

Supporting Information

Investigation of matrix effects in nitrogen microwave inductively coupled atmospheric-pressure plasma mass spectrometry (MICAP-MS) for trace elemental analysis in steels

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Table S1: Calibration range and corresponding IS used for aqueous and matrix-matched calibration.

Element	m/z	Internal standard	Calibration levels
			$\mu\text{g L}^{-1}$
Al	27	^{45}Sc	1 - 50
Ca	40, 44	^{45}Sc	0.1 - 5
V	50, 51	^{45}Sc	10 - 500
Cr	52, 53	^{45}Sc	10 - 500
Mn	55	^{45}Sc	10 - 250
Co	59	^{45}Sc	10 - 250
Ni	60, 61, 62	^{45}Sc	10 - 500
Cu	63, 65	^{45}Sc	10 - 500
Zn	66, 67, 68	^{89}Y	0.1 - 5
Ga	69, 71	^{89}Y	0.1 - 5
Nb	93	^{89}Y	1 - 50
Mo	95, 97, 98	^{89}Y	1 - 50
Sn	117, 118, 119	^{115}In	1 - 50
Sb	121, 123	^{115}In	1 - 50
W	182, 183	^{159}Tb	10 - 250
Pb	206, 207, 208	^{209}Bi	0.1 - 5

Table S2: Optimized voltages applied on the ion-optics used in MICAP-MS.

Ion Optics (V)	
First Extraction Lens Voltage	-110
Second Extraction Lens Voltage	-230
Third Extraction Lens Voltage	-520
Corner Lens Voltage	-500
Mirror Lens Left Voltage	54
Mirror Lens Right Voltage	48
Mirror Lens Bottom Voltage	60
Entrance Lens Voltage	9
Entrance Plate Voltage	-60
Fringe Bias	-4.5
Pole bias	0

Table S3: LODs and LOQs for aqueous and matrix-matched calibration. (* used for quantification)

Element	m/z	Aqueous calibration		Matrix-matched calibration	
		LOD ($\mu\text{g L}^{-1}$)	LOQ ($\mu\text{g L}^{-1}$)	LOD ($\mu\text{g L}^{-1}$)	LOQ ($\mu\text{g L}^{-1}$)
Al*	27	1.1	3.2	0.7	2.1
Ca	40	2.0	6.0	3.3	9.8
Ca	44	5.2	15.7	-	-
V	50	0.48	1.5	1.63	4.9
V*	51	0.014	0.041	0.068	0.20
Cr*	52	0.22	0.67	1.3	4.0
Cr	53	0.30	0.89	1.4	4.1
Cr	all	0.23	0.69	1.3	4.0
Mn*	55	0.17	0.52	0.14	0.43
Co*	59	0.11	0.32	0.11	0.34
Ni	60	1.2	3.6	2.4	7.1
Ni	61	1.6	4.7	2.8	8.5
Ni	62	1.4	4.1	2.2	6.6
Ni	all	1.2	3.6	2.4	7.1
Cu	63	0.42	1.3	0.42	1.3
Cu	65	0.39	1.2	0.40	1.2
Cu*	all	0.40	1.2	0.41	1.2
Zn	66	0.29	0.86	0.21	0.62
Zn	67	0.81	2.4	0.58	1.7
Zn	68	0.32	0.96	0.65	2.0
Zn	all	0.31	0.93	0.24	0.72
Ga	69	0.0080	0.024	0.032	0.097
Ga	71	0.0024	0.0071	0.05	0.16
Ga*	all	0.0043	0.013	0.016	0.048
Nb*	93	4.9	14.8	0.93	2.8
Mo	95	0.18	0.53	0.27	0.81
Mo	97	0.24	0.72	0.19	0.57
Mo	98	0.28	0.83	0.45	1.3
Mo*	all	0.20	0.61	0.29	0.88
Sn	117	0.017	0.052	0.015	0.044
Sn	118	0.0095	0.028	0.011	0.034
Sn	119	0.019	0.057	0.018	0.053
Sn*	all	0.0055	0.016	0.012	0.035
Sb	121	0.0036	0.011	0.0065	0.019
Sb	123	0.0046	0.014	0.0052	0.016
Sb*	all	0.0028	0.0084	0.0035	0.010
W	182	0.015	0.045	0.026	0.079
W	183	0.019	0.057	0.024	0.073
W	all	0.016	0.047	0.010	0.031
Pb	206	0.030	0.089	0.018	0.054
Pb	207	0.035	0.11	0.011	0.033
Pb	208	0.031	0.093	0.012	0.036
Pb*	all	0.031	0.094	0.013	0.039

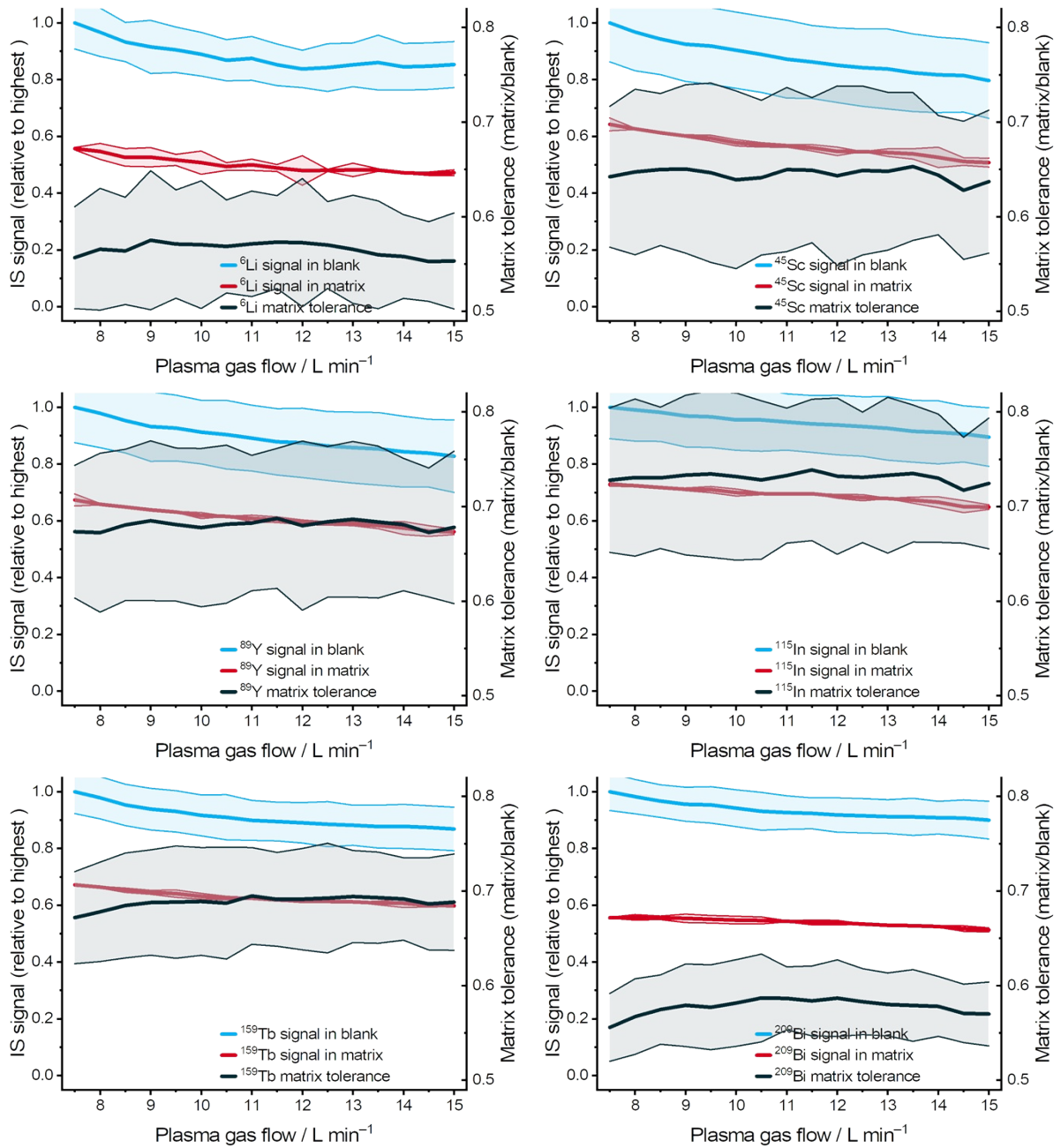


Figure S1: plasma gas flow – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

