Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Design strategy of ultrasmall Gd_2O_3 nanoparticles for T_1 MRI with high performance

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Supporting Information

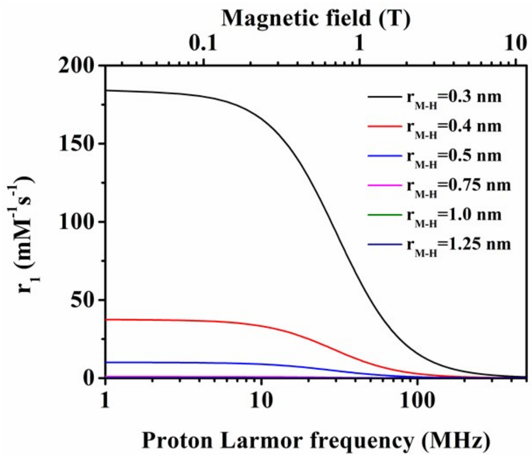

Fig. S1 The curves of r_1^{IS} modulated with $r_{M\text{-}H}$ as Larmor frequency in the range of 1-500 MHz.

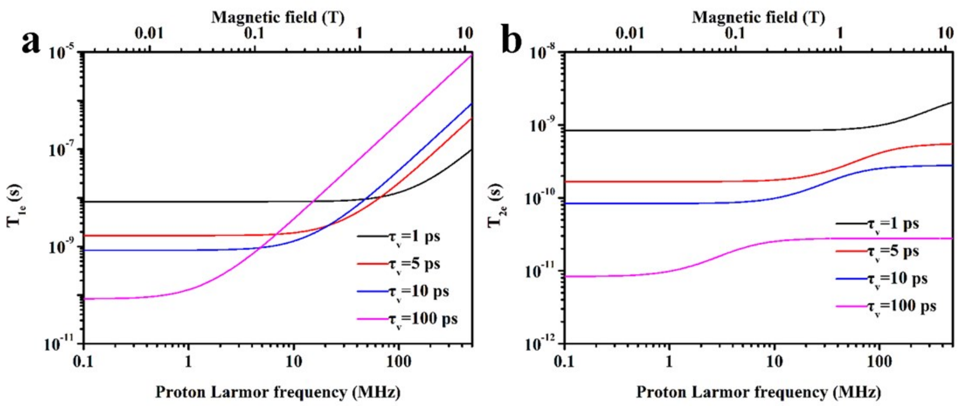

Fig. S2 Electronic relation time (a) T_{1e} and (b) T_{2e} as a function of proton Larmor frequency (0.1-500 MHz) with S = 7/2 (Gd).

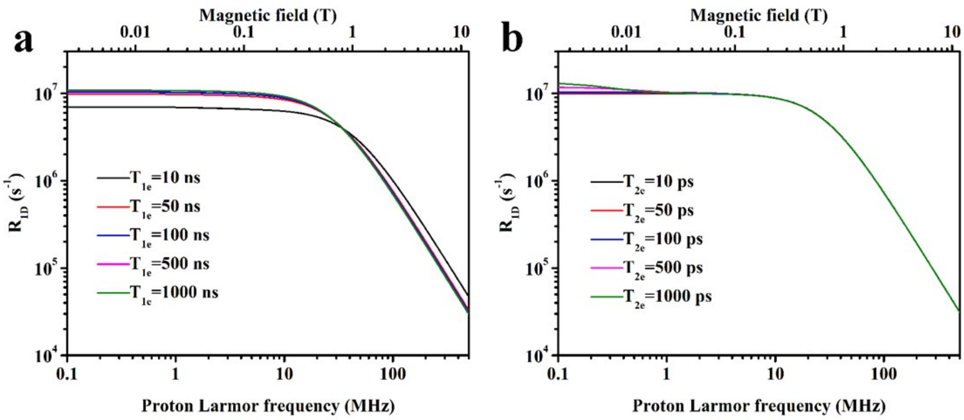

Fig. S3 The curves of R_{1D} modulated by (a) $T_{1e}$and (b) T_{2e} with increasing Larmor frequency.

