

Supporting information

Ultrasmall and Metabolizable PEGylated NaGdF₄:Dy Nanoparticle for High-performance T₁/T₂-weighted MR and CT multimodal Imaging

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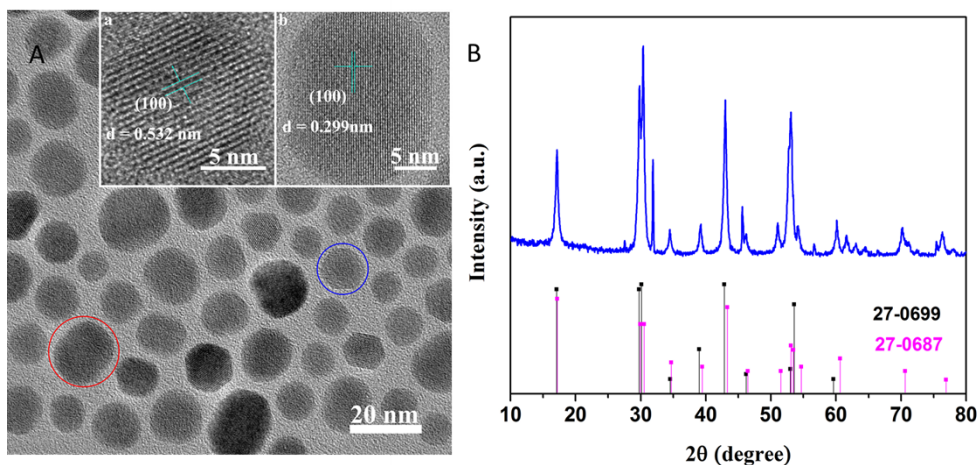


Fig. S1. Transmission electron microscopy (TEM) image (A) and XRD pattern of OA-NaGdF₄:Dy NPs obtained at 300 °C.

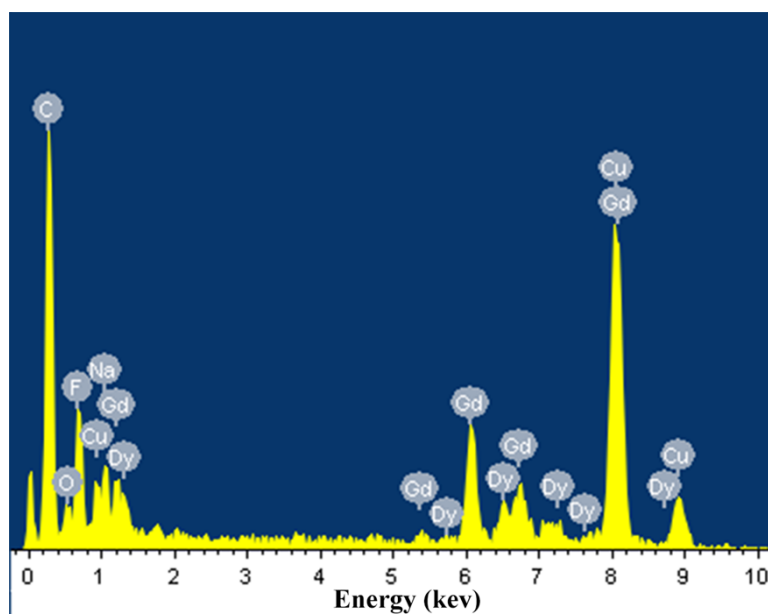


Fig. S2. X-ray energy dispersive spectroscopy (EDS) of the OA-NaGdF₄:Dy NPs.

Samples	NaGdF ₄ :Dy (20%)	NaGdF ₄ :Dy (30%)	NaGdF ₄ :Dy (40%)
Stoichiometric molar ratio of Gd/Dy	0.80:0.20	0.70:0.30	0.60:0.40
Actual molar ratio of Gd/Dy	0.766:0.234	0.659:0.341	0.528:0.472

Table S1. Stoichiometric and actual molar ratios of Gd/Dy in Dy-doped NaGdF₄ nanoparticles.

