

Supporting Information

Soft X-ray activated NaYF₄: Gd/Tb scintillating nanorods for *in vivo* dual-modal X-ray/X-ray-induced optical bioimaging

*Xiaolong Li,^a Zhenluan Xue,^a Mingyang Jiang,^a Youbin Li,^a Songjun Zeng,^{*a} and Hongrong Liu^{*a}*

^a College of Physics and Information Science and Key Laboratory of Low-dimensional Quantum Structures and Quantum Control of the Ministry of Education, Synergetic Innovation Center for Quantum Effects and Applications, and Hunan Normal University, Changsha, Hunan, People's Republic of China.

Email: songjunz@hunnu.edu.cn, hrliu@hunnu.edu.cn

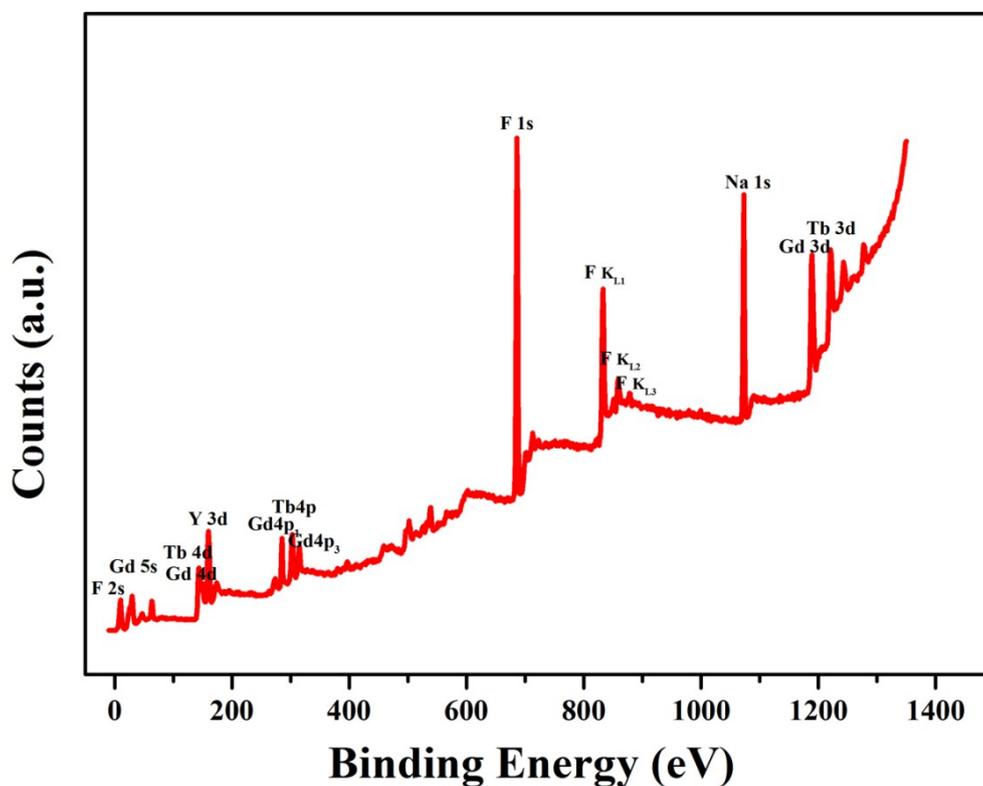


Fig. S1 The XPS spectra of the as-synthesized NaYF₄: 40%Gd/15%Tb NRs. The 2s level of F at 32 eV, 5s level of Gd at 38 eV, 4d level of Gd and Tb at 148 eV, 3d level of Y at 165 eV, 4p₃ level and 4p₁ of Gd at 272 eV and 303 eV, 4p level of Tb at 280 eV, 1s level of F at 691 eV, K_{L1}, K_{L2} and K_{L3} levels of F at 837, 864 and 882 eV, 1s level of Na at 1078 eV, 3d level of Gd at 1221 eV, 3d level of Tb at 1227 and 1243 eV.

