

## Support Information

### Gd<sup>3+</sup>-doped MoSe<sub>2</sub> nanosheets as a theranostic agent for bimodal imaging and high efficiency cancer photothermal therapy

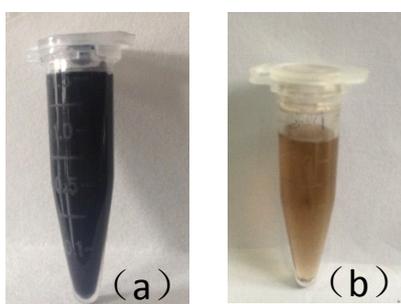
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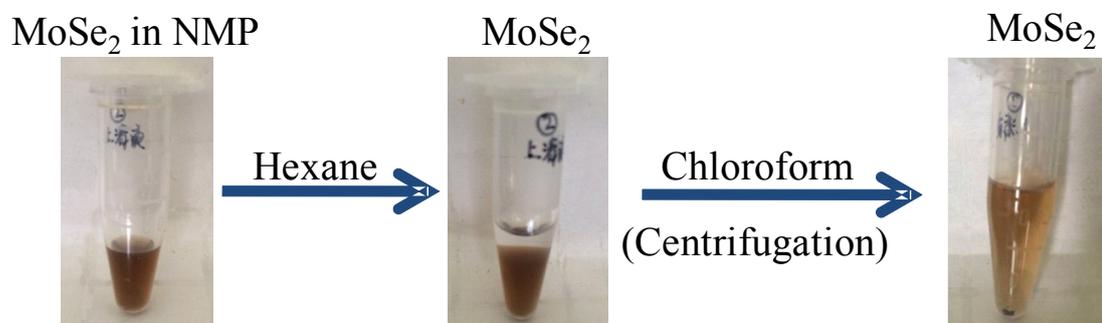
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<sup>1</sup> Both authors contributed equally to this work.

A



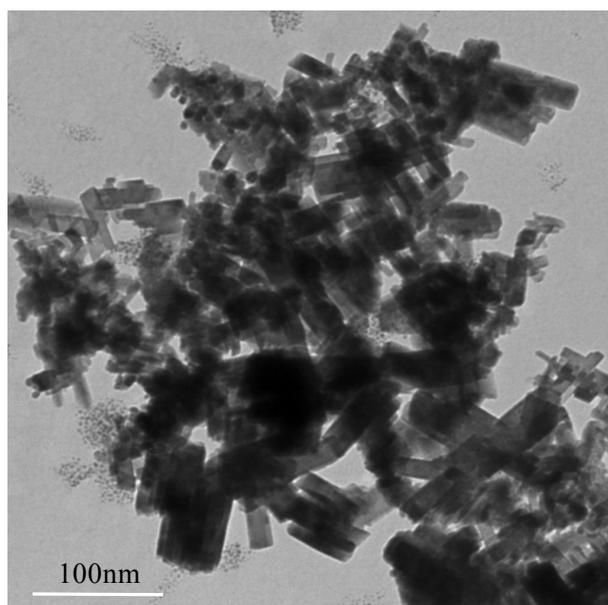
B



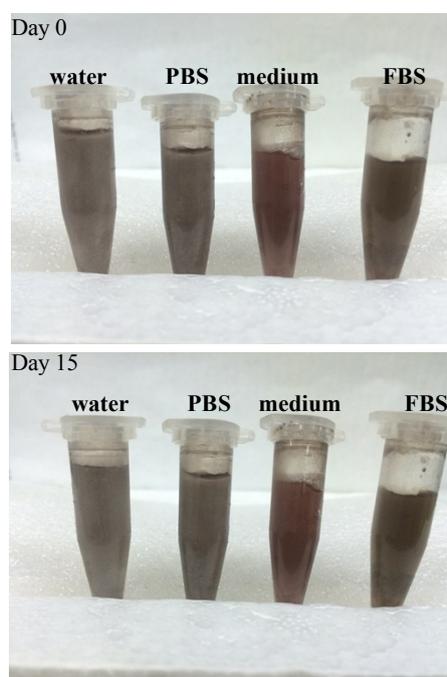
**Figure S1.** (A) Photographs of the suspensions of (a) raw MoSe<sub>2</sub> and (b) MoSe<sub>2</sub> treated with grinding and sonication.

