

Supporting Information

Multielement analysis in soils using nitrogen microwave inductively coupled atmospheric-pressure plasma mass spectrometry

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Table S1: Mass fractions (in mg kg⁻¹) of the elements in the reference soil samples (dry matter: 95%),

	V	Cr	Co	Ni	Cu	Zn	As	Cd	Hg	Pb
RV24-N2	12.85 ± 2.27	23.41 ± 3.48	7.57 ± 1.34	13.55 ± 2.01	96.69 ± 14.35	203.08 ± 30.14	16.26 ± 2.41	3.47 ± 0.51	0.9 ± 0.16	139.45 ± 20.69
RV25-N2	81.52 ± 11.32	687.33 ± 108.57	36.82 ± 5.11	245.68 ± 34.11	189.27 ± 22.62	959.34 ± 133.18	47.87 ± 6.65	5.48 ± 0.76	40.64 ± 6.42	273.28 ± 37.94
RV26-N1	16.39 ± 2.9	100.26 ± 15.83	6.27 ± 1.11	34.38 ± 4.77	117.91 ± 14.09	329.94 ± 45.8	81.15 ± 11.26	4.92 ± 0.68	1.64 ± 0.29	167.37 ± 23.23
RV26-N3	12.94 ± 2.29	146.36 ± 23.12	4.79 ± 0.85	36.64 ± 5.09	111.25 ± 13.3	357.12 ± 49.57	37.4 ± 5.19	7.68 ± 1.07	1.58 ± 0.28	143.01 ± 19.85
BRM09b	n.d.	16.4 ± 0.8	n.d.	6.53 ± 0.54	44.9 ± 3.3	144 ± 10	77.1 ± 2	23.1 ± 1.2	1.02 ± 0.17	85 ± 1.6
BRM10a	n.d.	403 ± 18	n.d.	209 ± 14	605 ± 29	2540 ± 45	34.2 ± 2.3	26.5 ± 1.5	26.9 ± 0.8	268 ± 12
BRM13	17.2 ± 1.1	27.4 ± 2.4	n.d.	12.8 ± 0.7	64 ± 2.2	210 ± 6	8.1 ± 0.44	1.32 ± 0.14	4.12 ± 0.28	230 ± 7

n.d. for not determined.

Table S2: Ti mass fractions (in mg kg⁻¹) in reference soil samples determined by MICAP-MS.

	Ti
RV24-N2	35.35 ± 3.54
RV25-N2	57.07 ± 3.52
RV26-N1	41.32 ± 3.03
RV26-N3	39.62 ± 2.65
BRM09b	23.22 ± 1.31
BRM10a	76.85 ± 5.94
BRM13	45.13 ± 3.42
En-Sample1	41.11 ± 3.31
En-Sample2	34.63 ± 2.94
En-Sample3	19.62 ± 1.42

Table S3: Zn mass fractions (in mg kg⁻¹) in reference soil samples determined by ICP-MS, MICAP-MS, and the reference values (st: standard deviation, En: metrological compatibility).

$$E_n = \frac{|W_{re} - W|}{\sqrt{st_{re}^2 - st^2}}$$

En: metrological compatibility; W_{re}: reference values; W: measured values; st_{re}: standard deviation of reference values; st: standard deviation of measured values

	W _{re}	st _{re}	W _{ICP-MS}	st	En	W _{MICAP-MS}	st	En
RV24-N2	203.08	30.14	198.14	23	0.12	212.83	8.84	0.29
RV25-N2	959.34	133.18	861.83	37.3	0.66	982.08	43.82	0.15
RV26-N1	329.94	45.8	301.84	8.19	0.56	328.76	9.87	0.02
RV26-N3	357.12	49.37	313.85	10.7	0.80	348.95	13.56	0.15
BRM09b	144	10	118.49	10.7	1.74	148.56	7.08	0.37
BRM10a	2540	45	2056	75.2	5.52	2395.62	50.67	2.13
BRM13	210	6	182.37	8.97	2.56	213.55	8.83	0.33

Table S4: As mass fractions (in mg kg⁻¹) in reference soil samples determined by ICP-MS, MICAP-MS, and the reference values (st: standard deviation, En: metrological compatibility).

