

**Speciation of gadolinium in gadolinium-based magnetic resonance
imaging agents by high-performance liquid chromatography inductively
coupled plasma optical emission spectrometry**

Chethaka L. Kahakachchi and Dennis A. Moore

Supplementary material

Table S1. Chromatographic parameters for Gd(III) complex analysis by HPLC-ICP-OES

Column	Gd(III) complex	t_R^a	k'^b	N^c	Asymmetry ^d
XTerra TM RP-C18 (4.6 × 250 mm; 5 μm)	Gd-DTPA-BMEA	7.8	2.12	319	1.00
	Gd-DTPA ²⁻	3.1	0.24	389	1.62
	Gd-HP-DO3A	4.6	0.84	1352	1.26
Synergi TM RP-Hydro (4.6 × 250 mm; 5 μm)	Gd-DTPA-BMA	7.8	2.12	1245	1.45
	Gd-DOTA ¹⁻	7.2	1.88	1255	1.00
BDS Hypersil TM C18 (4.6 × 50 mm; 3 μm)	Gd-BOPTA ²⁻	5.5	5.88	1629	1.20

^a Retention time (minutes); ^b Capacity factor; ^c Theoretical plates; ^d Peak symmetry

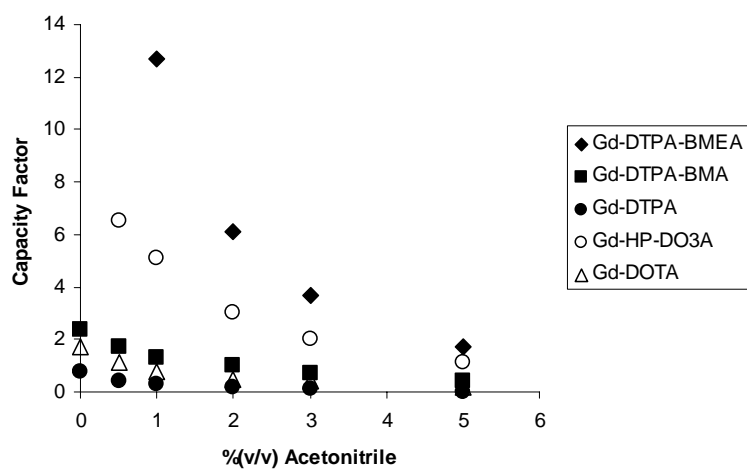
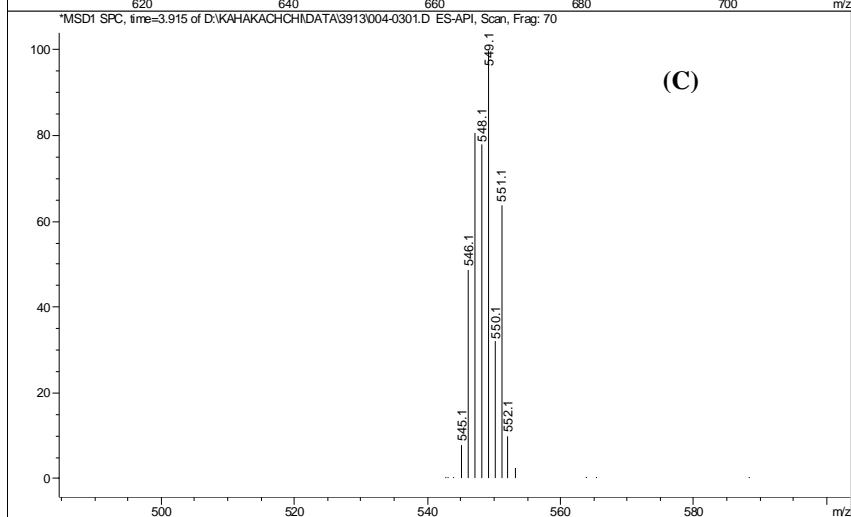
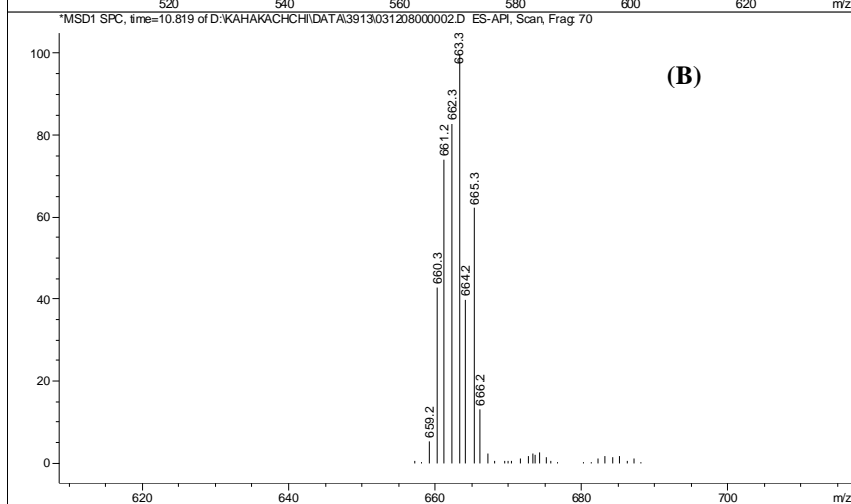
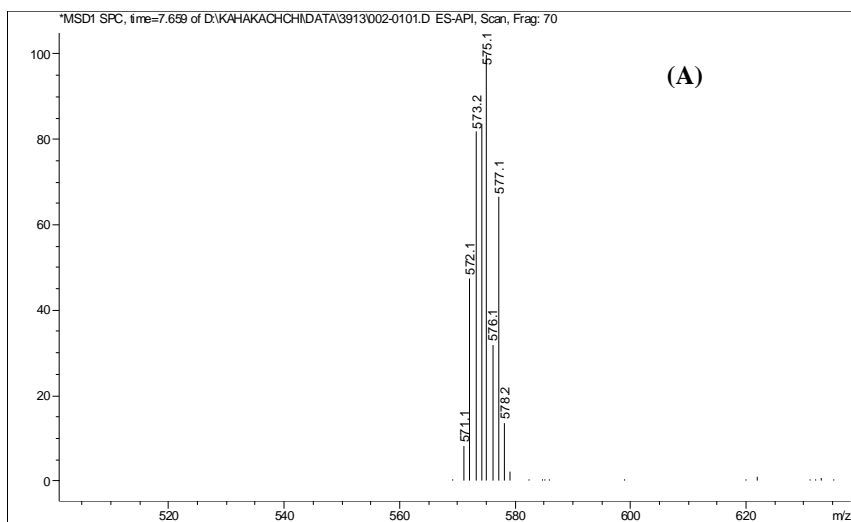