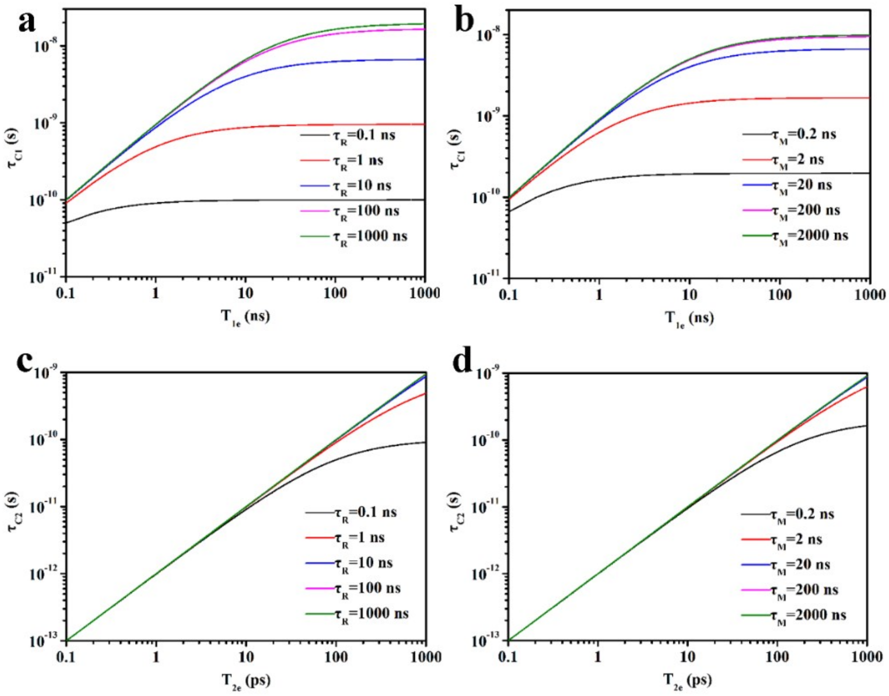

Fig. S4 (a) Dipolar correlation time τ_{c1} as a function of electronic relation time T_{1e} with various τ_R = 0.1-1000 ns and fixed τ_M = 20 ns, (b) τ_{c1} as a function of T_{1e} with various τ_M = 0.2-2000 ns and fixed τ_R = 10 ns; (c) Dipolar correlation time τ_{c2} as a function of electronic relation time T_{2e} with various τ_R = 0.1-1000 ns and fixed τ_M = 20 ns, (d) τ_{c2} as a function of T_{2e} with various τ_M = 0.2-2000 ns and fixed τ_R = 10 ns.

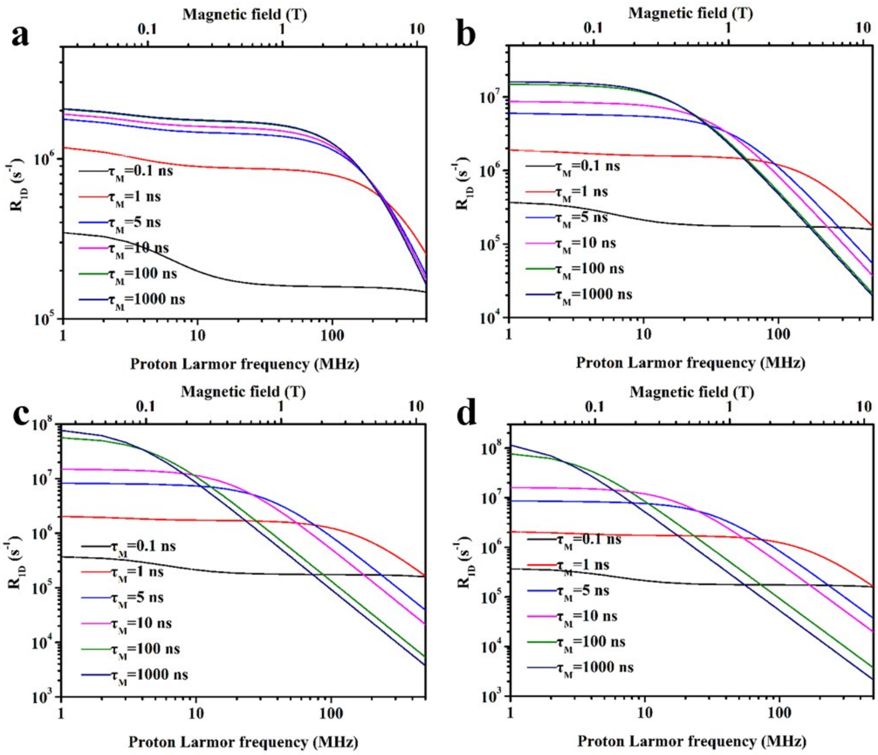

Fig. S5 The curves of R_{1D} modulated with τ_M (0.1-1000 ns) for (a) τ_R = 1 ns, (b) τ_R =10 ns, (c) τ_R =100 ns, (d) τ_R =1000 ns as Larmor frequency in the range of 1-500 MHz.

