Supporting Information

Surfactant-free Gd^{3+}-ion-containing Carbon Nanotube MRI Contrast Agents for Stem Cell Labeling

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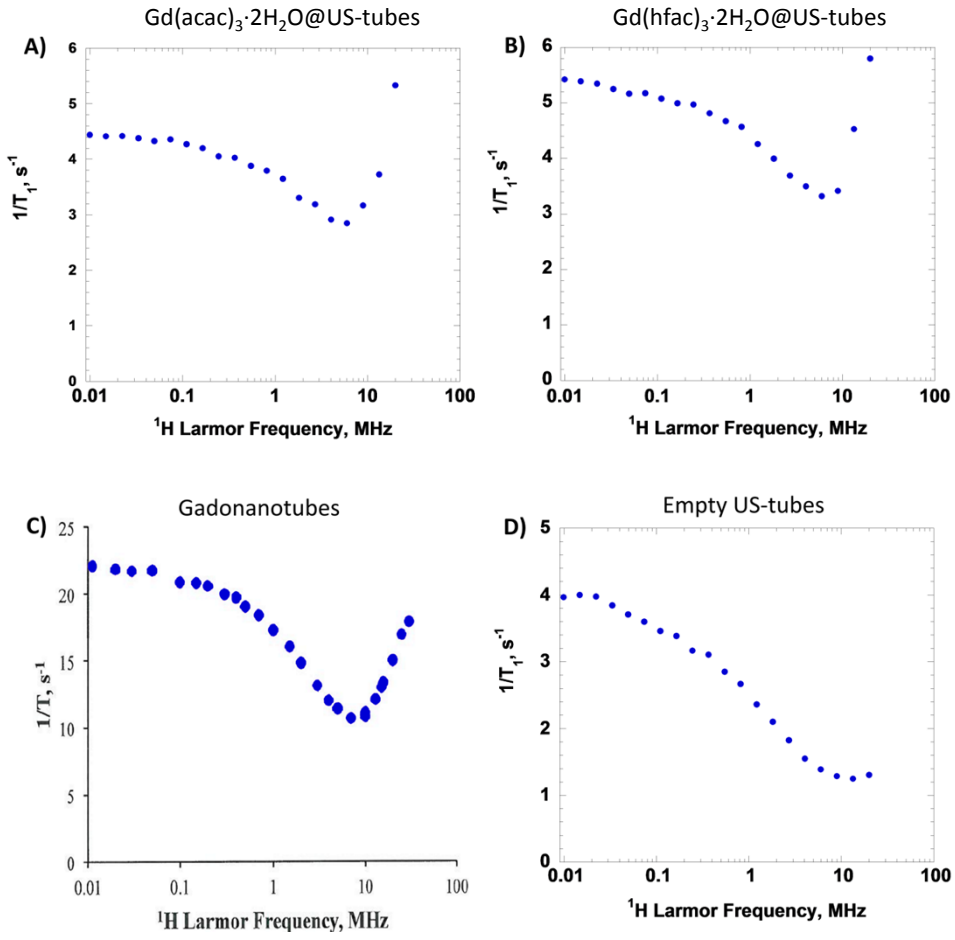

Figure S1. Nuclear Magnetic Resonance Dispersion profiles of A) $Gd(acac)_3{\cdot}2H_2O$@US-tubes (0.051 mM Gd^{3+}), B) $Gd(hfac)_3{\cdot}2H_2O$@US-tubes (0.064 mM Gd^{3+}), C) Gadonanotubes (0.11 mM Gd^{3+}), and D) Empty US-tubes. Low field contributions to relaxation arise from surface diffusion effects of water, while the high field dispersion Fig. S1 (A-C) exhibits classic T_{1e} limited relaxation which increases with increasing magnetic field. (Figure S1 C is reproduced from Sethi, R. Nanosystems: From their design to characterization as advanced MRI contrast agents, PhD Dissertation, Rice University, **2013**.)

