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Supporting Information

Biocompatible supramolecular dendrimers bearing gadolinium-substituted polyanionic core for MRI contrast agents

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Structure Characterization of the complexes

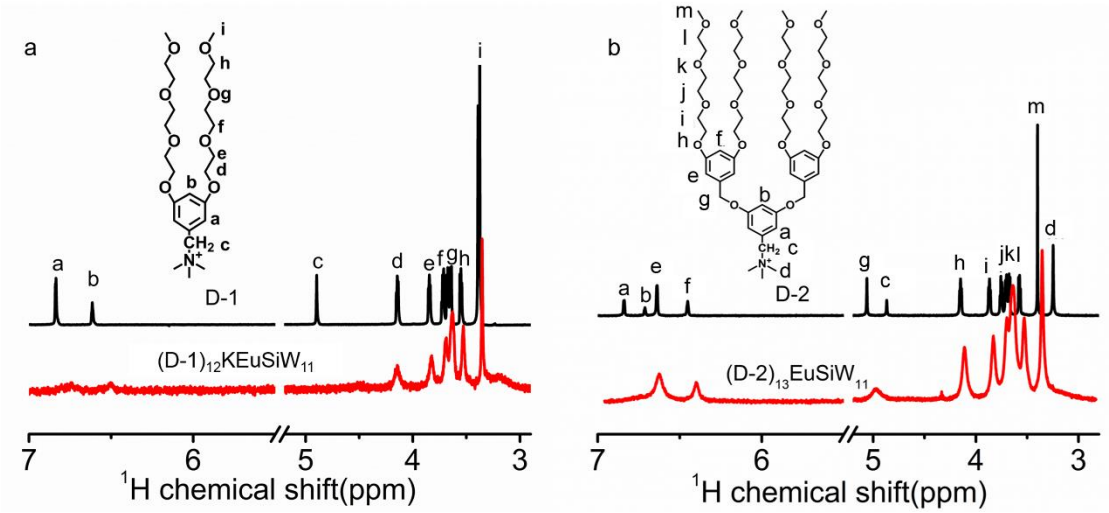

Fig. S1 ^{1}H NMR spectra of (a) D-1 and $(D\text{-}1)_{12}KEuSiW_{11}$, (b) D-2 and $(D\text{-}2)_{13}$ $EuSiW_{11}$ in $CDCl_3$, respectively.

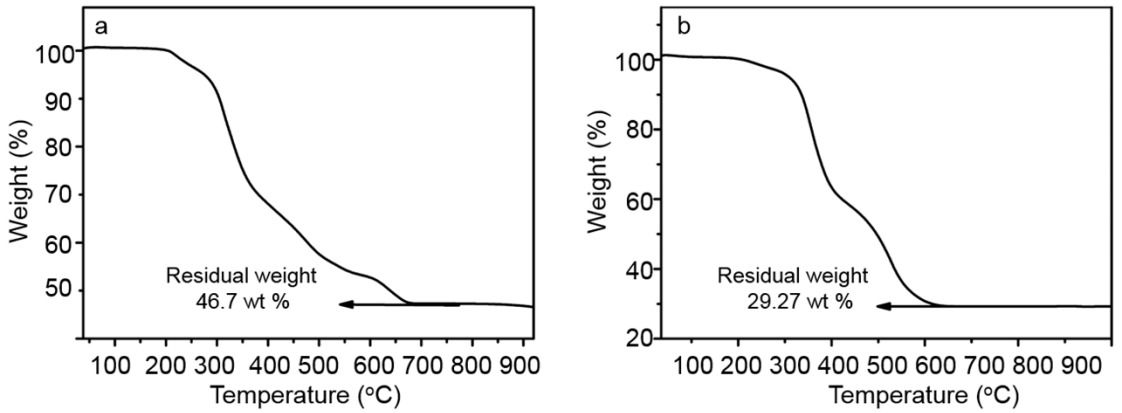

Fig. S2 TGA curves of (a) $(D\text{-}1)_{13}Gd(SiW_{11})_2$ and (b) $(D\text{-}2)_{13}Gd(SiW_{11})_2$, respectively.