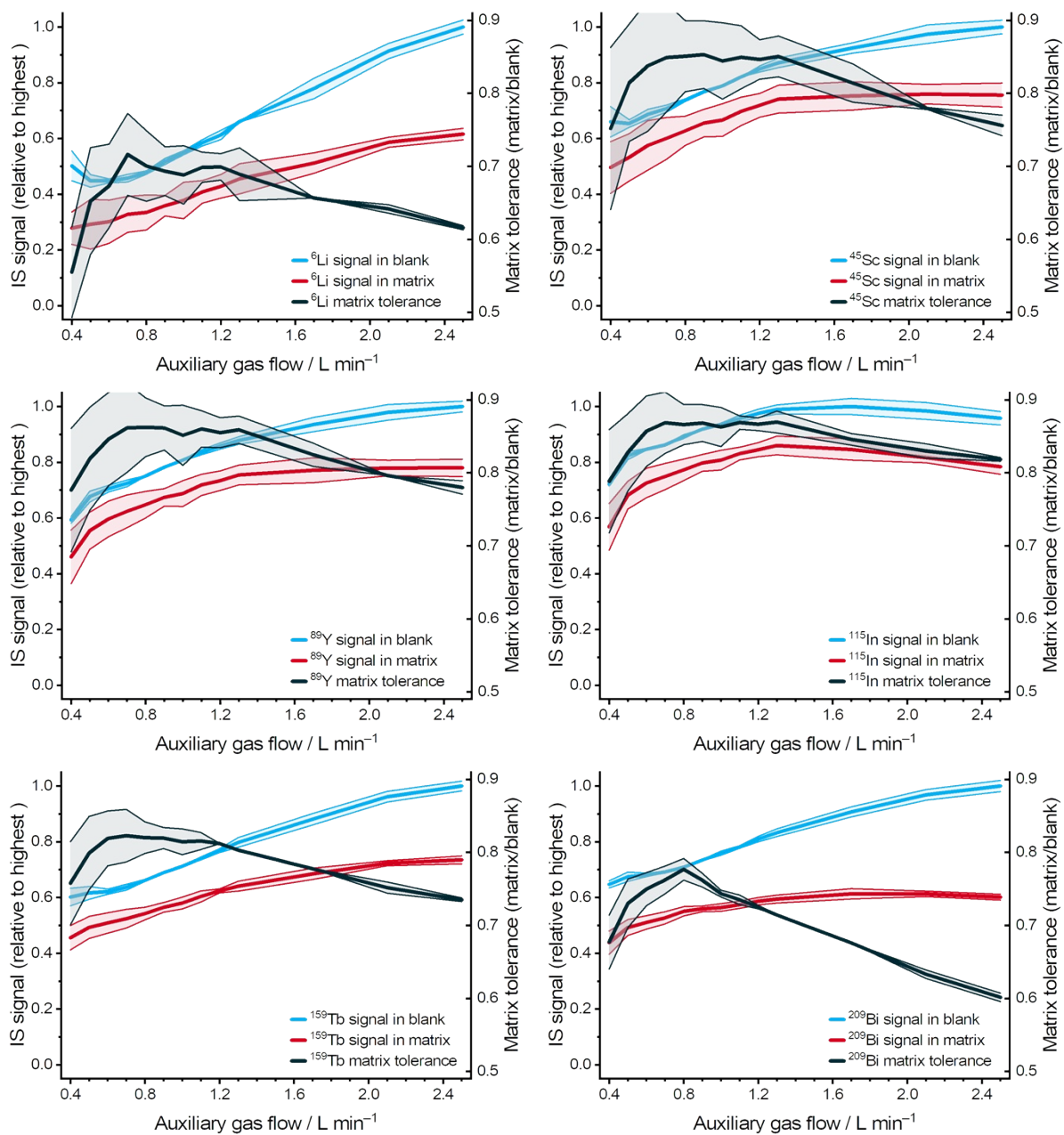


Figure S2: auxiliary gas flow – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

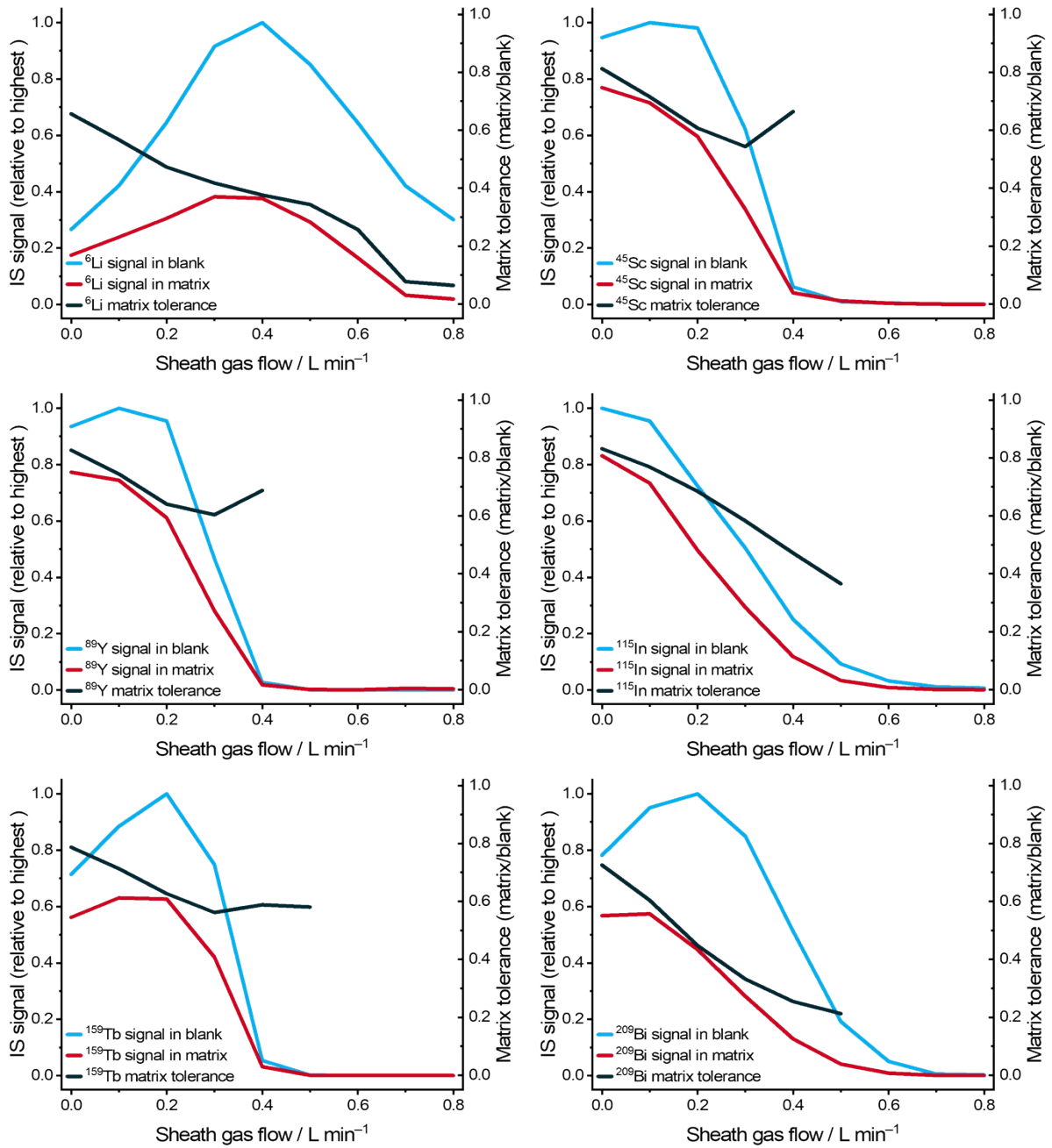


Figure S3: sheath gas flow – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