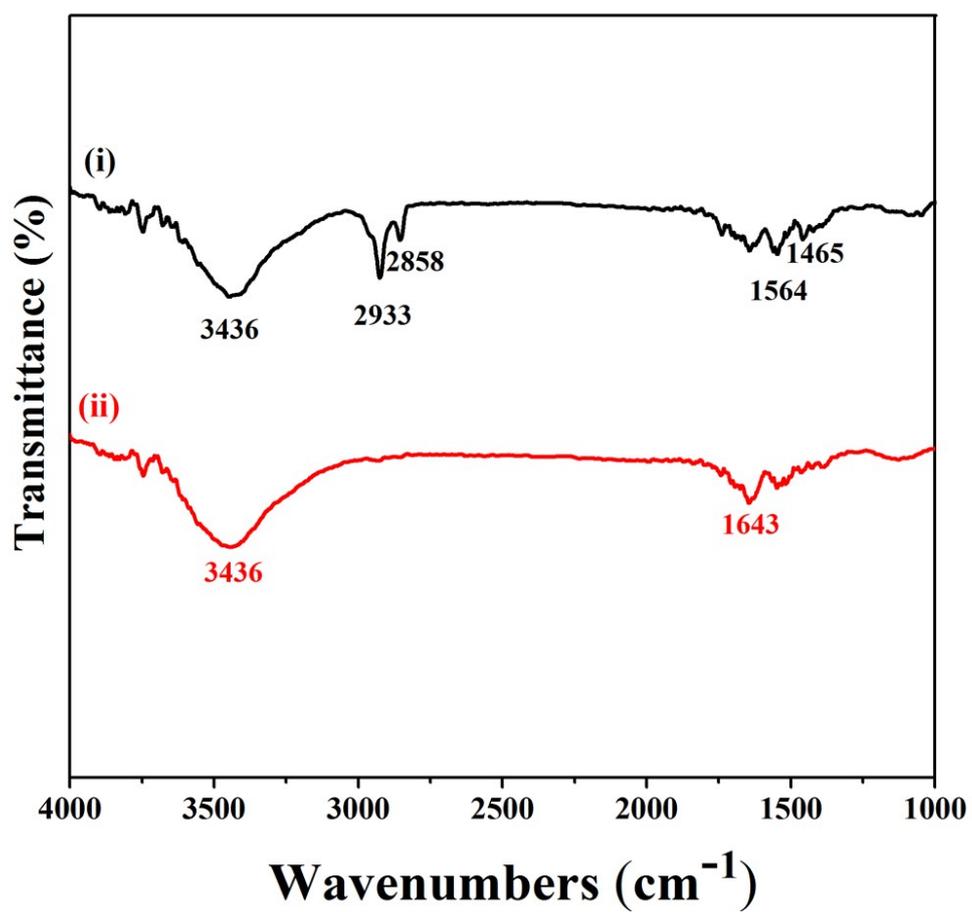


Fig. S2 The FTIR spectra of oleate-capped NRs (i) and LF-NRs (ii).