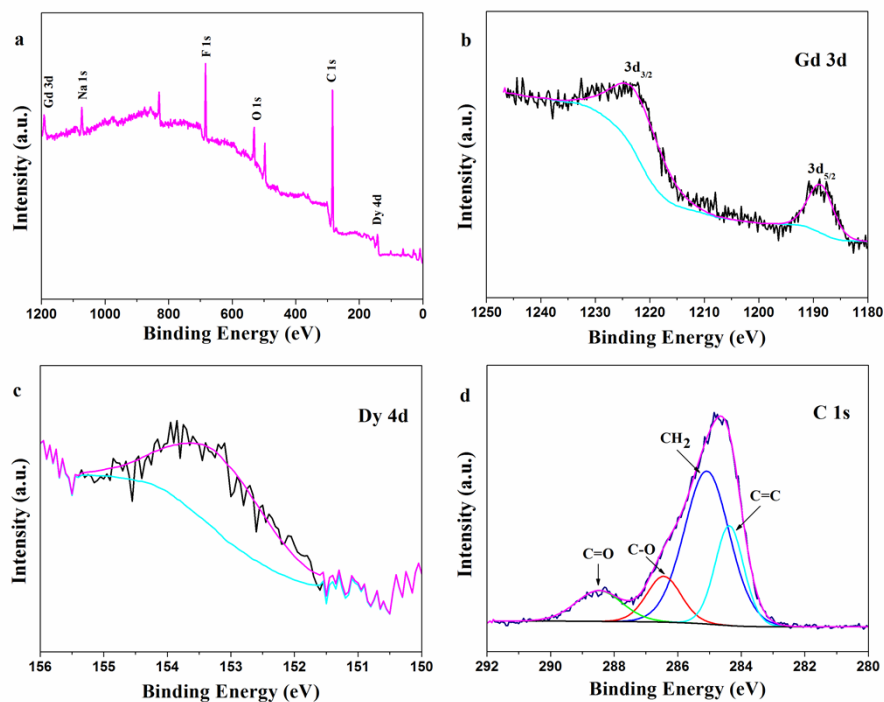


Fig. S3. XPS spectrum of prepared OA-NaGdF₄:Dy NPs (a). High resolution scan corresponding to Gd 3d (b), Dy 4d (c) and C 1s (d) region.

To further determine the successful doping of Dy ions into NaGdF₄ substrates, X-Ray photoelectron spectroscopy (XPS) was carried out.^{1,2} The survey spectrum of OA-NaGdF₄:Dy NPs mainly included carbon (C), oxygen (O), fluorine (F), sodium (Na), gadolinium (Gd) and dysprosium (Dy) (Fig. S3a). The peaks observed at 1224.2 and 1188.2eV can be assigned to the Gd 3d_{3/2} and Gd 3d_{5/2}, respectively. (Fig. S3b). The peak located at 153.7 eV corresponded to the binding energy of Dy 4d (Fig. S3c). Furthermore, for the C 1s peaks (Fig. S3d), the strongest peak could be separated into three characteristic peaks at 286.45 eV, 285.05 eV and 284.40 eV, corresponding well to C-O, C-H and C=C binding energy. The other peak located at 288.55 eV was attributed to the binding energy of C=O of OA molecules. These results further confirmed that the doping of Dy element into the NaGdF₄ substrates had successfully been performed.

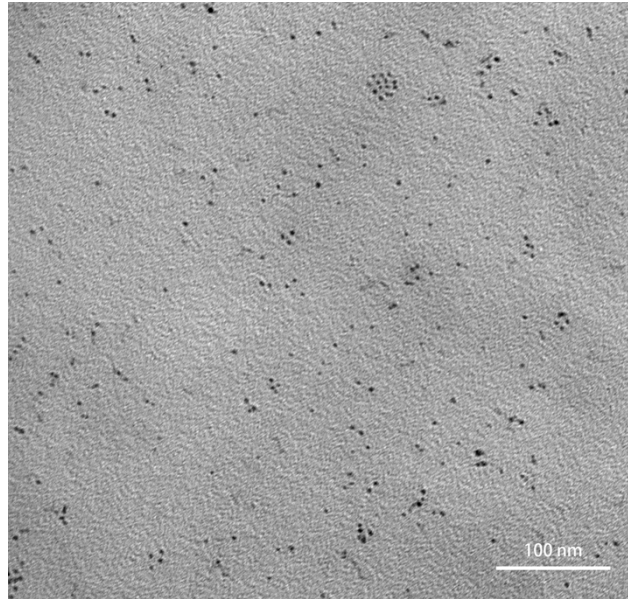


Fig. S4. Transmission electron microscopy (TEM) image of PEG-NaGdF₄ NPs obtained at 240 °C.

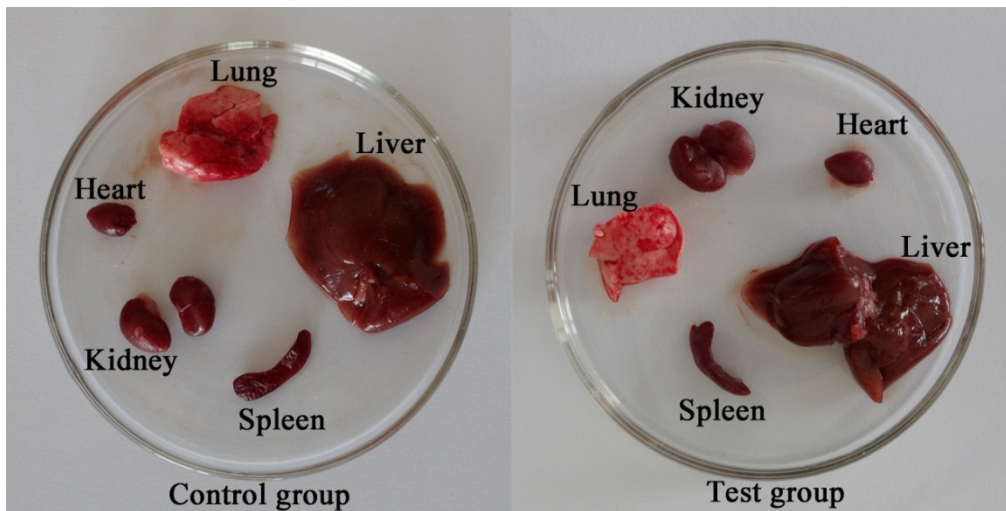


Fig. S5. The major organs (heart, liver, spleen, lung and kidney) of mice in the control and test group.