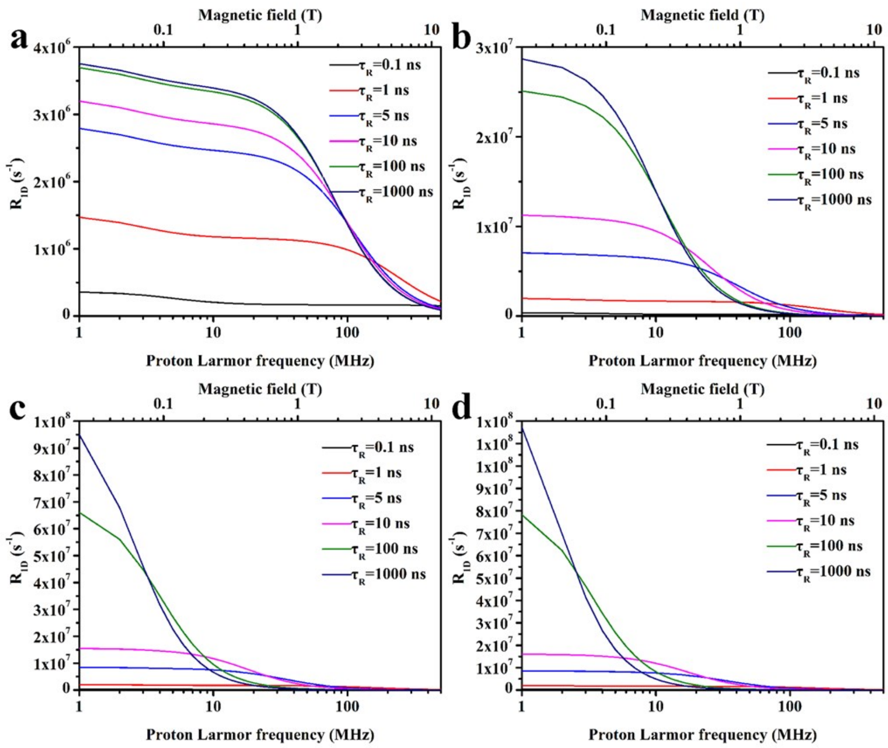

Fig. S6 The curves of R_{1D} modulated with τ_R (0.1-1000 ns) and (a) τ_M = 2 ns, (b) τ_M = 20 ns, (c) τ_M = 200 ns, (d) τ_M = 2000 ns as Larmor frequency in the range of 1-500 MHz.

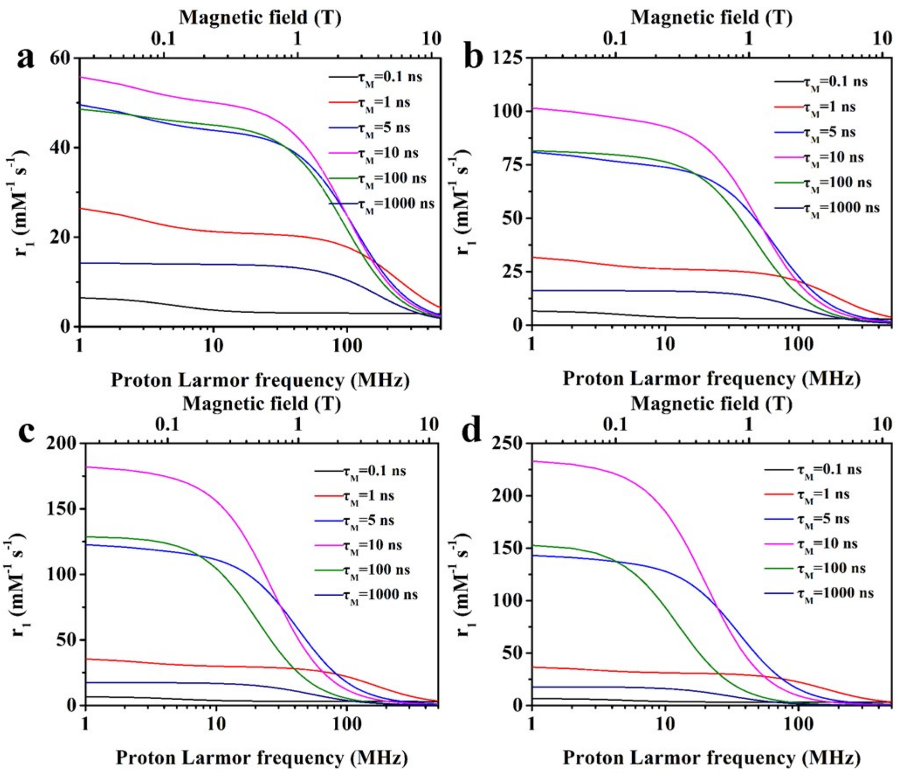

Fig. S7 The curves of r_1^{IS} modulated with τ_M (0.1-1000 ns) and (a) τ_R = 2 ns, (b) τ_R = 5 ns, (c) τ_R =20 ns, (d) τ_R =100 ns as Larmor frequency in the range of 1-500 MHz.

