Supplementary Information

Nanoassemblies with Gd-chelating lipids (GMO@DTPA-BSA-Gd) as potential new type of high molecular weight contrast agents

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Table S1 The space group and corresponding mean lattice constant obtained from the SAXS (Small Angle X-ray Scattering) spectra analysis.

Sample	Space group	Lattice constant / Å
2GMO-25F127	Pn3m	82.79 ± 0.17
2GMO-5DTPA-10F127	Pn3m	89.42 ± 0.86
2GMO-5DTPA-15F127	Pn3m	90.04 ± 0.40
2GMO-5DTPA-25F127	Pn3m	90.36 ± 0.02
2GMO-30DTPA-25F127	Im3m L_α	148.17 ± 0.51 62.93 ± 0.02
2GMO-40DTPA-25F127	L_α	63.15 ± 0.02
2GMO-50DTPA-25F127	L_α	63.29 ± 0.03

Table S2 ICP-MS instrument settings, data acquisition parameters and calibration data.

General conditions	
RF power, W	1600
Plasma gas flow, L min^{-1}	16
Auxiliary gas flow, L min^{-1}	1.2
Nebulizer gas flow, L min^{-1}	1.04
QID Fixed Voltage	-12
Hyperskimmer Park Voltage	4
OmniRing Park Voltage	-200
Nuclides monitored	^{158}Gd
Analysis parameters	
Dwell time, ms	50
Sweeps	40
Replicates	3
Integration time, ms	2000

Calibration data and instrumental limits of detection (LoDs) and limits of quantification (LoQs), obtained for m/z = 158 determination using ICP-MS.

Parameter	
Cor.Coeff.	0,999216
LoD (µg/L)	0,011
LoQ (ug/L)	0,019

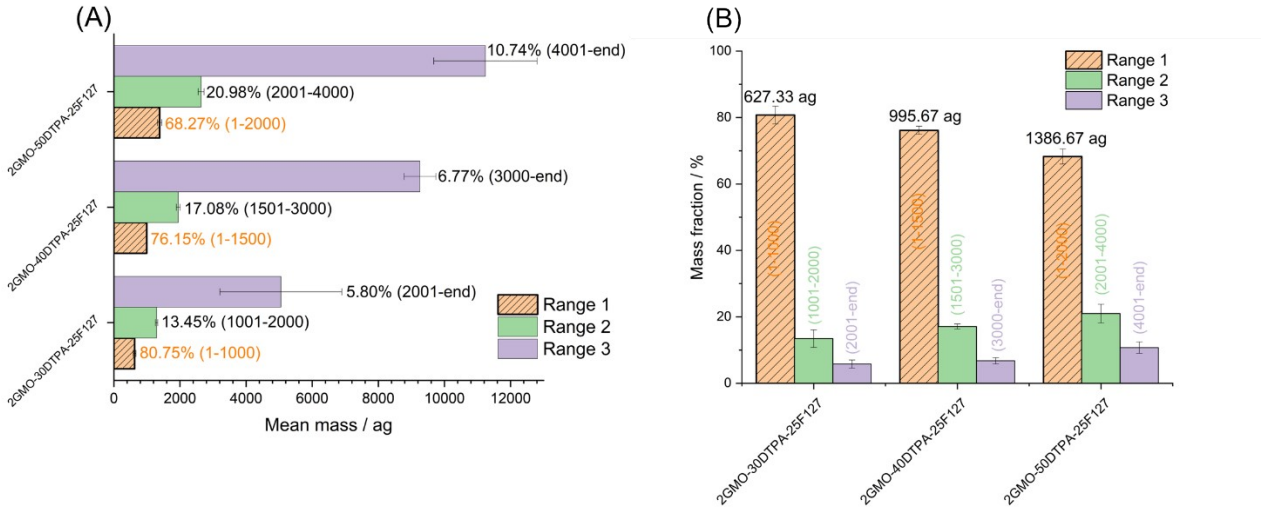

Fig. S1 Single Cell Inductively Coupled Plasma Mass Spectrometry ((SP)-ICP-MS)) uptake studies on HeLa cells treated with nanoassemblies of three different DTPA-BSA-Gd content (30, 40, 50% w/w) and 25% w/w of surfactant Pluronic F127. (A) Mean mass per analyzed nanoassemblies; (B) Percentage of mass fraction per analyzed nanoassemblies. Results show the mean mass of Gd per cell (expressed in attogram (ag)), accounted for the measured dominant single cell in terms of mean mass (Range 1, insert in the figure).

