Table 1: Treatment details for each group. Treatment times are referenced to the contamination with ^{153}Gd.

Group	Ligand	Time	Treatment
A	Saline	1 hr pre	100 μmol / kg
B	HOPO	24 hr pre	100 μmol / kg
C	HOPO	1 hr pre	100 μmol / kg
D	DTPA	1 hr pre	100 μmol / kg
E	HOPO	1 hr post	100 μmol / kg
F	DTPA	1 hr post	100 μmol / kg
G	HOPO	24 hr post	100 μmol / kg
H	HOPO	48 hr post	100 μmol / kg

Table 1: ^{153}Gd content of murine tissues and excreta for all groups. Data are reported as arithmatic means ± standard deviations in % of the recovered dose. Excreta were collected by group, therefore only the mean is reported

	Tissues										Excreta	
Group	Skeleton	Liver	Soft	ART	Kidneys	Heart	Lungs	Spleen	Brain	Thymus	Feces	Urine
A	40.5±1.3	10.5±1.4	3.71±0.29	0.998±0.18	0.622±0.09	0.0981±0.028	0.225±0.049	0.106±0.019	0.063±0.0032	0.0456±0.014	6.90	36.19
B	3.88±0.99	0.576±0.31	0.931±0.3	0.296±0.086	0.369±0.21	0.019±0.0074	0.0885±0.02	0.0422±0.012	0.0511±0.019	0.0138±0.014	66.00	28.02
C	0.0359±0.072	0.122±0.02	0.584±0.13	0.0865±0.014	0.0556±0.017	0.00633±0.0048	0.0584±0.011	0.0331±0.011	0.0373±0.016	0.0183±0.0054	74.00	24.80
D	7.59±1	0.781±0.33	0.63±0.061	0.167±0.027	0.0764±0.011	0.0117±0.0074	0.0798±0.0043	0.0315±0.013	0.0293±0.014	0.0209±0.0084	2.50	88.07
E	13.6±1.6	0.556±0.13	1.88±0.17	0.454±0.016	0.143±0.022	0.351±0.052	0.0971±0.0067	0.073±0.011	0.0328±0.0063	0.0296±0.009	46.00	36.50
F	31.4±1.7	6.32±1.6	2.59±0.3	0.881±0.12	0.253±0.027	0.201±0.055	0.133±0.015	0.0848±0.023	0.0407±0.011	0.0312±0.0096	8.80	49.20
G	29.2±1.2	0.81±0.073	2.42±0.22	0.655±0.14	0.179±0.058	0.219±0.016	0.14±0.011	0.0793±0.015	0.0254±0.0087	0.0165±0.0021	30.00	35.88
H	28.4±1	1.68±0.24	2.61±0.31	1.05±0.16	0.392±0.2	0.159±0.026	0.154±0.023	0.0778±0.0047	0.0276±0.0081	0.0405±0.021	26.00	39.69

Table S2: Equilibria and corresponding stability constants used in the speciation study.

