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

Supporting Information

Ultrasmall Gadolinium Hydrated Carbonate Nanoparticle: An Advanced T1 MRI Contrast Agent with Large Longitudinal Relaxivity

Guohai Liang[1], Lili Cao[1], Hui Chen[1], Zhengyong Zhang[1], Song Zhang[1], Shaoning Yu[1], Xianrong Shen[2] and Jilie Kong[1*]

[1]*Department of Chemistry and Institutes of Biomedical Sciences, Fudan University, Shanghai 200433, PR China*

[2]*Naval Medicine Institute, Shanghai 200433, PR China*

E-mail: jlkong@fudan.edu.cn

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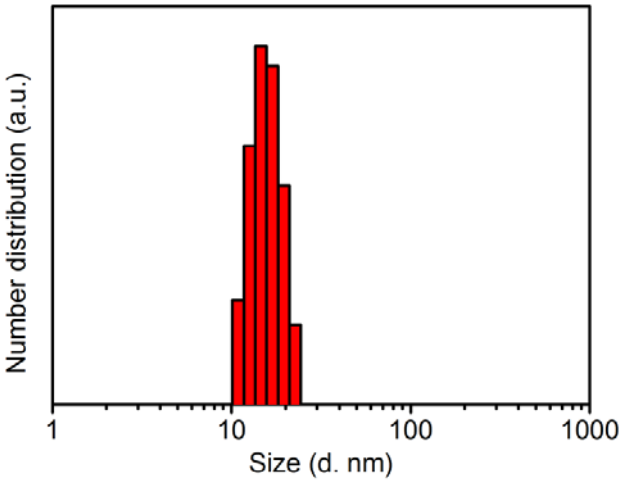

Fig. S1 Hydrodynamic diameter of GHC-1 in aqueous solution.

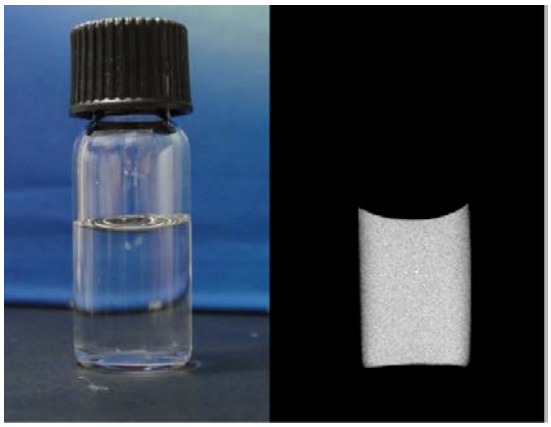

Fig. S2 GHC-1 in aqueous solution after 1 month. The gadolinium concentration in the solution was 1 mM. The image on the right was taken by MRI.