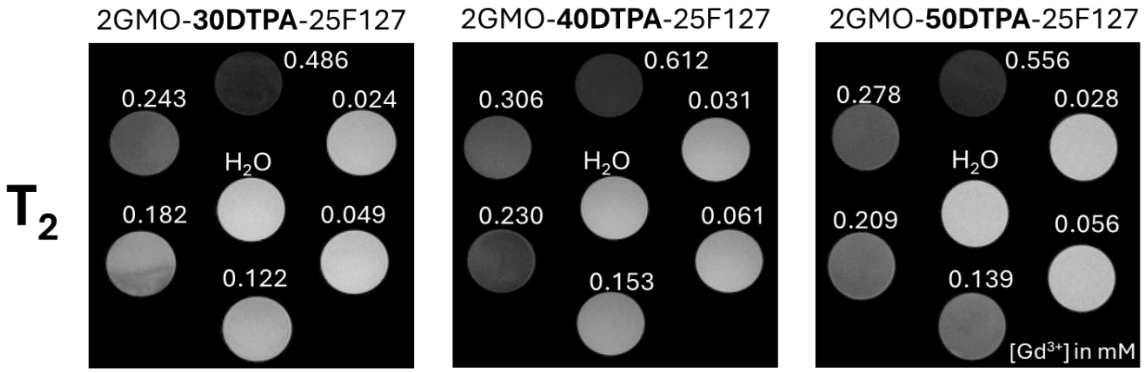

Fig. S2 T_2-weighted MR images of prepared nanoassemblies with high DTPA-BSA-Gd content (2GMO-30DTPA-25F127, 2GMO-40DTPA-25F127, 2GMO-50DTPA-25F127) at different Gd^{3+} ion concentrations ([Gd^{3+}] in mM), collected with a 9.4 T MRI horizontal scanner at room temperature.