Equilibrium	log K	Reference
$Gd^{3+} + PO_4^{3-} = [GdPO_4]_{(aq)}$	12.19	NIST
$Gd^{3+} + HPO_4^{2-} = [GdHPO_4]^+$	5.91	NIST
$Gd^{3+} + 2\ HPO_4^{2-} = [Gd(HPO_4)_2]^-$	9.97	NIST
$Gd^{3+} + H_2PO_4^- = [GdH_2PO_4]^{2+}$	2.74	NIST
$Gd^{3+} + C_2O_4^{2-} = [GdC_2O_4]^+$	4.77	NIST
$Gd^{3+} + 2\ C_2O_4^{2-} = [Gd(C_2O_4)]^-$	8.66	NIST
Gd^{3+} + Lactate$^-$ = [GdLactate]$^{2+}$	2.91	NIST
Gd^{3+} + 2 Lactate$^-$ = [GdLactate$_2$]$^+$	5.04	NIST
Gd^{3+} + 3 Lactate$^-$ = [GdLactate$_3$]	6.24	NIST
Gd^{3+} + Citrate^{3-} + H^+ = [GdHCitrate]	21.2	Heller 2012[a]
Gd^{3+} + 2 Citrate^{3-} + 3 H^+ = [Gd(H$_2$Citrate)(HCitrate)]$^{2-}$	43.6	Heller 2012[a]
Gd^{3+} + 2 Citrate^{3-} + 2 H^+ = [Gd(HCitrate)$_2$]$^{3-}$	38.5	Heller 2012[a]
Gd^{3+} + 2 Citrate^{3-} = [GdCitrate$_2$]$^{5-}$	21.0	Heller 2012[a]
$Gd^{3+} + CO_3^{2-} = [GdCO_3]^+$	7.64	NIST
$Gd^{3+} + 2\ CO_3^{2-} = [Gd(CO_3)_2]^-$	13.04	NIST
$Gd^{3+} + HCO_3^- = [GdHCO_3]^{2+}$	1.9	NIST
Gd^{3+} + DTPA^{5-} = [GdDTPA]$^{2-}$	22.39	NIST
[GdDTPA]$^{2-}$ + H^+ = [GdHDTPA]$^-$	2.39	NIST
Gd^{3+} + DOTA^{4-} = [GdDOTA]$^-$	24.0	NIST
Gd^{3+} + DTPA-BMA^{3-} = [GdDTPA-BMA]	16.86	NIST
Gd^{3+} + EDTA^{4-} = [GdEDTA]$^-$	17.35	NIST
[GdEDTA]$^-$ + H^+ = [GdHEDTA]	1.3	NIST
Gd^{3+} + HOPO^{4-} = [GdHOPO]$^-$	20.5	Sturzbecher-Hoehne 2011[b]