	W _{re}	st _{re}	W _{ICP-MS}	st	En	W _{MICAP-MS}	st	En
RV24-N2	16.26	2.41	18.67	0.84	0.88	17.54	0.75	0.47
RV25-N2	47.87	6.65	46.95	2.8	0.12	50.53	2.34	0.35
RV26-N1	81.15	11.26	80.35	1.72	0.07	79.9	2.54	0.10
RV26-N3	37.4	5.19	38.88	1.42	0.26	36.8	1.26	0.11
BRM09b	77.1	2	79.23	3.05	0.58	78.34	2.52	0.39
BRM10a	34.2	2.3	33.73	2.44	0.14	34.95	0.45	0.32
BRM13	8.1	0.44	11.48	0.64	4.35	8.88	0.27	1.51

Table S5: Cd mass fractions (in mg kg⁻¹) in reference soil samples determined by ICP-MS, MICAP-MS, and the reference values (st: standard deviation, En: metrological compatibility).

	W _{re}	st _{re}	W _{ICP-MS}	st	En	W _{MICAP-MS}	st	En
RV24-N2	3.47	0.51	3.41	0.16	0.10	3.65	0.11	0.32
RV25-N2	5.48	0.76	5.34	0.24	0.16	5.6	0.16	0.14
RV26-N1	4.92	0.68	4.88	0.05	0.05	4.75	0.14	0.23
RV26-N3	7.68	1.07	7.6	0.27	0.07	7.35	0.37	0.27
BRM09b	23.1	1.2	22.36	0.68	0.54	22.23	0.99	0.56
BRM10a	26.5	1.5	26	1	0.28	27.13	0.63	0.39
BRM13	1.32	0.14	1.53	0.1	1.22	1.62	0.07	1.92

Table S6: Pb mass fractions (in mg kg⁻¹) in reference soil samples determined by ICP-MS, MICAP-MS, and the reference values (st: standard deviation, En: metrological compatibility).

	W _{re}	st _{re}	W _{ICP-MS}	st	En	W _{MICAP-MS}	st	En
RV24-N2	139.45	20.69	132.1	4.26	0.32	130.52	4.83	0.39
RV25-N2	273.28	37.94	254.25	11.8	0.45	251.92	9.71	0.51
RV26-N1	167.37	23.23	156	3.24	0.45	155.39	4.37	0.47
RV26-N3	143.01	19.85	128.61	4.06	0.66	128	4.33	0.69

BRM09b	85	1.6	73.859	6.56	1.65	75.48	3.92	2.25
BRM10a	268	12	250.23	10.6	1.11	247.96	6.02	1.49
BRM13	230	7	222.99	6.93	0.71	216.23	7.27	1.36

Table S7: Comparisons of limits of detection (LODs) of ICP-MS and MICAP-MS for the selected elements in the soil samples (in ng L⁻¹).

	ICP-MS	MICAP-MS
⁵¹ V	1.96	2.11
⁵³ Cr	28.86	58.12
⁵⁹ Co	0.97	2.83
⁶⁰ Ni	2.74	102.70
⁶⁵ Cu	11.44	9.11
⁶⁶ Zn	107.63	84.23
⁷⁵ As	20.13	62.62
¹¹² Cd	0.39	3.31
²⁰⁷ Pb	7.25	5.12

	MICAP-MS	ICP-MS	
Table	first extraction lens	-150	5.6
	second extraction lens	-125	-88.5
	third extraction lens	-540	/
	corner lens	-516	/
	mirror lens left	57	/
	mirror lens right	50	/
	cell entrance	4	-22
	omega bias	/	-32
	omega lens	/	8.8
	quadrupol focus	/	2

S8:

Comparisons of potential applied on ion-transfer optics in MICAP-MS and ICP-MS (in V).