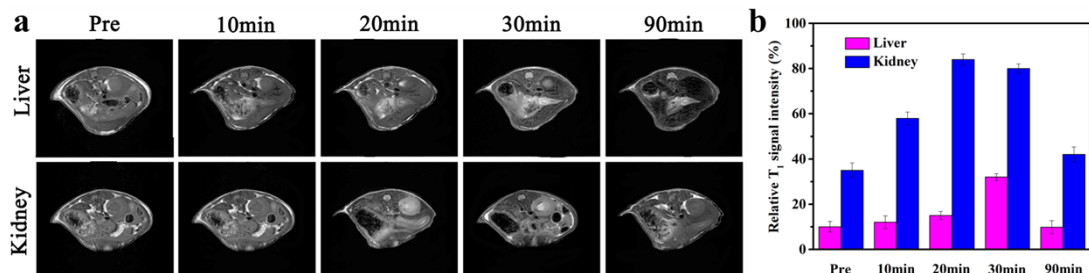


Fig. S6. *In vivo* T_1 -weighted MRI of Gd-DTPA (a), and the relative T_1 signal intensity of liver and kidney (b).

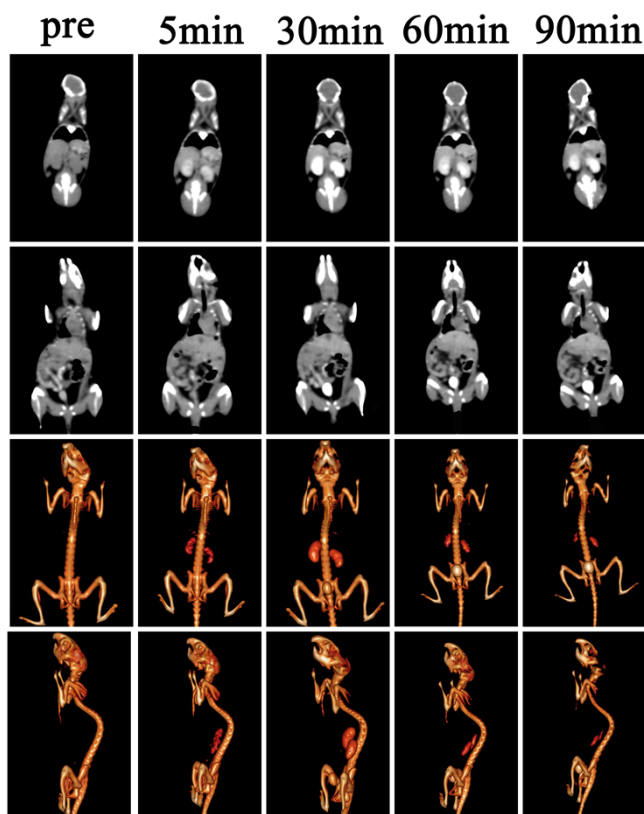


Fig. S7. *In vivo* CT coronal view images of the mice before and after intravenous injection of iohexol ($100 \mu\text{L}$, 50 mg I mL^{-1}) at different time intervals.

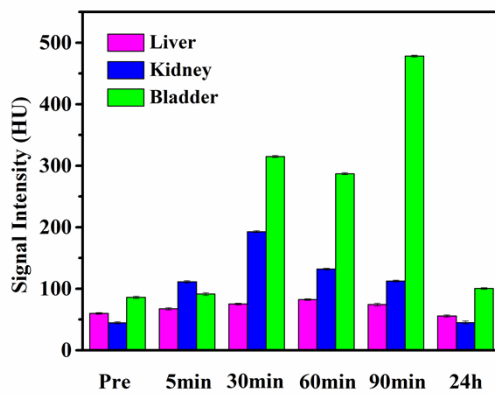


Fig. S8. The relative CT values of liver, spleen and bladder before and after injection of iohexol ($100 \mu\text{L}$, 50 mg I mL^{-1}) at different time intervals.

References

1. G. Gao, C. L. Zhang, Z. J. Zhou, X. Zhang, J. B. Ma, C. Li, W. L. Jin and D. X. Cui, *Nanoscale*, 2013, 5, 351-362.
2. Y. L. Liu, K. L. Ai, J. H. Liu, Q. H. Yuan, Y. Y. He and L. H. Lu, *Angew. Chem. Int. Ed.*, 2012, 51, 1437-1442.