[GdHOPO]$^-$ + H^+ = [GdHHOPO]	1.2	Sturzbecher-Hoehne 2011[b]
$Gd^{3+} + H_2O = [GdOH]^{2+} + H^+$	-8.1	Sturzbecher-Hoehne 2011[b]
$Gd^{3+} + 2\ H_2O = [Gd(OH)_2]^+ + 2\ H^+$	-14.5	Sturzbecher-Hoehne 2011[b]
$Gd^{3+} + 3\ H_2O = [Gd(OH)_3] + 3\ H^+$	-24.1	Sturzbecher-Hoehne 2011[b]
Zn^{2+} + DTPA^{5-} = [ZnDTPA]$^{3-}$	18.2	NIST
[ZnDTPA]$^{3-}$ + H^+ = [ZnHDTPA]$^{2-}$	5.6	NIST
[ZnDTPA]$^{3-}$ + Zn^{2+} = [Zn$_2$DTPA]$^-$	4.48	NIST
Zn^{2+} + EDTA^{4-} = [ZnEDTA]$^{2-}$	16.5	NIST
[ZnEDTA]$^{2-}$ + H^+ = [ZnHEDTA]$^-$	3.0	NIST
Zn^{2+} + DTPA-BMA^{3-} = [ZnDTPA-BMA]$^-$	12.04	NIST
$Zn^{2+} + HPO_4^{2-} = [ZnHPO_4]$	2.46	NIST
$Zn^{2+} + H_2PO_4^- = [ZnH_2PO_4]^+$	1.2	NIST
Zn^{2+} + Oxalate^{2-} = [ZnOxalate]	4.0	NIST
Zn^{2+} + 2 Oxalate^{2-} = [ZnOxalate$_2$]$^{2-}$	6.45	NIST
Zn^{2+} + Lactate$^-$ = [ZnLactate]$^+$	1.86	NIST
Zn^{2+} + 2 Lactate$^-$ = [ZnLactate$_2$]	2.6	NIST
Zn^{2+} + 3 Lactate$^-$ = [ZnLactate$_3$]$^-$	3.4	NIST
$Zn^{2+} + CO_3^{2-} = [ZnCO_3]$	3.9	NIST
$Zn^{2+} + 2\ CO_3^{2-} = [Zn(CO_3)_2]^{2-}$	7.3	NIST
$Zn^{2+} + HCO_3^- = [ZnHCO_3]^+$	1.5	NIST
Zn^{2+} + Citrate^{3-} = [ZnCitrate]$^-$	4.93	NIST
Zn^{2+} + 2 Citrate^{3-} = [ZnCitrate$_2$]$^{4-}$	6.8	NIST
Zn^{2+} + HCitrate^{2-} = [ZnHCitrate]	3.00	NIST
Zn^{2+} + H$_2$Citrate$^-$ = [ZnH$_2$Citrate]$^+$	1.2	NIST
$Zn^{2+} + HO^- = [ZnOH]^+$	4.6	NIST

