Electronic supplementary information

Design of high-relaxivity polyelectrolyte nanocapsules based on citrate complexes of gadolinium(III) of unusual composition

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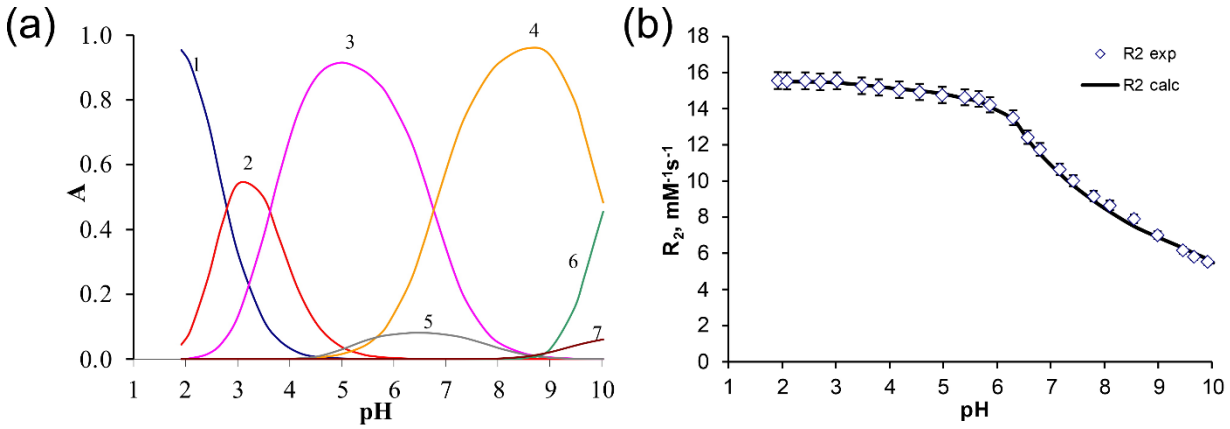

Figure S1: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand ratio 1 : 1 (1-Gd, 2-GdH_2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2)

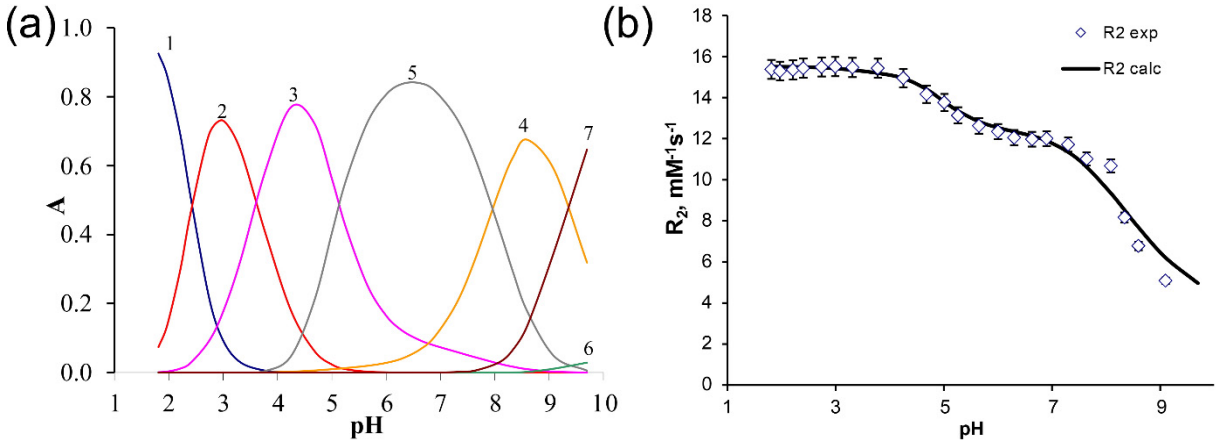

Figure S2: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand ratio 1 : 3; (1-Gd, 2-GdH_2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)2$, 7-GdL_2)