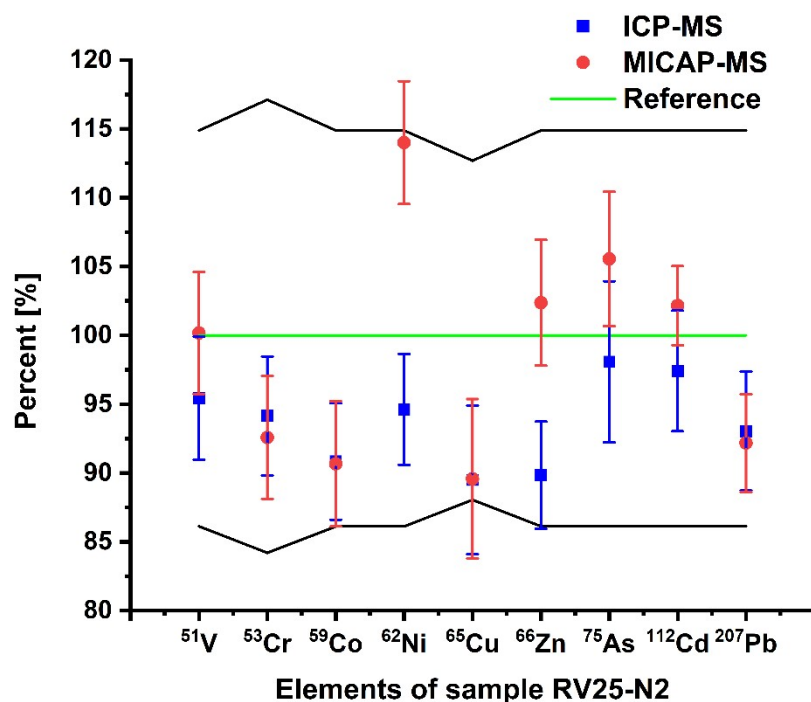


Figure S1. Percentage deviation of the mass fractions of selected elements in soil samples RV25-N2 determined by ICP-MS (blue) and MICAP-MS (red) compared to their reference values (green). The black lines represent the upper and lower limits of the reference ranges.

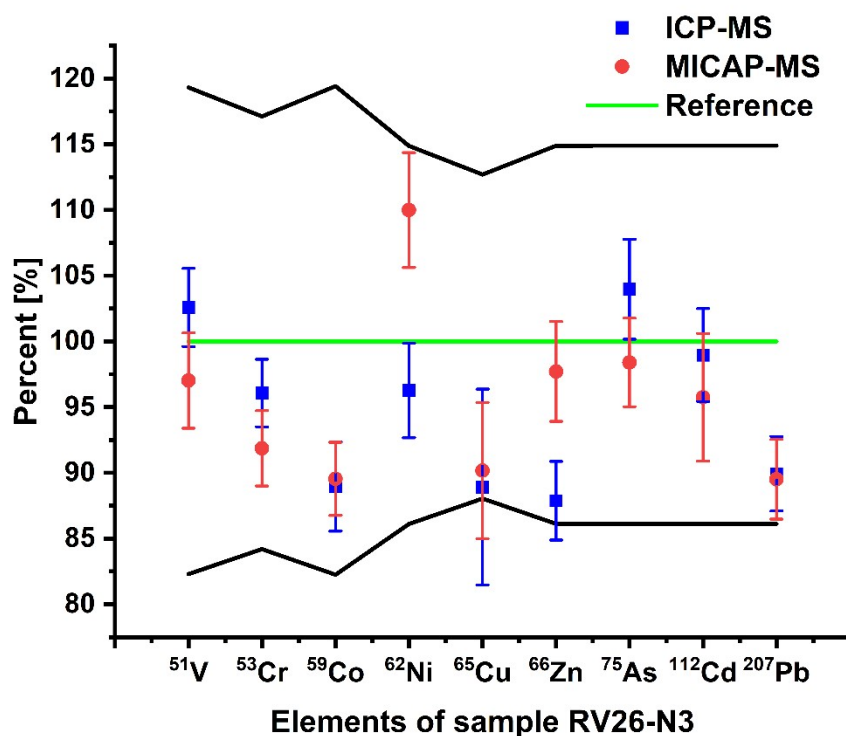


Figure S2. Percentage deviation of the mass fractions of selected elements in soil samples RV26-N3 determined by ICP-MS (blue) and MICAP-MS (red) compared to their reference values (green). The black lines represent the upper and lower limits of the reference ranges.