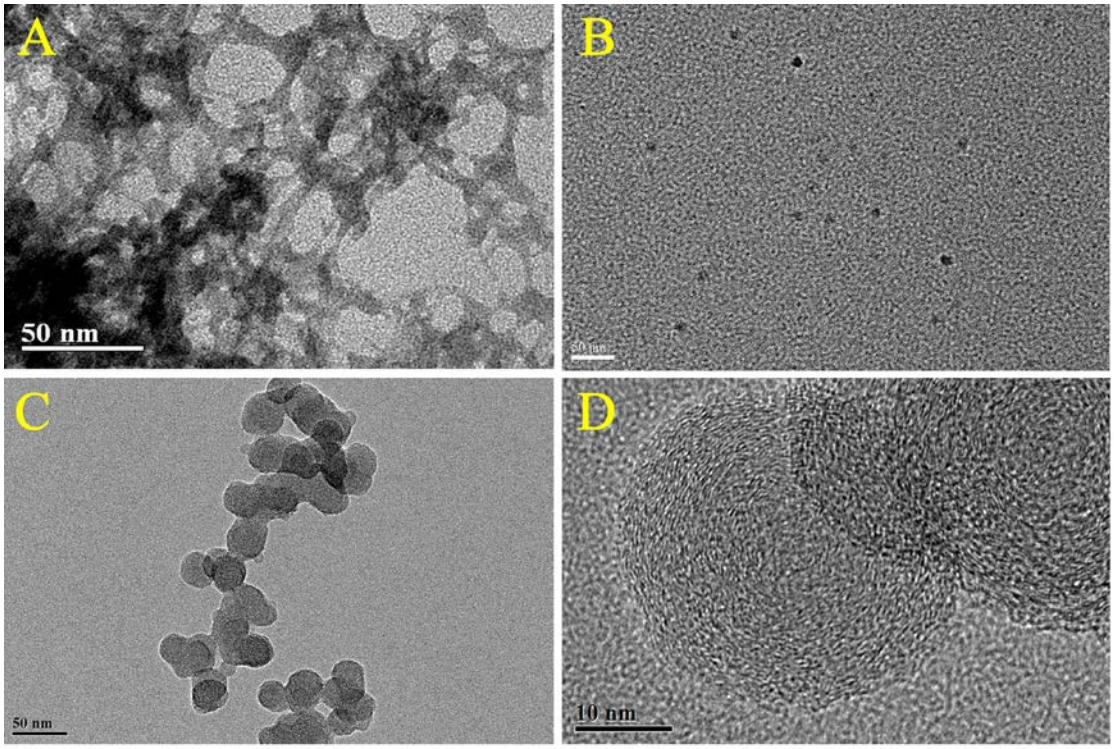

Fig. S3 TEM image of gadolinium hydrated carbonate nanoparticles synthesized (A) without PAA, (B) with 0.2g PAA, (C) and (D) with 0.1g PAA.

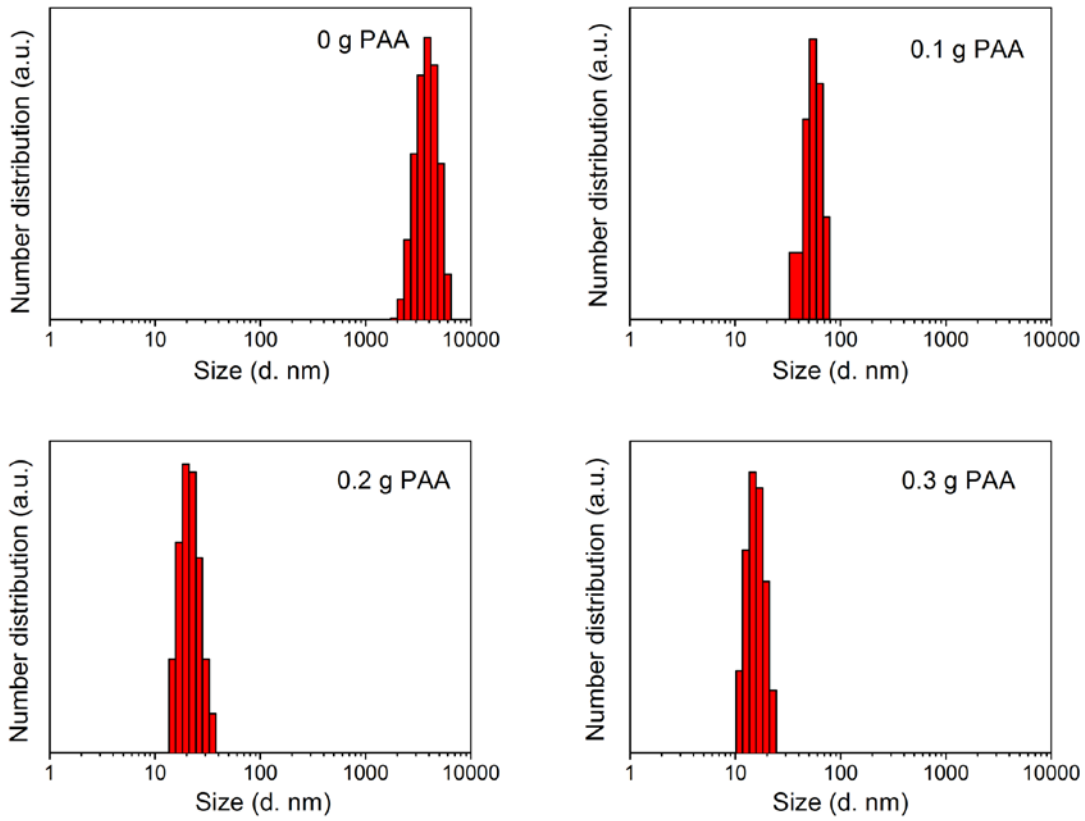

Fig. S4 Hydrodynamic sizes of gadolinium hydrated carbonate nanoparticles synthesized with different initial amount of PAA.

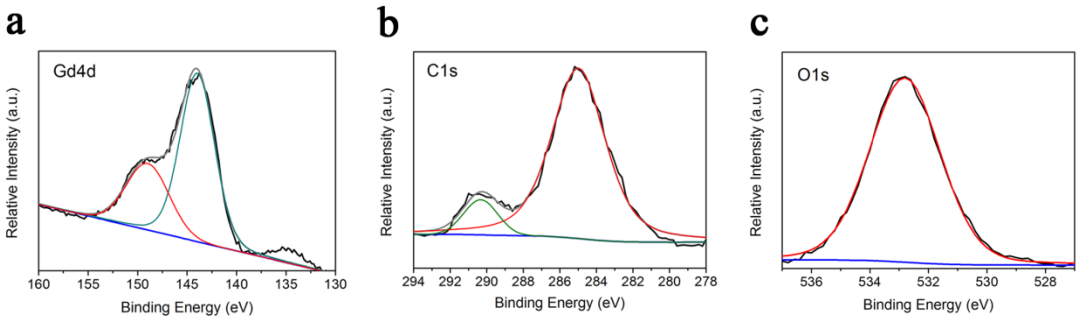

Fig. S5 XPS spectra for naked gadolinium hydrated carbonate nanoparticles: (a) Gd 4d, (b) C 1s, and (c) O 1s.