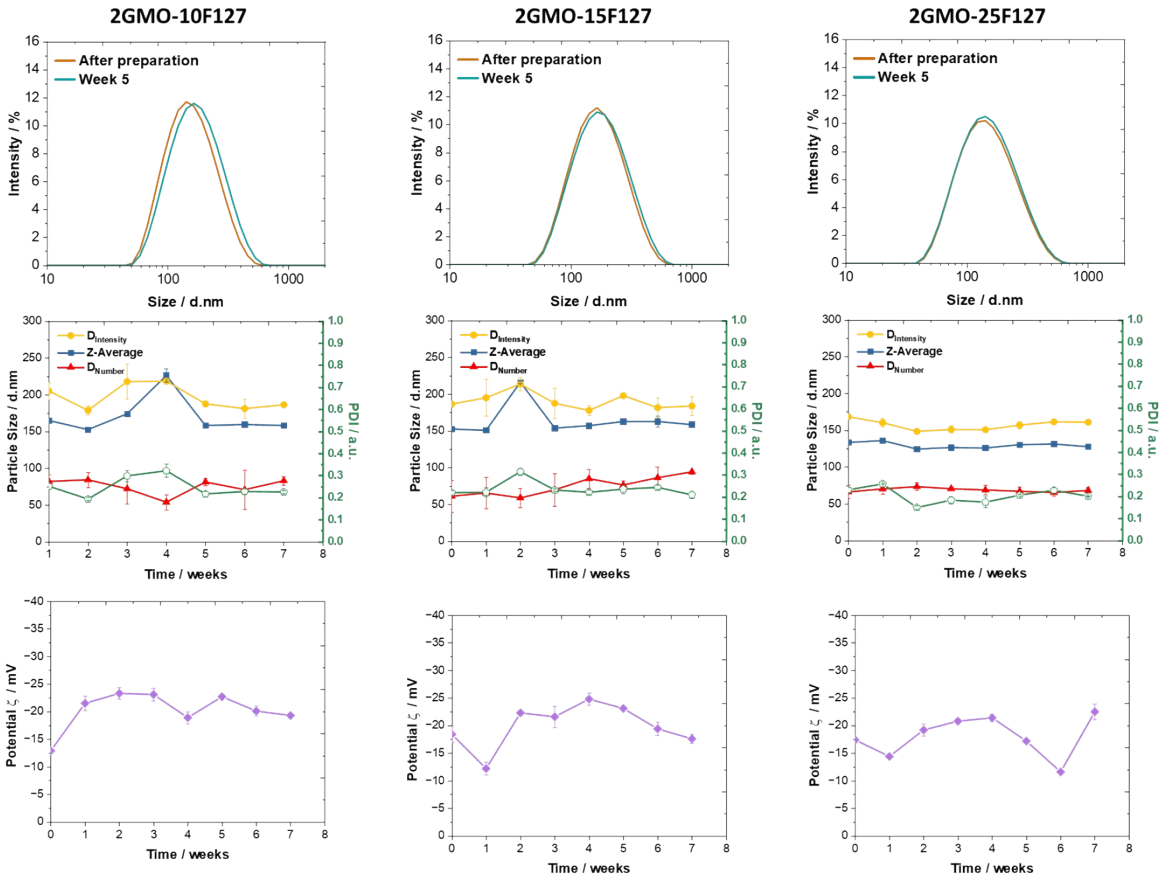

Fig. S3 Dynamic Light Scattering (DLS) results: (top row) particle size distribution curves weighed by intensity for chosen time points (0 – after preparation and after 5 weeks), (middle row) particle size distribution weighed by intensity ($D_{Intensity}$) and by number (D_{Number})), polydispersity index (PDI), (bottom row) potential ζ over the 7 weeks for un-modified nanoassemblies: 2GMO-10F127, 2GMO-15F127, 2GMO-25F127.