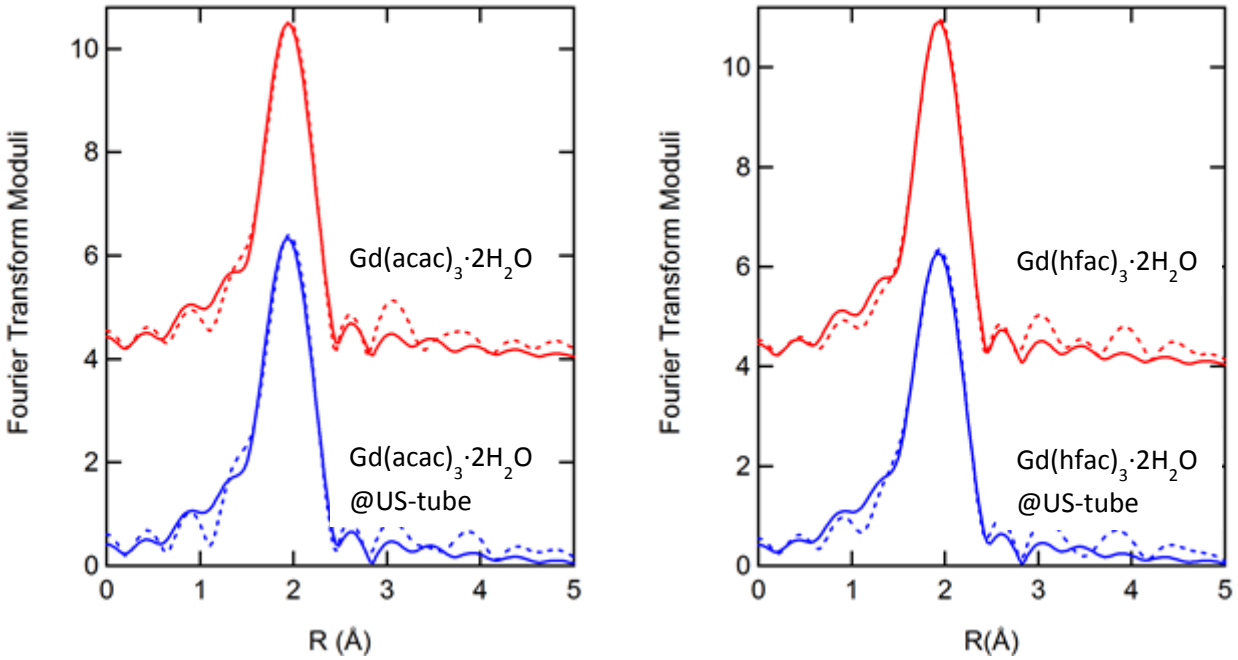

Figure S2. The Fourier transforms of the EXAFS data (dashed lines) and their fittings (full lines). On the left: $Gd(acac)_3 \cdot 2H_2O$ and $Gd(acac)_3 \cdot 2H_2O$@US-tubes; on the right: $Gd(hfac)_3 \cdot 2H_2O$ and $Gd(hfac)_3 \cdot 2H_2O$@US-tubes.

Samples	N (N=8)	R (Å)	σ^2 (Å^2)	E_0 (eV)	R-factor
$Gd(acac)_3 \cdot 2H_2O$@US-tubes	9.9	2.43	0.0113	6.8	0.008
$Gd(acac)_3 \cdot 2H_2O$	9.9	2.43	0.0110	6.6	0.005
$Gd(hfac)_3 \cdot 2H_2O$@US-tubes	10.9	2.42	0.0126	6.3	0.004
$Gd(hfac)_3 \cdot 2H_2O$	10.7	2.42	0.0110	6.4	0.002

Table S1. EXAFS curve fitting data for $Gd(acac)_3 \cdot 2H_2O$@US-tubes, $Gd(acac)_3 \cdot 2H_2O$, $Gd(hfac)_3 \cdot 2H_2O$@US-tubes, and $Gd(hfac)_3 \cdot 2H_2O$. – Amplitude scaling factor, N – Coordination number from crystalline structures, R – Bond distances, σ^2 – Debye-Waller factor, E_0 – Energy shift, R-factor – factor of merit.

