

Supporting Information

Relaxometric Properties and Biocompatibility of a Novel Nanostructured Fluorinated Gadolinium Metal-Organic Framework

Letizia Trovarelli ^{*a#}, Alessandra Mirarchi ^{b#}, Cataldo Arcuri ^{b*}, Stefano Bruscoli ^b, Oxana Bereshchenko ^b, Marta Febo ^b, Fabio Carniato ^{*c}, Ferdinando Costantino ^{*a}

a. Department of Chemistry, Biology and Biotechnologies, University of Perugia

Via Elce Di Sotto n 8, 06123, Perugia, Italy

b. Department of Medicine and Surgery, University of Perugia

Piazza Lucio Severi n 1, 06132 Perugia, Italy

c. Department of Science and Technology, University of Eastern Piedmont "A.Avogadro"

Viale Teresa Michel 11, 15121, Perugia, Italy

Identification code	GdF4BDC
Empirical formula	C15 H8 F6 Gd N O8
Formula weight	601.47
Temperature (K)	293(2)
Wavelength (Å)	0.71069
Crystal System	monoclinic
Space Group	P 21/a
Unit Cell Dimensions (Å, °)	a=7.7894(2), b=21.8151(6) c=10.1789(3) β=98.800(1)
Volume (Å ³)	1709.30(8)
Z	4
Density (calculated) (Mg/m ³)	2.337
Absorption coefficient (mm ⁻¹)	3.994
F(000)	1148
Crystal size (mm)	0.57 x 0.12 x 0.10
Theta range for data collection (°)	2.236 to 30.560
Index ranges	-11 ≤ h ≤ 11, -31 ≤ k ≤ 31, -14 ≤ l ≤ 14
Reflections collected	5243
Independent reflections	38028 [R(int) = 0.0478]
Completeness	99.8 % (to theta= 30.560°)
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4683 / 2 / 288
Goodness-of-fit on F ²	1.111
Final R indices [I > 2σ(I)]	R1 = 0.0247, wR2 = 0.0577

Table S1. Crystallographic data for **GdF4BDC**

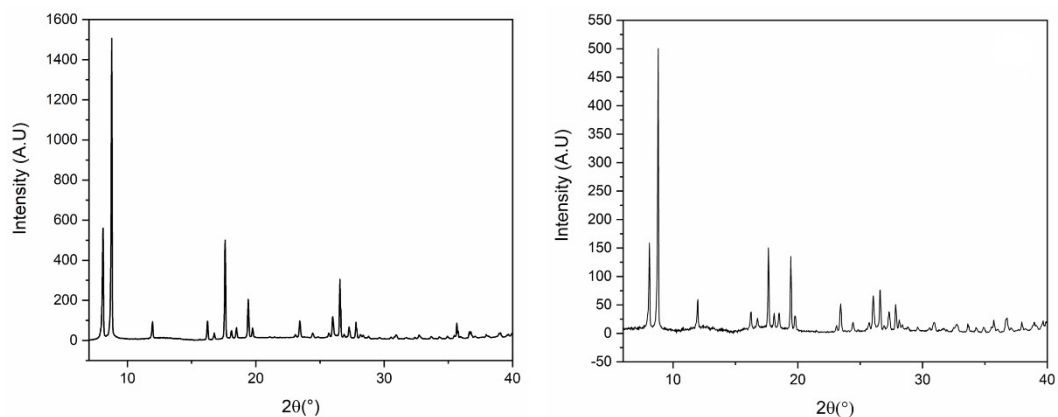


Figure S1: PXRD patterns of Gd-F₄BDC nanoparticles obtained using: (sx) CTABr (Cetyltrimethylammonium Bromide) and (dx) Acetic acid as modulators.

