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## Photosensitizer Loaded MoS<sub>2</sub>-Au Hybrid for NIRF/CT Imaging-Guided Stepwise

## Photothermal and Photodynamic Therapy

Li Liu, Jingping Wang, Xiaoxiao Tan, Xiaojuan Pang, Qi sun, Qing You, Fengping Tan, and Nan

Li\*

\*Corresponding author at: School of Pharmaceutical Science and Technology, Tianjin University,

300072, Tianjin, PR China.

Tel.:+86-022-27404986

E-mail address: linan19850115@163.com



Figure S1. Calibration curve between the absorbance and the concentration of Ce6.



Figure S2. Size distribution of Au NPs.



Figure S3. Fluorescence emission spectra of free Ce6, the  $MoS_2$ -Au-Ce6 nanocomposite and  $MoS_2$ -Au hybrid at the same concentration (Ce6: 1.5 µg mL<sup>-1</sup>) and (MoS<sub>2</sub>-Au: 45 µg mL<sup>-1</sup>).



Figure S4. Photos of  $MoS_2$ -Au-Ce6 in water, PBS and cell medium after 5,000 rpm centrifugation, respectively.



Figure S5. UV-Vis spectrum of  $MoS_2$ -Au-Ce6 in cell medium over time.



Figure S6. a) Temperature evolution curve of PEG-MoS<sub>2</sub>+Au over a period of 10 min following exposure to the NIR laser (808 nm, 1.5 W cm<sup>-2</sup>). b) Photothermal image of PEG-MoS<sub>2</sub>+Au over following exposure to the NIR laser (808nm, 1.5 W cm<sup>-2</sup>, 10 min).



Figure S7. Biodistribution (heart, liver, spleen, lung and kidneys) of PEG-MoS<sub>2</sub>-AuNPs-Ce6 in 4T1 tumorbearing mice at different postinjection time points (0.5, 2, 4, 6, 12, 24 and 48 h). Data were presented as percent injected dose per gram (%ID/g)  $\pm$  standard deviation, n = 3.