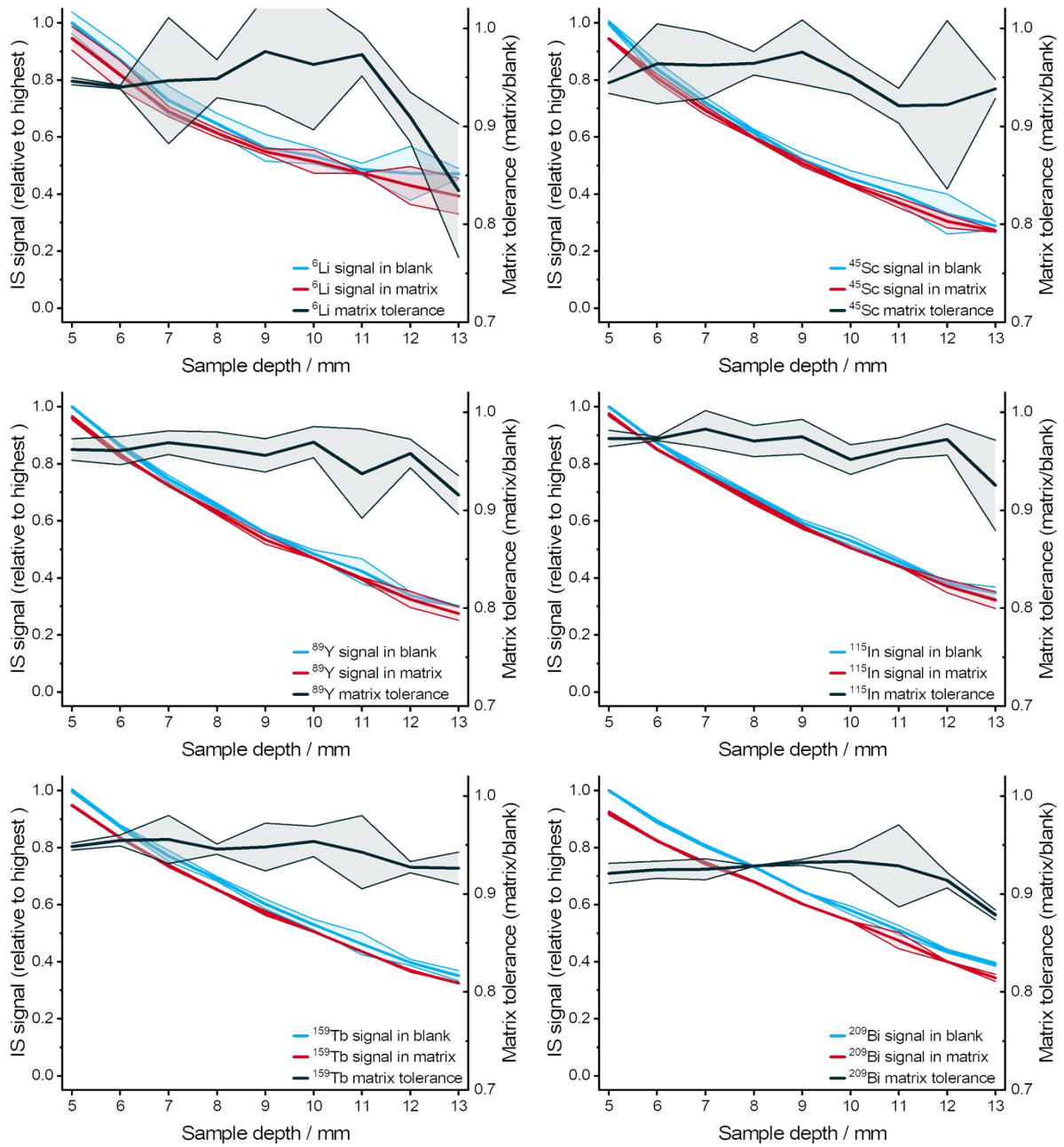


Figure S4: sample depth – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

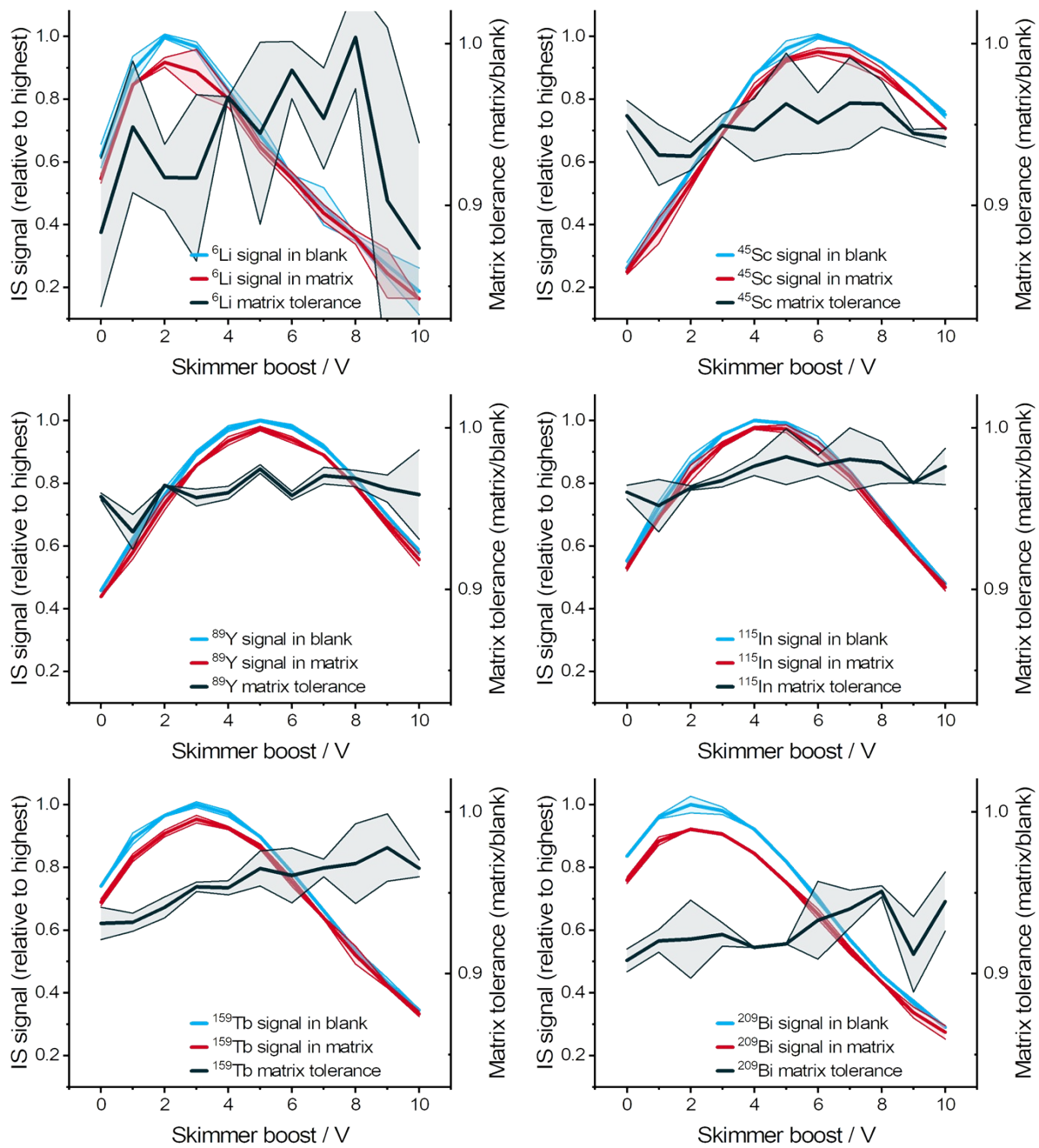


Figure S5: skimmer boost voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

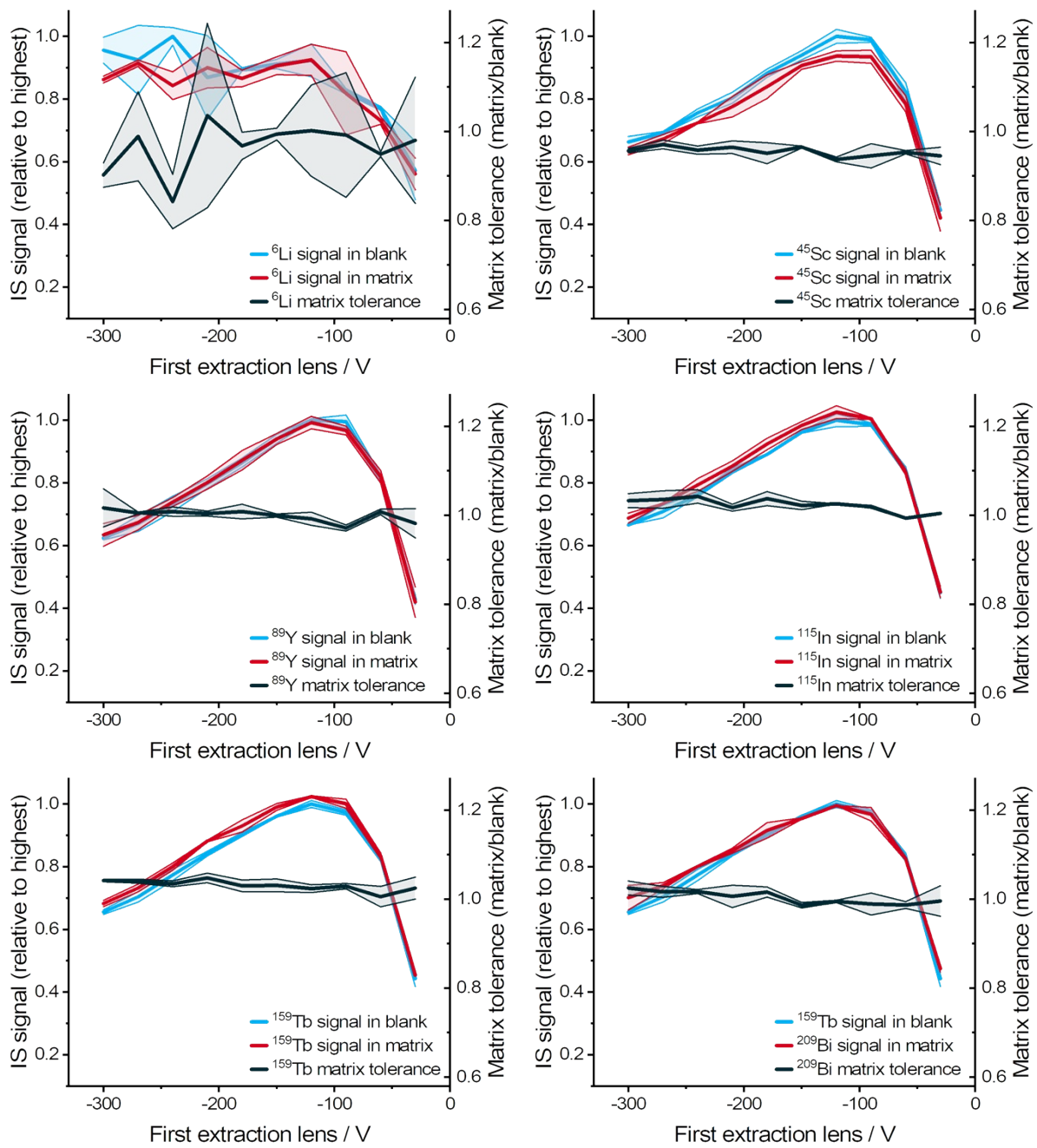