Zn^{2+} + 2 HO^- = $[Zn(OH)_2]$	11.1	NIST
Zn^{2+} + 3 HO^- = $[Zn(OH)_3]^-$	13.6	NIST
Zn^{2+} + 4 HO^- = $[Zn(OH)_4]^{2-}$	14.8	NIST
Ca^{2+} + $DTPA^{5-}$ = $[CaDTPA]^{3-}$	10.75	NIST
$[CaDTPA]^{3-}$ + H^+ = $[CaHDTPA]^{2-}$	6.11	NIST
$[CaDTPA]^{3-}$ + Ca^{2+} = $[Ca_2DTPA]^-$	1.6	NIST
Ca^{2+} + $EDTA^{4-}$ = $[CaEDTA]^{2-}$	10.65	NIST
Ca^{2+} + $DTPA\text{-}BMA^{3-}$ = $[CaDTPA\text{-}BMA]^-$	7.17	NIST
Ca^{2+} + HPO_4^{2-} = $[CaHPO_4]$	1.62	NIST
Ca^{2+} + $H_2PO_4^-$ = $[CaH_2PO_4]^+$	0.6	NIST
Ca^{2+} + $Oxalate^{2-}$ = [CaOxalate]	2.46	NIST
Ca^{2+} + CO_3^{2-} = $[CaCO_3]$	3.22	NIST
Ca^{2+} + HCO_3^- = $[CaHCO_3]^+$	0.29	NIST
Ca^{2+} + $Citrate^{3-}$ = $[CaCitrate]^-$	3.48	NIST
Ca^{2+} + $HCitrate^{2-}$ = [CaHCitrate]	2.07	NIST
Ca^{2+} + $Lactate^-$ = $[CaLactate]^+$	1.12	NIST
Ca^{2+} + 2 $Lactate^-$ = $[CaLactate_2]$	1.62	NIST
Ca^{2+} + HO^- = $[CaOH]^+$	1.3	NIST
PO_4^{3-} + H^+ = HPO_4^{2-}	11.8	NIST
HPO_4^{2-} + H^+ = $H_2PO_4^-$	6.88	NIST
$H_2PO_4^-$ + H^+ = = H_3PO_4	1.99	NIST
CO_3^{2-} + H^+ = HCO_3^-	9.9	NIST
HCO_3^- + H^+ = H_2CO_3	6.13	NIST
$Oxalate^{2-}$ + H^+ = $HOxalate^-$	3.82	NIST
$HOxalate^-$ + H^+ = $H_2Oxalate$	1.2	NIST
$Lactate^-$ + H^+ = HLactate	3.67	NIST
$Citrate\text{-}O^-$ + H^+ = $Citrate^{3-}$ (Hydroxyl proton)	13.5	Heller 2012[a]
$Citrate^{3-}$ + H^+ = $HCitrate^{2-}$	5.7	Heller 2012[a]
$HCitrate^{2-}$ + H^+ = $H_2Citrate^-$	4.4	Heller 2012[a]
$H_2Citrate^-$+ H^+ = $H_3Citrate$	2.9	Heller 2012[a]
$DOTA^{4-}$ + H^+ = $HDOTA^{3-}$	11.2	NIST
$HDOTA^{3-}$ + H^+ = H_2DOTA^{2-}	9.73	NIST
H_2DOTA^{2-} + H^+ = H_3DOTA^-	4.44	NIST
H_3DOTA^- + H^+ = H_4DOTA	4.34	NIST
H_4DOTA + H^+ = H_5DOTA^+	2.35	NIST
$DTPA^{5-}$ + H^+ = $HDTPA^{4-}$	10.4	NIST
$HDTPA^{4-}$ + H^+ = H_2DTPA^{3-}	8.55	NIST
H_2DTPA^{3-} + H^+ = H_3DTPA^{2-}	4.28	NIST
H_3DTPA^{2-} + H^+ = H_4DTPA^-	2.7	NIST
H_4DTPA^- + H^+ = H_5DTPA	2.0	NIST
H_5DTPA + H^+ = H_6DTPA^+	1.6	NIST
H_6DTPA^+ + H^+ = H_7DTPA^2	0.7	NIST
$DTPA\text{-}BMA^{3-}$ + H^+ = $HDTPA\text{-}BMA^{2-}$	9.37	NIST
$HDTPA\text{-}BMA^{2-}$ + H^+ = $H_2DTPA\text{-}BMA^-$	4.38	NIST
$H_2DTPA\text{-}BMA^-$+ H^+ = $H_3DTPA\text{-}BMA$	3.31	NIST
$HOPO^{4-}$ + H^+ = $HHOPO^{3-}$	6.64	Abergel 2009[c]
$HHOPO^{3-}$ + H^+ = H_2HOPO^{2-}	5.68	Abergel 2009[c]
H_2HOPO^{2-} + H^+ = H_3HOPO^-	5.01	Abergel 2009[c]
H_3HOPO^- + H^+ = H_4HOPO	3.87	Abergel 2009[c]
H_2O = H^+ + HO^-	-13.77	NIST