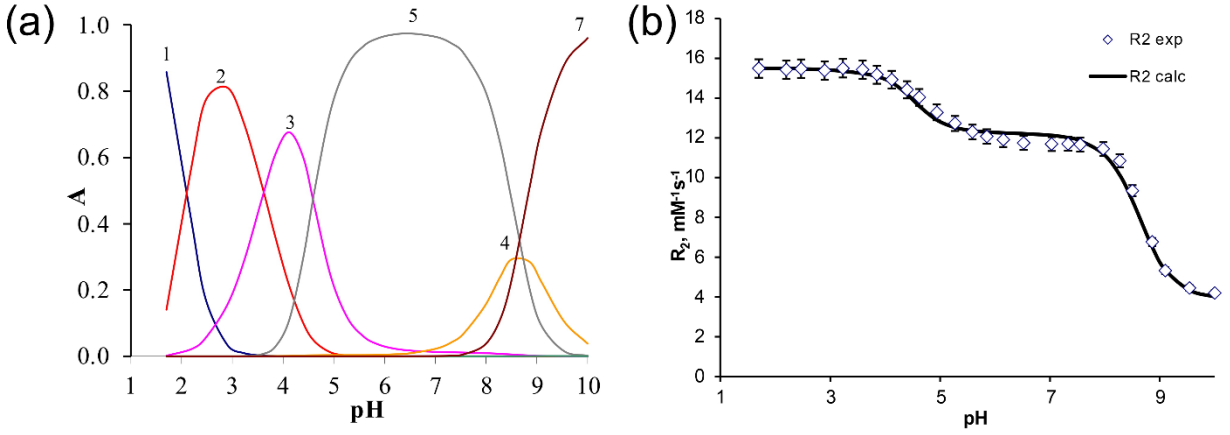

Figure S3: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand ratio 1 : 10; (1-Gd, 2-GdH_2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2)

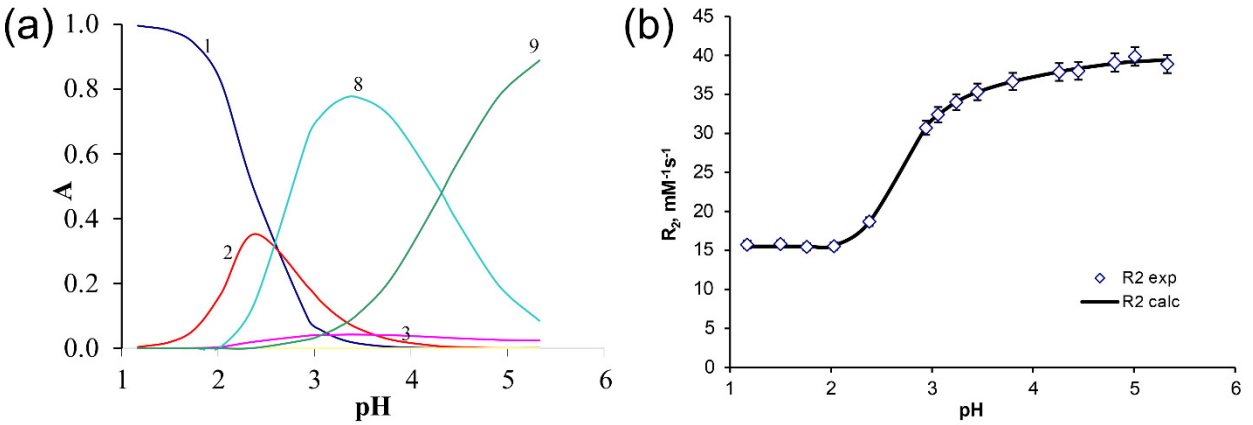

Figure S4: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid - PEI0 system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI0 ratio 1 : 3 : 10. (1-Gd, 2-GdH_2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)