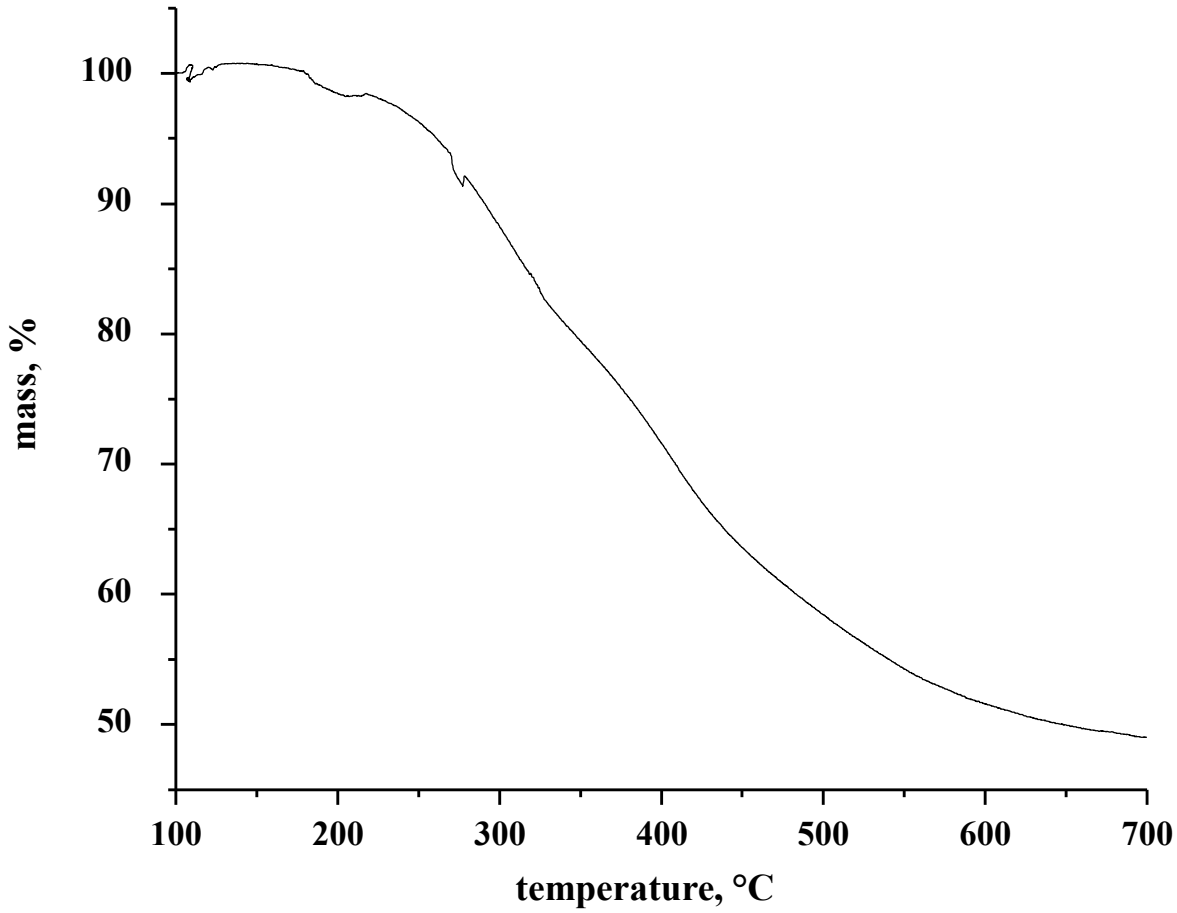

Figure S3. Thermal gravimetric analysis (TGA) of the PCP-Gd(acac)$_3$•2H$_2$O@US-tubes (functionalized 4 times) in an Ar atmosphere at a 10 °C min^{-1} scan rate, from 100 to 700 °C.

