological changes in main organs of Kunming mice via H&E staining after intravenous injection of physiological saline (control) or G-TiO$_2$-TPP (8 mg Ti/kg) at different time points (i.e., 0, 3, 15, 30 days). All the scale bars are 50 μm.
Figure S14. *In vivo* brain toxicity evaluation of G-TiO$_2$-x-TPP. H&E-stained main brain tissues sections of cortex, hippocampus and striatum, which were collected from mice treated with intravenous injection of physiological saline (control) or G-TiO$_2$-x-TPP (8 mg Ti/kg) at different time points (*i.e.*, 0, 3, 15, 30 days), to monitor the histological changes. All the scale bars are 50 μm.