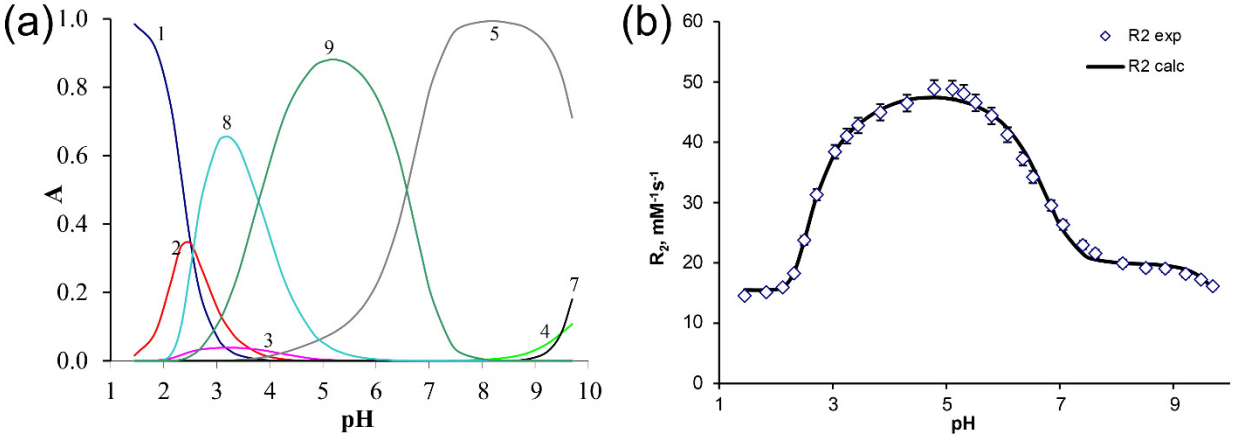

Figure S5: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid - PEI0 system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI0 ratio 1 : 3 : 20 (1-Gd, 2-GdH_2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)

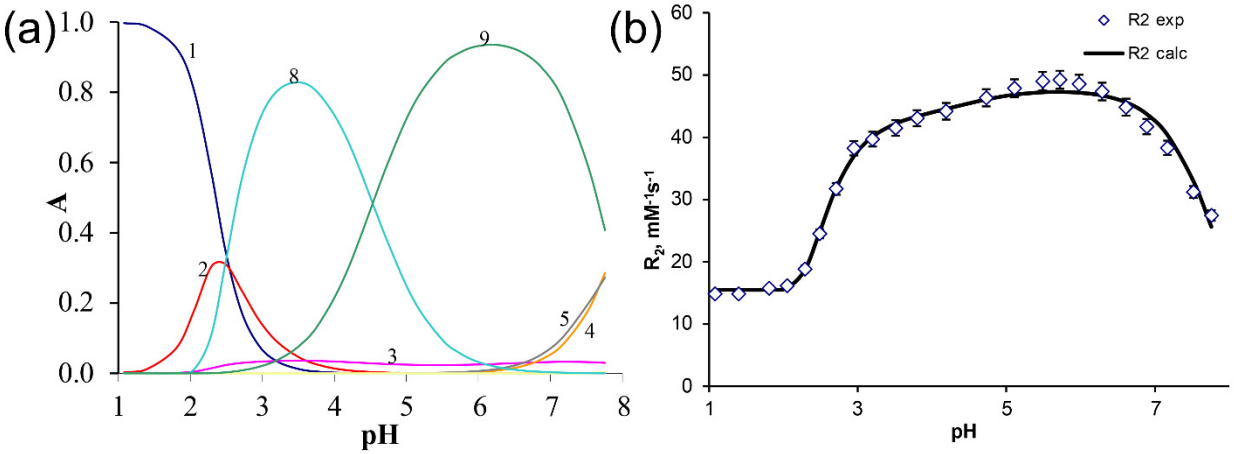

Figure S6: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid - PEI0 system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI0 ratio 1 : 3 : 50 (1-Gd, 2-GdH2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)

