Supplementary Information

## Possible Gadolinium Ions Leaching and MR Sensitivity Over-Estimation in Mesoporous Silica-Coated Upconversion Nanocrystals

Shengjian Zhang, ‡ Zhaoxia Jiang, ‡ XiaoHang Liu, Liangping Zhou, Weijun Peng\*

Department of Radiology, Fudan University Shanghai Cancer Center; Department of

Oncology, Shanghai Medical College, Fudan University, Shanghai 200032, China

E-mail: weijunpeng@yahoo.cn



**Figure S1.** High resolution TEM image of highly crystalline  $NaYF_4$ :Er/Yb@NaGdF<sub>4</sub>. White line represents the boundary of  $NaYF_4$  and  $NaGdF_4$ .



**Figure S2.** (A) T<sub>2</sub>-map of free Gd<sup>3+</sup> ions. (B) Plot of  $R_2$  (1/s) versus Gd<sup>3+</sup> ion concentration (mM), the slop indicates the specific relaxivity ( $r_2$ ).  $r_2/r_1 = 2.2$ .



**Figure S3.** (A) T<sub>2</sub>-map of Core@NaGdF<sub>4</sub>@m-SiO<sub>2</sub> (inner core damaged). (B) Plot of  $R_2$  (1/s) versus Gd<sup>3+</sup> ion concentration (mM), the slop indicates the specific relaxivity ( $r_2$ ).  $r_2/r_1 = 9.6$ .



**Figure S4.** (A) T<sub>2</sub>-map of Core@NaGdF<sub>4</sub>@m-SiO<sub>2</sub> obtained by calcination. (B) Plot of  $R_2$  (1/s) versus Gd<sup>3+</sup> ion concentration (mM), the slop indicates the specific relaxivity ( $r_2$ ).  $r_2/r_1 = 59.3$ .



**Figure S5.** (A) T<sub>2</sub>-map of Core@NaGdF<sub>4</sub>@d-SiO<sub>2</sub>. (B) Plot of  $R_2$  (1/s) versus Gd<sup>3+</sup> ion concentration (mM), the slop indicates the specific relaxivity ( $r_2$ ).  $r_2/r_1 = 9.6$ .



Figure S6. MTT cell viability assay of UCNP@m-SiO<sub>2</sub> after different treatments to extract CTAB on HeLa cells for 24 h incubation. To decrease the cytotoxicity of calcined nanoparticles, they were subject to centrifuge at 3000 r/min for 3 min to exclude large-sized nanoparticles.



Figure S7. DLS measurements of  $Core@NaGdF_4@m-SiO_2$  before and after calcinations.