Notes: Most log K values are given for an ionic strength of 0.1M and at 25°C, see corresponding reference for more information. NIST: A. E. Martell, R. M. Smith, R. J. Motekaitis, NIST Critically Selected Stability Constants of Metal Complexes: Version 8.0. a: Heller et al. *Dalton Trans.*, 2012, 41, 13969. Values for the Gd-citrate complexes were considered identical to those of the Eu-citrate complexes. b: Sturzbecher-Hoehne et al., *Dalton Trans.*, 2011, 40, 8340-8346. The protonation constant of the $[GdHOPO]^-$ complex was considered similar to that of the $[EuHOPO]^-$ complex. c: Abergel et al. *Inorg. Chem*. 2009, 48, 10868–10870.

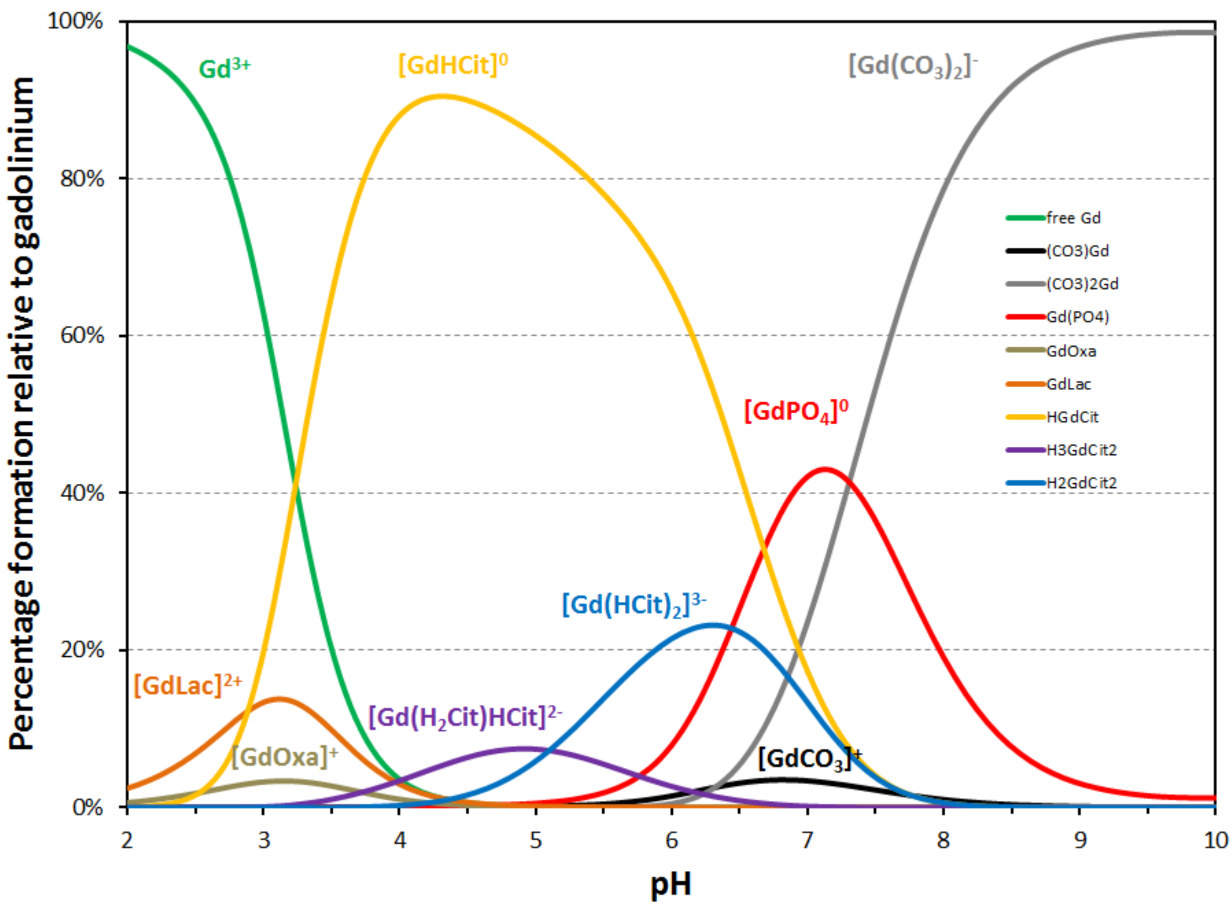

Figure Sx: Calculated speciation of gadolinium under physiological conditions and for a concentration of Gd corresponding to 5% of the typical amount of GBCA injected to a patient. [Gd] = 7.15 µM. [Phosphate] = 1.1 mM, [Carbonate] = 25 mM, [Oxalate] = 9.2 µM, [lactate] = 1.5 mM, [Citrate] = 160 µM. pH = 7.4. Citrate species are displayed in yellow, the phosphate species in red, and the carbonate species in blue.

