

Supporting information

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

Juan Mou, Tianquan Lin, Fuqiang Huang, Jianlin Shi and Hangrong Chen✉

Supplementary figures

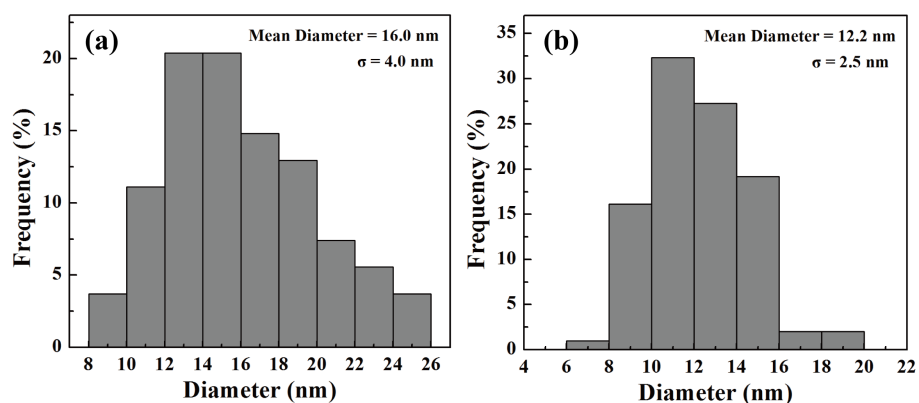


Figure S1. Nanocrystal size distribution histograms of $B\text{-TiO}_{2-x}$ (a) and $G\text{-TiO}_{2-x}$ (b).

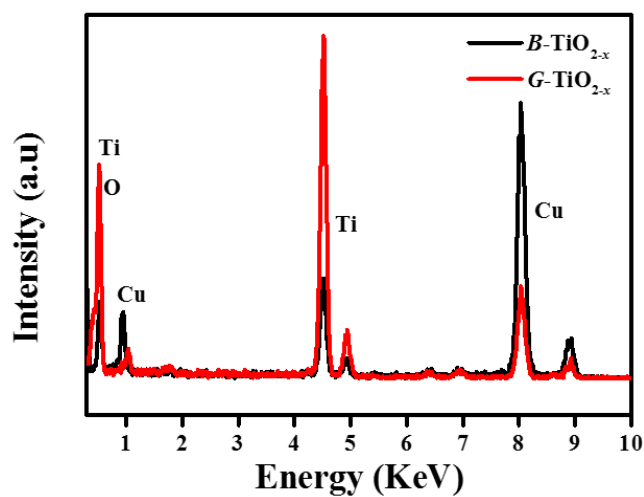


Figure S2. Energy dispersive X-ray spectrum of the as-synthesized $B\text{-TiO}_{2-x}$ and $G\text{-TiO}_{2-x}$.

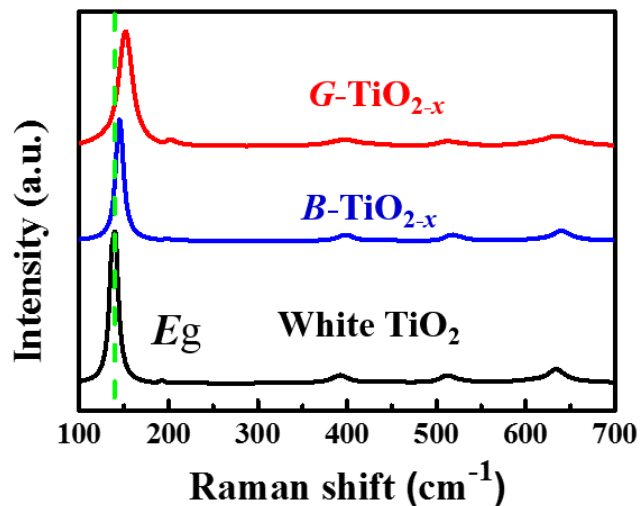


Figure S3. Raman spectra of white TiO_2 , as-synthesized $B\text{-TiO}_{2-x}$ and $G\text{-TiO}_{2-x}$.