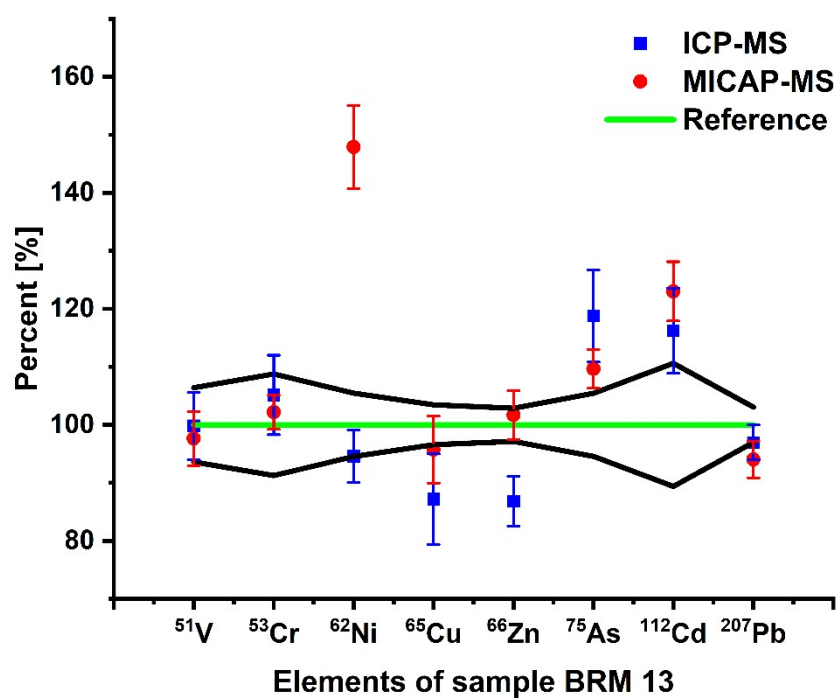


Figure S3. Percentage deviation of the mass fractions of selected elements in soil samples BRM13 determined by ICP-MS (blue) and MICAP-MS (red) compared to their reference values (green). The black lines represent the upper and lower limits of the reference ranges.

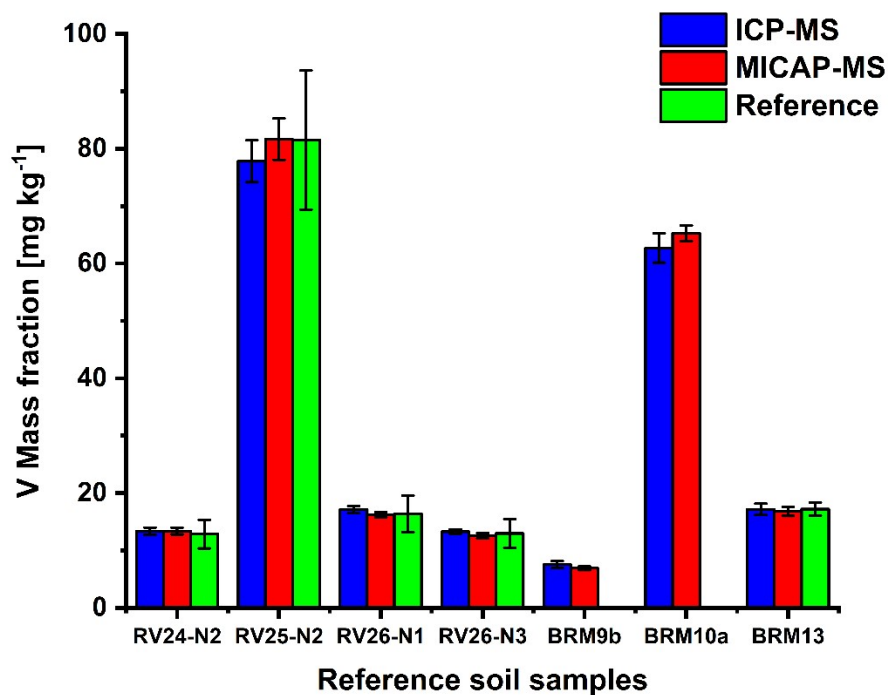


Figure S4. Mass fractions of V in reference soil samples determined by ICP-MS (blue), MICAP-MS (red) and its comparison with reference values (green).

