## **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

Yu-Chen Lu, Cheng-Xiong Yang, and Xiu-Ping Yan\*

College of Chemistry, Research Center for Analytical Sciences, State Key Laboratory of Medicinal Chemical Biology (Nankai University), Tianjin Key Laboratory of Molecular Recognition and Biosensing, and Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University, 94 Weijin Road, Tianjin 300071, China-

\*Corresponding author. Fax: (86)22-23506075. E-mail: xpyan@nankai.edu.cn

## **Table of Contents**

Experimental Details Figure S1-Figure S7

## **Experimental Details**

**Histopathology**. The histological changes in the main organs of mice injected with PEG-ZGGO:Cr,Pr@TaO<sub>x</sub>@SiO<sub>2</sub> (300  $\mu$ L, 1 mg mL<sup>-1</sup>) or PBS (300  $\mu$ 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  $\mu$ 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<sub>x</sub>@SiO<sub>2</sub> or PEG-ZGGO:Cr,Pr@TaO<sub>x</sub>@SiO<sub>2</sub> (200  $\mu$ g mL<sup>-1</sup>) 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<sub>x</sub>@SiO<sub>2</sub>; PEG-ZGGO:Cr,Pr@TaO<sub>x</sub>@SiO<sub>2</sub> and NGR-ZGGO:Cr,Pr@TaO<sub>x</sub>@SiO<sub>2</sub>.



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<sub>x</sub>@SiO<sub>2</sub> 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<sub>x</sub>@SiO<sub>2</sub> 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<sub>x</sub>@SiO<sub>2</sub> (0.3 mL, 1.0 mg mL<sup>-1</sup>) injected mice (n = 3) and the control mice (n = 3, injected with PBS) at 7 day after administration. The scale bars is100  $\mu$ m for all images.



**Figure S7.** In vivo CT imaging of HepG2 tumor-bearing mice with PEG-ZGGO:Cr,Pr@TaO<sub>x</sub>@SiO<sub>2</sub> through tail vein injection; (a) pre-injection, (b) 10 min post-injection, (c) 2 h post-injection.