Figure S1. Effect of acetonitrile concentration in the mobile phase on the capacity factors of gadolinium(III) complexes. Mobile phase: 10 mM ammonium acetate at pH 7; stationary phase: Phenomenex SynergiTM 4 μ m RP-Hydro C18 (4.6 x 250 mm)



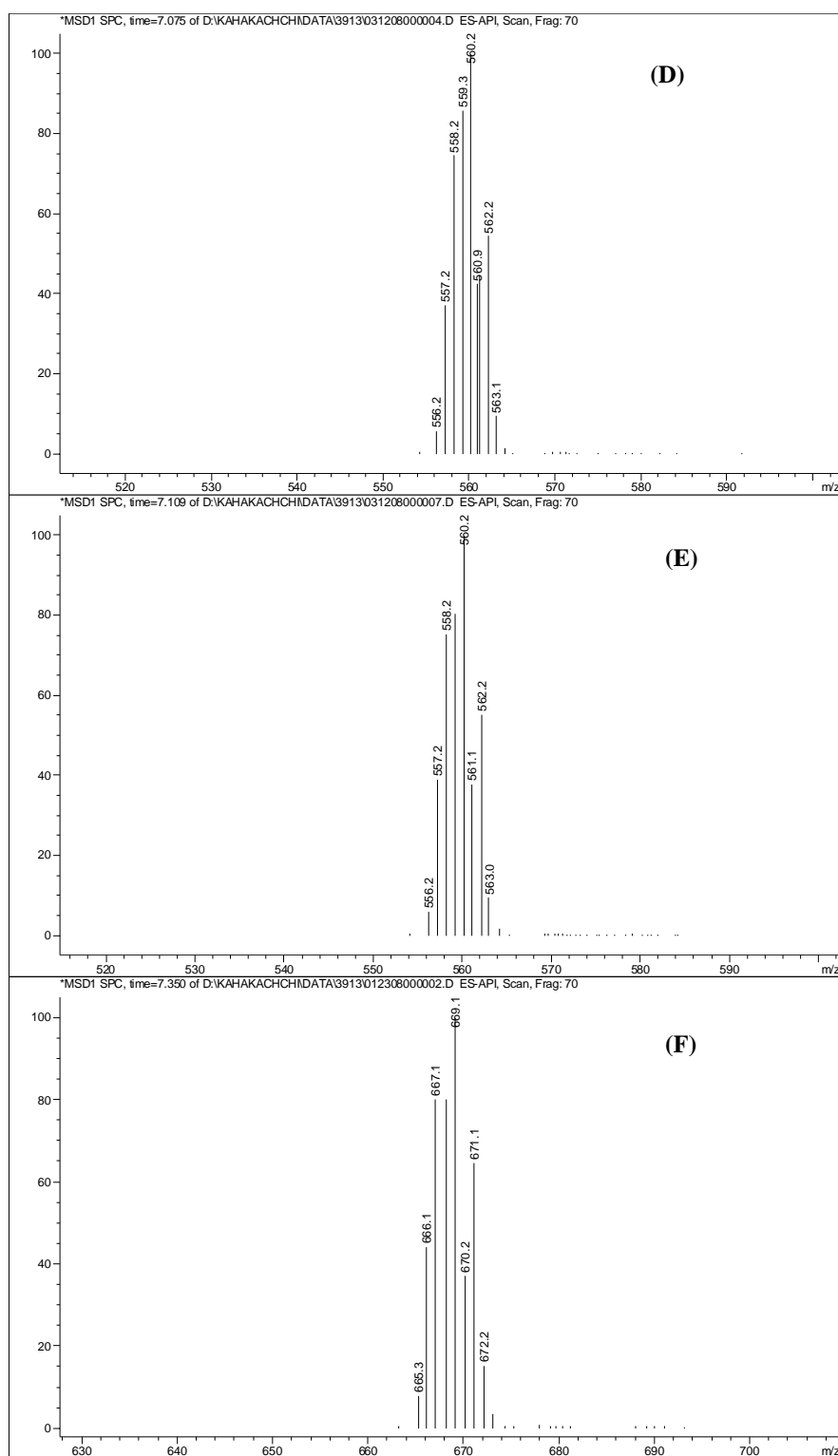


Figure S2. Electrospray ionization mass spectra: (A) Gd-DTPA-BMA; (B) Gd-DTPA-BMEA; (C) Gd-DTPA²⁻; (D) Gd-HP-DO3A; (E) Gd-DOTA¹⁻ and (F) Gd-BOPTA²⁻