## **Supporting Information**

Aqueous Phase Synthesis of Upconversion Nanocrystals through Layer-by-layer Epitaxial

Growth for in-vivo X-Ray Computed Tomography

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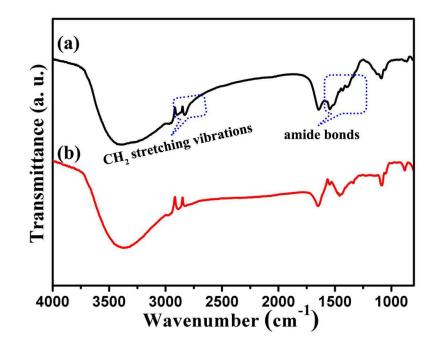
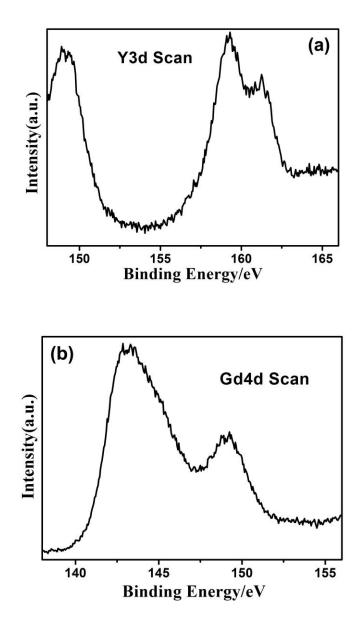


Figure S1. FT-IR spectrum of (a) pure NaYF<sub>4</sub>:Yb, Er@NaGdF<sub>4</sub> core-shell UCNCs

and (b) PEI capped NaYF<sub>4</sub>:Yb, Er@NaGdF<sub>4</sub> core-shell UCNCs.



**Figure S2**. X-ray photoelectron spectra of 4-layer NaYF<sub>4</sub>:Yb, Er@NaGdF<sub>4</sub> core-shell UCNCs. (a) Y3d Scan; (b) Gd4d Scan.

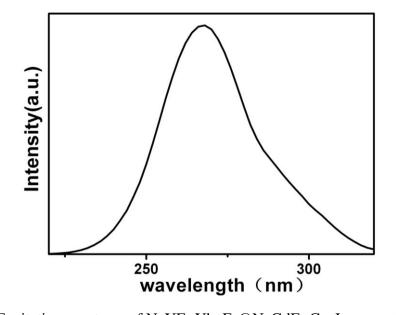
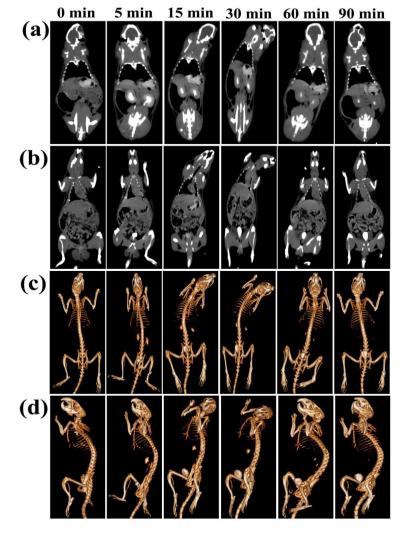


Figure S3. Excitation spectrum of NaYF4:Yb, Er@NaGdF4:Ce, Ln core-shell

UCNCs.



**Figure S4**. *In vivo* upconversion luminescence digital photos of a rat by intravenous NaYF<sub>4</sub>:Yb, Er@NaGdF<sub>4</sub> core-shell UCNCs injection irradiated under 980 nm laser.



**Figure S5**. *In vivo* CT coronal view images of a rat before and after intravenous injection of 0.3 mL of Iobitridol (350 mg I mL<sup>-1</sup>) at timed intervals. (a) Spleen and kidney. (b) Heart, liver and bladder. (c,d) The corresponding 3D-renderings of *in vivo* CT images.

**Table S1** CT values of the heart, liver, spleen and kidney of a rat before and after intravenous administration of 1 mL of 4-layer core/shell UCNCs solution (480 mg Gd mL<sup>-1</sup>) at timed intervals. 237.6 was the CT value of renal pelvis.

Time	heart	liver	spleen	kidney
Pre-injection	50	67.3	58.0	40.0
5 min	69.1	151.2	100	69.6
15 min	54.5	178.2	104.5	78.1
30 min	50.5	201.6	111.0	87.9
60 min	50.3	220.2	116.8	84.4
90 min	50.0	196.4	112.3	80.0

**Table S2.** CT values of the heart, liver and kidney of a rat before and after intravenous administration of 0.3 mL of Iobitridol ( $350 \text{ mg I mL}^{-1}$ ) at timed intervals. 599.9 and 703.8 were the CT values of renal pelvis.

Time	heart	liver	bladder	kidney
Pre-injection	46.4	58.7	52.1	43.5
5 min	63.0	73.9	951.0	106.5, 707.5
15 min	59.1	77.6	1462.8	86.2, 528.2
30 min	53.0	55.6	2731.7	70.4, 412.5
60 min	49.1	78.0	2975.5	62.0, 182.2
90 min	49.0	66.8	1937.0	48.7, 217.2