Figure S6: first extraction lens voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

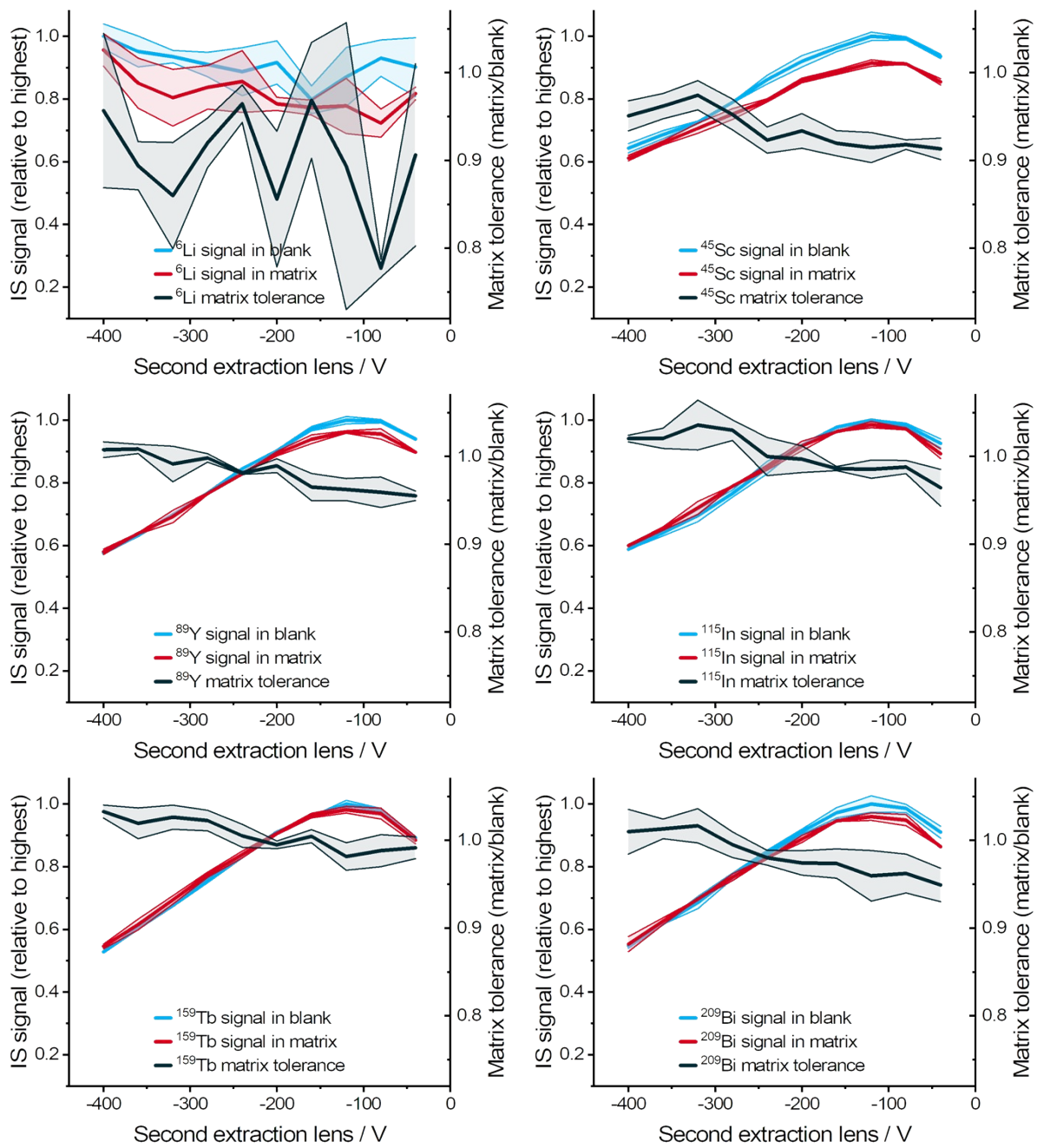


Figure S7: second extraction lens voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

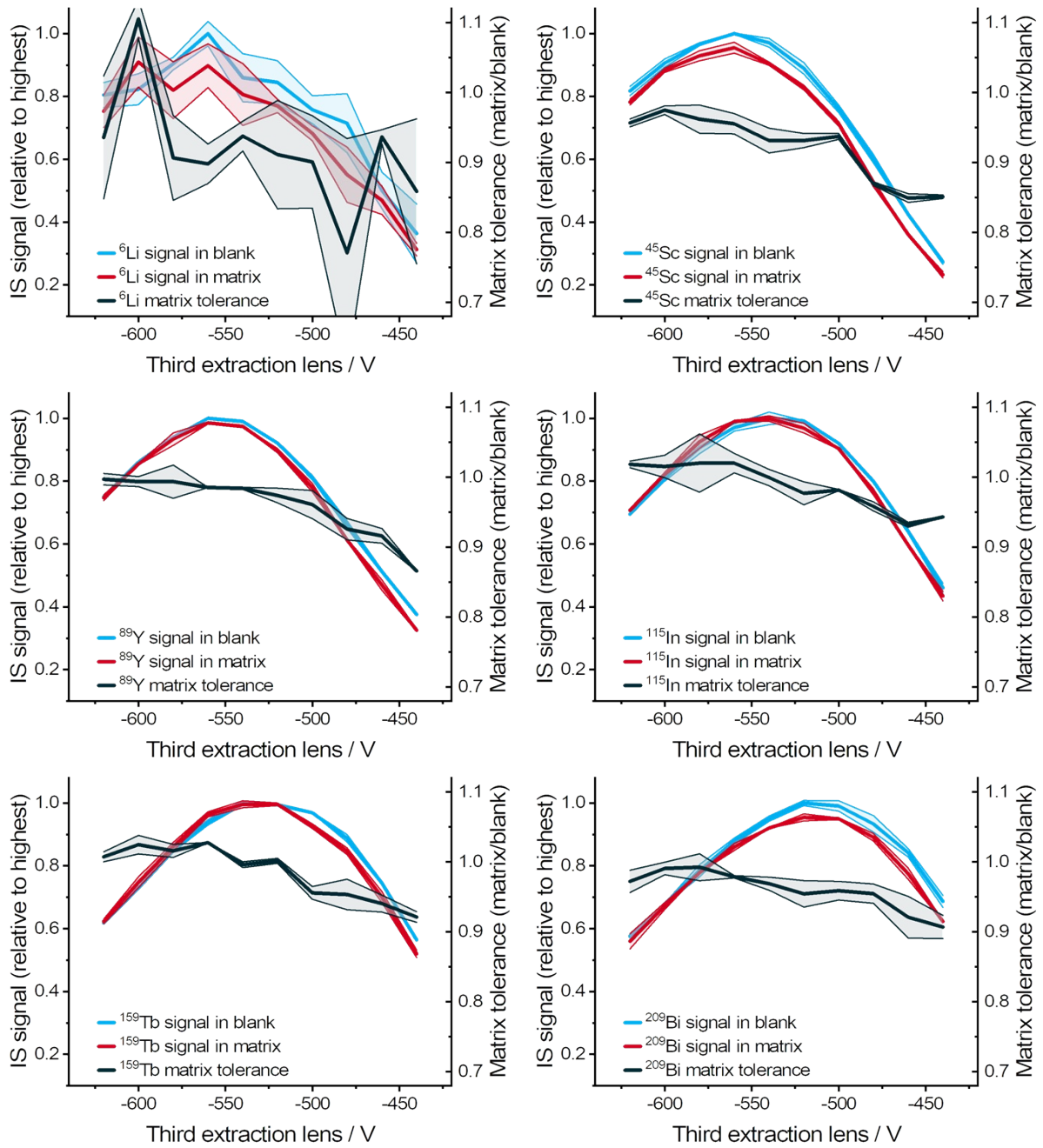


Figure S8: third extraction lens voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