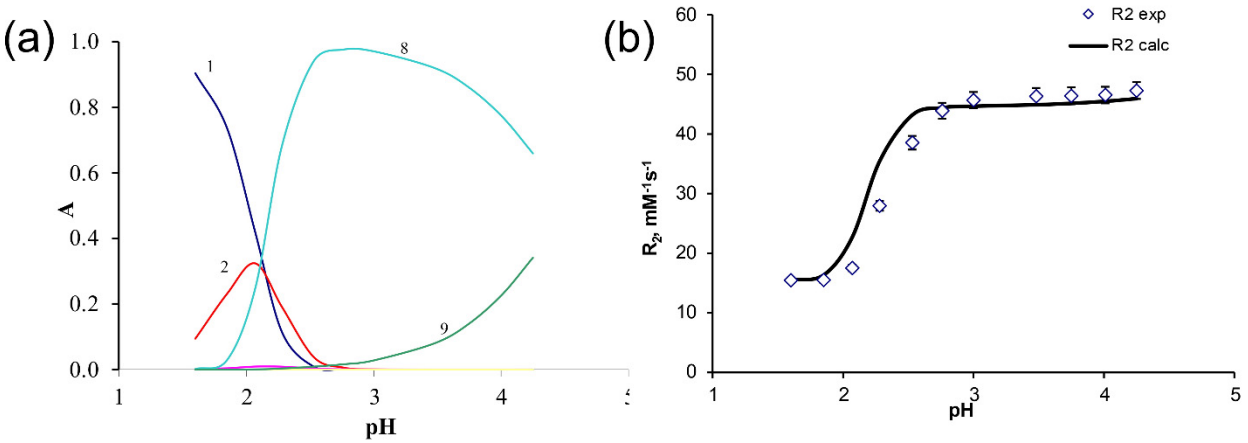

Figure S7: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid - PEI0 system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI0 ratio 1 : 10 : 20; (1-Gd, 2-H_4L, 3-H_3L, 4-H_2L, 5-HL, 6-L, 7-GdH_2L, 8-GdHL, 9-GdL, 10-$Gd(HL)_2$, 11-$Gd_3L_3(OH)_2$, 12-GdL_2, 13-$Gd(H_2L)_3$, 14-$Gd(H_2L)_2HL$)

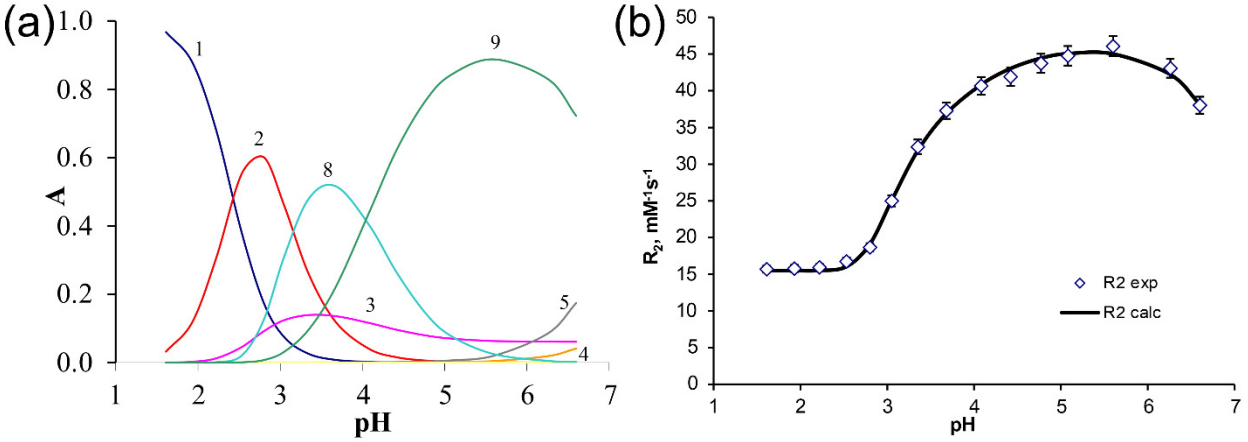

Figure S8: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid - PEI0 – NaCl system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI0-NaCl ratio 1 : 3 : 20:300; (1-Gd, 2-GdH2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)

