Supporting Information

Facile Preparation of Uniform FeSe₂ Nanoparticles for PA/MR Dual-modal

Imaging and Photothermal Cancer Therapy

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Supporting Figure S1. High magnification TEM images of FeSe₂ nanoparticles prepared by different reaction time (10 min, 30 min, and 60 min) under 150°C (**a**), and under different reaction temperatures (120 °C, 150 °C, and 300 °C) for the same period of time (30 min) (**b**).



Supporting Figure S2. DLS size of FeSe₂-PEG in various solutions including water, phosphate buffered saline (PBS), RMPI-1640 cell medium, and fetal bovine serum (FBS).



Supporting Figure S3. Even at lower pH value solution (pH=5.0), the PEGylated FeSe₂ nanoparticles still showed high stability (**Supporting Figure S3**).



Supporting Figure S4. A TEM image of as-synthesized Fe₃O₄ nanoparticles. The average nanoparticle diameter was *ca*. 6 ± 2.2 nm.



Supporting Figure S5. IR thermal images of $FeSe_2$ -PEG solutions at different concentrations and a Fe_3O_4 -DA solution at 0.4 mg/mL under irradiation by an 808 nm laser (0.8 W cm²) for 5 min.



Supporting Figure S6. Temperature variations of $FeSe_2$ -PEG (0.4 mg/mL) and Fe_3O_4 -DA (0.4 mg/mL) under irradiation by the 808-nm laser at the power density of 0.8 W/cm² for 5 cycles (6 min of irradiation for each cycle). It could be found the $FeSe_2$ -PEG should excellent photothermal stability and better photothermal effect than Fe_3O_4 -DA.



Supporting Figure S7. Representative photos of mice after various different treatments indicated taken 10 days after treatment.



Supporting Figure S8. Representation Prussian blue stained images of spleen collected from untreated control mice and FeSe₂-PEG (20 mg /kg) injected mice at different time points (1, 7, 14, and 30 days) post-injection.



Supporting Figure S9. H&E stained images of major organ (liver, spleen, kidney, heart, and lung) collected from untreated control mice and FeSe₂-PEG (20 mg/kg) injected mice at different time points (1 day, 7 days, 14 days and 30 days) post-injection.