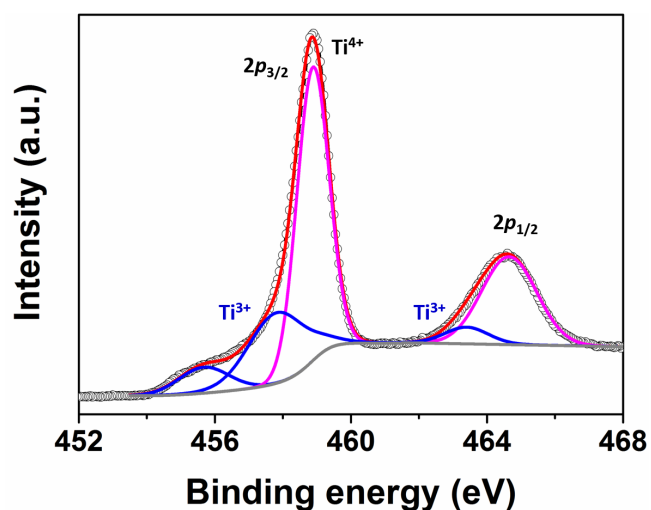


Figure S4. X-ray Photoelectron Spectroscopy spectra of the $G\text{-TiO}_{2-x}$. The shoulder peaks (in blue) at ~ 457 eV in the $\text{Ti } 2p_{3/2}$ and at 463 eV in $\text{Ti } 2p_{1/2}$ XPS spectra are correlated with Ti^{3+} while the main peak (in magenta) at 458.9 and 464.6 eV corresponding to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

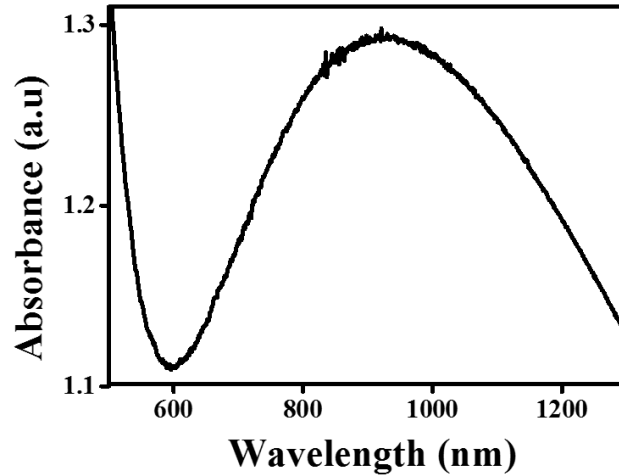


Figure S5. UV-vis absorbance spectrum of aqueous solutions containing $G\text{-TiO}_{2-x}$ (Ti concentration: 50 ppm).

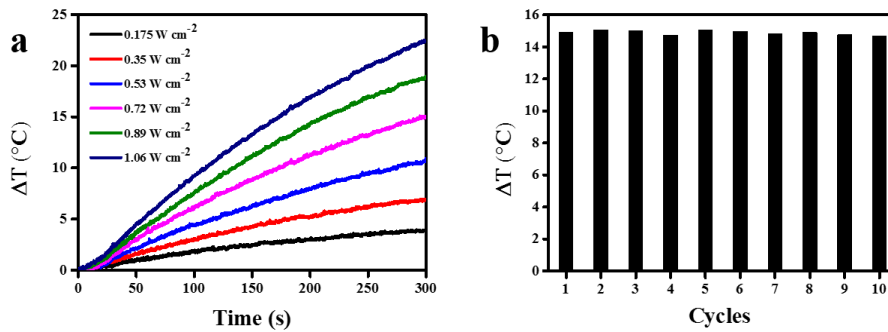


Figure S6. (a) Temperature elevation of the aqueous solution containing $G\text{-TiO}_{2-x}$ at determined Ti concentration (2 mL, 50 ppm) as a function of irradiation time and power densities (980 nm). (b) Photothermal stability investigation after laser irradiation for 10 cycles (980 nm, 0.72 W cm^{-2}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

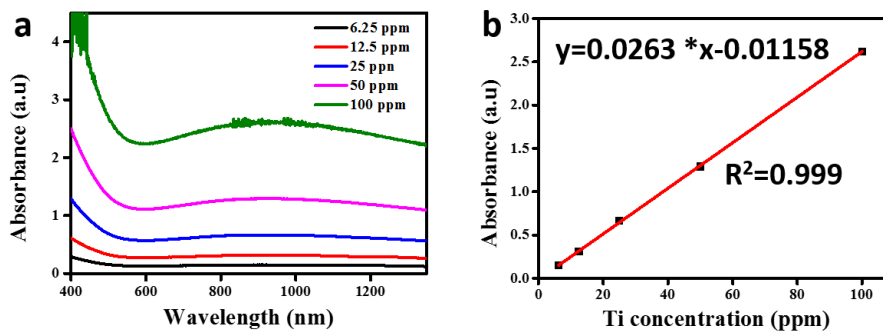


Figure S7. (a) UV-vis absorbance spectra of aqueous solutions containing $G\text{-TiO}_{2-x}\text{-TPP}$ at varied concentrations and (b) the corresponding linear plot of absorbance vs concentrations at 920 nm.