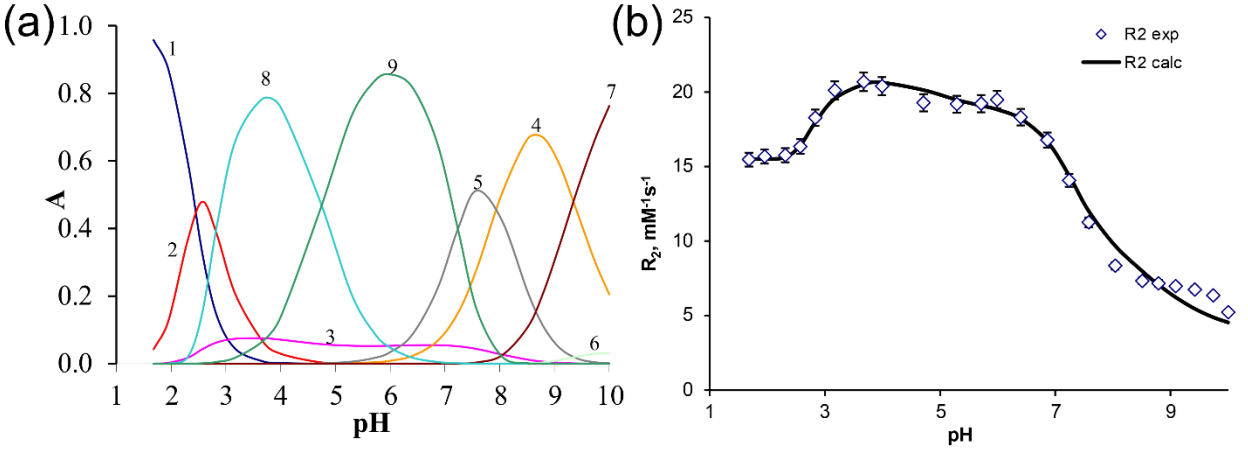

Figure S9: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid – PEI3 system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI3 ratio 1 : 3 : 20; (1-Gd, 2-GdH2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)

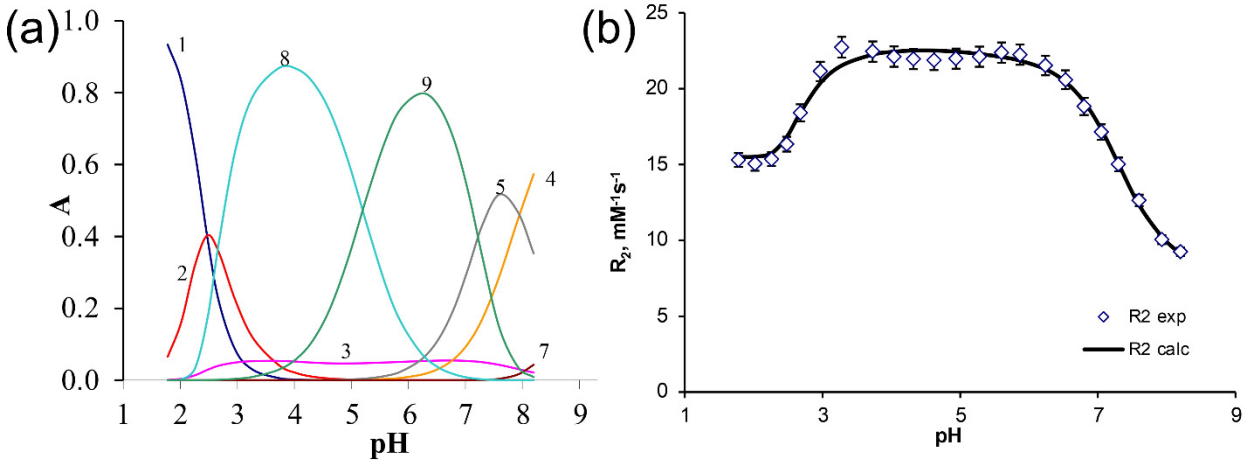

Figure S10: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid – PEI2 system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI2 ratio 1 : 3 : 20; (1-Gd, 2-GdH2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)