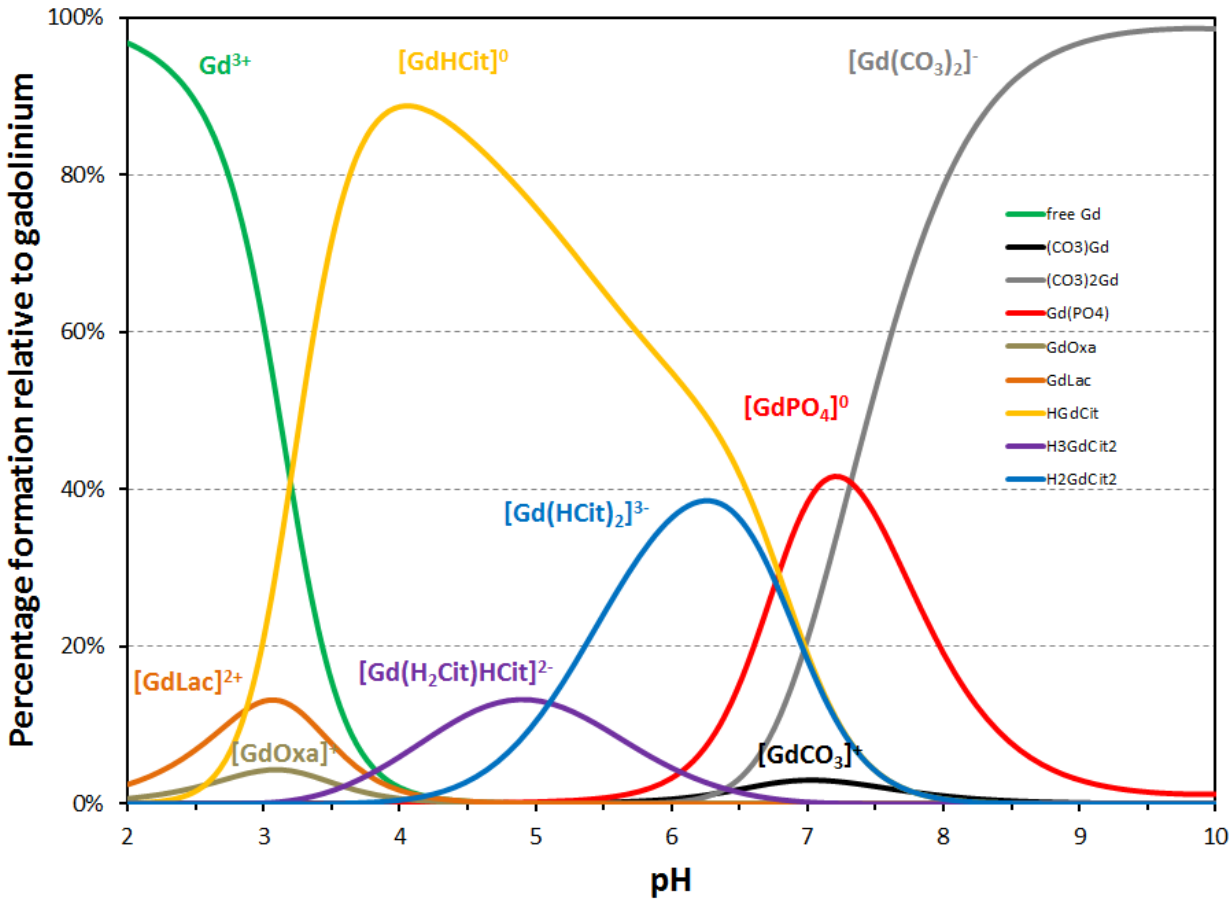

Figure Sx: Calculated speciation of gadolinium under physiological conditions and for a concentration of Gd corresponding to 0.05% of the typical amount of GBCA injected to a patient. [Gd] = 715 nM. [Phosphate] = 1.1 mM, [Carbonate] = 25 mM, [Oxalate] = 9.2 µM, [lactate] = 1.5 mM, [Citrate] = 160 µM. pH = 7.4. Citrate species are displayed in yellow, the phosphate species in red, and the carbonate species in blue.