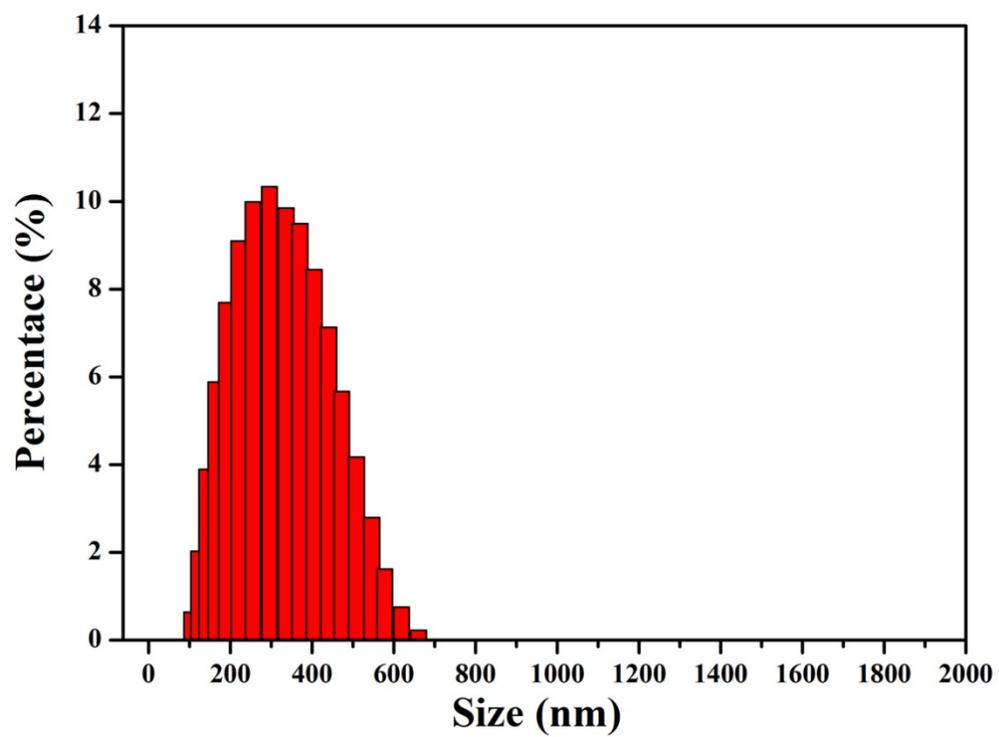


Fig. S3 The size distribution of LF-NRs determined by DLS.

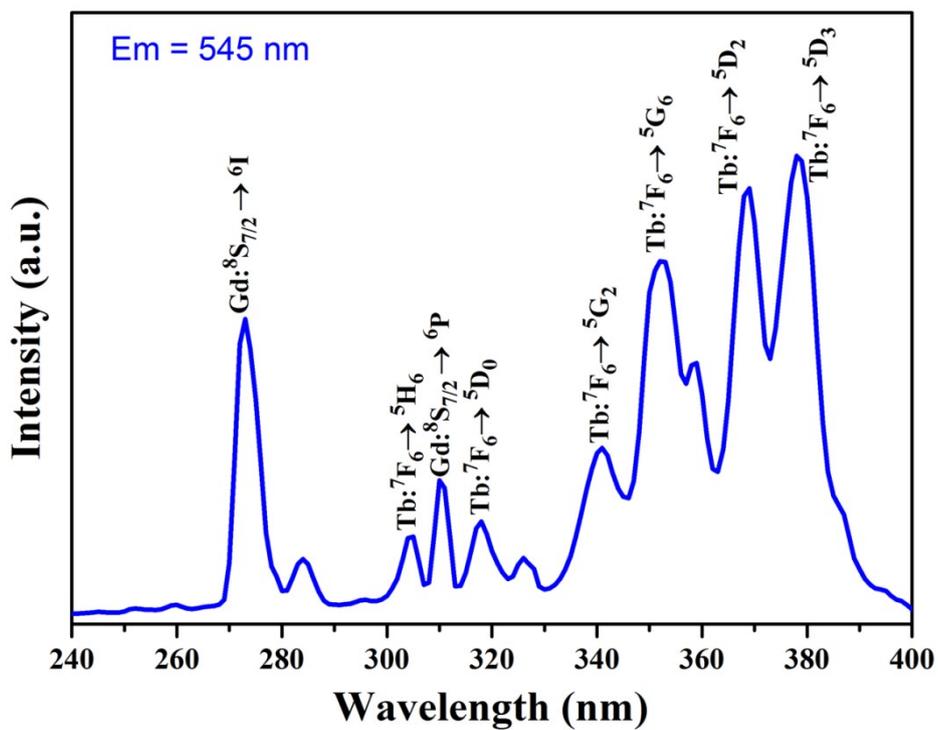


Fig. S4 Photoluminescence excitation spectrum of NaYF₄: 40%Gd/15%Tb NRs.