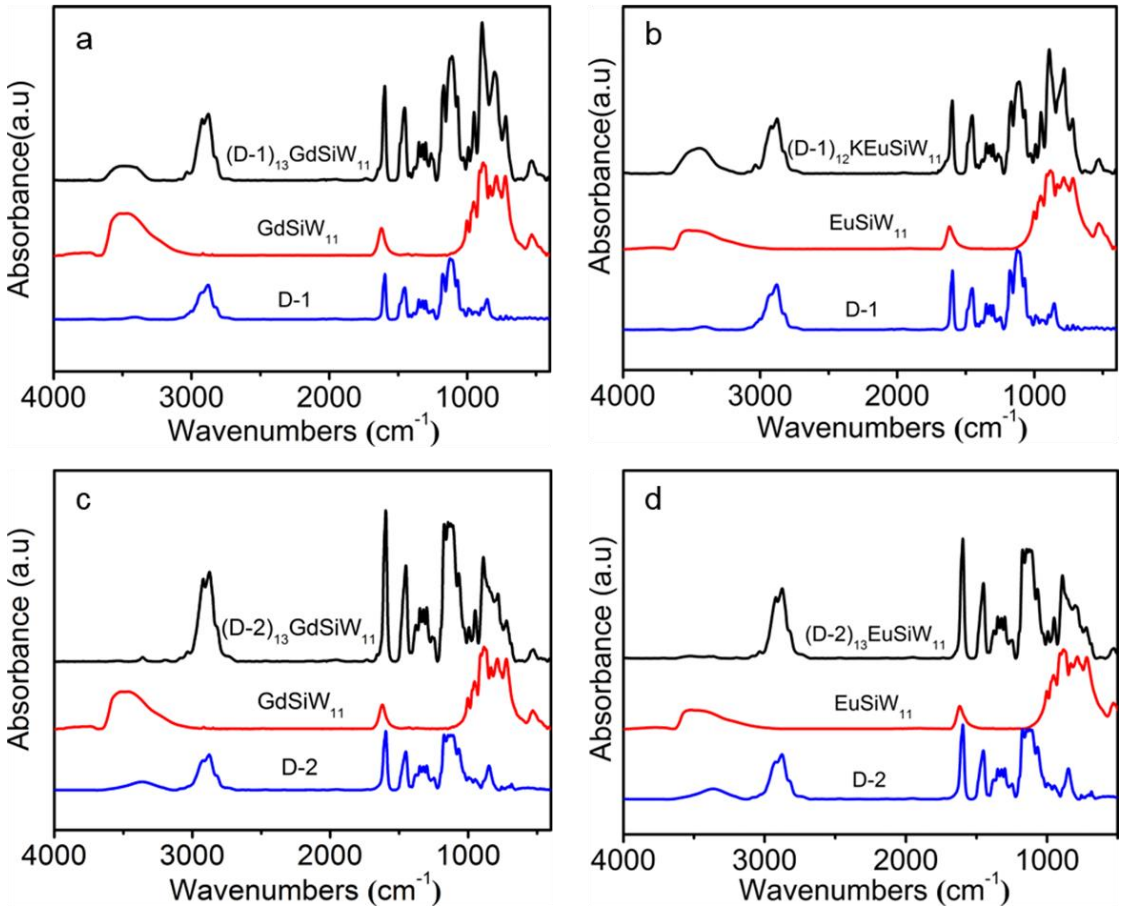

Fig. S3 IR spectra of (a) pure $K_{13}[Gd(SiW_{11}O_{39})_2]$, D-1, and $(D\text{-}1)_{13}Gd(SiW_{11})_2$, (b) pure $K_{13}Eu(SiW_{11}O_{39})_2]$, D-1, $(D\text{-}1)_{12}KEu(SiW_{11})_2$, (c) pure $K_{13}[Gd(SiW_{11}O_{39})_2]$, D-2, and $(D\text{-}2)_{13}Gd(SiW_{11})_2$, (d) pure $K_{13}Eu(SiW_{11}O_{39})_2]$, D-2, and $(D\text{-}2)_{13}Eu(SiW_{11})_2$ in KBr pellets.