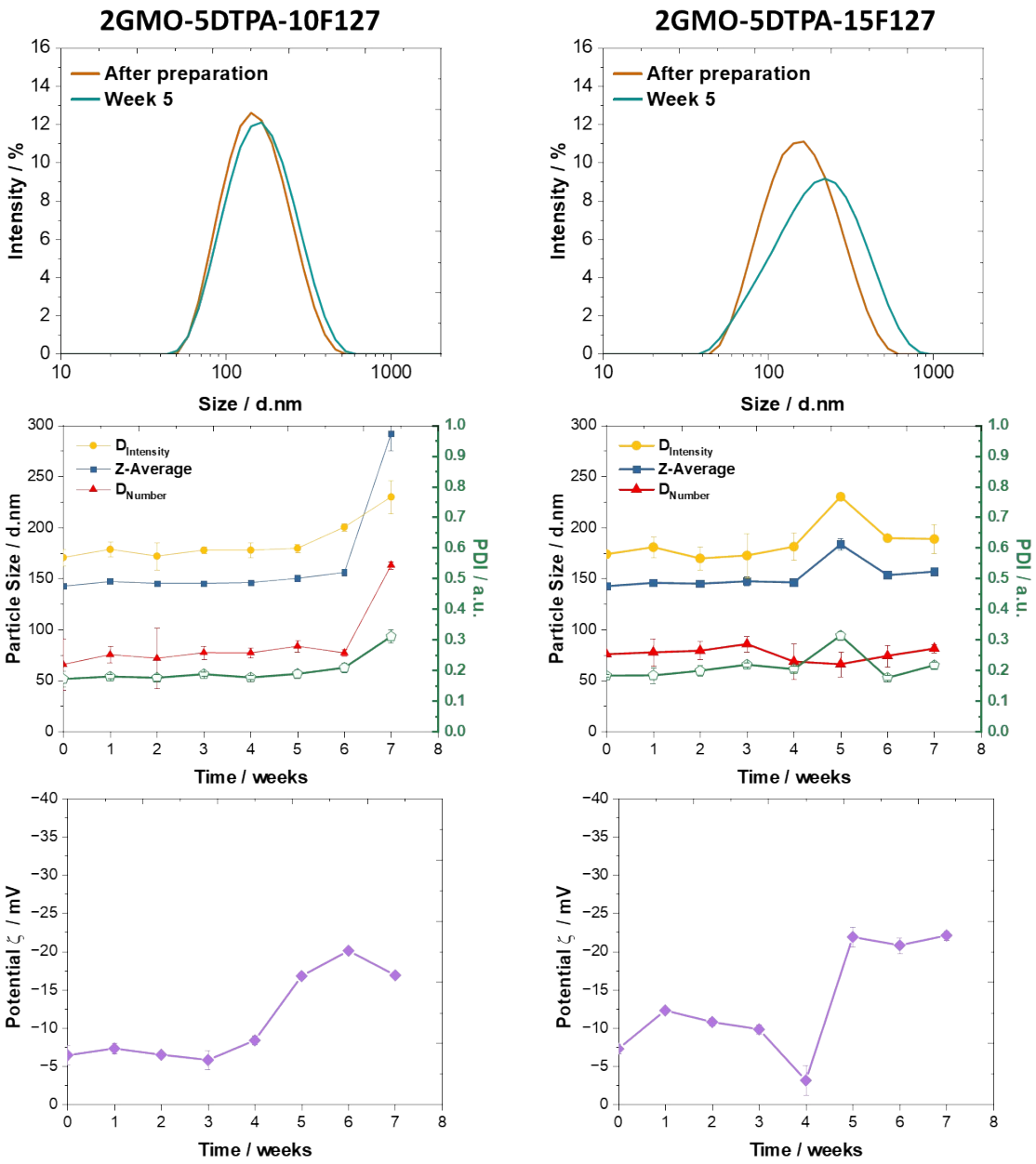

Fig. S4 Dynamic Light Scattering (DLS) results: (top row) particle size distribution curves weighed by intensity for chosen time points (0 – after preparation and after 5 weeks), (middle row) particle size distribution weighed by intensity ($D_{Intensity}$) and by number (D_{Number})), polydispersity index (PDI), (bottom row) potential ζ over the 7 weeks for nanoassemblies with 5% w/w of DTPA-BSA-Gd and 10% w/w (2GMO-5DTPA-10F127) and with 15% w/w (2GMO-5DTPA-15F127) of surfactant Pluronic F127.

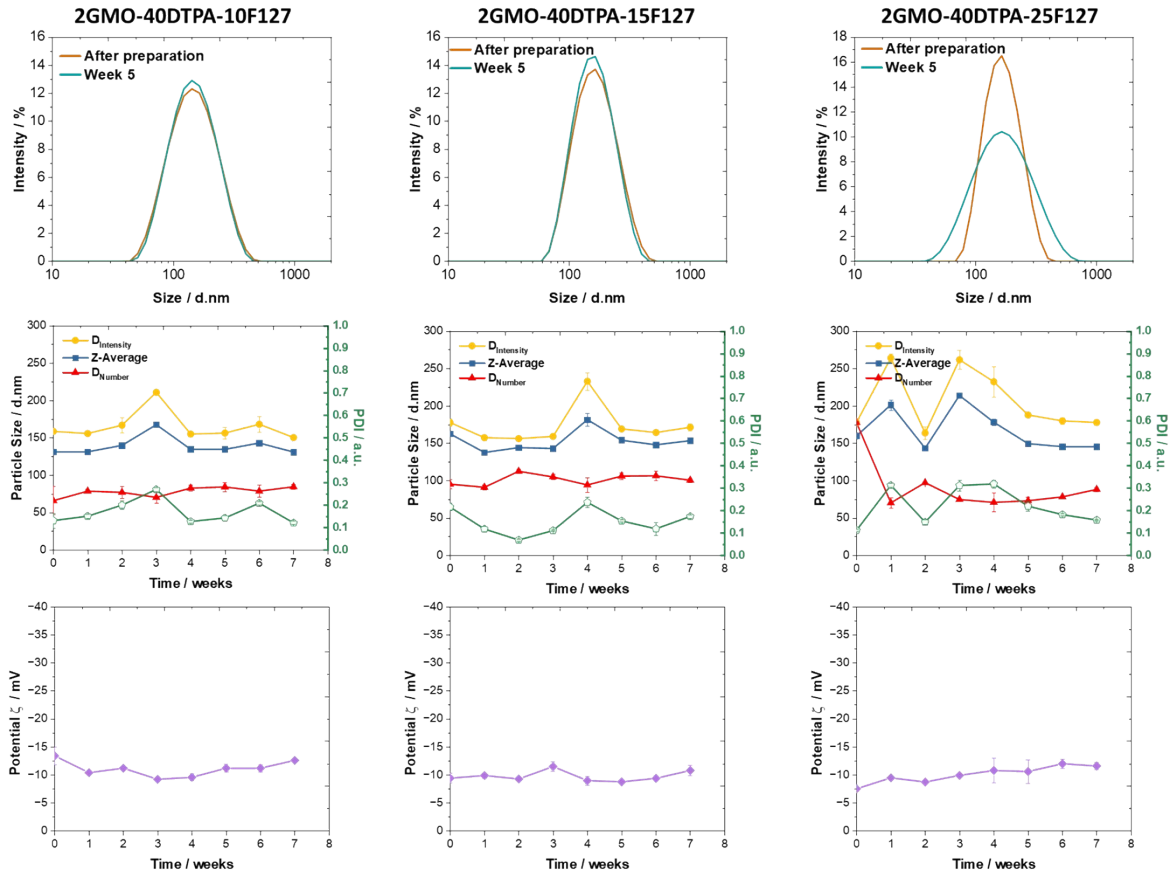

Fig. S5 Dynamic Light Scattering (DLS) results: (top row) particle size distribution curves weighed by intensity for chosen time points (0 – after preparation and after 5 weeks), (middle row) particle size distribution weighed by intensity ($D_{Intensity}$) and by number (D_{Number})), polydispersity index (PDI), (bottom row) potential ζ over the 7 weeks for nanoassemblies with 40% w/w of DTPA-BSA-Gd and 10% w/w (2GMO-5DTPA-10F127), 15% w/w (2GMO-5DTPA-15F127), 25% w/w (2GMO-40DTPA-25F127) of surfactant Pluronic F127.