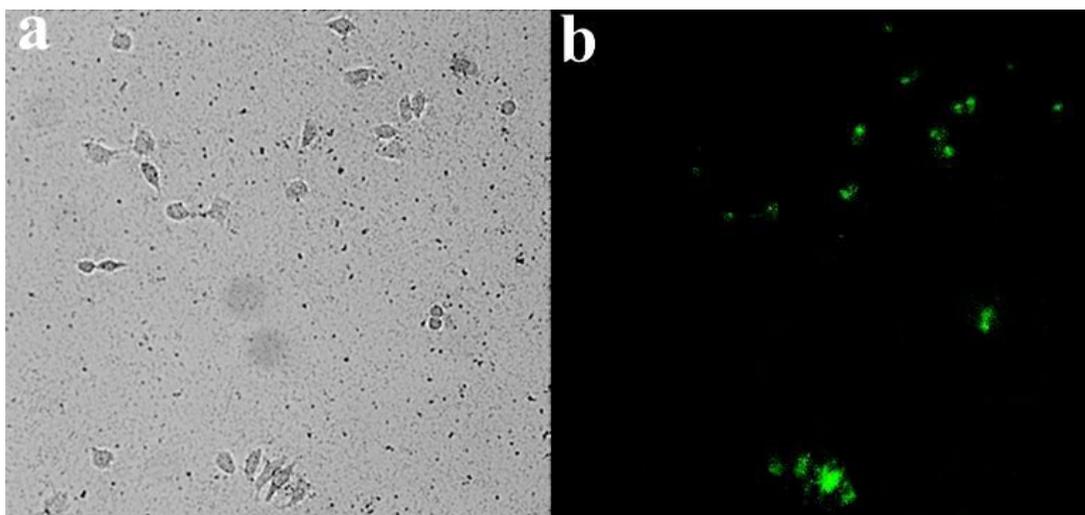


Fig. S5 *In vitro* optical bioimaging of HeLa cell treated with the LF-NRs: (a) bright field image; (b) green fluorescence emission image;

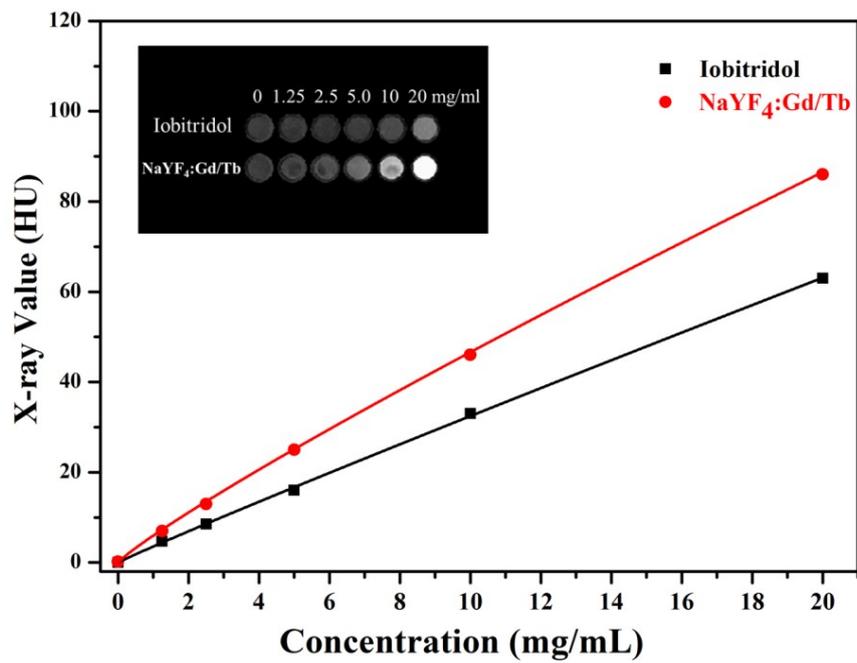


Fig. S6 The X-ray value (HU) of LF-NRs (red line) and Iobitridol (black line) as a function of concentration of the two agents, respectively. The inset shows X-ray imaging based on LF-NRs and iobitridol with different concentrations.