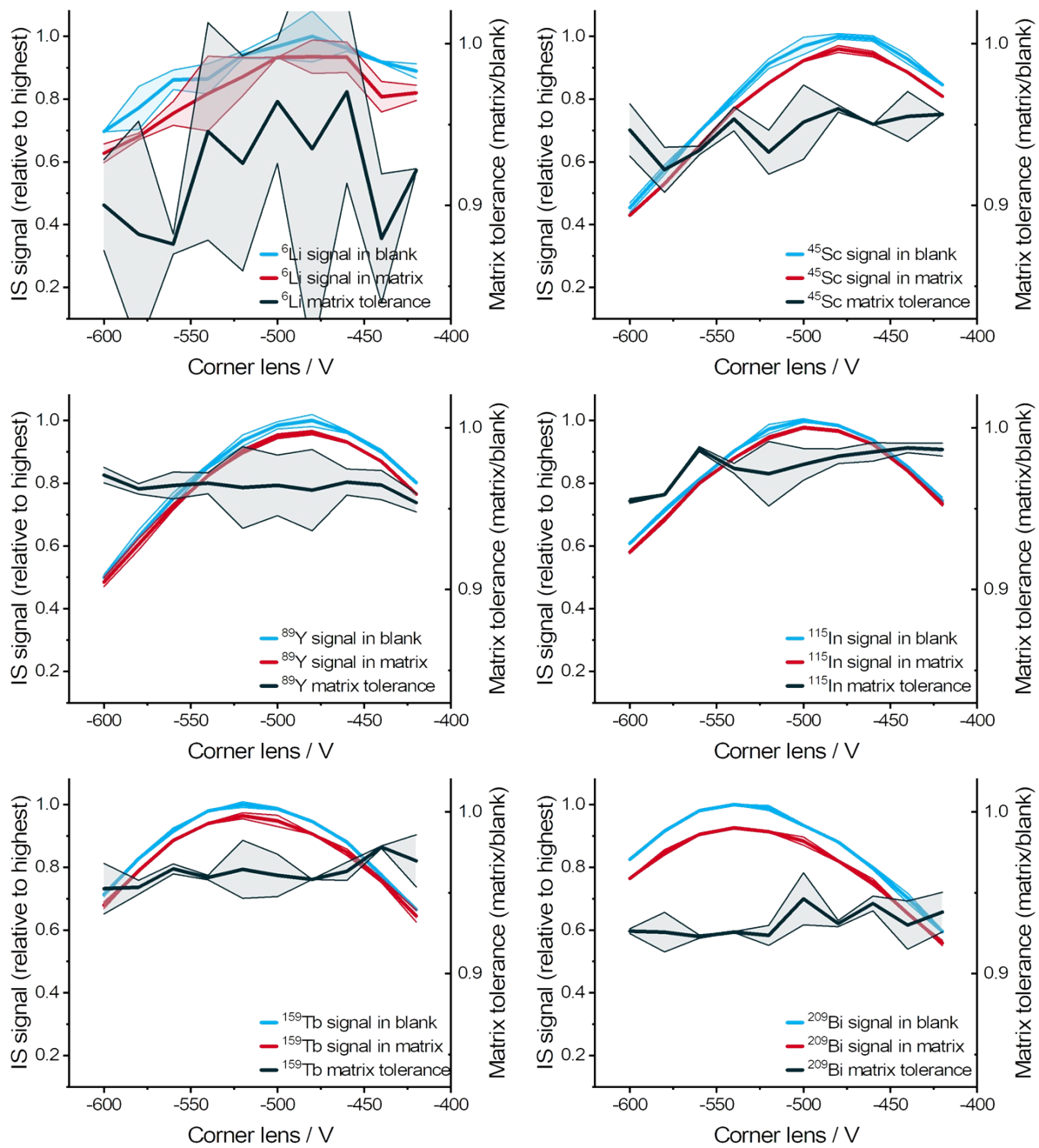


Figure S9: corner lens voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

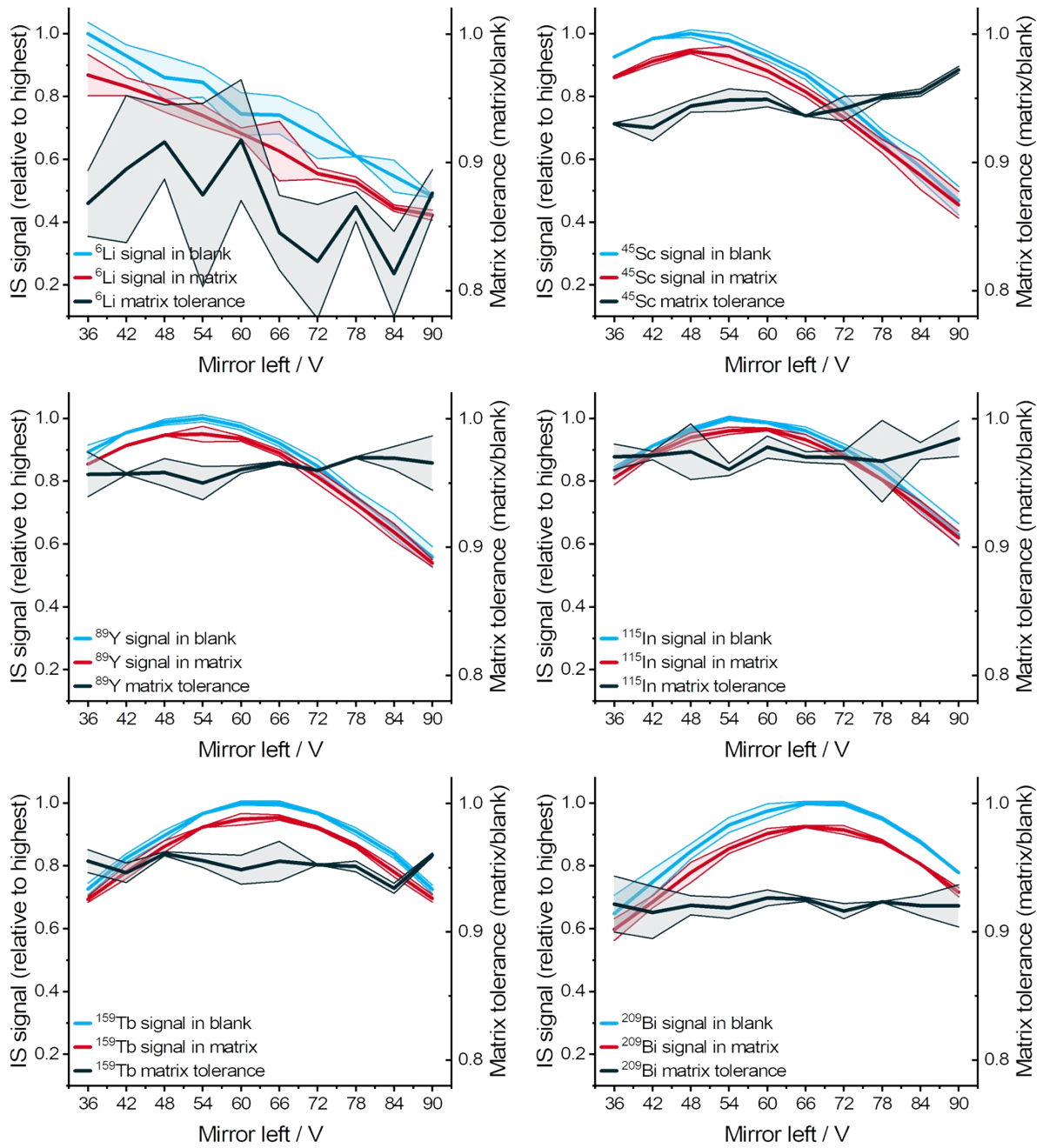


Figure S10: left mirror voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