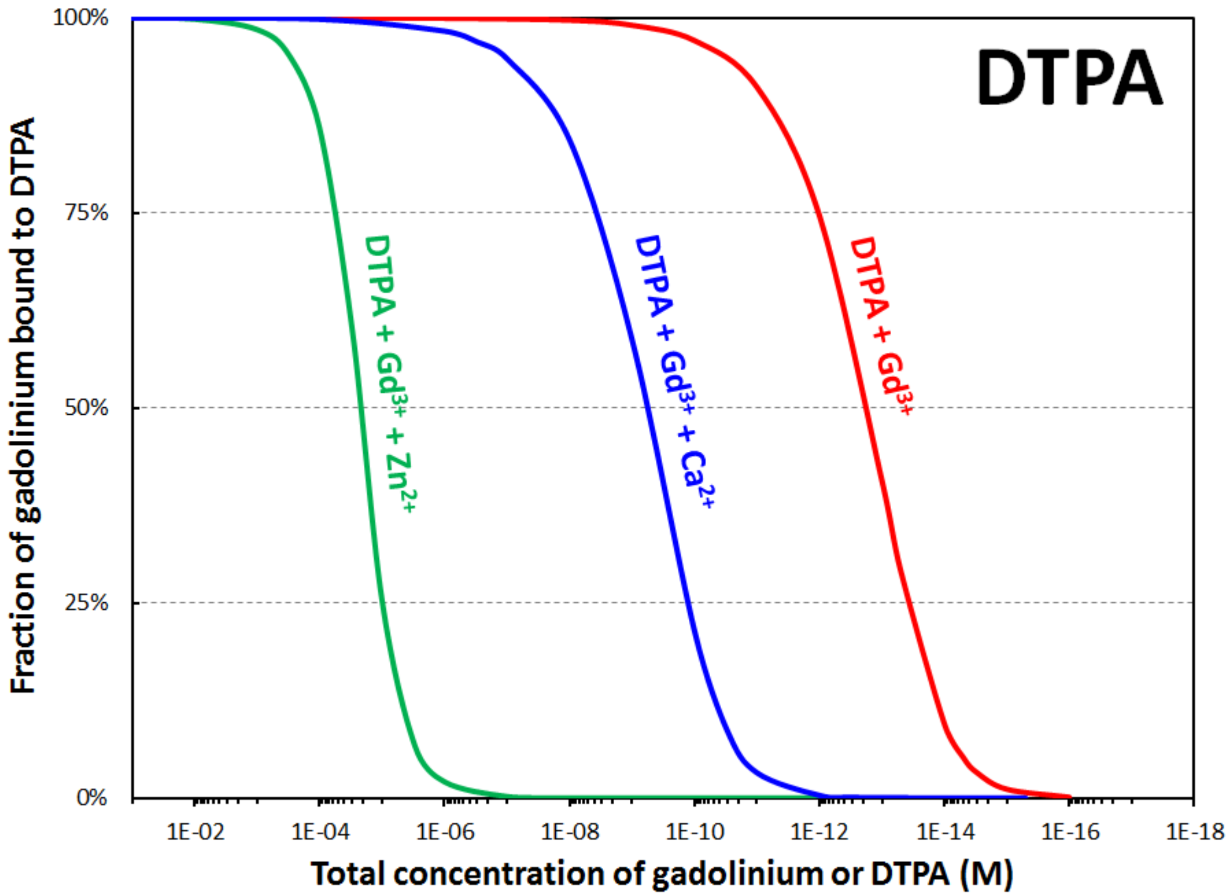

Figure Sx: Calculated percentage of gadolinium bound to DTPA as a function of dilution and in the presence of bio-relevant chelators. Calculations in the presence of calcium (1.1 mM) or zinc (15 µM) ions are also given for comparison. Total concentrations of phosphates (1.1 mM), carbonates (25 mM), oxalates (9.2 µM), lactates (1.5 mM), and citrates (160 µM) held constant to match physiological conditions. Ratio Gd/DTPA = 1.0 mol/mol. pH = 7.4. See Table S2 for stability constants used in these speciation simulations.