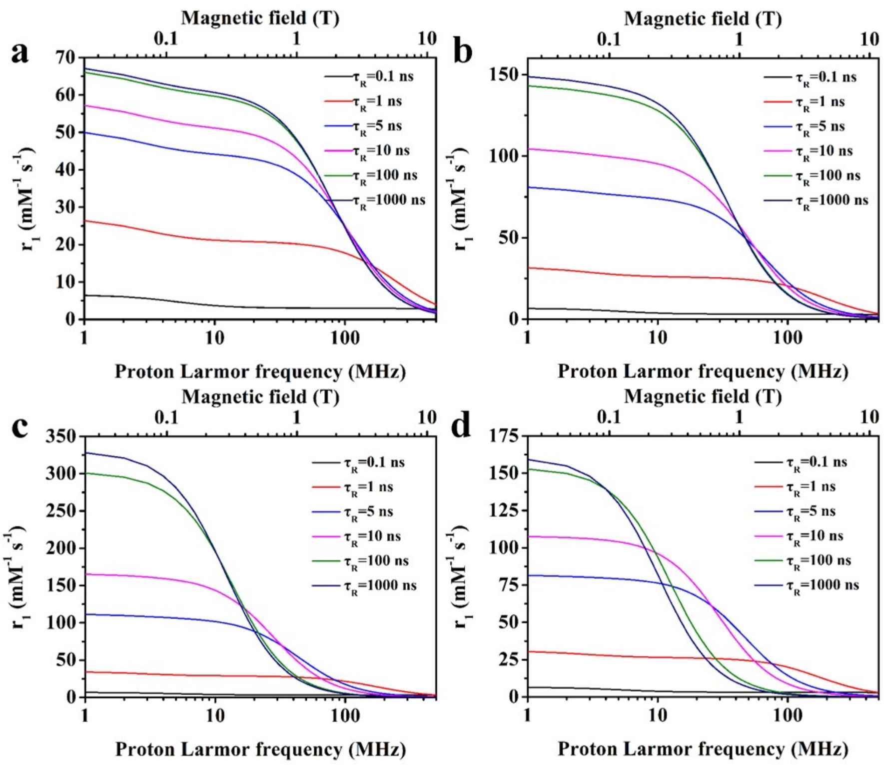

Fig. S8 The curves of r_1^{IS} modulated with τ_R (0.1-1000 ns) and (a) τ_M = 2 ns, (b) τ_M =5 ns, (c) τ_M =20 ns, (d) τ_M =100 ns as Larmor frequency in the range of 1-500 MHz.

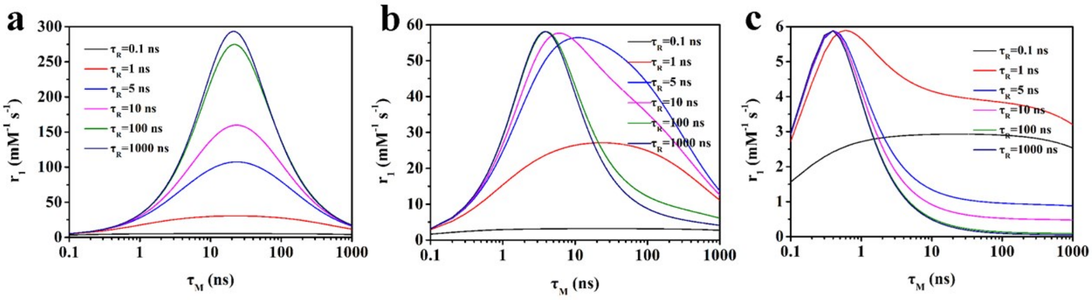

Fig. S9 r_1^{IS} as a function of τ_M (0.1-1000 ns) with various τ_R = 0.1-1000 ns and (a) B_0 = 0.1 T, (b) B_0 = 1 T, and (c) B_0 = 10 T.

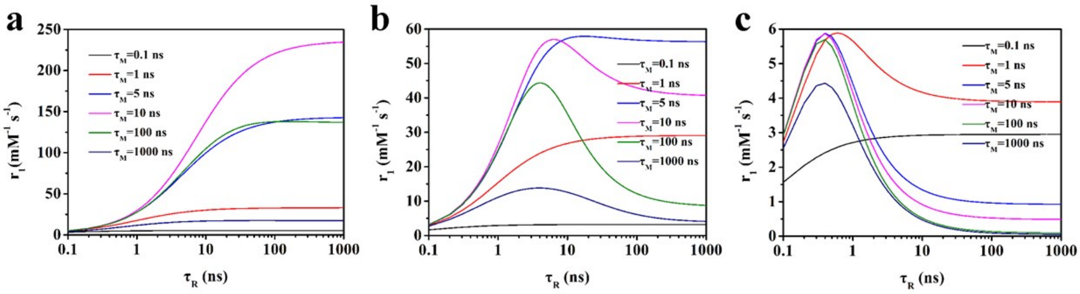

Fig. S10 r_1^{IS} as a function of τ_R (0.1-1000 ns) with various τ_M = 0.1-1000 ns and (a) B_0 = 0.1 T, (b) B_0 = 1 T, and (c) B_0 = 10 T.