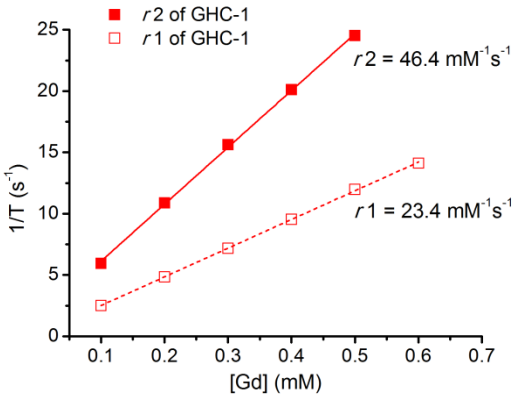

Fig. S6 The r_2 (solid) and r_1 (dashed) relaxivity curves of GHC-1 at 3.0 T field strength.

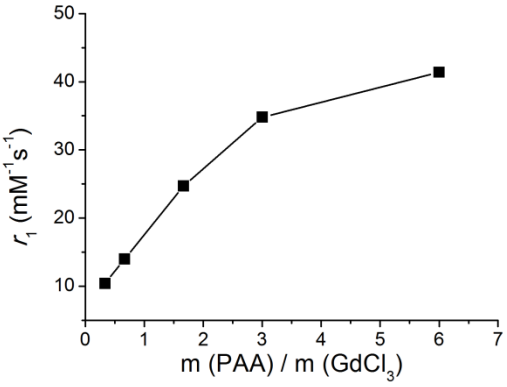

Fig. S7 The r_1 relaxivity of PAA-coated gadolinium hydrated carbonate nanoparticles synthesized in the presence of different amounts of PAA. r_1 was plotted as a function of m(PAA)/m($GdCl_3$). The nanoparticles were synthesized using the same method except for the amount of PAA added.

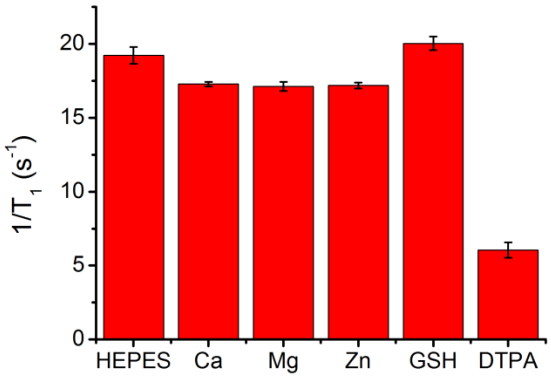

Figure S8. Influence of endogenous metal ions and small chelating ligands on the relaxivity of GHC-1. GSH stands for L-glutathione. All metal ions and chelating ligands were tested with a 5-fold higher concentration than Gd.

The formation of gadolinium hydrated carbonate nanoparticles

The main reactions in the formation of gadolinium hydrated carbonate nanoparticles can be expressed as follows [Eqs. (1)-(5)]:

$2\ HOCH_2CH_2OH \rightarrow 2\ CH_3CHO + 2\ H_2O$ (1)

$CO(NH_2)_2 \rightarrow NH_3 + HNCO$ (2)

$CNO^- + 2H_2O \rightarrow NH_4^+ + CO_3^{2-}$ (3)

$NH_3 + H_2O \rightarrow NH_4^+ + OH^-$ (4)

$Gd^{3+} + OH^- + CO_3^{2-} + 2H_2O \rightarrow Gd(OH)CO_3{\cdot}2H_2O$ (5)

Calculation of tumbling time

Tumbling time of GHC-1 (τ_R) can be calculated using the following formula[1]:

$\tau_R = 4\pi\eta a^3/3k_BT$

Where η represents dynamic viscosity = 10^{-3} pa·s, $k_BT = 4.2\times10^{-21}$ J, a is the hydrodynamic radius of GHC-1, which is 8.45 nm, and T = 305 K.

1. N. J. J. Johnson, W. Oakden, G. J. Stanisz, R. S. Prosser and F. C. J. M. van Veggel, *Chem. Mater.*, 2011, **23**, 3714-3722.