Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B

Supporting Information

High Payload Gd(III) Encapsulated in Hollow Silica Nanospheres for High Resolution Magnetic Resonance Imaging

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Calculation on the number of Gd per Gd@SiO_2-PEG_{500}:

Using the following data, we calculated the number of Gd per particle:

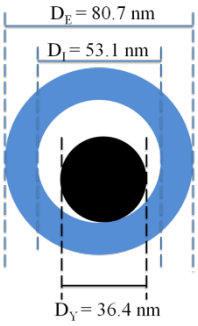
1. Gd content in Gd@SiO_2-PEG_{500} is 11.4 wt%.

2. Density of amorphous silica (d1) is 2.2 g/cm^3.

3. Density of yolk (d2) is firstly assumed to be 2.5 g/cm^3.

4. The external (D_E), interior (D_I) and yolk (D_Y) diameter of Gd@SiO_2-PEG_{500} are 80.7 nm, 53.1 nm and 36.4 nm, respectively.

Calculation:



1. The weight per Gd@SiO_2-PEG_{500}:

$4/3\pi(D_E/2)^3\times$ (d1)–$4/3\pi(D_I/2)^3\times$ (d1) + $4/3\pi(D_Y/2)^3\times$ (d2)

$= 4.96 \times 10^{-16}$ (g)

2. The number of Gd@SiO_2-PEG_{500} per gram:

$1/4.96 \times 10^{-16} = 2.02 \times 10^{15}$

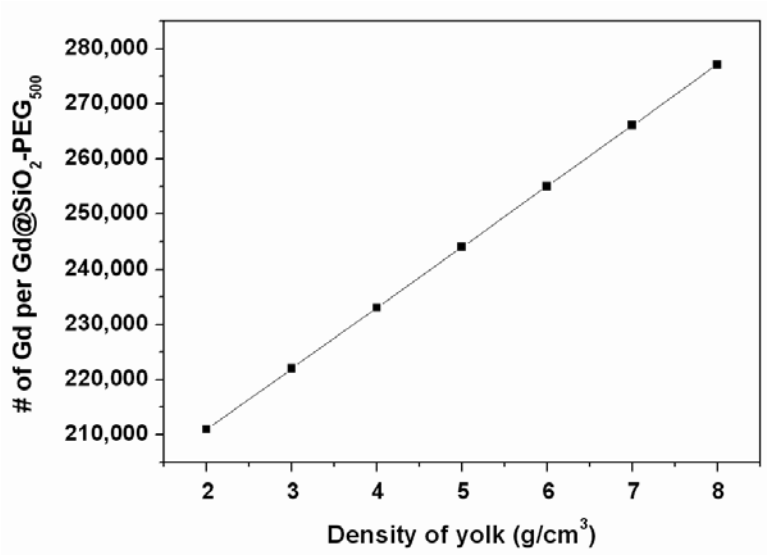
3. The number of Gd per gram of Gd@SiO_2-PEG_{500}:

$1 \times 11.4\% \div 157.25 \times 6.02\times10^{23} = 4.36\times10^{20}$

4. The number of Gd per Gd@SiO_2-PEG_{500}:

$4.36\times10^{20} \div 2.02 \times 10^{15} = 2.16\times 10^{5}$

In addition, the number of Gd per Gd@SiO_2-PEG_{500} was also calculated from various densities of yolk (between 2 to 8 g/cm^3) and the results are shown in the following figure. (The boundary of densities are assumed based on polymeric lanthanum citrate (d=2.5 g/cm^3, *Inorg. Chem.* 2004, *43*, 6965-6968) and Gd metal (7.9 g/cm^3).