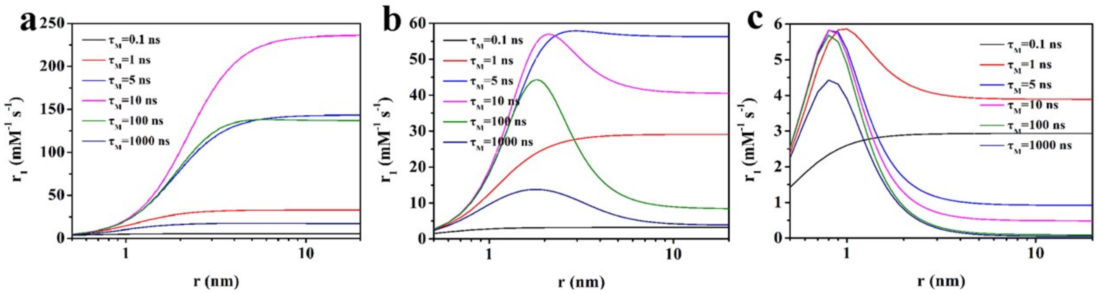

Fig. S11 r_1^{IS} as a function of r (0.5-20 nm) with various τ_M = 0.1-1000 ns and (a) B_0 = 0.1 T, (b) B_0 = 1 T, and (c) B_0 = 10 T.

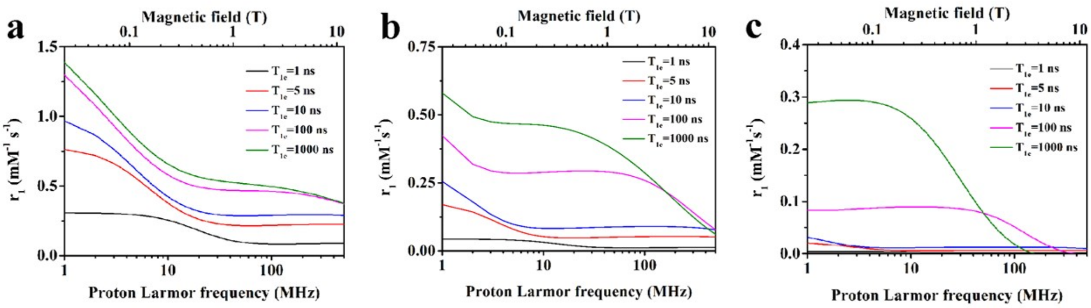

Fig. S12 r_1^{OS} as a function of proton Larmor frequency (1-500 MHz) with various T_{1e} = 1-1000 ns and (a) τ_d = 10 ns, (b) τ_d =100 ns, and (c) τ_d = 1000 ns.

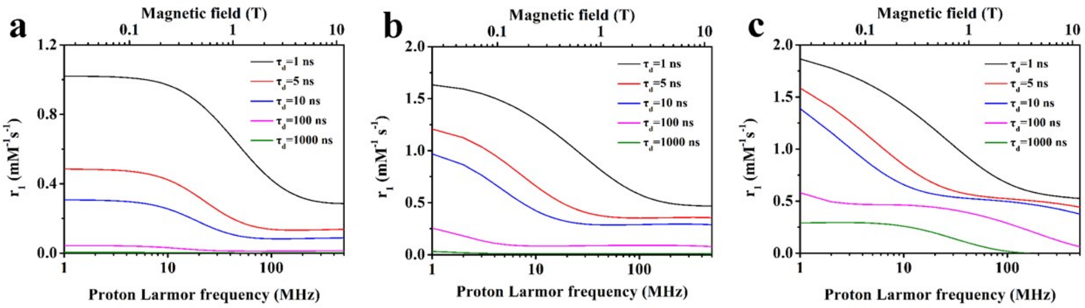

Fig. S13 r_1^{OS} as a function of proton Larmor frequency (1-500 MHz) with various τ_d = 1-1000 ns and (a) T_{1e} = 1 ns, (b) T_{1e} = 10 ns, and (c) T_{1e} = 1000 ns.

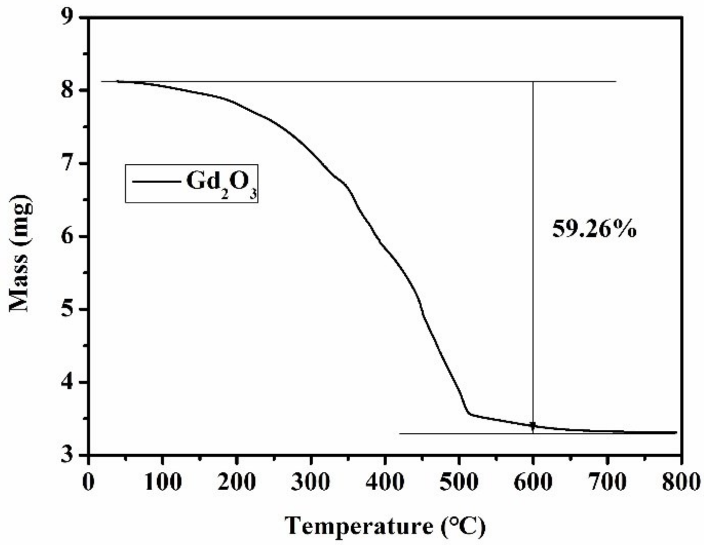

Fig. S14 TGA curve of the OA-Gd_2O_3 NPs with temperature increasing from RT to 800 °C.

