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 NaYF₄:Eu/Yb@NaGdF₄. White line represents the boundary of NaYF₄ and NaGdF₄.
Figure S2. (A) T₂-map of free Gd³⁺ ions. (B) Plot of $R_2$ (1/s) versus Gd³⁺ ion concentration (mM), the slop indicates the specific relaxivity ($r_2$). $r_2/r_1 = 2.2$. 

$r_2 = 19.69 \text{ mM}^{-1} \text{s}^{-1}$
Figure S3. (A) T₂-map of Core@NaGdF₄@m-SiO₂ (inner core damaged). (B) Plot of $R_2$ (1/s) versus Gd³⁺ ion concentration (mM), the slope indicates the specific relaxivity ($r_2$). $r_2/r_1 = 9.6$. 

$r_2 = 62 \text{ mM}^{-1} \text{s}^{-1}$
**Figure S4.** (A) $T_2$-map of Core@NaGdF$_4$@m-SiO$_2$ obtained by calcination. (B) Plot of $R_2$ (1/s) versus Gd$^{3+}$ ion concentration (mM), the slop indicates the specific relaxivity ($r_2$). $r_2/r_1 = 59.3$. 

$$r_2 = 181 \text{ mM}^{-1} \text{s}^{-1}$$
**Figure S5.** (A) T$_2$-map of Core@NaGdF$_4$@d-SiO$_2$. (B) Plot of $R_2$ (1/s) versus Gd$^{3+}$ ion concentration (mM), the slope indicates the specific relaxivity ($r_2$). $r_2/r_1 = 9.6$. 
**Figure S6.** MTT cell viability assay of UCNP@m-SiO$_2$ 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.