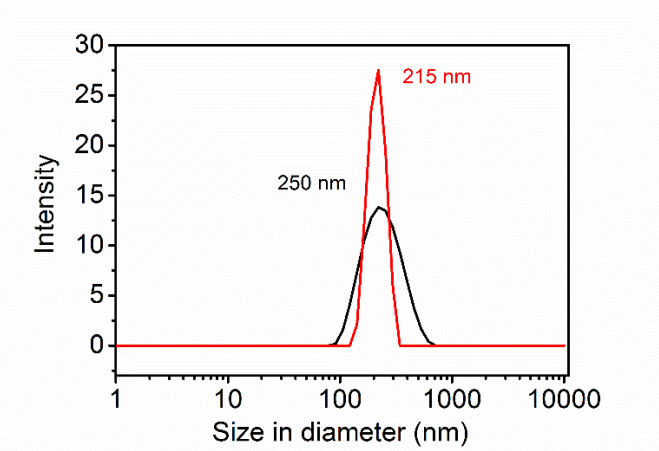

Fig. S4 DLS curves of (a) D-1 (black) and (b) D-2 (red) in aqueous solution at 25°C with the concentration of 0.39 mM.

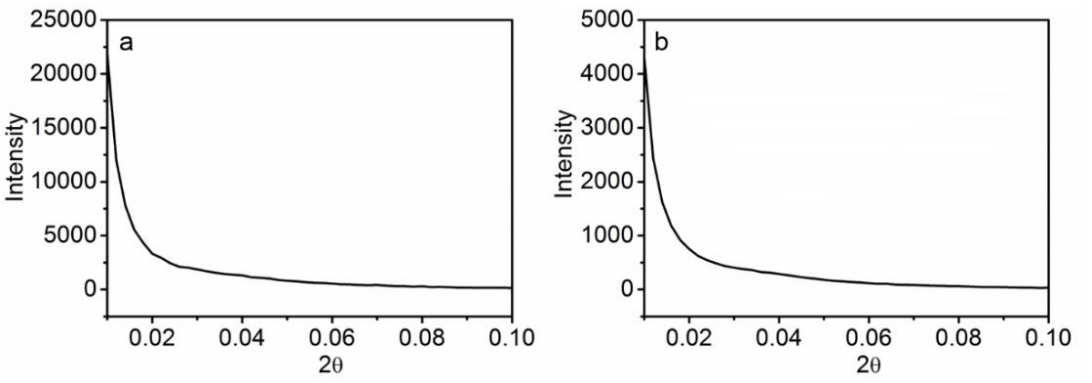

Fig. S5 USAXS pattern of (a) $(D\text{-}1)_{13}GdSiW_{11}$ and (b) $(D\text{-}2)_{13}GdSiW_{11}$ in aqueous solution.