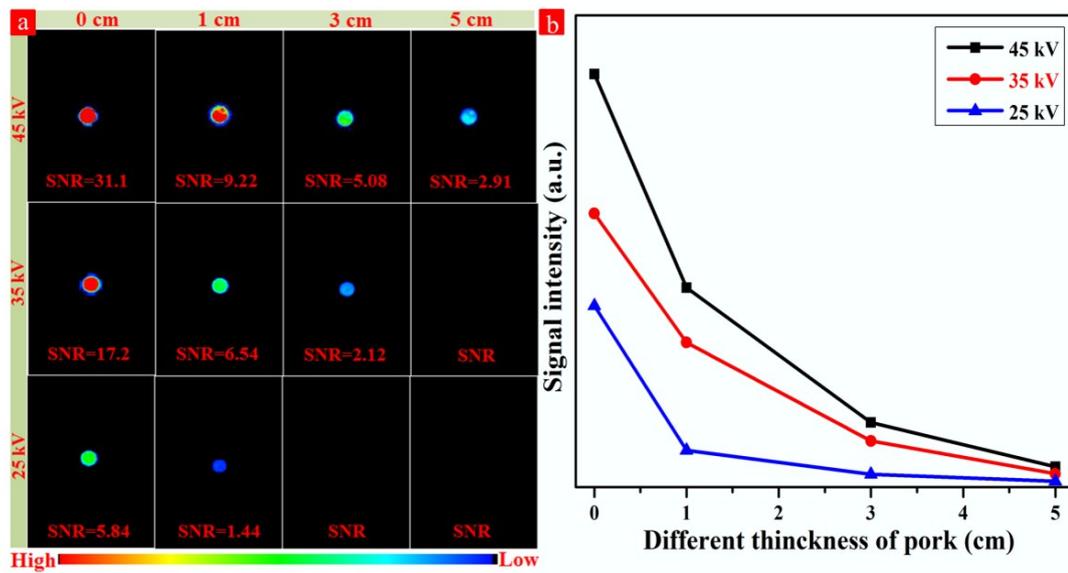


Fig. S7 (a) *In vitro* phantom optical imaging of NaYF₄: 40%Gd/15%Tb covered with different thicknesses of pork tissue between the sample and light source under the excitation of different voltages of soft X-ray (1 min). (b) The average signal intensity curves of different thicknesses of pork tissue under different excited voltages.

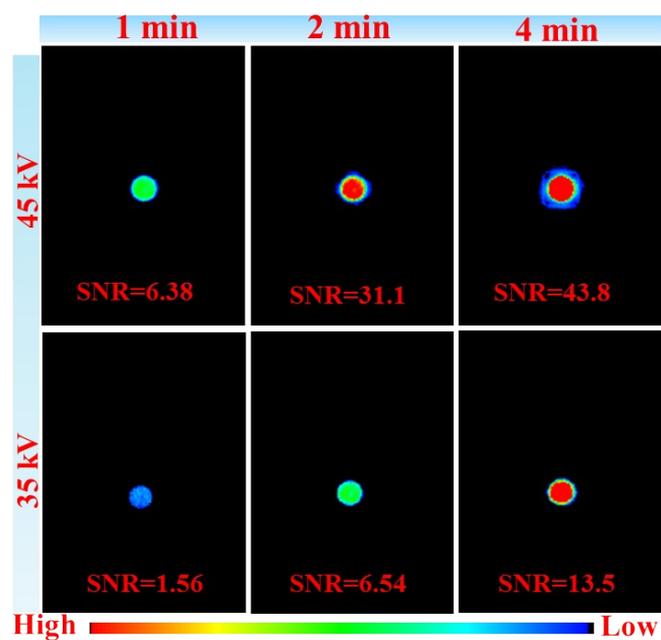


Fig. S8 *In vitro* phantom optical imaging of NaYF₄: 40%Gd/15%Tb covered with 2 cm thicknesses of pork tissue (between sample and light source) excited by different voltages and different times of soft X-ray.