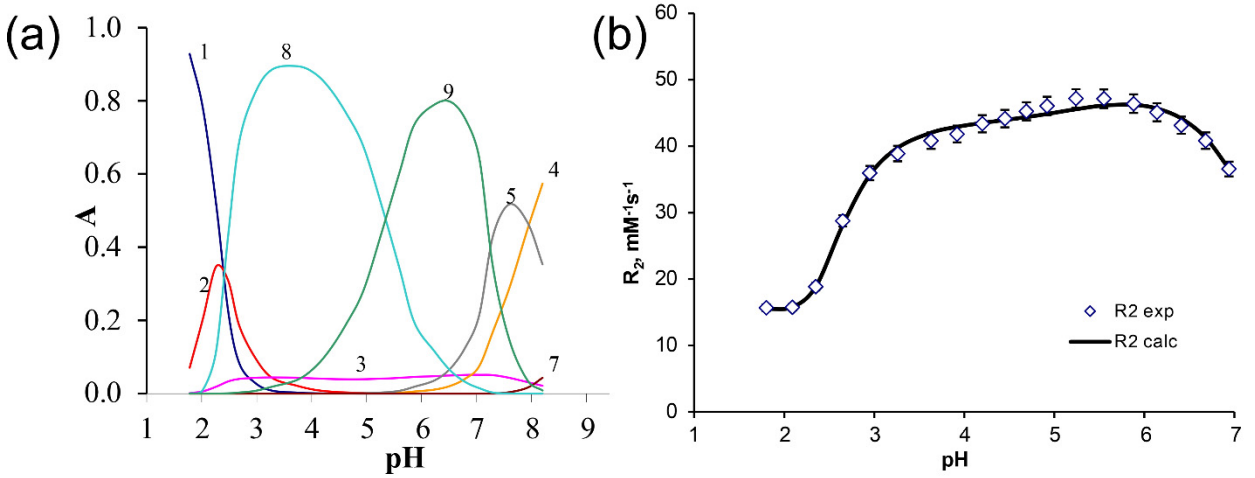

Figure S11: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid – PEI1 system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PEI1 ratio 1 : 3 : 20; (1-Gd, 2-GdH2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)

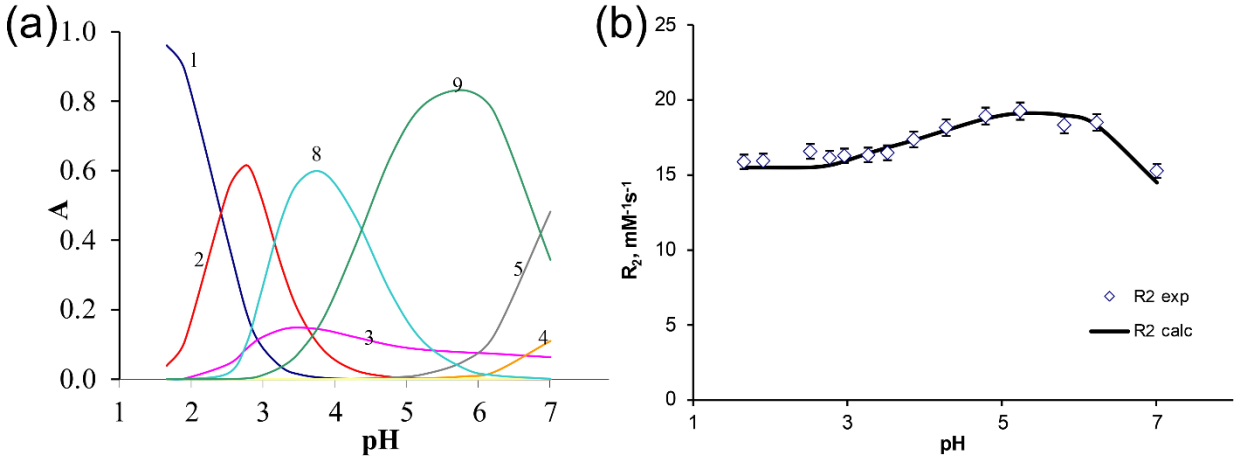

Figure S12: Diagrams of the proportional distribution of complex forms accumulating in the gadolinium(III) - citric acid – PDDC system (a) and Relaxivity vs pH experimental and fitted curves (b) at a metal-ligand-PDDC ratio 1 : 3 : 20. (1-Gd, 2-GdH2L, 3-GdHL, 4-GdL, 5-$Gd(HL)_2$, 6-$Gd_3L_3(OH)_2$, 7-GdL_2, 8-$Gd(H_2L)_3$, 9-$Gd(H_2L)_2HL$)