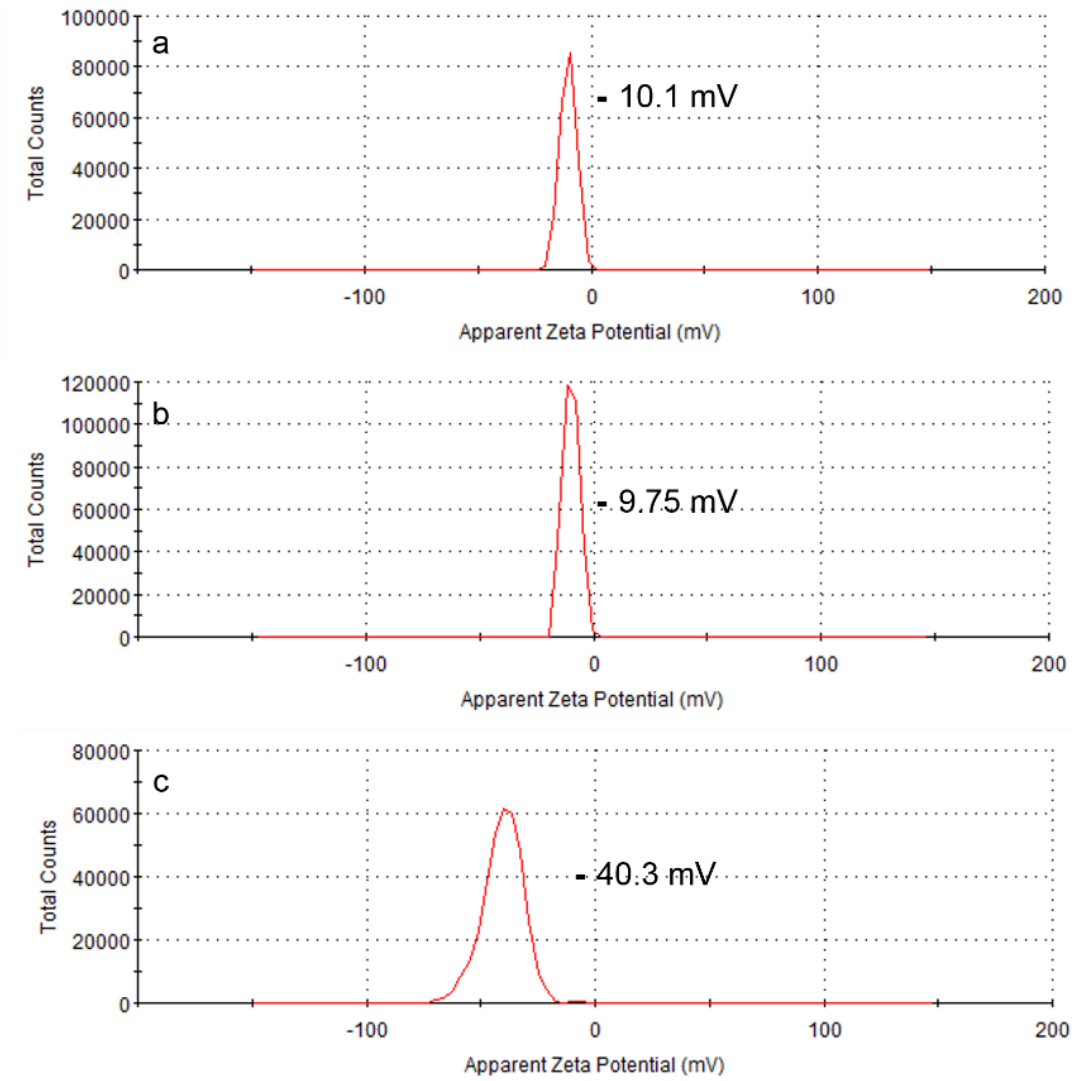

Fig. S6 Zeta potential of (a) $(D\text{-}1)_{13}GdSiW_{11}$, (b) $(D\text{-}2)_{13}GdSiW_{11}$ and (c) pure $GdSiW_{11}$ in aqueous solution, where the concentration is fixed at 0.03 mM.