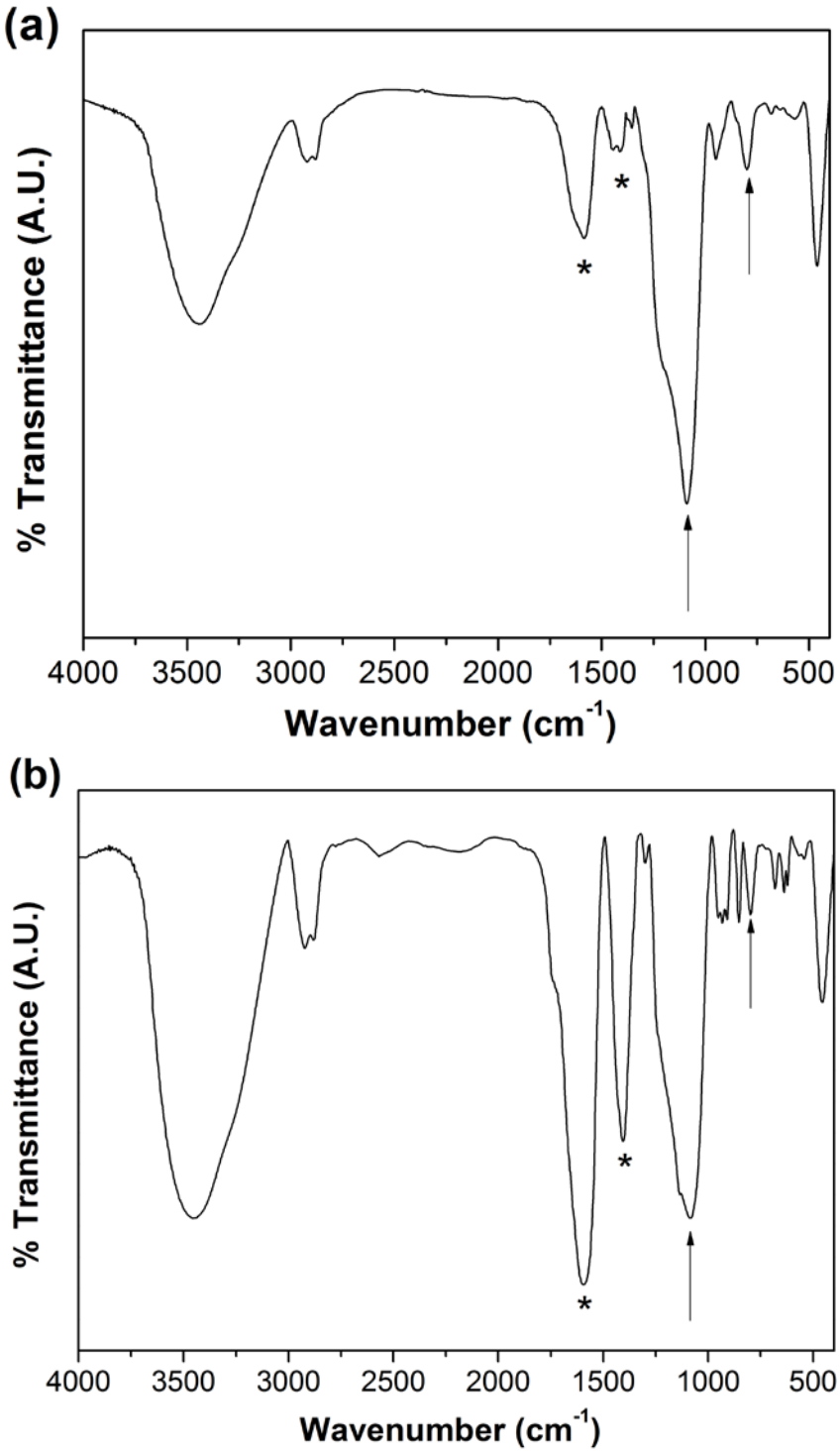


Figure S1 FT-IR spectrum of (a) Gd@SiO_2-PEG_{500} (b) the removed material. The removed material was obtained by concentrating the supernatant collected from the reaction mixture of Gd@SiO_2 PEGylation after centrifugation. The peaks near 1590 and 1405 cm^{-1} (indicated by stars) can be assigned to the anti-symmetric and symmetric carboxylate stretches ($\nu as(COO^-)$,$\nu s(COO^-)$), respectively. The Δ value ($\nu as(COO^-)-\nu s(COO^-)$) can be interpreted as Gd complex of carboxylate bridges. The peaks near 1085 and 798 cm^{-1} (indicated by arrows) are the characteristic peaks of silicate. The small peak shoulder around 1100 cm^{-1} is due to PEG. About 0.4 wt% Gd was removed during PEGylation of Gd@SiO_2 by ICP-MS measurement.

