Electronic Supplementary Information for

Radiopaque tantalum oxide coated persistent luminescent nanoparticles as a multimodal probe for in vivo near-infrared luminescence and computed tomography bioimaging

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Experimental Details

Histopathology. The histological changes in the main organs of mice injected with PEG-ZGGO:Cr,Pr@TaO_x@SiO₂ (300 μ L, 1 mg mL⁻¹) or PBS (300 μ L, 10 mM, pH 7.4) were observed after 7 days of injection. The selected organs (heart, liver, spleen, lung and kidney) were fixed in 10% neutral buffered formalin, embedded in paraffin, sectioned (5 μ m thick), and stained with hematoxylin and eosin (H&E). The histological sections were observed under an optical microscope.

Procedures for cell imaging. The HepG2 cells and 3T3 cells were cultured for 24 h, and then incubated with NGR-ZGGO:Cr,Pr@TaO_x@SiO₂ or PEG-ZGGO:Cr,Pr@TaO_x@SiO₂ (200 μ g mL⁻¹) in the 24-well plate for 24 h. The resulting cells were washed with PBS (10 mM, pH 7.4) three times before imaging. The cell images were observed on an IX81 motorized inverted microscope (Olympus, Japan) (ocular, WHN 10×; objective, UPLFLN 10×/0.30; excitation filter, BP330-385; dichroic beamsplitter, DM400; barrier filter, BA420) with X-cite series 120 illuminator (Lumen Dynamics Co., Ontario, Canada) and Retiga 2000R cooled CCD.



Figure S1. The UV-vis spectra of TaO_x powder.



Figure S2. The zeta potential of ZGGO:Cr,Pr; ZGGO:Cr,Pr@TaO_x@SiO₂; PEG-ZGGO:Cr,Pr@TaO_x@SiO₂ and NGR-ZGGO:Cr,Pr@TaO_x@SiO₂.



Figure S3. FT-IR spectra of cyclic (disulfide bond between cysteines) CNGRCGG peptide.

Figure S4. NIR afterglow decay images of PEG-ZGGO:Cr,Pr@TaO_x@SiO₂ powder recorded by CCD camera at different times after stopping 5 min UV irradiation.

Figure S5. *In vitro* cell viability of 3T3 cells and HepG2 cells incubated with PEG-ZGGO:Cr,Pr@TaO_x@SiO₂ at different concentrations for 24 h.

Figure S6.Representative H&E stained images of major organs including heart, liver, spleen, lung, and kidney collected from PEG-ZGGO:Cr,Pr@TaO_x@SiO₂ (0.3 mL, 1.0 mg mL⁻¹) injected mice (n = 3) and the control mice (n = 3, injected with PBS) at 7 day after administration. The scale bars is100 μ m for all images.

Figure S7. In vivo CT imaging of HepG2 tumor-bearing mice with PEG-ZGGO:Cr,Pr@TaO_x@SiO₂ through tail vein injection; (a) pre-injection, (b) 10 min post-injection, (c) 2 h post-injection.