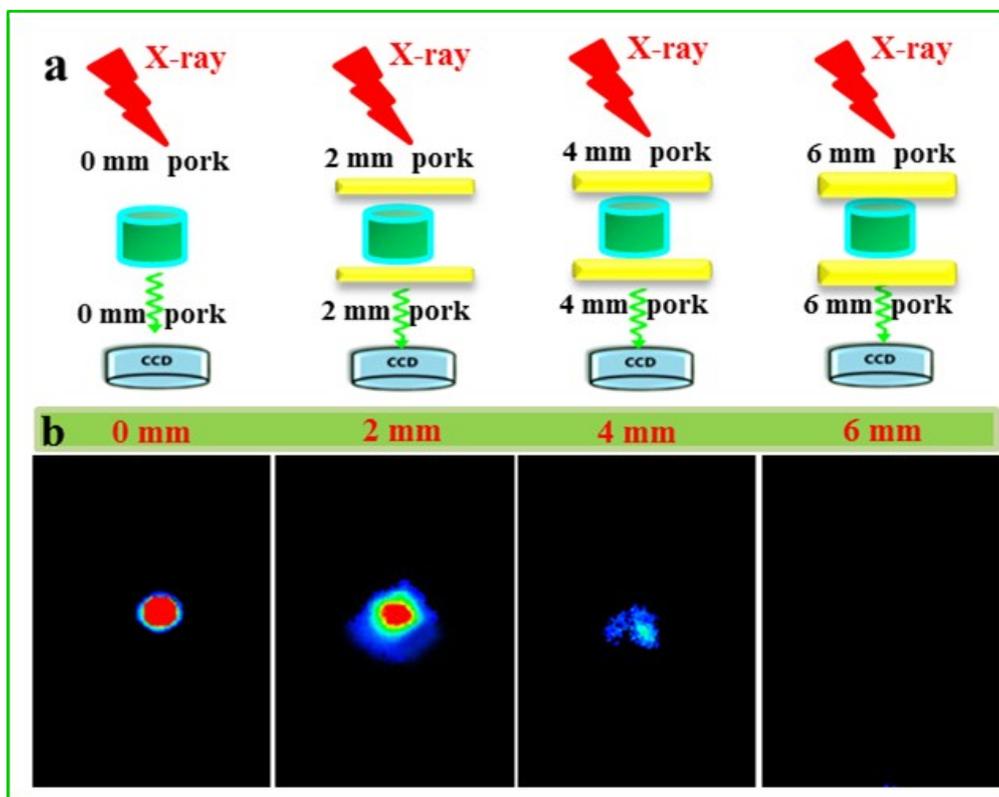


Fig. S9 (a) A schematic illustration of excitation/emission-related penetration depth of NRs covered with various thicknesses of pork slices. (b) *In vitro* phantom optical imaging of NaYF₄: 40%Gd/15%Tb covered with different thicknesses of pork tissues excited by soft X-ray (45 kVp, 1min).

Table S1: The average lengths and widths of NaYF₄: Gd/x% Tb NRs (x % Tb, x = 1, 2, 5, 10, 15, 25, and 35).

Size (X% Tb)	1 %	2 %	5 %	10 %	15 %	25 %	35 %
Length	263 nm	284 nm	272 nm	280 nm	286 nm	304 nm	310 nm
width	20 nm	21 nm	19nm	18 nm	18 nm	16 nm	15 nm

Table S2: List of the operated voltage and current of the X-ray source.

X-ray	this work	Xing's work ^[s1]	clinical X-ray ^[s2]
voltage	45 kVp	320 kVp	120 – 140 kVp
current	0.5 mA	12.5 mA	100 – 320 mA

[s1] D. J. Naczynsk, C. Sun, S. Türkcan, C. Jenkins, A. L. Koh, D. Ikeda, G. Pratz and L. Xing, *Nano Lett.*, 2015, **15**, 96.

[s2] J. M. Boone, T. R. Nelson, K. K. Lindfors, and J. A. Seibert, *Medical Physics*, 2001, **221**, 657.