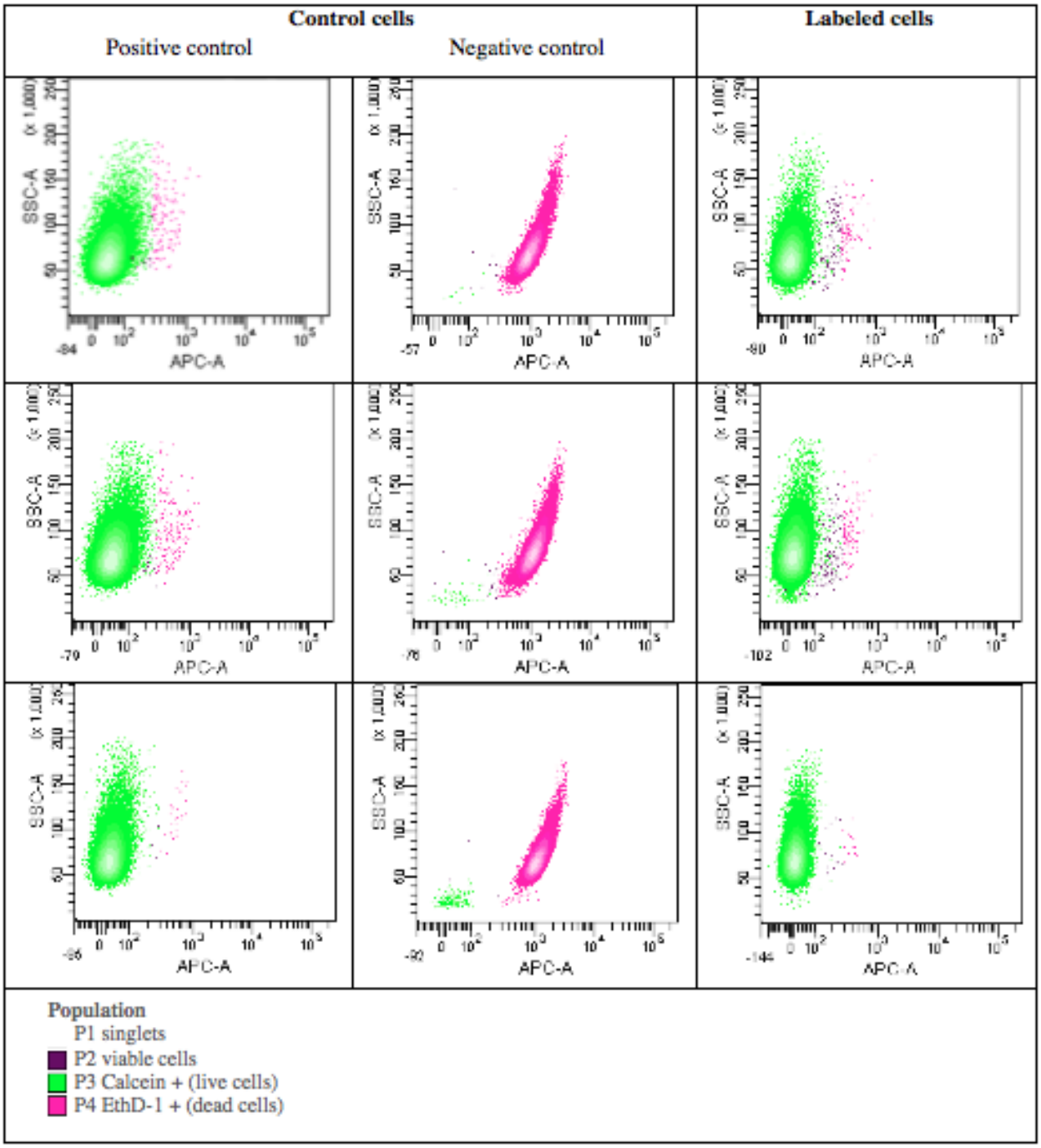

Figure S4. Diagram of the side-scattered light (SSC) and Allophycocyanin (APC-A) of the viable cells population for three different cell samples, each from different animals, with their respective controls. Positive controls are unlabeled live cells, while negative control are unlabeled dead cells which were incubated with MeOH for 15-20 min. >98 % of dead cells were obtained for negative controls.

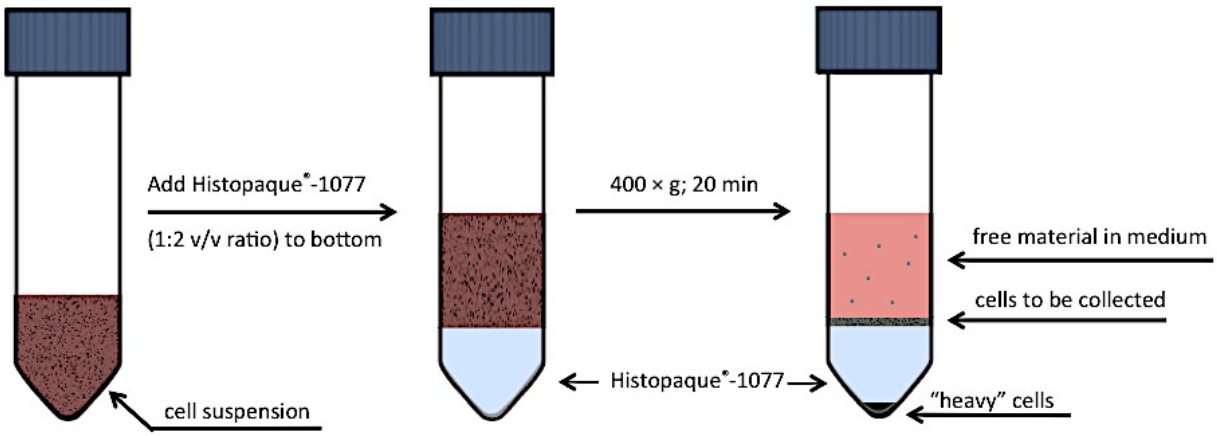

Figure S5. Scheme showing the density gradient separation using Histopaque®-1077 performed to separate free PCP-Gd(acac)$_3$·2H$_2$O@US-tubes in the medium from labeled cells and "heavy cells", which are cells with PCP-Gd(acac)$_3$·2H$_2$O@US-tubes on the outside membrane of the cells.