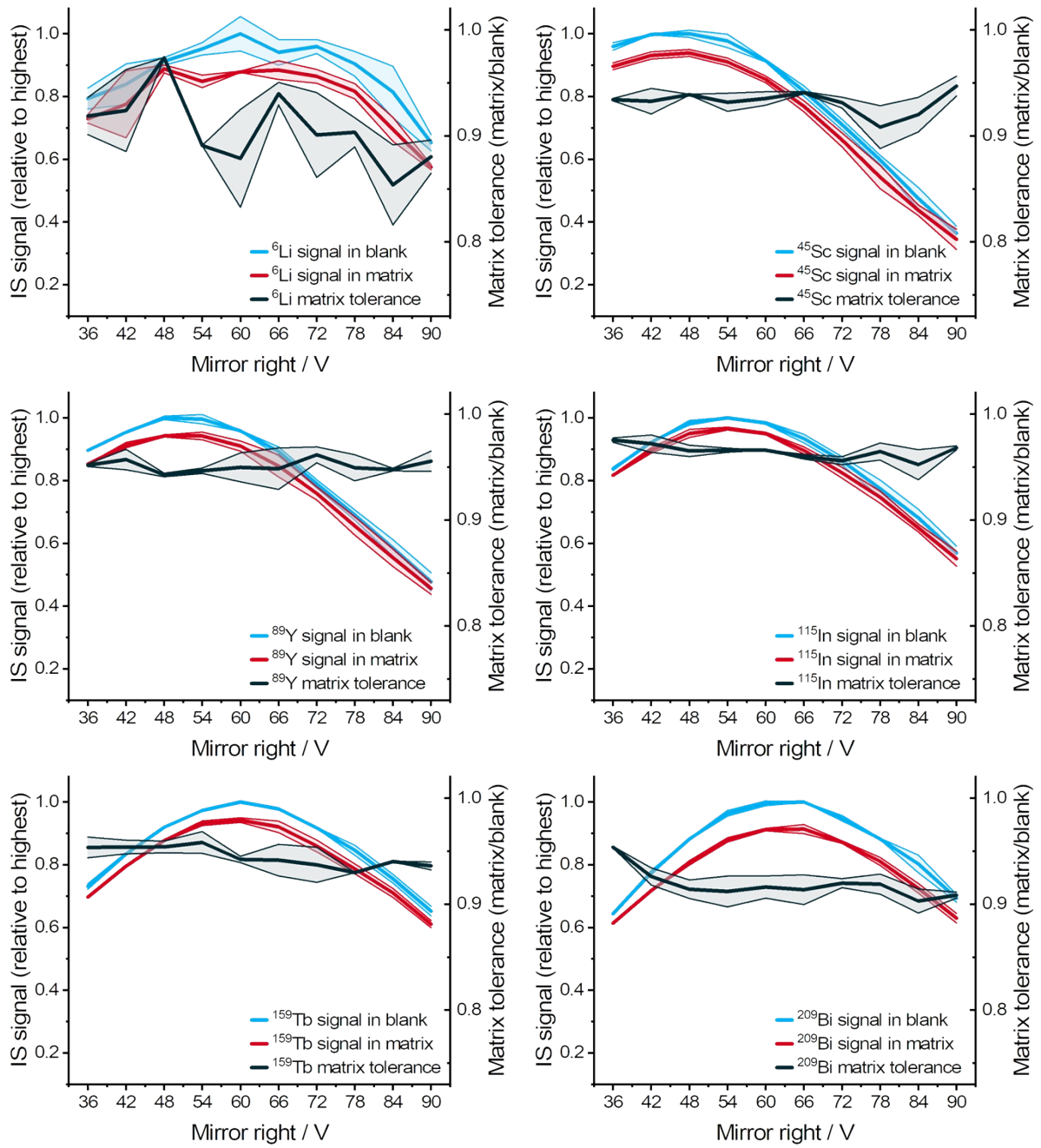


Figure S11: right mirror voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

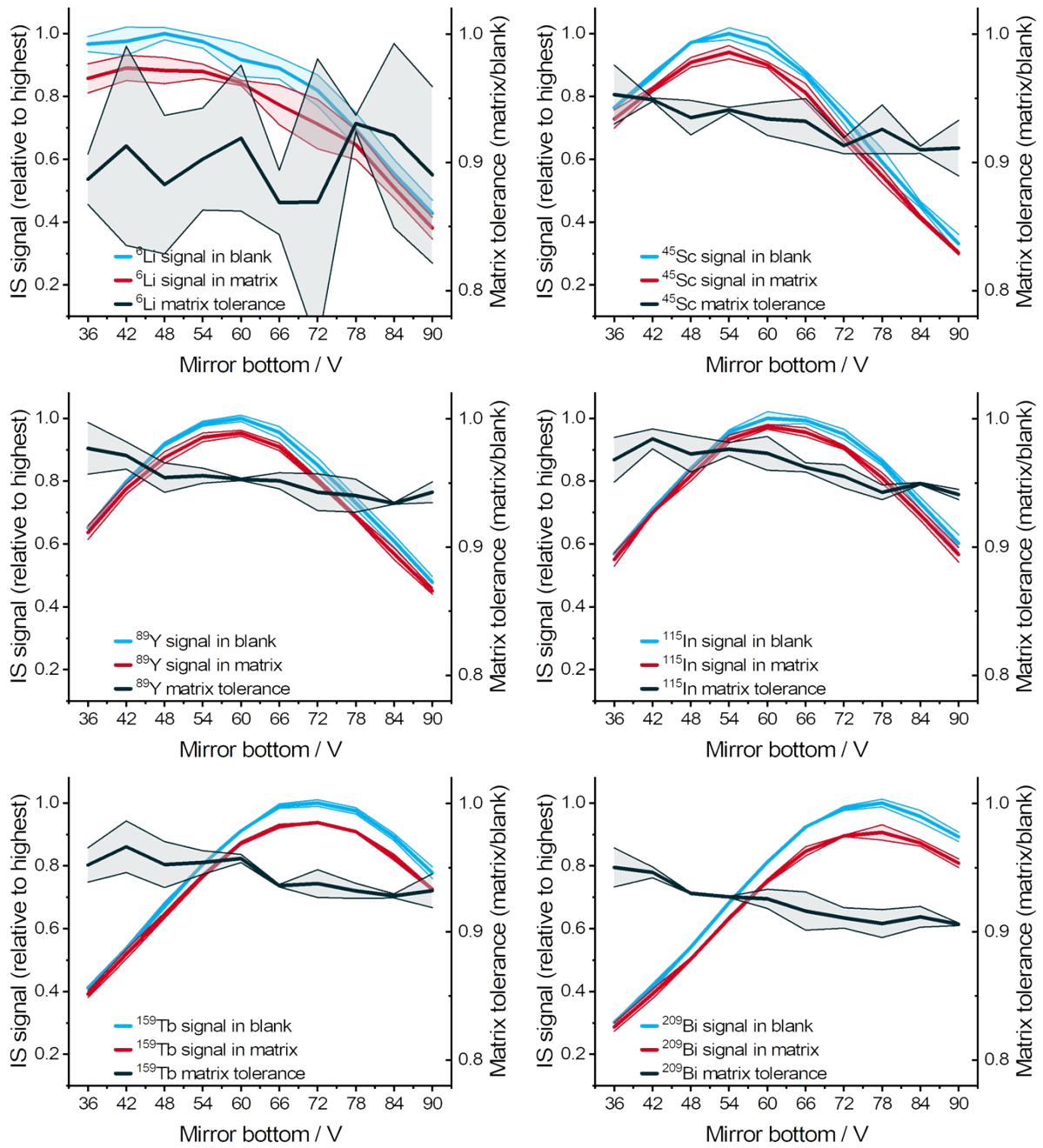


Figure S12: bottom mirror voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