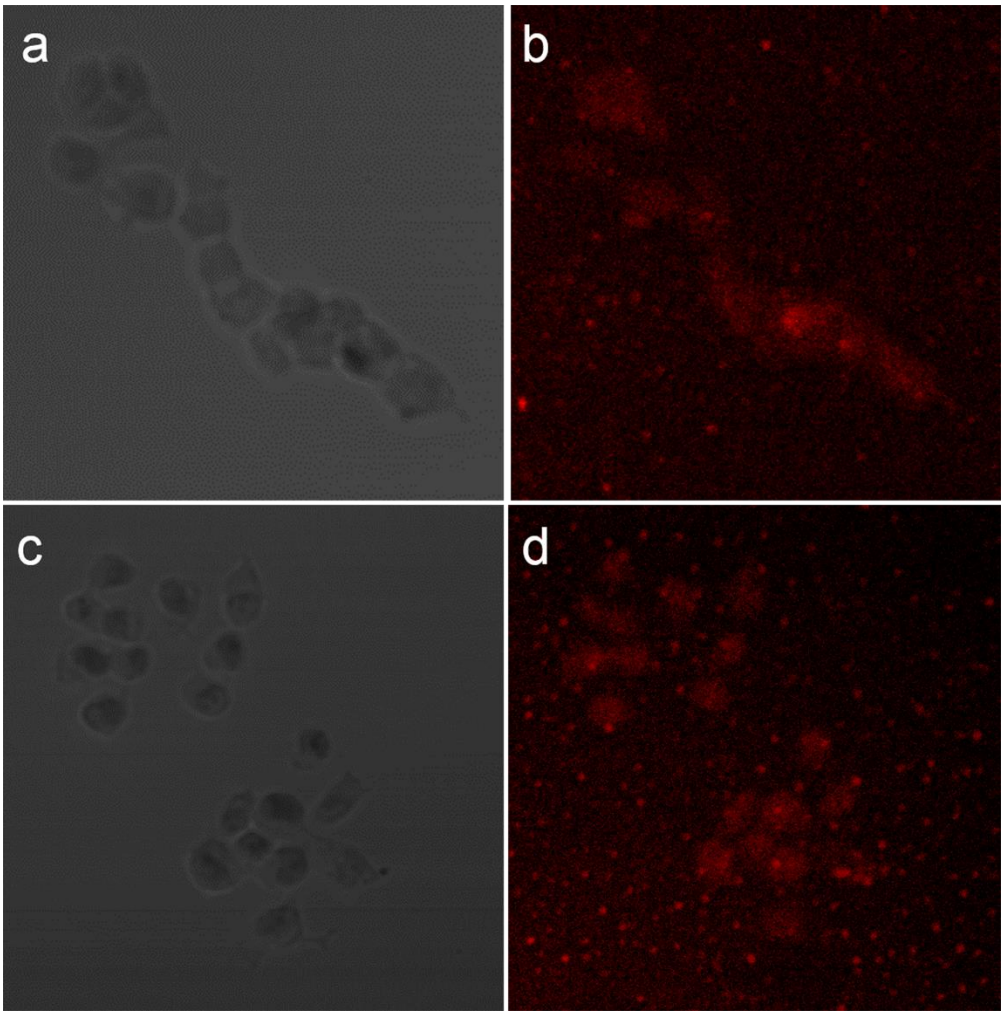

Fig. S7 Confocal laser scanning microscopic (CLSM) images of 293T cells after incubation with 0.01 mM (a, b) $(D\text{-}1)_{13}GdSiW_{11}$ and (c, d) $(D\text{-}2)_{13}GdSiW_{11}$ aggregations that loaded rhodamine B for 4 h under (a, c) bright-field, and (b, d) excitation at 541 nm.