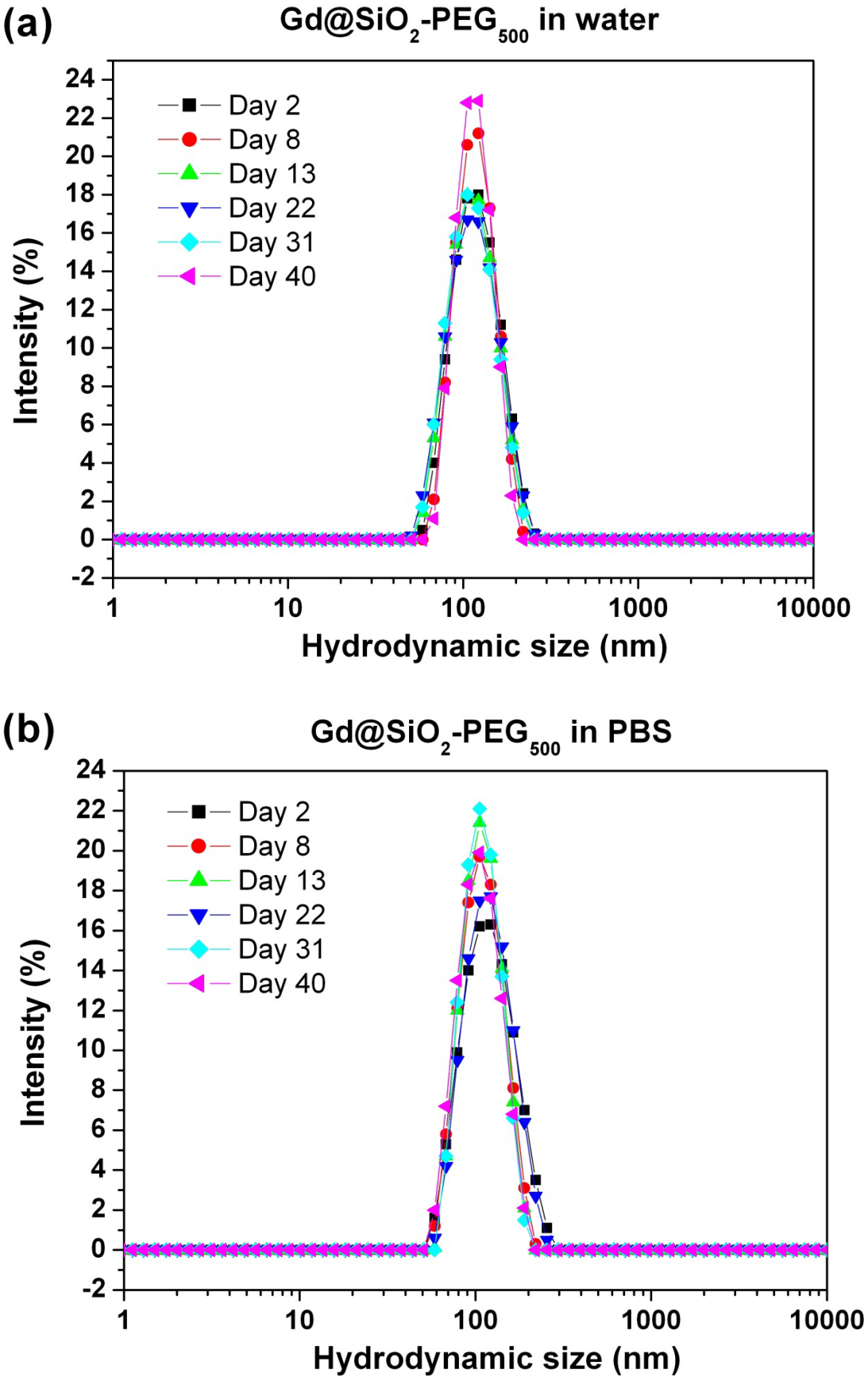


Figure S2 Hydrodynamic size distribution of $Gd@SiO_2$-PEG_{500} suspended in (a) water (b) PBS.