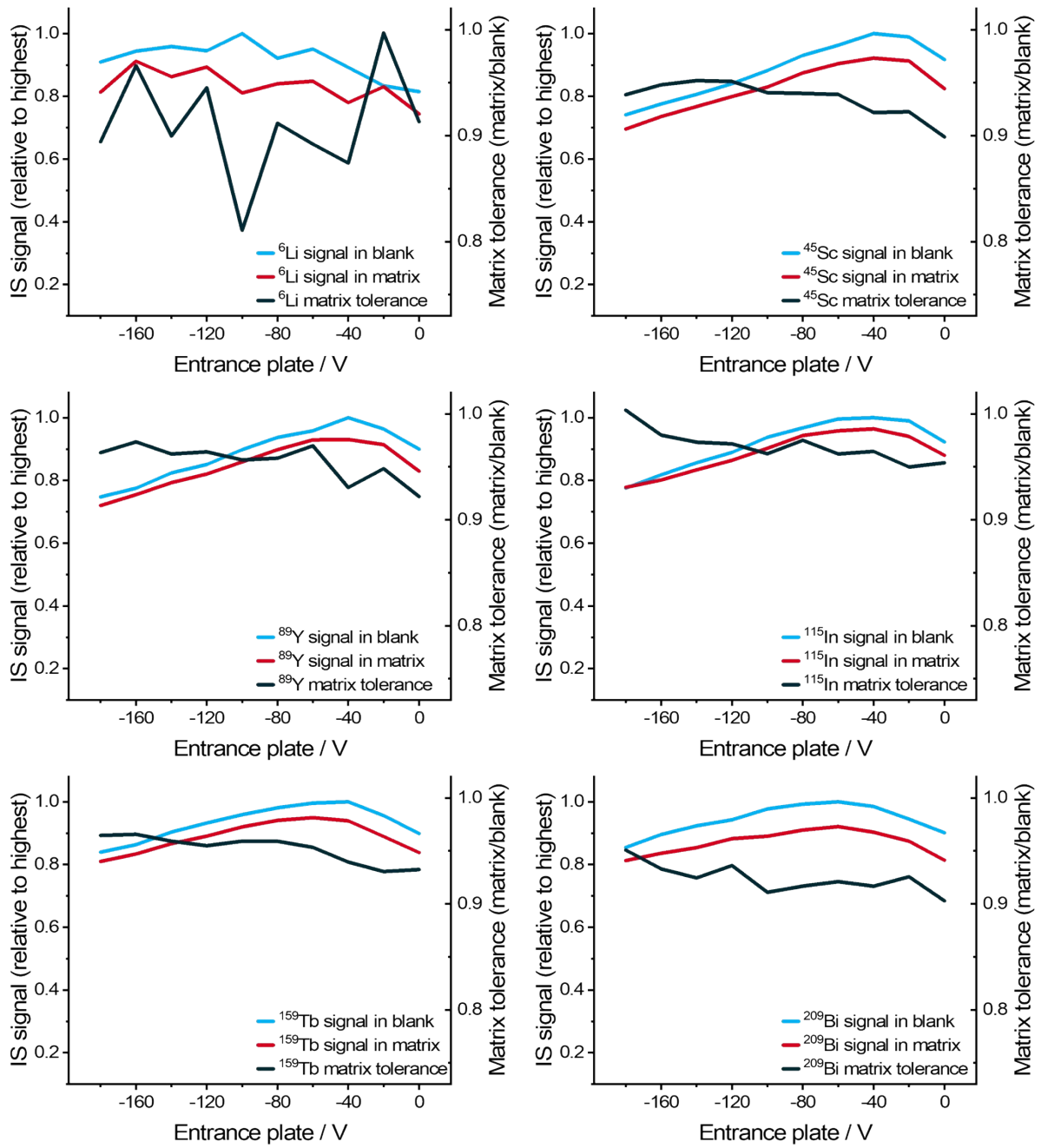


Figure S13: entrance plate voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

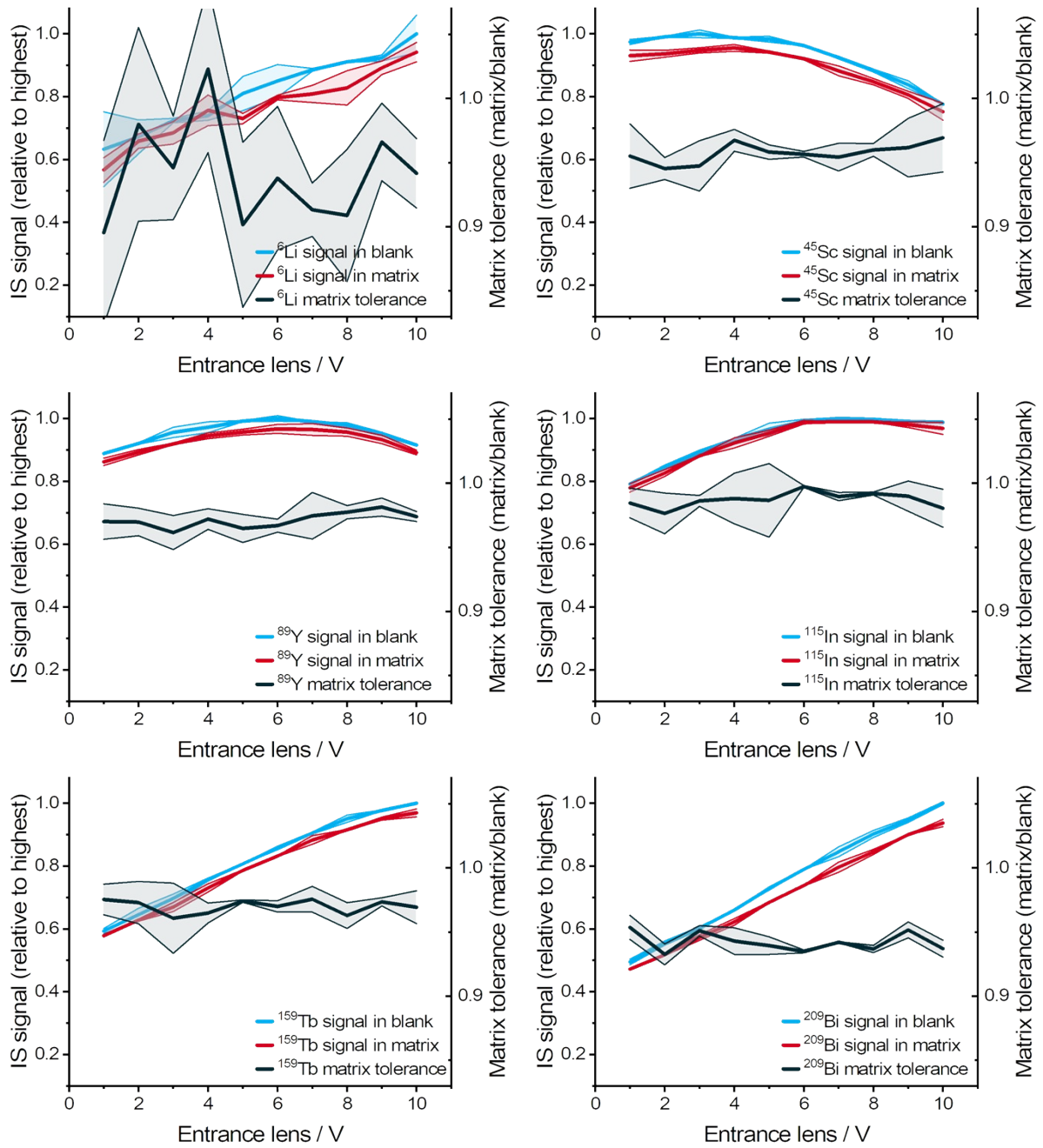


Figure S14: entrance lens voltage – internal standard signal recovery (relative to highest signal in blank) in blank and matrix, and matrix tolerance.