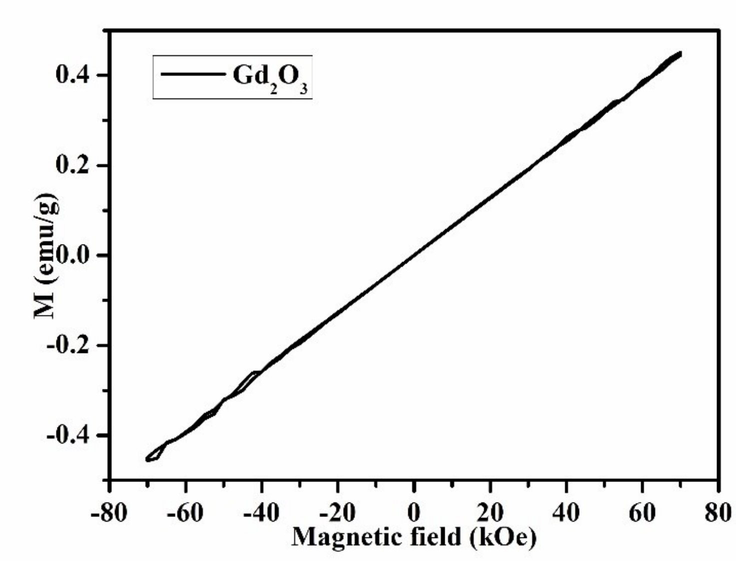

Fig. S15 Magnetization curve of OA-Gd_2O_3 NPs in the magnetic field from -7 to 7 T.

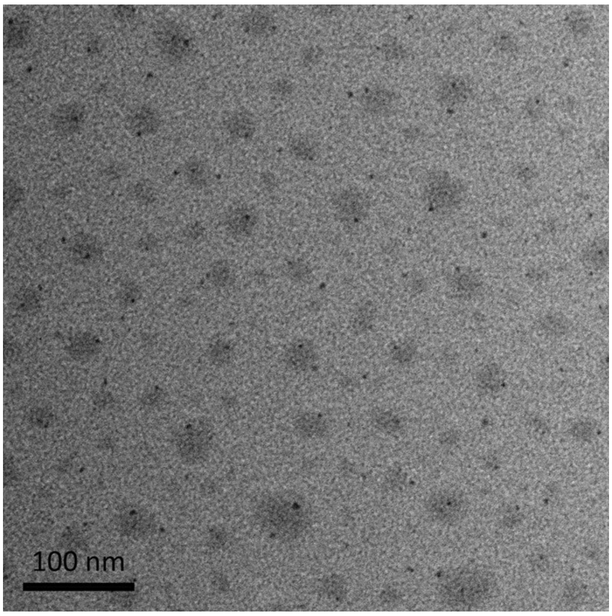

Fig. S16 TEM image of Gd_2O_3 NPs coated with PVP.

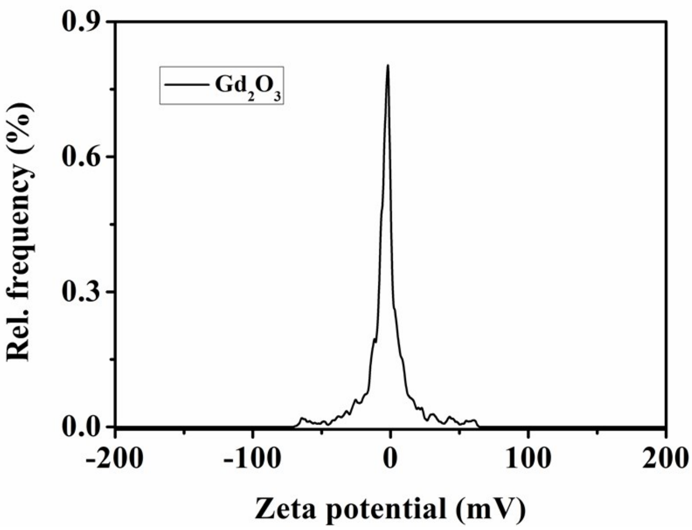

Fig. S17 Zeta potential of Gd_2O_3 NPs coated with PVP.

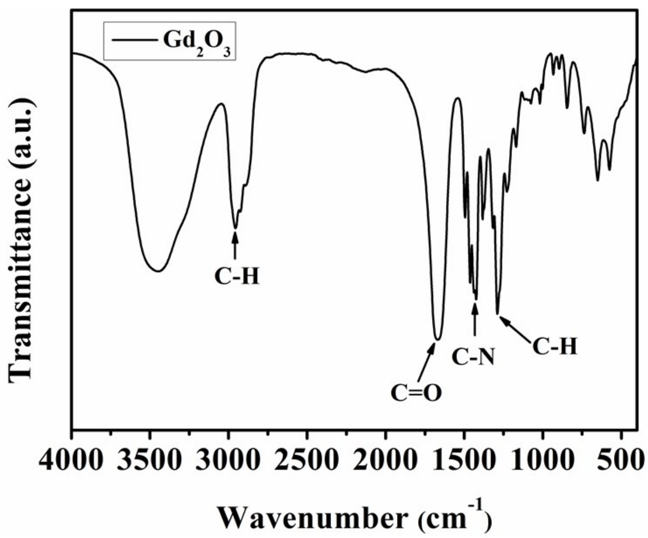

Fig. S18 FT-IR spectrum of Gd_2O_3 NPs coated with PVP.

