Supporting Information For

Gadolinium Nicotinate Clusters for Potential MRI Contrast Agents

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Table S1. Crystal data and details of data collection and refinement for **1** and **3**.

Compound	**1**	**3**
Formula	$C_{36}H_{34}Gd_2N_6O_{17}$	$C_{72}H_{88}Cl_4Gd_8N_{12}O_{64}$
Mr	1119.18	3545.34
Crystal colour	colorless	colorless
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$p2_1/n$
a/Å	9.6007(4)	15.9574(8)
b/Å	11.5481(5)	19.0647(11)
c/Å	17.5905(8)	18.6238(8)
α/deg	90	90
β/deg	92.476(4)	103.514(4)
γ/deg	90	90
V/Å^3	1948.45(15)	5508.9(5)
Dc/g cm^{-3}	1.908	2.137
Z	2	2
T/K	100	100
θ /deg	3.53-25.00	3.49 – 28.39
μ(Mo-Kα)/mm^{-1}	3.456	4.949
Data/params	3413/287	9671/721
Obs reflns	8097	45596
R_1 [I> 2σ(I)]	0.0361	0.0774
wR_2(All data)	0.0613	0.1214

[a] $R_1 = \sum||F_O| - |F_C||/\sum|F_O|$ [b] $wR_2 = \{\sum[w(F_O^2 - F_C^2)^2]/\sum[w(F_O^2)^2]\}^{1/2}$

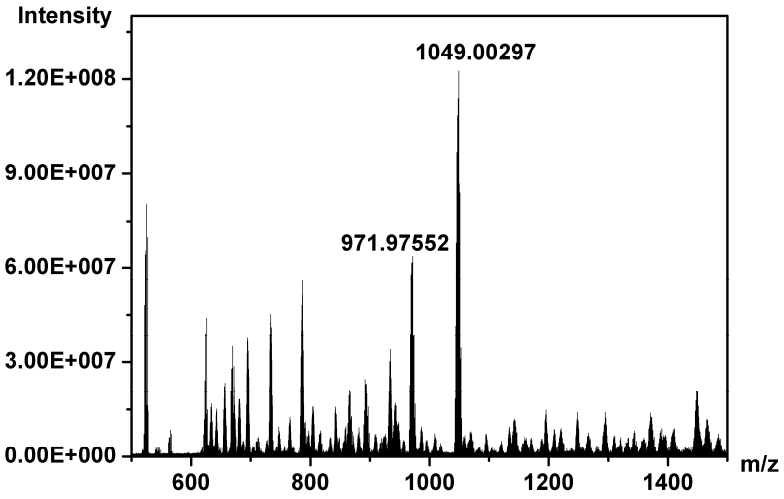


Figure S1. Electrospray mass spectrum of the cluster **1**.

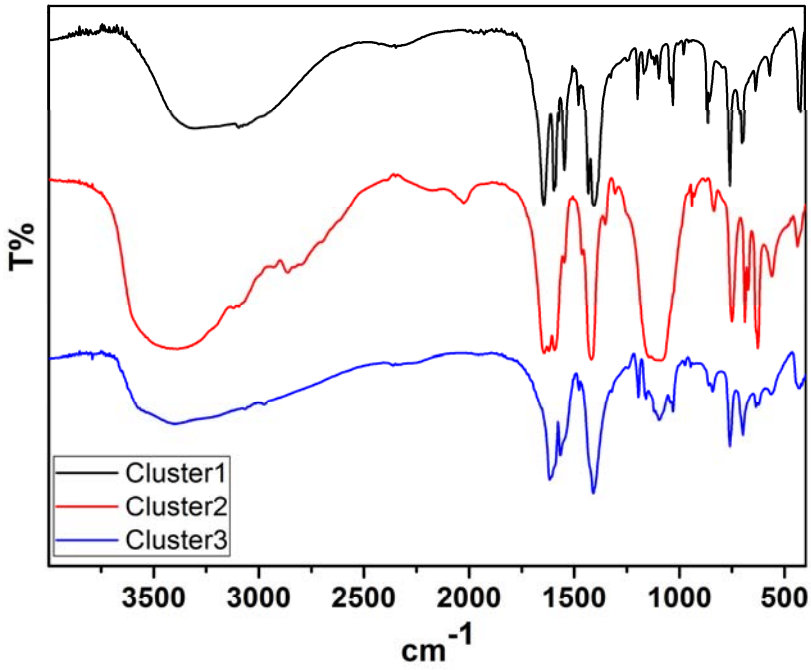


Figure S2. IR spectra for the clusters **1- 3**.

