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Supporting Information

Nd³⁺-doped LiYF₄ nanocrystals for the bio-imaging in the second near-infrared window

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Fig. S1 (a-e) TEM images of LiYF₄: x% Nd³⁺ NPs, x = 1.0, 3.0, 5.0, 7.0, 10.0. Scale bar = 100 nm. Inset: size distribution. Red bars represent the length and blue bars represent the width of the NPs. (f) TEM image of NaYF₄: 5% Nd³⁺. Scale bar = 100 nm. (g) XRD pattern of LiYF₄: x% Nd³⁺ NPs, x = 1.0, 3.0, 5.0, 7.0, 10.0., and the standard PDF card of tetragonal LiYF₄.



Fig. S2. EDXA analysis of LiYF₄: Nd³⁺ NPs.



Fig. S3. The testing result of the quantum yield of LiYF_4 : 5% Nd³⁺ NPs. The blank solution was pure cyclohexane. Inset: the enlarged spectrum from 850 nm to 1150 nm.



Fig. S4. Fluorescence spectra of cyclohexane solution of OA-NaYF₄: x% Nd³⁺ NPs, x=3.0, 5.0, 7.0.



Fig. S5. Dynamic light scattering (DLS) analysis of EDTMP-LiYF₄: 5% Nd³⁺ NPs.



Fig. S6 The quantum efficiency of the CCD. This figure was obtained from the instrument manual.



Fig. S7 The transmittance of the 980 nm long-pass edge filter. This figure was obtained from the website of manufacturer. (<u>http://www.semrock.com/FilterDetails.aspx?id=BLP01-980R-25</u>)



Fig. S8 NIR II images of a (a) nude mouse, (b) nude mouse after removal of skin and fat tissues above, (c) Kunming mouse, (d) Kunming mouse after removal of skin and fat tissues above, (e) mouse food..



Fig. S9. (a)*In vivo* blood vessel NIR II imaging of a Kunming mouse immediately after intravenous injection. (b) The NIR II imaging after removal of skin and fat tissues. (c) The NIR II imaging of removed heart, liver, spleen, lung and kidneys. Scale bar = 1 cm. The regions of interest (ROI) are marked using blue areas. The mean intensity of ROI 1(specific uptake), ROI 2 (nonspecific uptake) and ROI 3 (background) were collected for the signal-to-noise ratio (SNR) calculation (see Table S1)



Fig. S10. Histology test of LiYF₄: Nd³⁺ NPs. (a-j) 1 day after injection, (k-t) 7 days after injection.



Fig. S11. Histology analysis of the lymph nodes taken out in lymphatic imaging.(a) The axillary lymph node, (b-c) the lymph nodes at leg.

| Fig. | ROI | Intensity | SNR |
|----------|-------|-----------|-------|
| Fig. 5. | a-1 | 43756.300 | 14.8 |
| | a-2 | 7085.399 | / |
| | a-3 | 4422.621 | / |
| | b-1 | 56193.610 | 18.9 |
| | b-2 | 5853.926 | / |
| | b-3 | 3035.600 | / |
| | c-1 | 60492.190 | 113.9 |
| | c-2 | 1156.357 | / |
| | c-3 | 630.939 | / |
| | d-1-1 | 35599.050 | 13.2 |
| | d-1-2 | 28844.880 | 10.5 |
| | d-2 | 5144.828 | / |
| | d-3 | 2651.378 | / |
| | e-1-1 | 42494.360 | 11.0 |
| | e-1-2 | 44104.910 | 11.4 |
| | e-2 | 5966.592 | / |
| | e-3 | 2303.210 | / |
| | f-1-1 | 50666.520 | 51.1 |
| | f-1-2 | 51395.770 | 51.9 |
| | f-2 | 2186.726 | / |
| | f-3 | 1219.451 | / |
| Fig. S9. | a-1 | 4332.542 | 12.8 |
| | a-2 | 1538.827 | / |
| | a-3 | 1301.266 | / |
| | b-1 | 6289.621 | 9.8 |
| | b-2 | 1607.336 | / |
| | b-3 | 1077.212 | / |
| | c-1 | 6247.757 | 27.4 |

| Fig. | ROI | Intensity | SNR |
|------|-----|-----------|-----|
| | c-2 | 985.229 | / |
| | c-3 | 785.677 | / |

Table S1.The SNR (signal-to-noise ratio) of bio-imaging in Fig. 5 and Fig. S6. The regions of interest (ROI) are marked using blue areas in the figures. The mean intensity of ROI 1(specific uptake), ROI 2 (nonspecific uptake) and ROI 3 (background) were collected for the SNR calculation. SNR = ($I_{ROI1} - I_{ROI3}$) / ($I_{ROI2} - I_{ROI3}$).