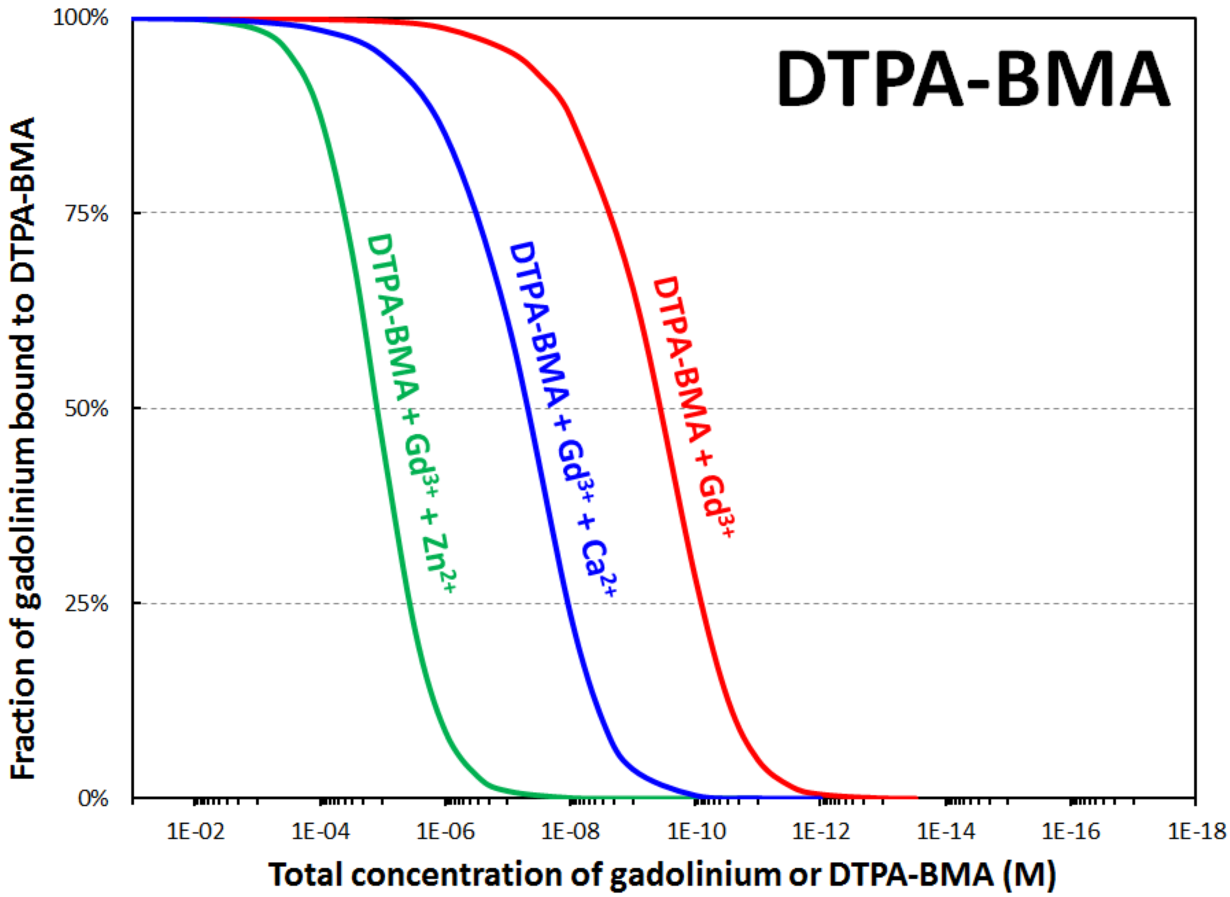

Figure Sx: Calculated percentage of gadolinium bound to DTPA-BMA as a function of dilution and in the presence of bio-relevant chelators. Calculations in the presence of calcium (1.1 mM) or zinc (15 µM) ions are also given for comparison. Total concentrations of phosphates (1.1 mM), carbonates (25 mM), oxalates (9.2 µM), lactates (1.5 mM), and citrates (160 µM) held constant to match physiological conditions. Ratio Gd/DTPA-BMA = 1.0 mol/mol. pH = 7.4. See Table S2 for stability constants used in these speciation simulations.