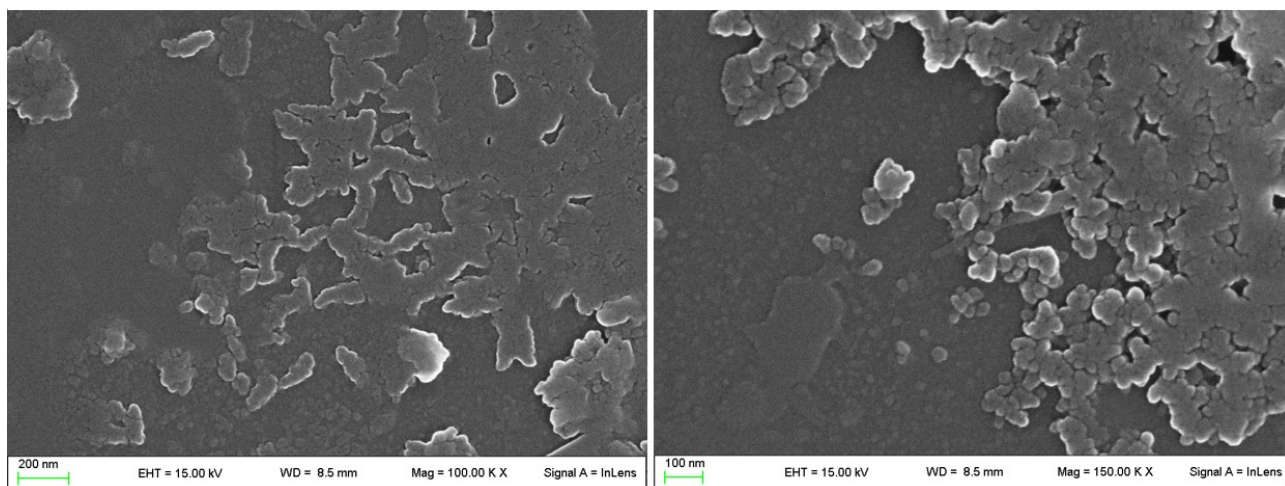


Figure S2: SEM images of Gd-F₄BDC nanoparticles obtained using CTABr (Cetyltrimethylammonium Bromide) as modulator.

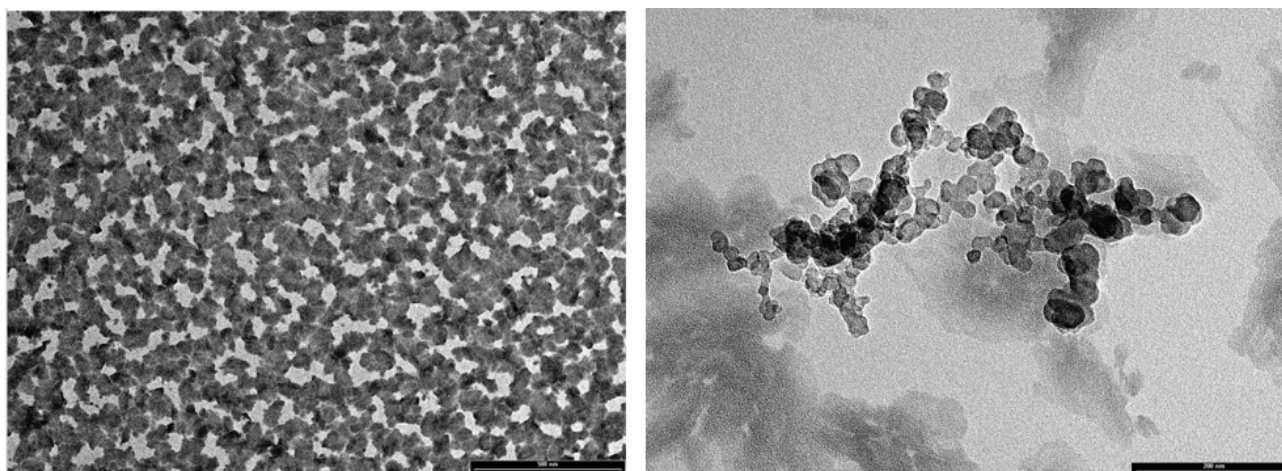


Figure S3: TEM images of Gd-F₄BDC nanoparticles obtained using CTABr (Cetyltrimethylammonium Bromide) as modulator.

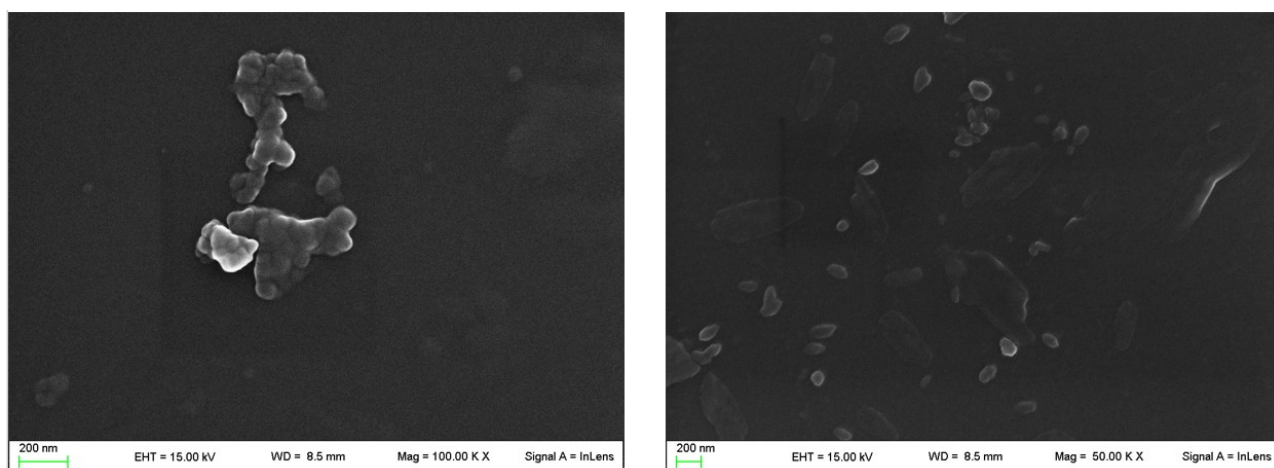


Figure S4: SEM images of Gd-F₄BDC nanoparticles obtained using A.A (Acetic acid) as modulator.