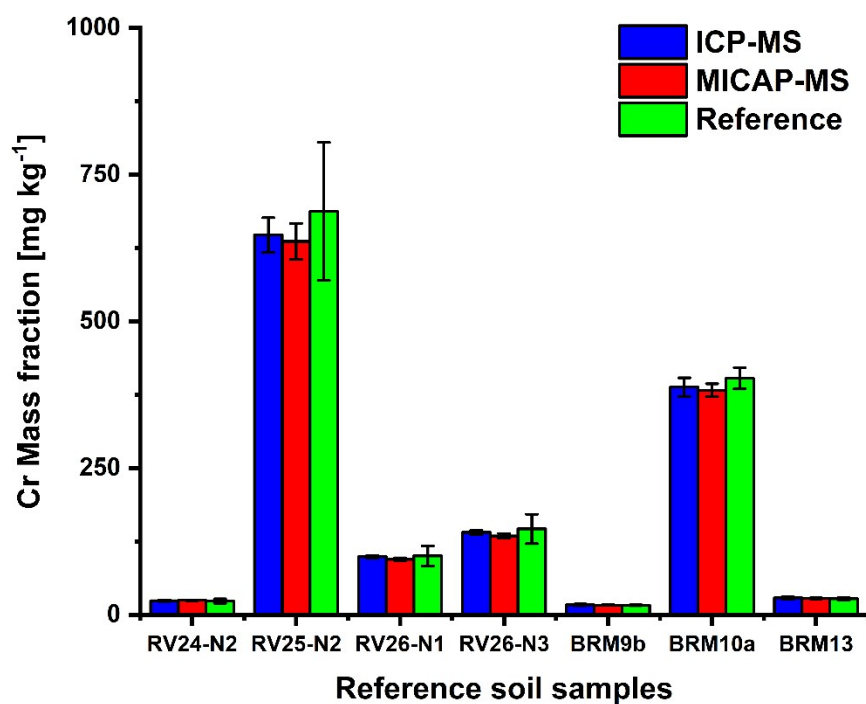


Figure S5. Mass fractions of Cr in reference soil samples determined by ICP-MS (blue), MICAP-MS (red) and its comparison with reference values (green).

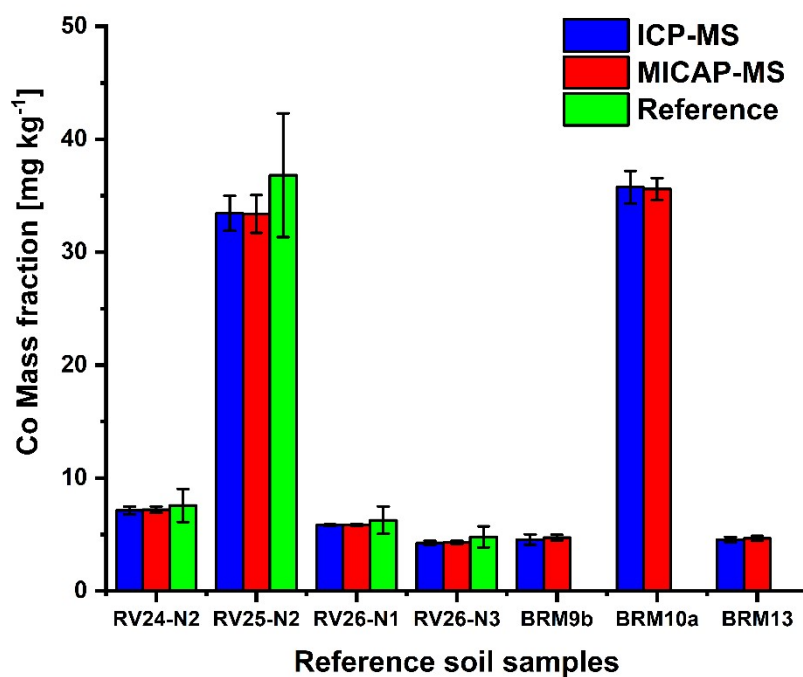


Figure S6. Mass fractions of Co in reference soil samples determined by ICP-MS (blue), MICAP-MS (red) and its comparison with reference values (green).

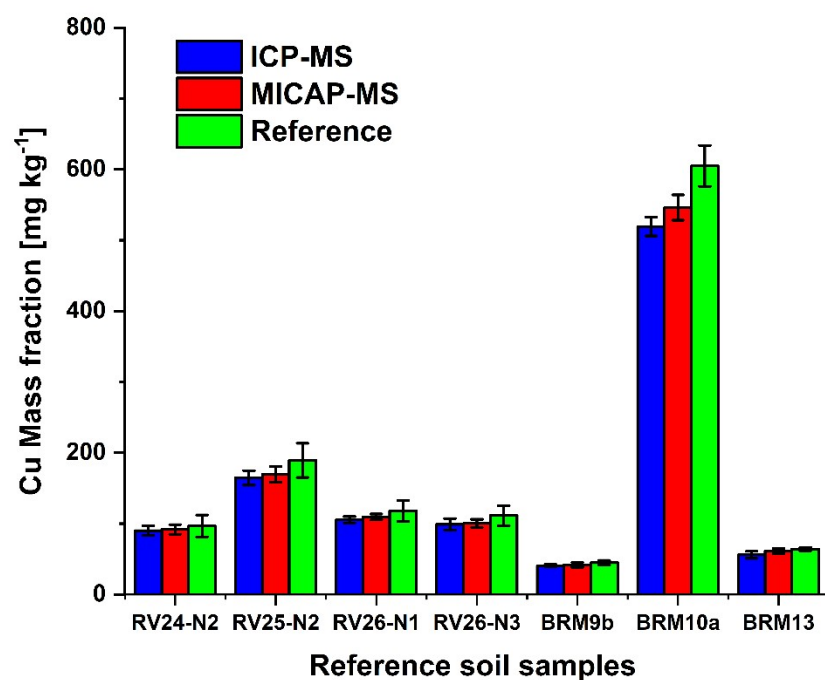


Figure S7. Mass fractions of Cu in reference soil samples determined by ICP-MS (blue), MICAP-MS (red) and its comparison with reference values (green).