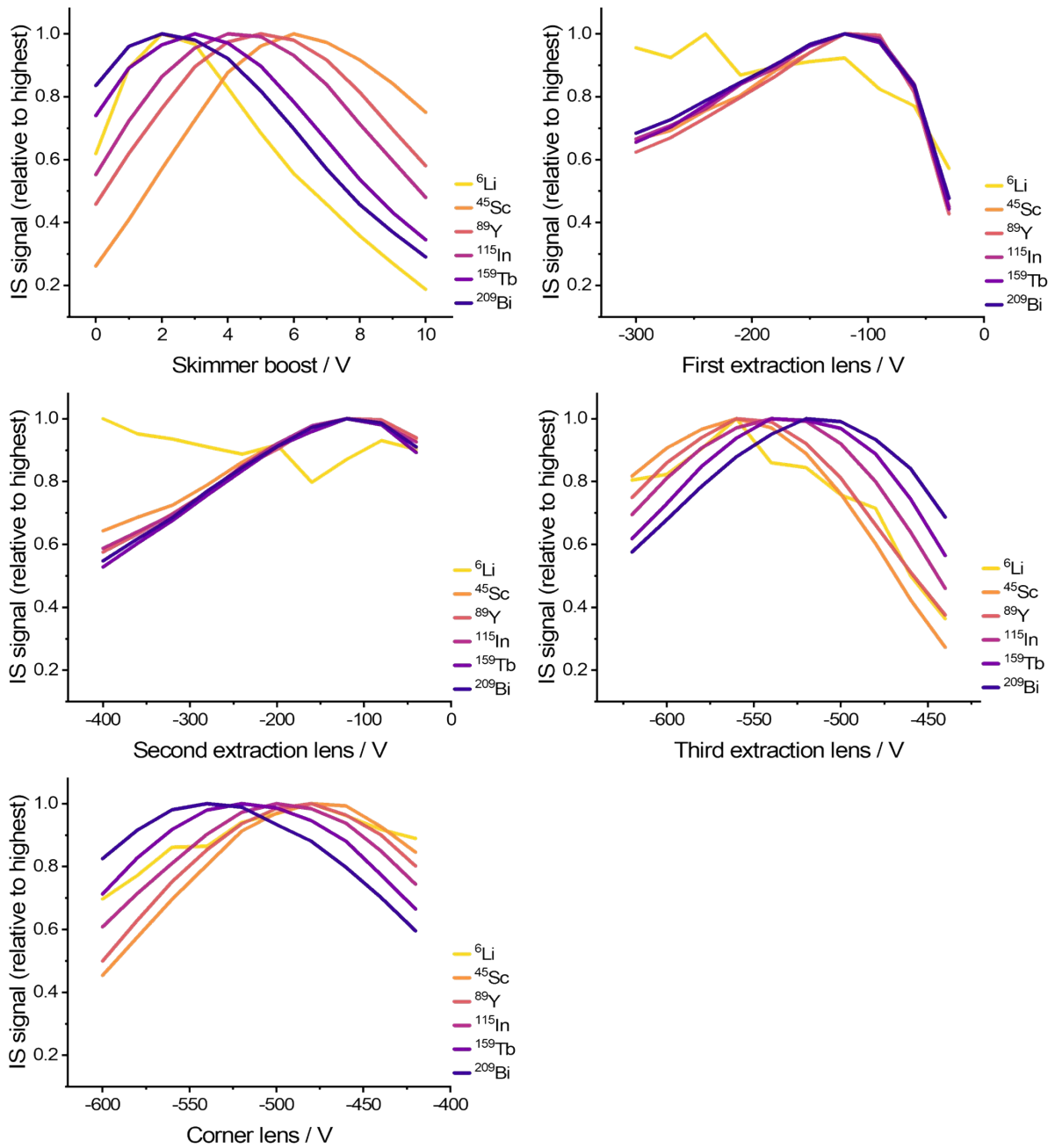


Figure S15: mass shift – internal standard signal recovery in blank (relative to highest in blank) with varying skimmer boost, extraction lenses and corner lens voltages.

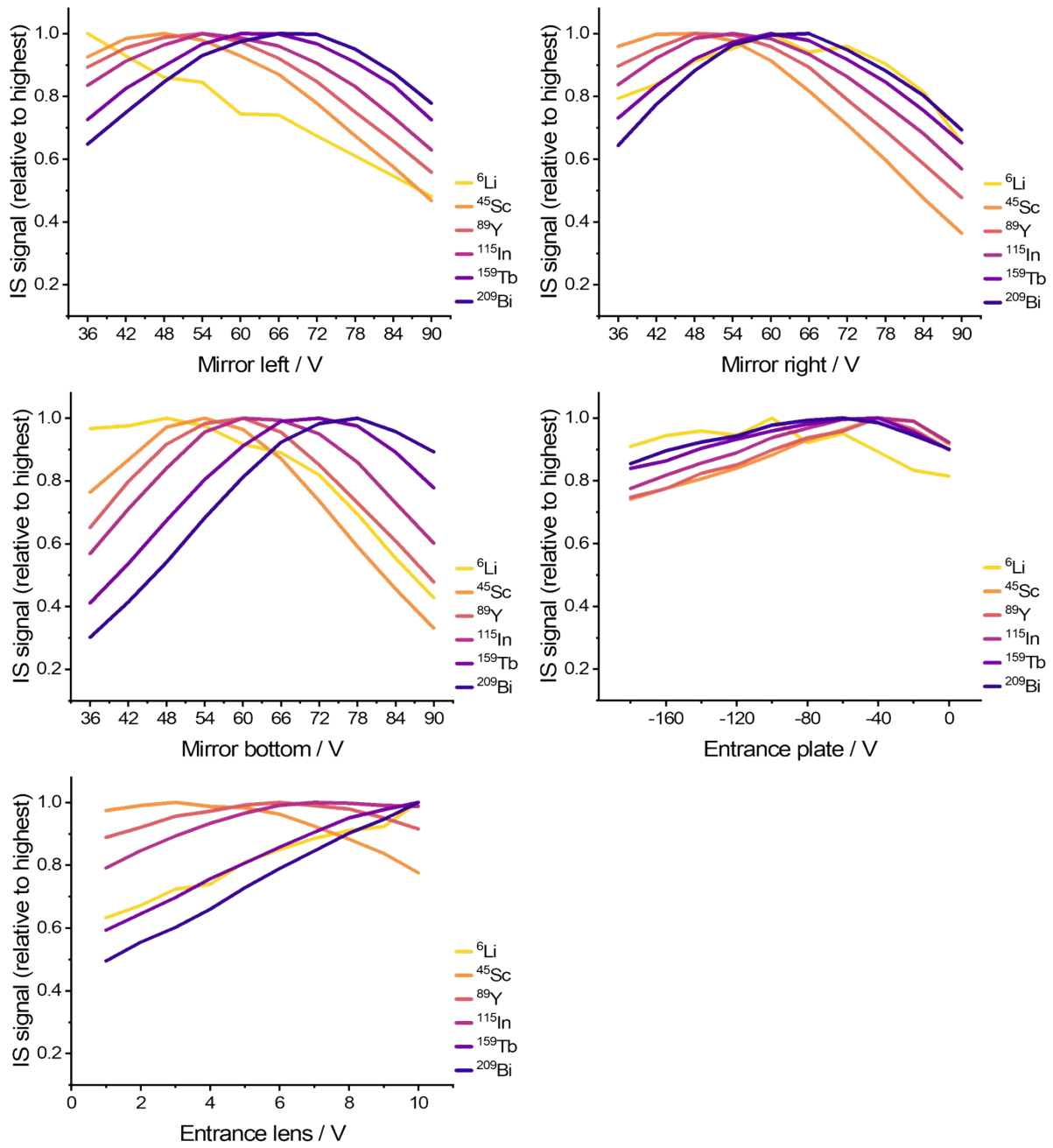


Figure S16: mass shift – internal standard signal recovery in blank (relative to highest in blank) with varying mirrors, entrance plate and lens voltages.

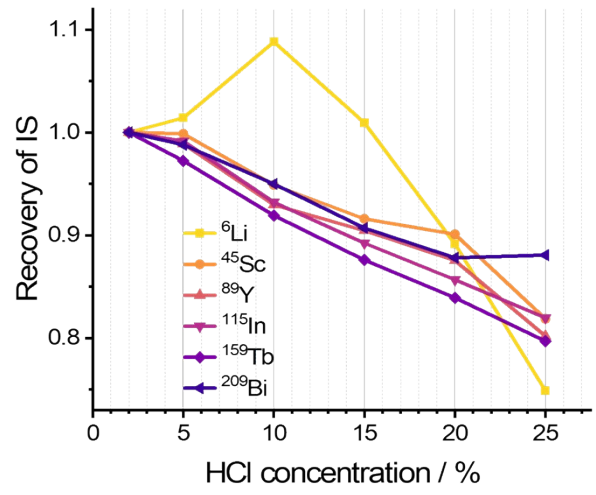
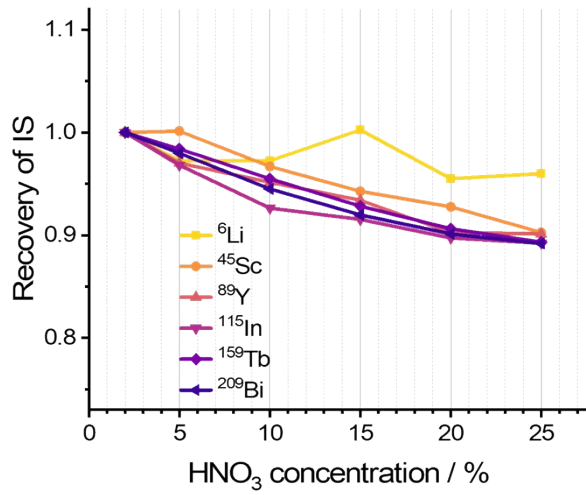


Figure S17: acid matrix effect – internal standard signal recovery with increasing acid concentration compared to 2 % for nitric and hydrochloric acid.