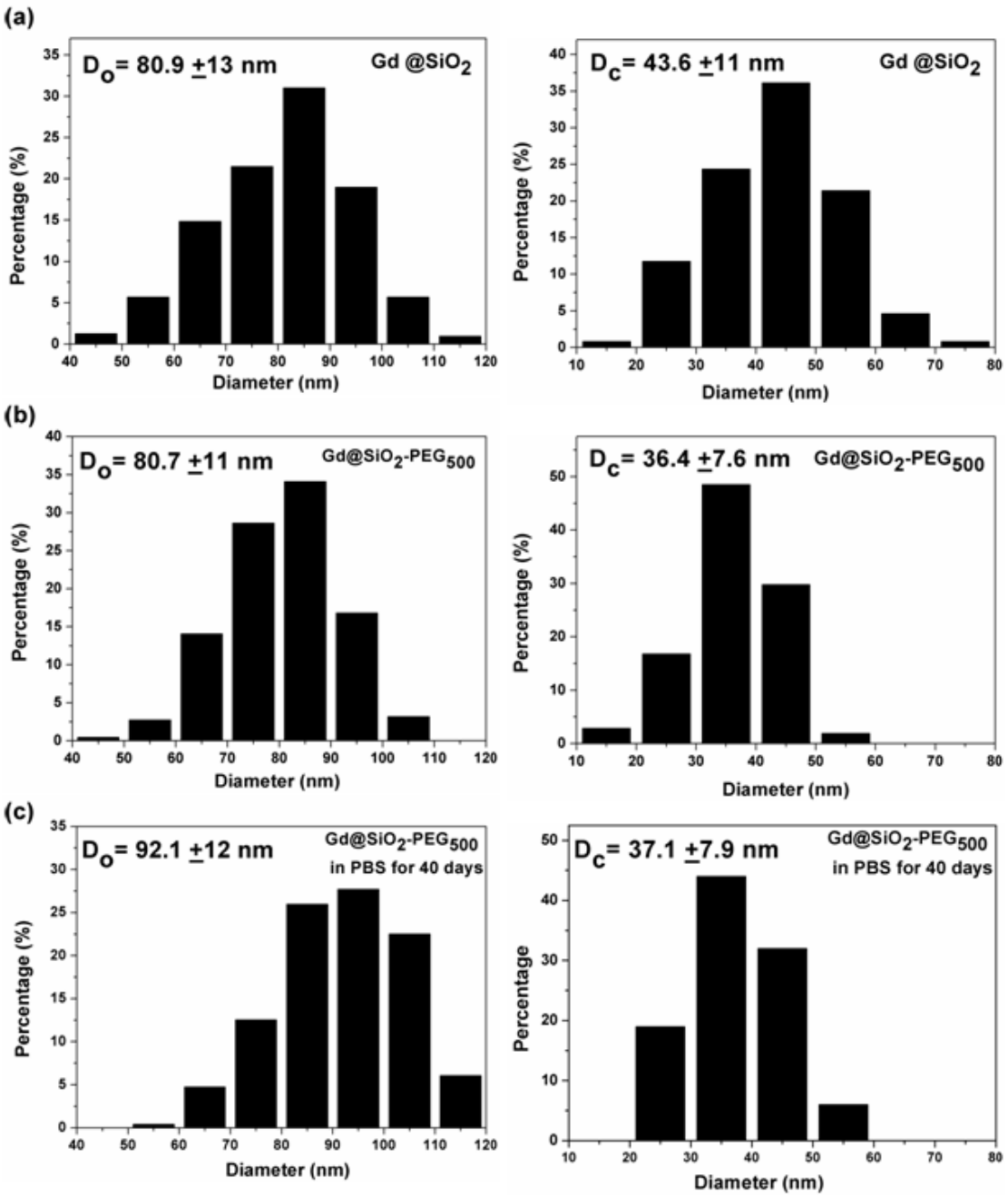


Figure S3 Histograms of particle size distributions of (a) Gd@SiO_2, (b) Gd@SiO_2-PEG_{500}, and (c) Gd@SiO_2-PEG_{500} suspended in PBS for 40 days. Data are from TEM micrographs. D_o and D_c represents overall diameter of nanoparticles and internal core diameter inside nanoparticles, respectively.

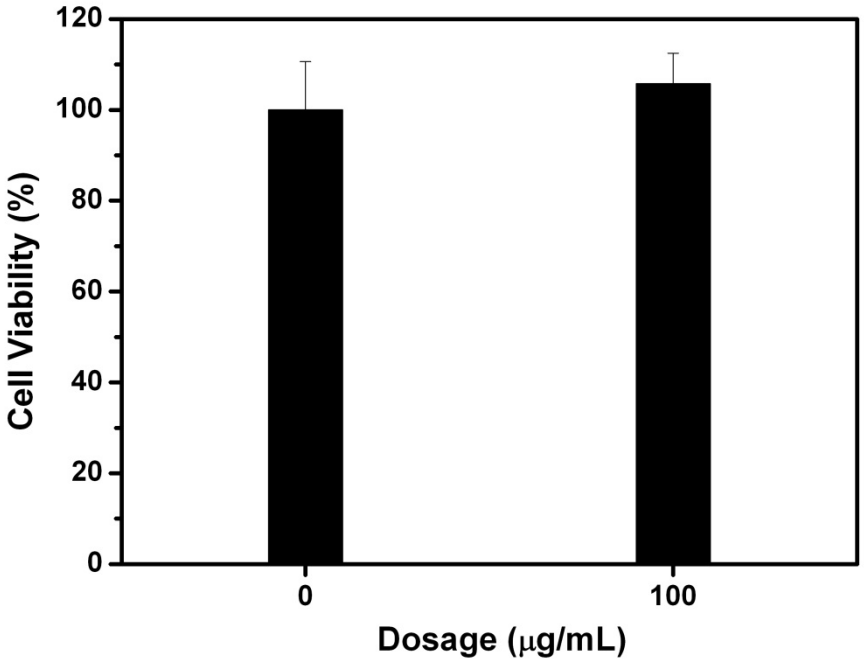


Figure S4 The effect of Gd@SiO_2-PEG_{500} on NIH3T3cell proliferation.

Cell proliferation assay

2×10^4 NIH3T3 cells per well were seeded in 96-well plates for proliferation assays. After incubation with different amounts of Gd@SiO_2-PEG_{500} suspension in culture medium for 4 h, cells were allowed to grow in regular growth medium for 24 h followed by incubation with WST-1 reagent (Clontech) for 4 h at 37 °C for proliferation assay. The dark blue formazan dye generated by the live cells was proportional to the number of live cells and the absorbance at 450 nm was measured using a microplate reader (Bio-Rad, model 680).