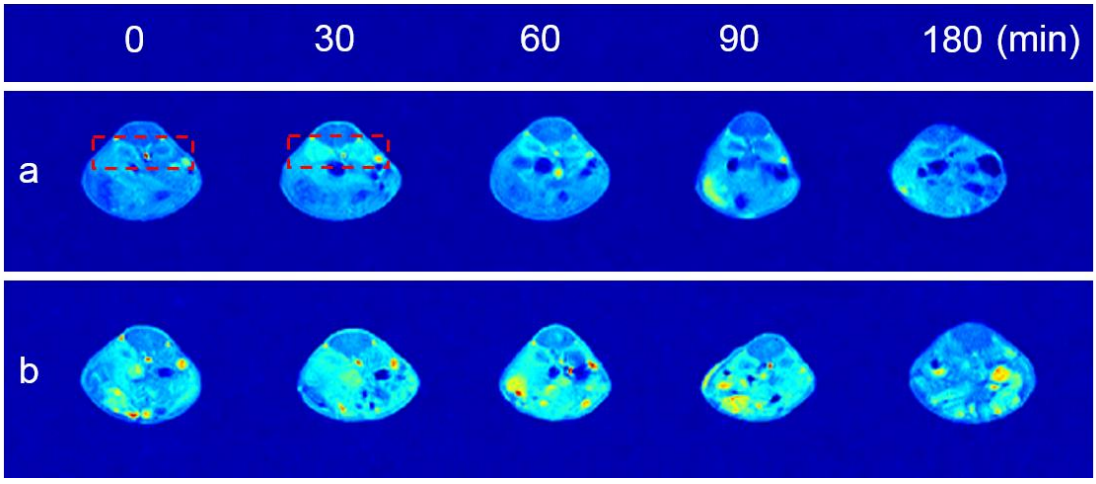

Fig. S8 T_1-weighted images of Wistar rat at kidney after post intravenous injection of (a) $(D\text{-}1)_{13}GdSiW_{11}$ and (b) $(D\text{-}2)_{13}GdSiW_{11}$ for 30, 60, 90 and 180 min.

Table S1. The assignments of infrared spectra of $(D\text{-}1)_{13}GdSiW_{11}$ and $(D\text{-}2)_{13}GdSiW_{11}$ in sold state.

D-1 (cm^{-1})	$(D\text{-}1)_{13}GdSiW_{11}$ (cm^{-1})	D-2 (cm^{-1})	$(D\text{-}2)_{13}GdSiW_{11}$ (cm^{-1})	Assignments
				O–H asym. str.
2936	2923	2928	2921	CH_3 asym. str.
2874	2877	2872	2875	CH_2 asym. str.
2825	2819	2823	2821	CH_2 sym. str.
1596	1598	1595	1596	C=C framework str.
1454	1456	1451	1450	CH_2 scissoring
1387	1384	1380	1379	CH_3 scissoring
1350	1350	1352	1350	CH_2 wagging
1322	1325	1328	1325	CH_2 wagging
1301	1301	1300	1299	CH_2 twisting
1248	1248	1246	1248	CH_2 twisting
1176	1175	1176	1174	=C–O–C asym. str.
1116	1112	1110	1112	C–O–C stretching
-	891	-	889	$Si–O_a$ asym. str.
1071	1071	1072	1071	=C–O–C asym. str.
-	991		995	$W–O_d$ sym. str.
-	950		948	$W–O_d$ asym. str.
	867		867, 835	$W–O_b–W$ asym. str.
846	845	840	842	CH str.
-	789, 761, 721		784, 757, 721	$W–O_c$-W asym. str.
758		758		CH_2 rocking

Table S2. Summary of elemental analysis.[a]

		C	H	N	Gd/Eu	W
$(D\text{-}1)_{13}GdSiW_{11}$	Calcd. (%)	31.99	4.96	1.55	1.34	34.53
	Found (%)	31.56	4.96	1.50	1.31	34.25
$(D\text{-}2)_{13}GdSiW_{11}$	Calcd. (%)	43.53	5.90	0.97	0.84	21.68
	Found (%)	43.67	5.85	0.96	0.83	21.54
$(D\text{-}1)_{12}KEuSiW_{11}$	Calcd. (%)	30.78	4.74	1.50	1.35	36.00
	Found (%)	30.66	4.70	1.47	1.38	36.12
$(D\text{-}2)_{13}EuSiW_{11}$	Calcd. (%)	43.54	5.90	0.97	0.82	21.69
	Found (%)	43.41	6.04	0.85	0.83	21.83

[a]Elemental analytical results of C, H and N were obtained from organic elemental analysis, and the elemental analysis of Gd, Eu and W were performed on inductive coupled plasma emission spectrometer.