## **Supporting Information of:**

## PEG-capped, lanthanide doped GdF<sub>3</sub> nanoparticles: luminescent and T<sub>2</sub> contrast agents for optical and MRI multimodal imaging

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**Figure SF1.** XRPD pattern (black line) and Rietveld refinement (red line) for PEG-capped  $GdF_3$ :  $Er^{3+}$ ,  $Yb^{3+}$  NPs ( $R_w$ =0.0801). Lower line: residuals between experimental and calculated data.



**Figure SF2.** XRPD pattern for uncapped GdF<sub>3</sub>: $Er^{3+}$ , Yb<sup>3+</sup> NPs. Similar pattern has been obtained for the GdF<sub>3</sub>: $Tm^{3+}$ , Yb<sup>3+</sup> NPs.



**Figure SF3**. X-ray powder diffraction patterns for  $\text{Er}^{3+}/\text{Yb}^{3+}$  doped GdF<sub>3</sub> NPs prepared under different heat treatments: (a) 140 °C; (b) 160 °C; (c) 180 °C. Similar results have been found for the Tm<sup>3+</sup>/Yb<sup>3+</sup> doped GdF<sub>3</sub> NPs.



**Figure SF4**. Short edge size distribution for the  $GdF_3$ : $Tm^{3+}$ , $Yb^{3+}$  NPs. Similar distribution is found for the  $GdF_3$ : $Er^{3+}$ , $Yb^{3+}$  NPs.



**Figure SF5**. Aspect ratio distribution for the  $GdF_3$ : $Tm^{3+}$ , $Yb^{3+}$  NPs. A similar distribution is found for the  $GdF_3$ : $Er^{3+}$ , $Yb^{3+}$  NPs.



**Figure SF6.** Upconversion spectrum ( $\lambda_{exc}$ =980 nm) for the uncapped GdF<sub>3</sub>:Er<sup>3+</sup>,Yb<sup>3+</sup> NPs in powder form. A similar spectrum has been obtained for the PEG-capped GdF<sub>3</sub>:Er<sup>3+</sup>,Yb<sup>3+</sup> NPs.



**Figure SF7.** Upconversion power study ( $\lambda_{exc}$ =980 nm) for water dispersion of (a) GdF<sub>3</sub>:Er<sup>3+</sup>, Yb<sup>3+</sup> (0.60 g/l) (green:  $\lambda_{em}$ =550 nm, red:  $\lambda_{em}$ =660 nm); (b) GdF<sub>3</sub>:Tm<sup>3+</sup>, Yb<sup>3+</sup> (0.47 g/l) ( $\lambda_{em}$ =810 nm).



**Figure SF8**. Schematic representation of upconversion processes for  $\text{Er}^{3+}/\text{Yb}^{3+}$  ions ( $\lambda_{exc}$ =980 nm).



Figure SF9. Schematic representation of upconversion processes for  $Tm^{3+}/Yb^{3+}$  ions ( $\lambda_{exc}=980$  nm).