Table S2 FT-IR assignment for clusters **1-3**

Cm^{-1}	**Assignment**
1645,1643,1617,1597, 1593,1566	υ (C=C)
1405,1417,1409	υ (C=C , C=N)
1195,1089	υ (C-O)
759, 702,750, 688,759, 698	υ (C-H)

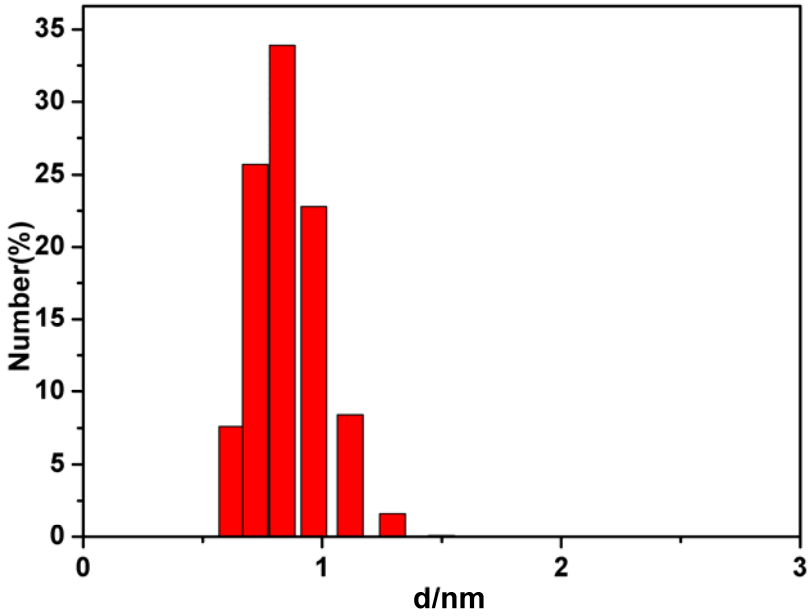


Figure S3. DLS of the cluster **2**.

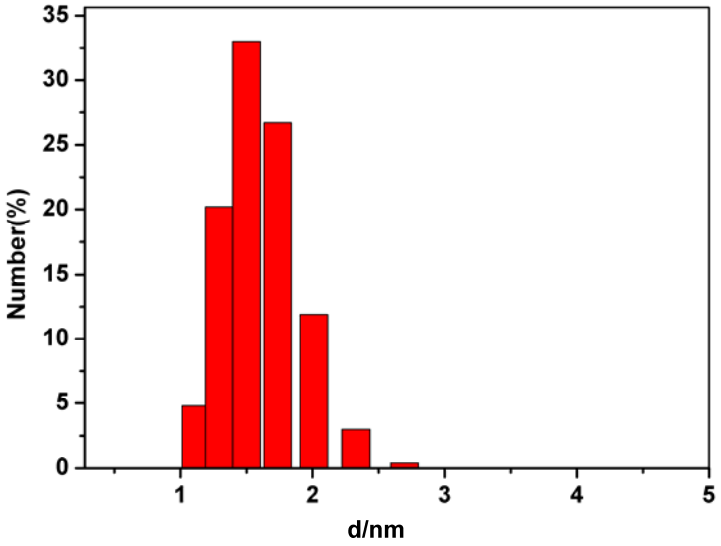


Figure S4. DLS of the cluster **3**.

MR relaxivity measurements at 0.5 T and 7T. To measure the T_1 relaxivitythe clusters with different Gd concentrations were dispersed in water or in 1% agarose solution. The relaxivity r_1 values were determined by the 0.5T NMI20-Analyst NMR Analyzing & Imaging system (Niumag Corporation, Shanghai, China) or on a 7T MRI scanner (at 300 K).