(B) The separation process by addition of hexane and then chloroform, maybe followed by centrifugation..

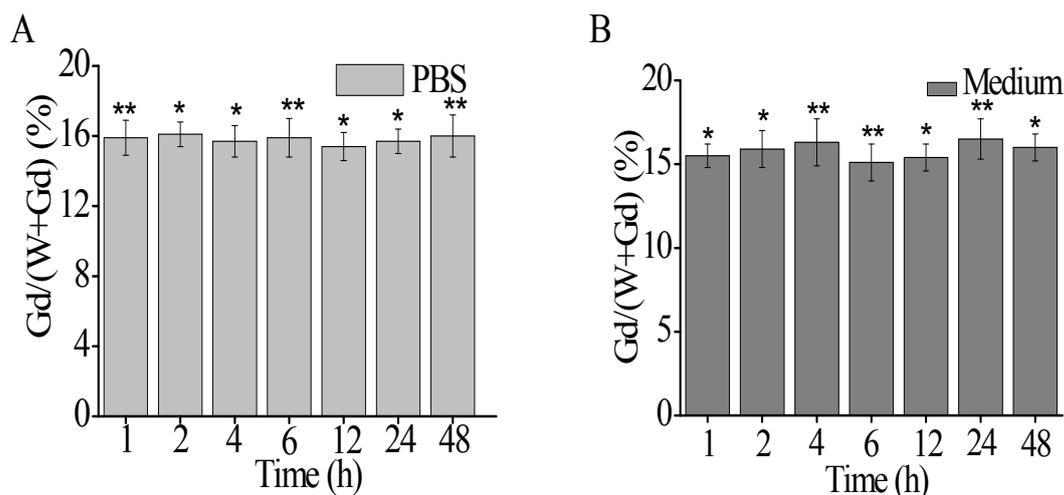
- (a) MoSe<sub>2</sub> dispersed in NMP after addition of hexane (NMP:hexane=1:1, v:v).
- (b) The dispersion in after addition of chloroform (NMP:chloroform=1:1, v:v), maybe accompanied by a small amount of precipitation.
- (c) Samples after centrifuging at 5,000 rpm for 10 min.



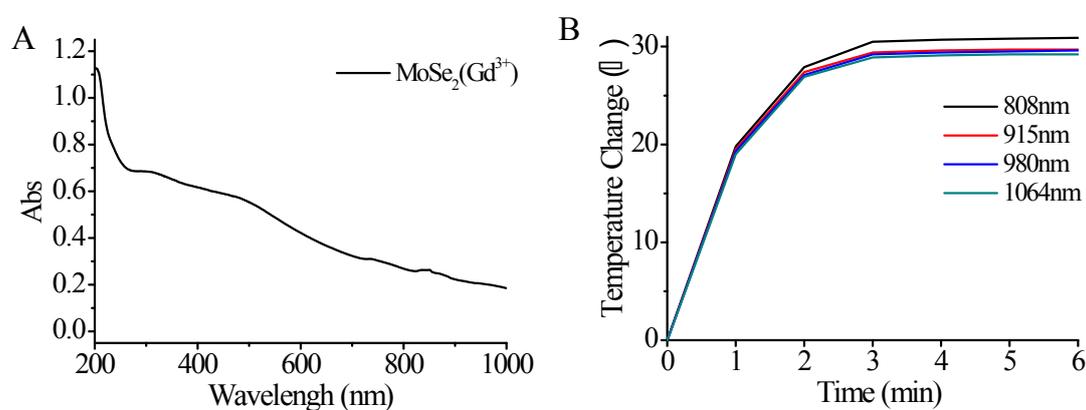
**Figure S2.** TEM image of PEGylated  $\text{MoSe}_2(\text{Gd}^{3+}\text{-3})$  nanosheets.