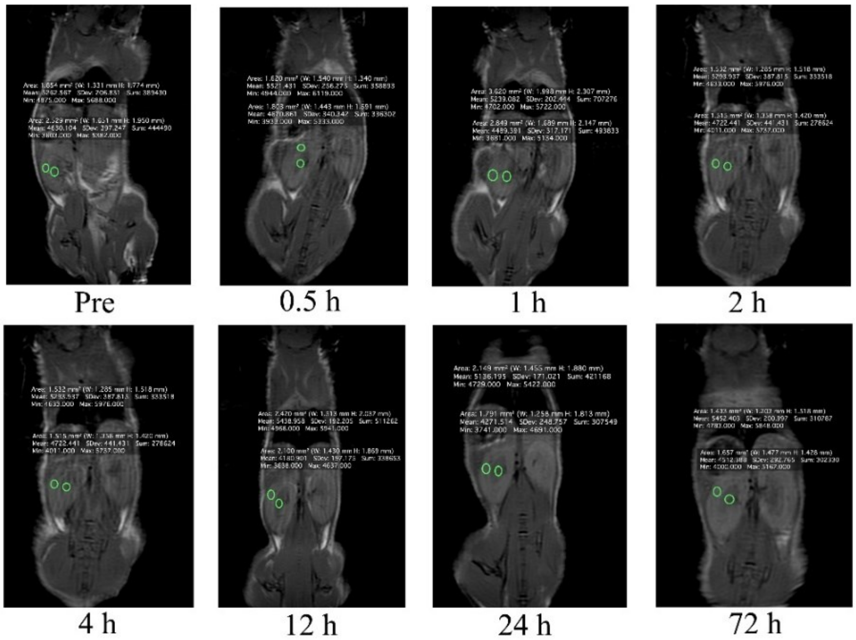

Fig. S19 In vivo T_1 MR images of mice for kidney after injection with different times.

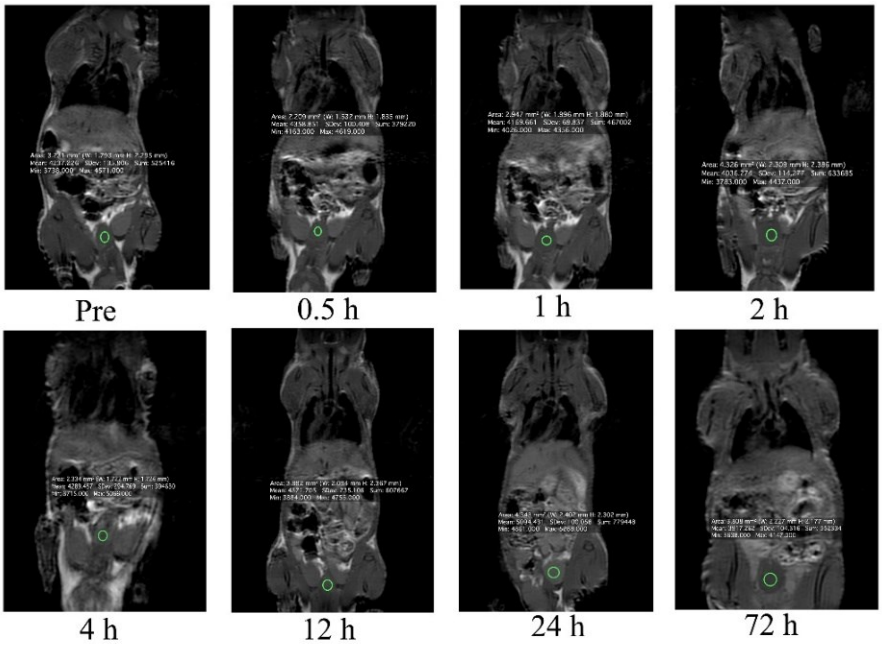

Fig. S20 In vivo T_1 MR images of mice for bladder after injection with different times.