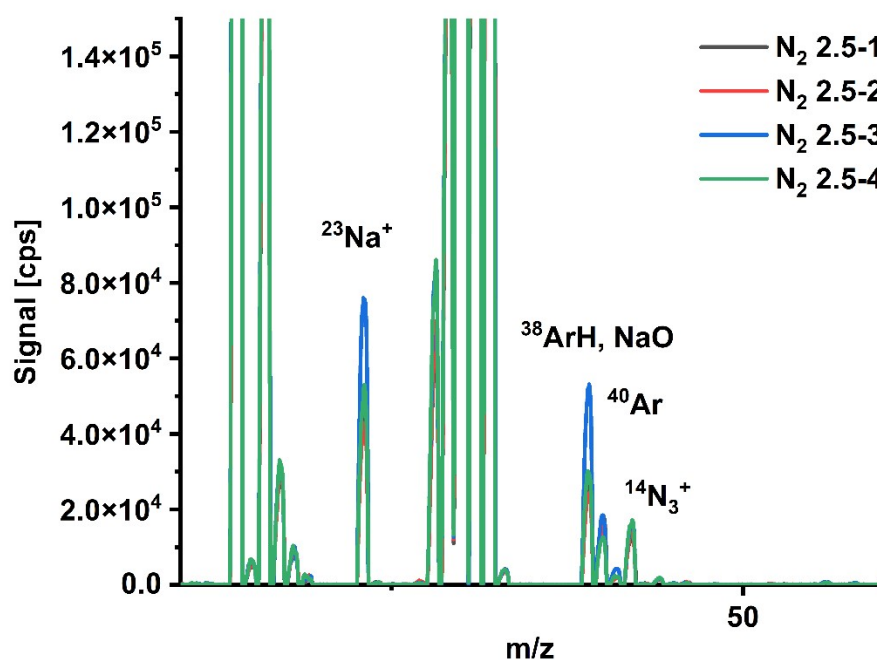


Figure S8. Comparison of MICAP-MS mass scans for a 2% HNO_3 solution obtained using N_2 2.5 from four different gas bottles.

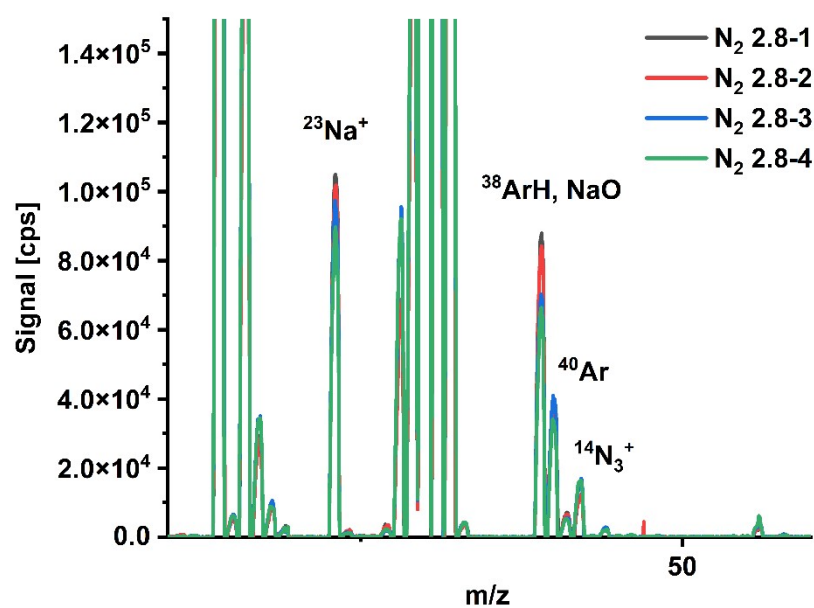


Figure S9. Comparison of MICAP–MS mass scans for a 2% HNO₃ solution obtained using N₂ 2.8 from four different gas bottles.