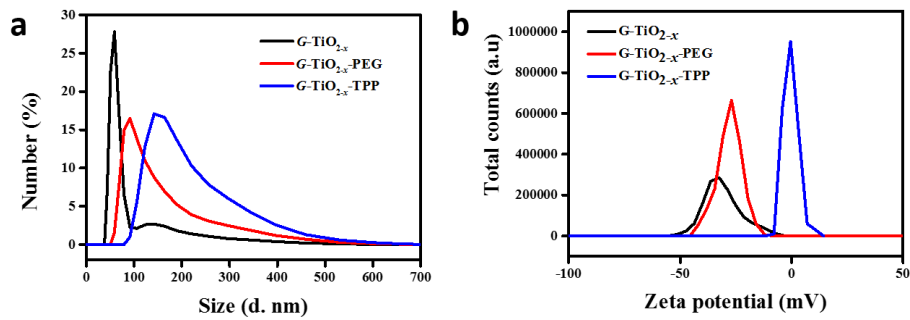


Figure S8. Hydrodynamic diameter distribution (a) and Zeta potential (b) of the as-synthesized $G-TiO_{2-x}$ and after PEG, TPP modification.

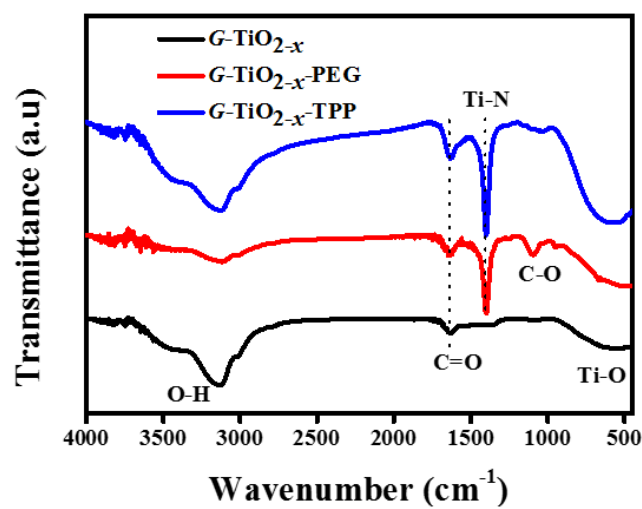


Figure S9. FT-IR spectra of the $G-TiO_{2-x}$ and after PEG, TPP modification.

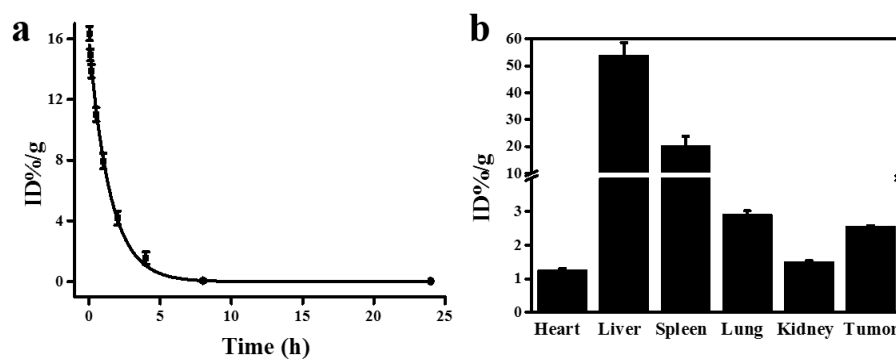


Figure S10. (a) Pharmacokinetic profile of $G-TiO_{2-x}-TPP$ following intravenous administration. (b) Biodistribution of $G-TiO_{2-x}-TPP$ at 24 h after intravenous injection in mice. Each experiment was repeated three times in triplicate. Data were shown as the means \pm SD.