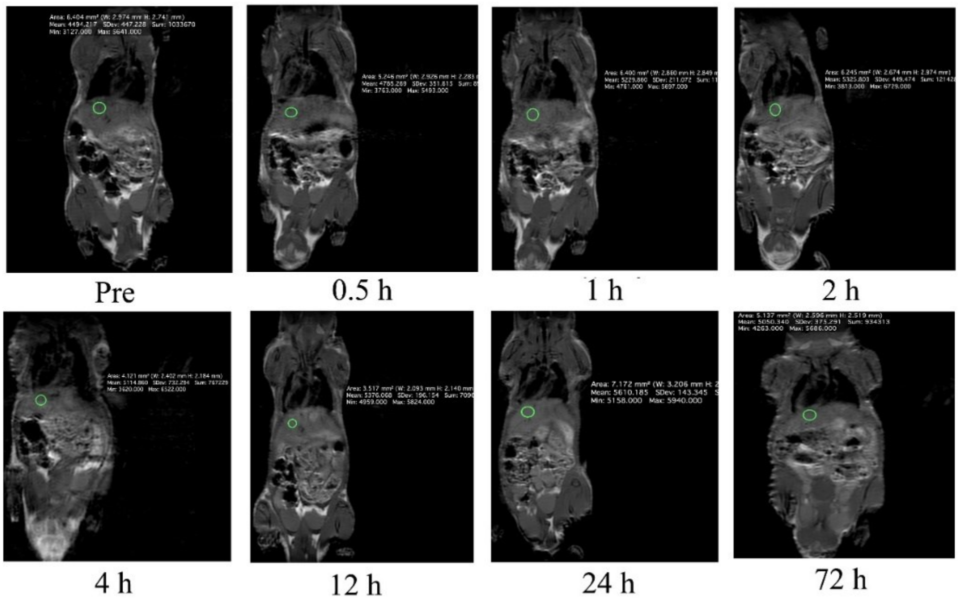

Fig. S21 In vivo T_1 MR images of mice for liver after injection with different times.

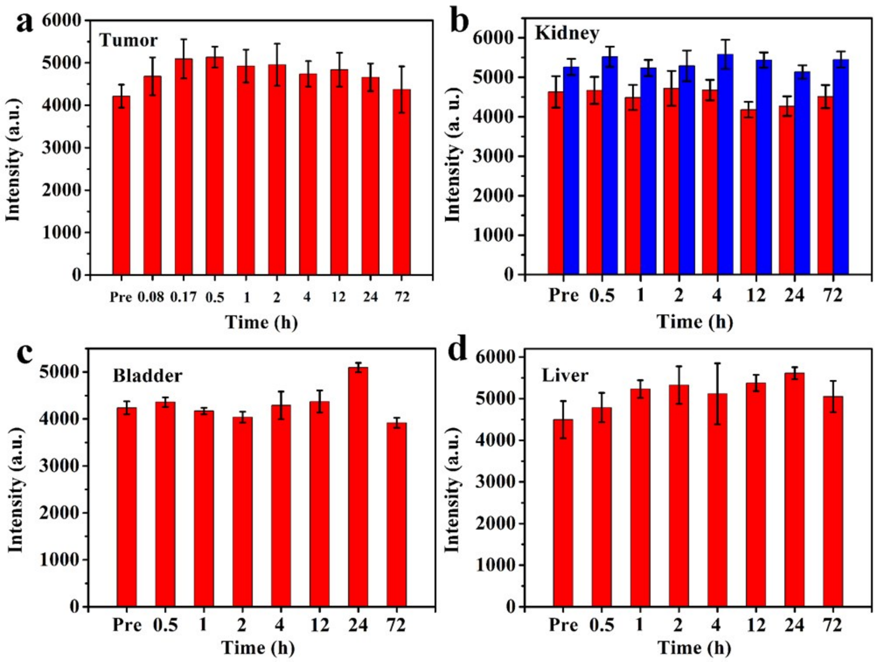

Fig. S22 In vivo T_1 MR signal intensity of mice after injection with different times for (a) tumor, (b) kidney, (c) bladder, and (d) liver.

Table S1. The rotation times of nanoparticles with different radii (0.5-10 nm) at 310 K.

r/nm	0.5	1.0	1.5	2.0
τ_R/ns	0.08506	0.6805	2.2960	5.4452
r/nm	2.5	4.0	5.0	10
τ_R/ns	10.632	45.291	88.483	707.86

Table S2 Relationship between optimal r_1^{IS} and r_1^{OS} under different magnetic fields.

B_0/T	1	3	7	10
r_1^{IS}	τ_R=6 ns τ_M=10 ns r_1^{IS}=56.98 mM^{-1} s^{-1}	τ_R=2 ns τ_M=5 ns r_1^{IS}=19.54 mM^{-1} s^{-1}	τ_R=1 ns τ_M=1 ns r_1^{IS}=8.41 mM^{-1} s^{-1}	τ_R=0.6 ns τ_M=1 ns r_1^{IS}=5.89 mM^{-1} s^{-1}
r_1^{OS}	τ_d=1 ns r_1^{OS}=0.92 mM^{-1} s^{-1}	τ_d=1 ns r_1^{OS}=0.63 mM^{-1} s^{-1}	τ_d=1 ns r_1^{OS}=0.55 mM^{-1} s^{-1}	τ_d=1 ns r_1^{OS}=0.53 mM^{-1} s^{-1}
r_1^{IS}/r_1	98.41%	96.88%	93.86%	91.74%
r_1^{OS}/r_1	1.59%	3.12%	6.14%	8.26%