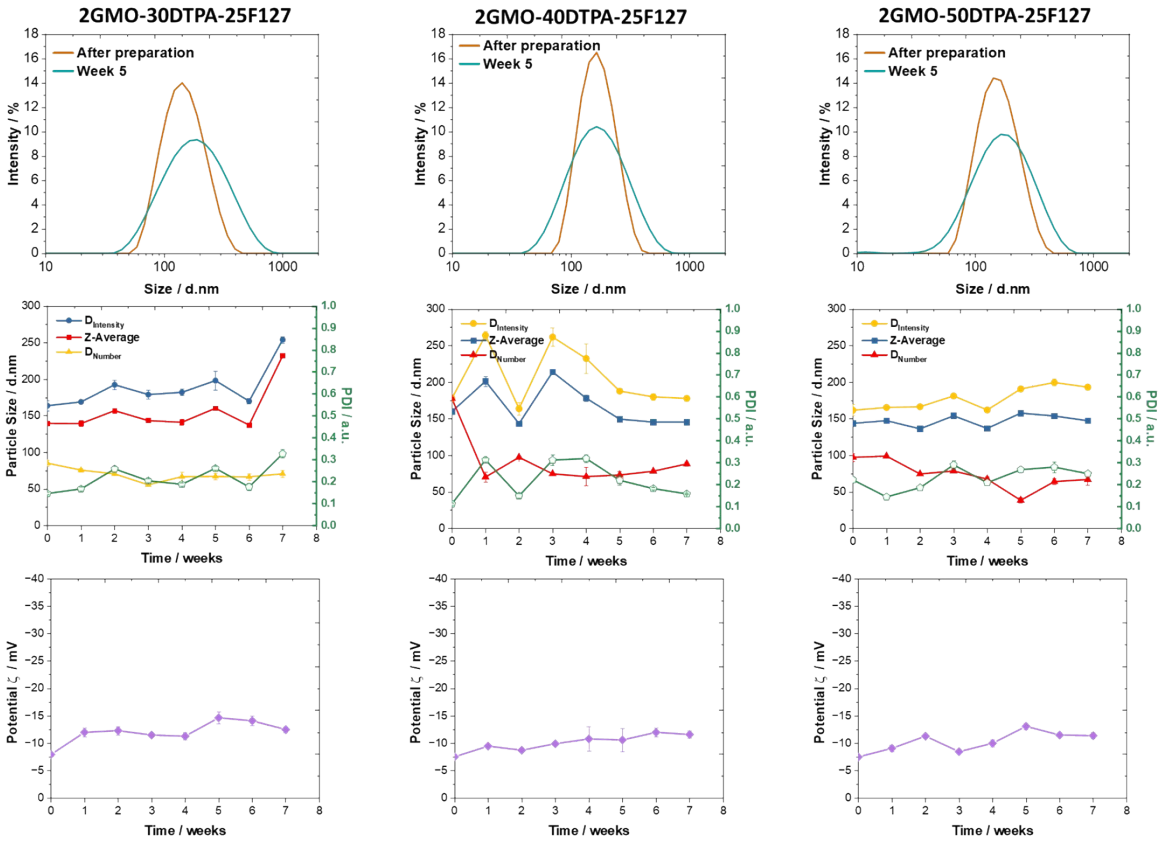

Fig. S6 Dynamic Light Scattering (DLS) results: (top row) particle size distribution curves weighed by intensity for chosen time points (0 – after preparation and after 5 weeks), (middle row) particle size distribution weighed by intensity ($D_{Intensity}$) and by number (D_{Number})), polydispersity index (PDI), (bottom row) potential ζ over the 7 weeks for nanoassemblies with 30% w/w (2GMO-30DTPA-25F127), 40% w/w (2GMO-40DTPA-25F127) and 50% w/w (2GMO-50DTPA-25F127) of DTPA-BSA-Gd and 25% w/w of surfactant Pluronic F127.