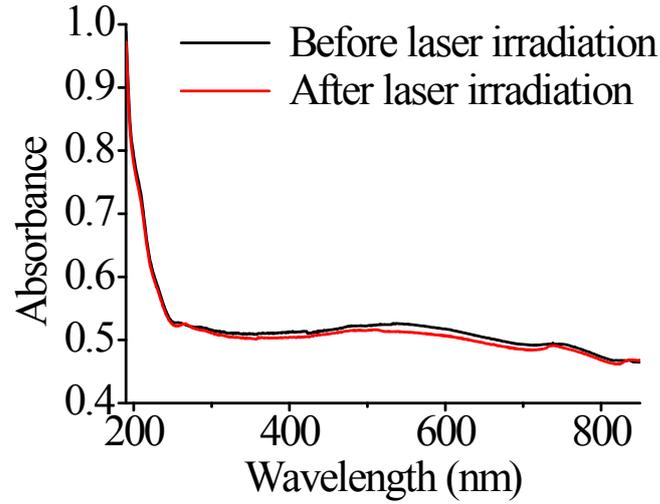
**Figure S3.** Photos of  $\text{MoSe}_2(\text{Gd}^{3+})$ -PEG nanosheets in water and physiological solutions, including phosphate buffered saline (PBS), cell culture medium, and fetal bovine serum(FBS) , after 0 (upper) or 15 days (bottom).



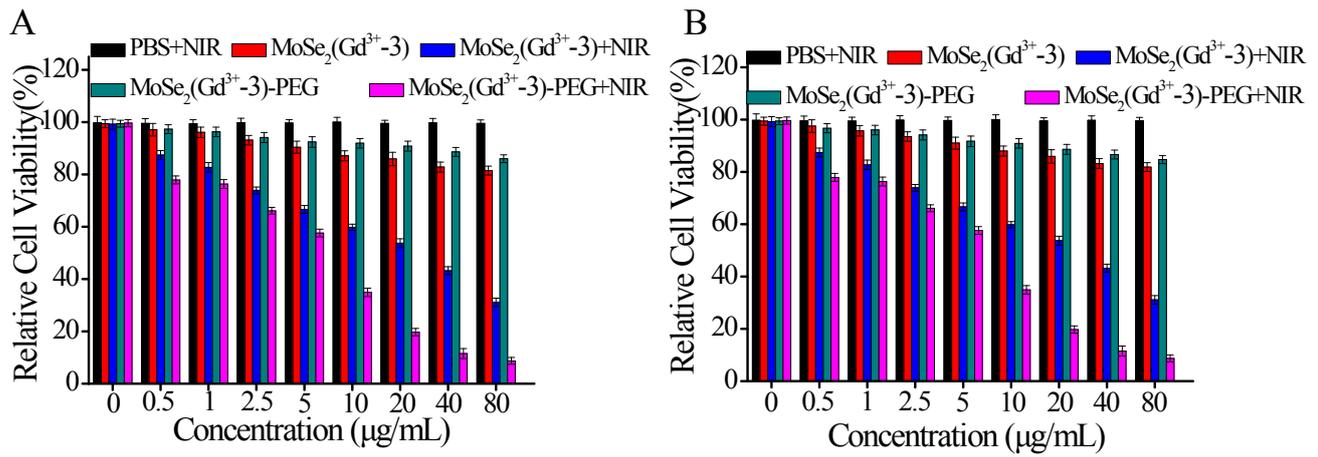
**Figure S4.** Stability of doped Gd<sup>3+</sup> in of MoSe<sub>2</sub>(Gd<sup>3+</sup>-3)-PEG nanosheets in PBS(A) or in cell culture medium(B) for different stored time. Those samples were determined by the ICP-AES to measure Gd<sup>3+</sup> percentages. No abrupt change of Gd<sup>3+</sup>-content in those samples was observed, suggesting no obvious leakage of doped Gd<sup>3+</sup> from of MoSe<sub>2</sub>(Gd<sup>3+</sup>-3)-PEG nanosheets. p values: \*p < 0.05, \*\*p < 0.01.