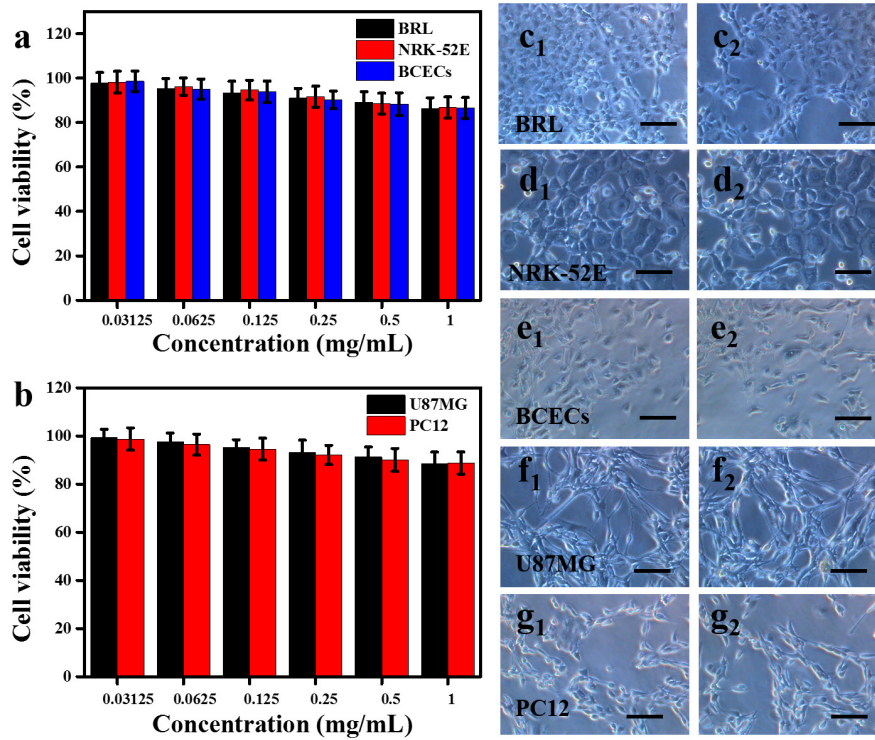


Figure S11. *In vitro* cell viabilities of three types of normal cells (BRL, NRK-52E, BCECs) and two types of brain-related cancer cells (U87MG and PC12) incubated with $G\text{-TiO}_{2-x}\text{-TPP}$ at different concentrations for 24 h, evaluated by a standard MTT assay. Corresponding optical microscopic images of the *in vitro* cell morphology of five types of cells incubated without ($c_1\text{-}g_1$) or with $G\text{-TiO}_{2-x}\text{-TPP}$ ($c_2\text{-}g_2$) (Ti concentration: 100 ppm) for 24 h. Each experiment was repeated three times in triplicate. Data were shown as the means \pm SD. All the scale bars in (c-g) are 100 μm .

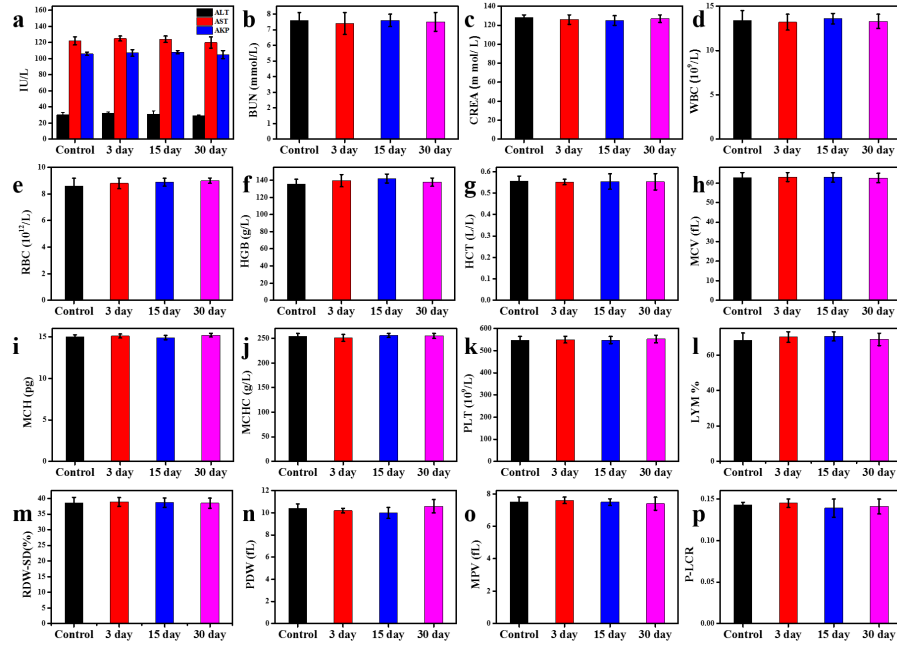


Figure S12. The variations of blood indexes of Kunming mice after intravenous injection of physiological saline (control) or $G\text{-TiO}_{2-x}\text{-TPP}$ (8 mg Ti/kg) at different time points (*i.e.*, 0, 3, 15, 30 days). Each experiment was repeated three times in triplicate. Data were shown as the means \pm SD.