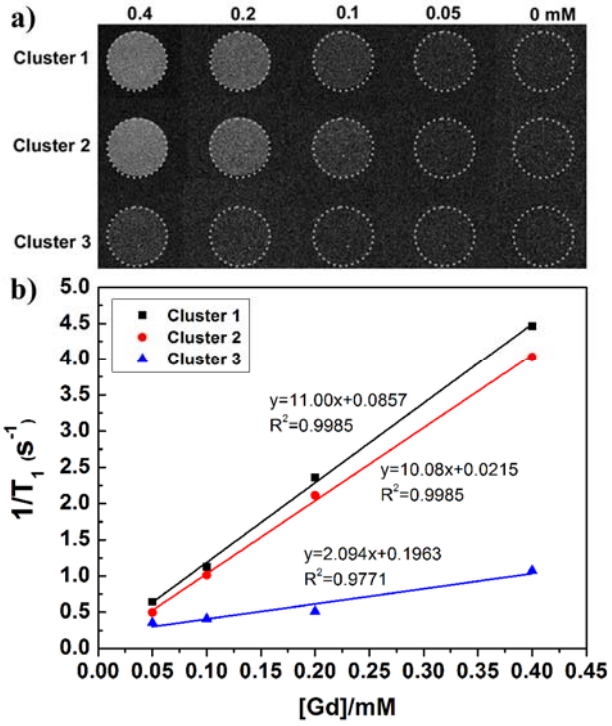
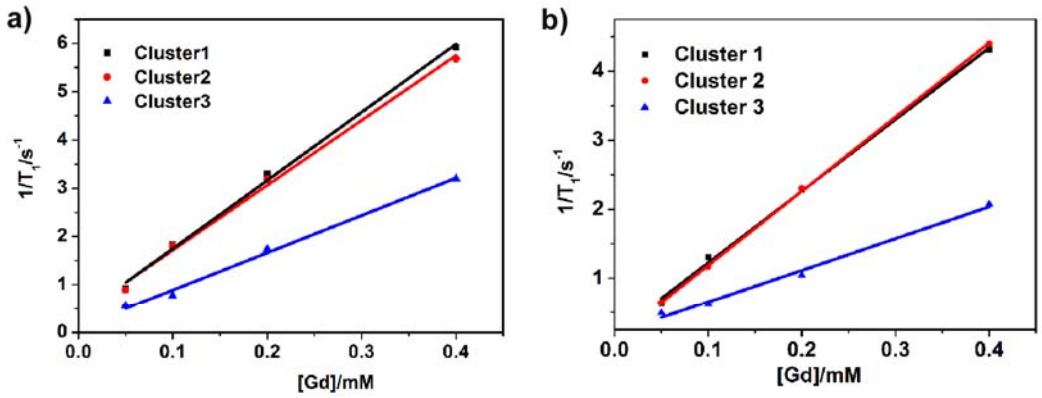


Figure S5. The r_1 relaxivity values of the three clusters dispersed in water solution at 0.5 T.



	R_1(mM^{-1} s^{-1})	R^2
Cluster 1	14.12	0.9973
Cluster 2	13.44	0.9997
Cluster 3	7.74	0.9878

	R_1(mM^{-1} s^{-1})	R^2
Cluster 1	10.37	0.9973
Cluster 2	10.74	0.9997
Cluster 3	4.60	0.9878

Figure S6. The r_1 relaxivity values of the three clusters dispersed in 1% agarose solution at 0.5T (a) and 7 T (b)

Table S3. Unit-cell and space group of powdery sample of **3** *

Space Group	*P2₁/n*
a (Å)	16.03
b (Å)	19.56
c (Å)	18.59
β (°)	104.27

*Derived by indexing the PXRD data

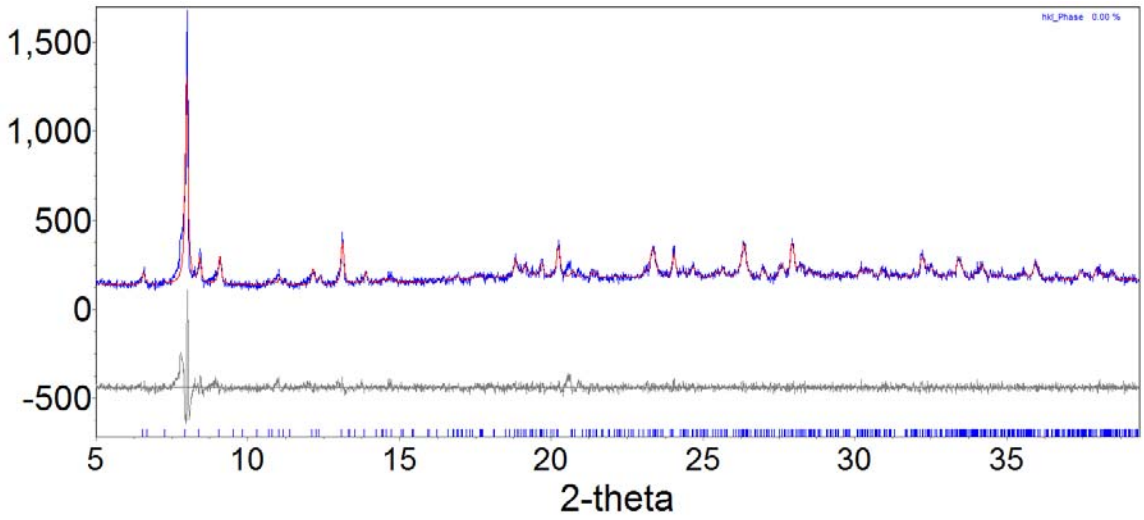


Figure S7. The Rietveld refinement of PXRD pattern of powdery sample of **3**. Blue: experiment data; Red: fitting; Gray: residue