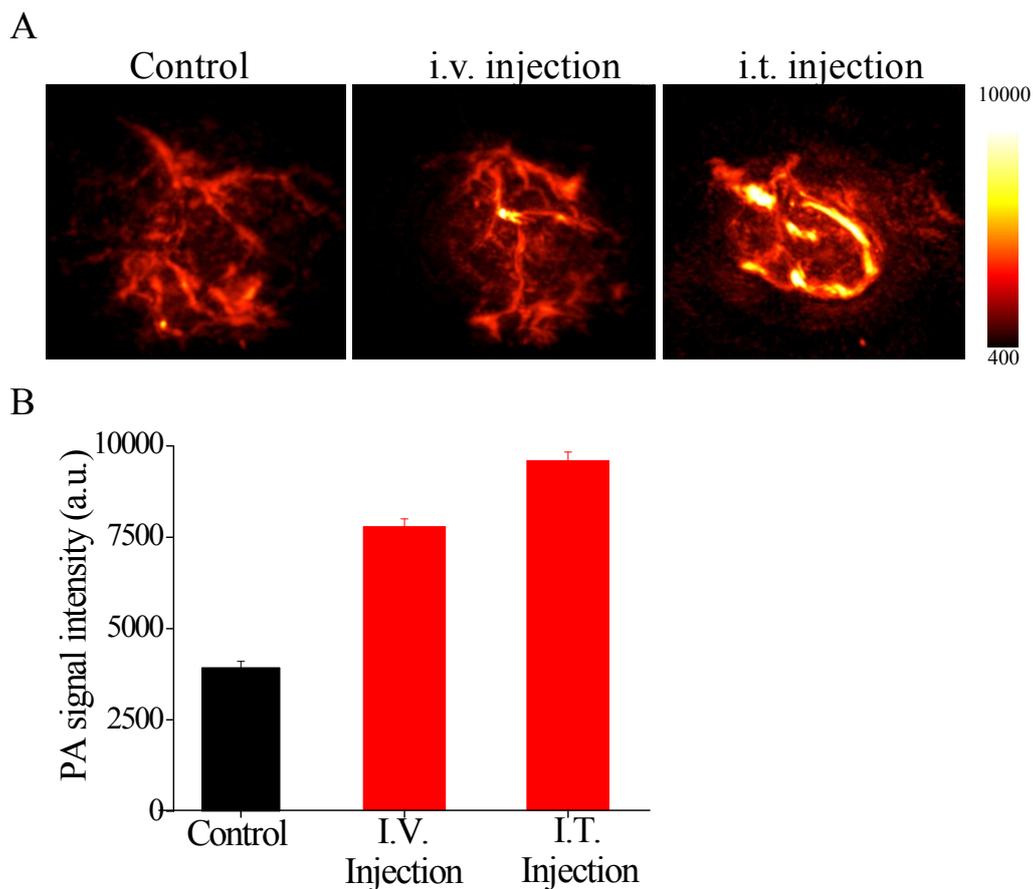
**Figure S5.** (A) UV-vis-NIR absorption spectrum of MoSe<sub>2</sub>(Gd<sup>3+</sup>)-PEG. (B) Photothermal heating curves of MoSe<sub>2</sub>(Gd<sup>3+</sup>)-PEG at the same concentrations under different NIR laser irradianations.



**Figure S6.** UV-vis-NIR spectra of the  $\text{MoSe}_2(\text{Gd}^{3+})$ -PEG nanosheets under 808 nm laser before and after irradiation at  $2 \text{ W/cm}^2$  for 60 min.



**Figure S7.** (A&B) Cell relative viabilities of 4T1 cells and SGC-7901 cells after being incubated with different concentrations of  $\text{MoSe}_2(\text{Gd}^{3+})$  or  $\text{MoSe}_2(\text{Gd}^{3+})$ -PEG for 24 h and then being exposed to the 808 nm NIR laser for 5 min.



**Figure S8.** (A) PA images of tumors on mice before and after i. t. or i. v. injection with  $\text{MoSe}_2(\text{Gd}^{3+}\text{-3})\text{-PEG}$ . (B) Photoacoustic signals inside the tumors before and after i. t. injections or i. v. injections of  $\text{MoSe}_2(\text{Gd}^{3+}\text{-3})\text{-PEG}$ . The injection dosages of i,t. injection and i.v. injection were 10 or 100  $\mu\text{L}$  at the concentration of 0.2 mg/mL, respectively.



**Figure S9.** Corresponding photographs of mice before treatment and after 14 days various treatments. Group (i): saline as the control; Group (ii): Only NIR laser irradiation; Group (iii): i.v. injection with  $\text{MoSe}_2(\text{Gd}^{3+}\text{-3})\text{-PEG}$ ; Group (iv): i.v. injection with  $\text{MoSe}_2(\text{Gd}^{3+}\text{-3})\text{-PEG+NIR}$ .