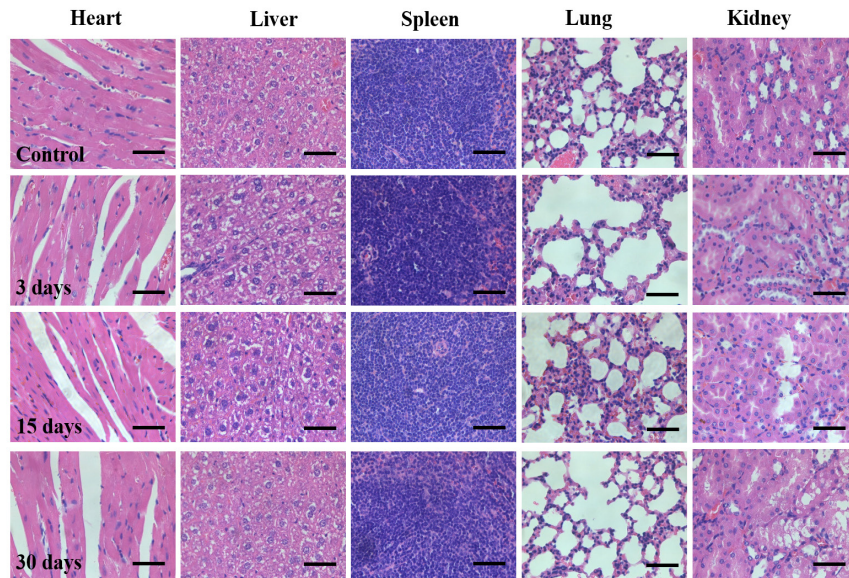


Figure S13. Time courses of histological changes in main organs of Kunming mice *via* H&E staining after intravenous injection of physiological saline (control) or $G\text{-TiO}_{2-x}\text{-TPP}$ (8 mg Ti/kg) at different time points (*i.e.*, 0, 3, 15, 30 days). All the scale bars are 50 μm .

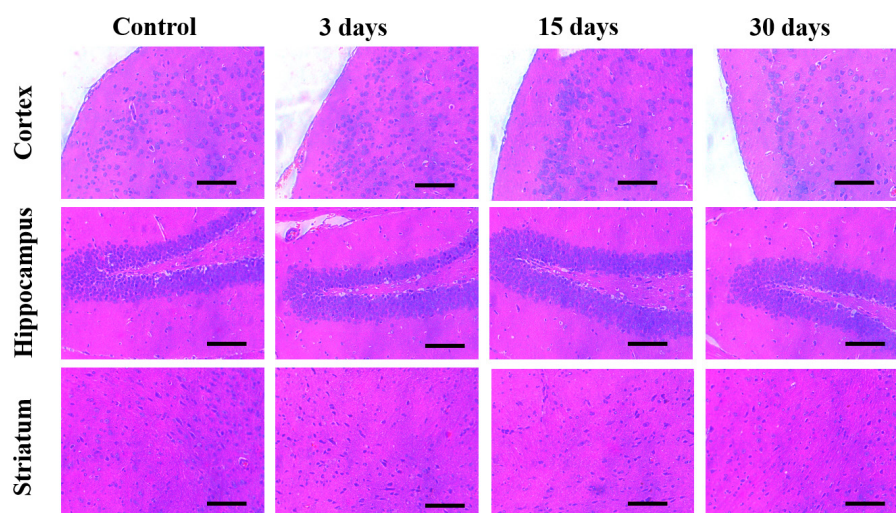


Figure S14. *In vivo* brain toxicity evaluation of $G\text{-TiO}_{2-x}\text{-TPP}$. H&E-stained main brain tissues sections of cortex, hippocampus and striatum, which were collected from mice treated with intravenous injection of physiological saline (control) or $G\text{-TiO}_{2-x}\text{-TPP}$ (8 mg 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 .