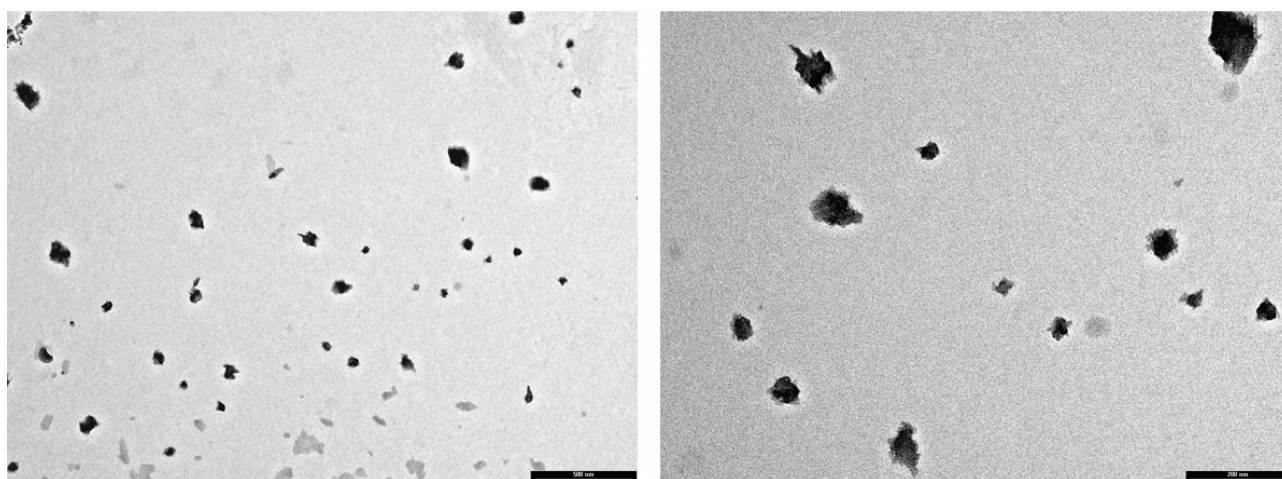


Figure S5: TEM images of Gd-F₄BDC nanoparticles obtained using A.A (Acetic acid) as modulator.

	Gd ³⁺ (ppm)	V (mL)	% Gd ³⁺ _{diss} / Gd ³⁺ _{tot}
Gd-F ₄ BDC	0.09968	5	0.02 %

Table S2: Gd³⁺ leaching evaluated from ICP-OES: Gd³⁺ concentration in ppm, sample volume and the metal percentage released.

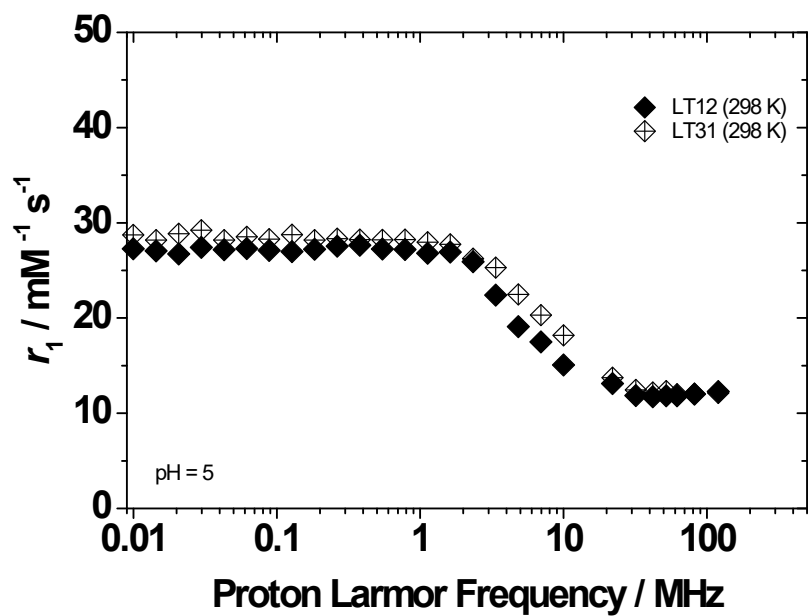


Figure S6: ^1H T_1 NMRD profiles of Gd- F_4BDC NPs (LT31) compared to Gd- F_4BDC Single crystals (LT12)