

Supplementary material 1

LOQ given as a range from individual LOQs from all runs.

CRM means and standard deviations calculated from averages from each run. Run averages only based on data above LOQ for that specific run.

Accuracy and method precision calculated for average CRM values from the runs.

Table 1: Replicate analyses of IAPSO seawater reference material during ICP-OES measurements (n=29 measurements, 8 ICP-OES runs)

LOQ [#] [mg/kg]	Element	IAPSO (OSIL) reference [mg/kg]	IAPSO measured [mg/kg]	Accuracy (%)	Method precision (%RSD)
0.11-0.96	B	4.5	4.5±0.12	0	3
0.83-9.83	Br	67	65±2	-2	3
0.34-14.36	Ca	412	430±8	4	2
2.19-10.43	K	399	401±8	1	2
0.36-12.10	Mg	1290	1427±41	11	3
1.11-72.53	S	904	914±16	1	2
0.42-2.82	Si	<0.02-5	1.4±0.2	---	17
0.20-2.98	Sr	7.9	7.5±0.3	-5	3

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

Table 2: Replicate analyses of MESS-3 reference material during ICP-OES measurements (n=38 measurements, 11 digested samples, 9 ICP-OES runs)

LOQ [#] [mg/kg]	Element	MESS-3 reference [mg/kg]	MESS-3 measured [mg/kg]	Accuracy (%)	Method precision (%RSD)
28-401	Al	85900±2300	74546±15405	-13	21
23-183	Ca	14700±600	13757±1095	-6	8
5-37	Cu	33.9±1.6	33.7±1.2	-1	4
98-808	Fe	43400±1100	40447±2277	-7	6
76-542	K	26000 ^a	25425±1273	-2	5
1-62	Mg	16000 ^a	15874±2059	-1	13
3-100	Mn	324±12	311±16	-4	5
86-741	P	1200 ^a	1306±125	9	10
4-15	Zn	159±8	149±4	-7	3

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

^a information value

Table 3: Replicate analyses of BHVO-2 reference material during ICP-OES measurements (n=24 measurements, 11 digested samples, 9 ICP-OES runs)

LOQ [#] [mg/kg]	Element	BHVO-2 reference [mg/kg]	BHVO-2 measured [mg/kg]	Accuracy (%)	Method precision (%RSD)
28-401	Al	71600±800	74874±1842	5	2
23-183	Ca	81700±1200	82833±1115	1	1
5-37	Cu	127±7	133±4	5	3
98-808	Fe	86300±1400	87784±1633	2	2
76-542	K	4300±100	4309±80	0	2
1-62	Mg	43600±700	44625±986	2	2
3-100	Mn	1290±40	1354±28	5	2
86-741	P	1200±100	1338±167	12	13
4-15	Zn	103±6	115±5	12	4

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

Table 4: Replicate analyses of IAPSO seawater reference material during ICP-MS measurements (n=25, 8 ICP-MS runs)

LOQ [#] [µg/kg]	Element	IAPSO (OSIL) reference [µg/kg]	IAPSO measured [µg/kg]	Accuracy (%)	Method precision (%RSD)
0.12-1.58	Mo	10.5	13.07±0.99	25	8
0.004-0.452	U	3.3	3.09±0.15	-6	5

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

Table 5: Replicate analyses of NASS-6 seawater reference material during ICP-MS measurements (n=50, 8 ICP-MS runs)

LOQ [#] [µg/kg]	Element	NASS-6 reference [µg/kg]	NASS-6 measured [µg/kg]	Accuracy (%)	Method precision (%RSD)
0.12-1.58	Mo	9.66±0.70	11.17±0.89	16	8
0.001-0.040	Cd	0.0303±0.0019	0.0480±0.0054	58	11
0.004-0.452	U	3 ^a	2.81±0.16	-6	6

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

^a information value

Table 6: Replicate analyses of NASS-6 seawater reference material during ICP-MS measurements (n=24, 7 ICP-MS runs)

LOQ [#] [µg/kg]	Element	NASS-6 reference [µg/kg]	NASS-6 measured [µg/kg]	Accuracy (%)	Method precision (%RSD)
0.20-0.90	V (KED)	1.42±0.16	1.42±0.06	0	4
0.73-3.34	Mn (KED)	0.516±0.047	Below LOQ	---	---
0.08-0.22	Co (KED)	0.015 ^a	Below LOQ	---	---
0.21-1.35	Cu (KED)	0.242±0.025	Below LOQ	---	---
0.17-1.65	As (KED)	1.40±0.12	1.28±0.10	-9	8

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

^a information value

Table 7: Replicate analyses of SLEW-3 estuarine water reference material during ICP-MS measurements (n=15, 7 ICP-MS runs)

LOQ [#] [µg/kg]	Element	n	SLEW-3 reference [µg/kg]	SLEW-3 measured [µg/kg]	Accuracy (%)	Method precision (%RSD)
0.38-3.55	Mn	8 (5 runs)	1.59±0.22	1.90±0.39	19	21
0.20-0.90	V (KED)	15 (7 runs)	2.54±0.31	2.94±0.12	16	4
0.73-3.34	Mn (KED)	8 (4 runs)	1.59±0.22	1.57±0.13	-2	9
0.08-0.22	Co (KED)		0.040±0.010	Below LOQ	---	---
0.21-1.35	Cu (KED)	15 (7 runs)	1.53±0.12	1.34±0.39	-13	29
0.17-1.65	As (KED)	12 (6 runs)	1.34±0.09	1.39±0.17	4	13

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

Table 8: Replicate analyses of SLRS-6 river water reference material during ICP-MS measurements (n=12, 7 ICP-MS runs)

LOQ [#] [µg/kg]	Element	n	SLRS-6 reference [µg/kg]	SLRS-6 measured [µg/kg]	Accuracy (%)	Method precision (%RSD)
0.20-0.90	V (KED)		0.352±0.006	Below LOQ	---	---
0.73-3.34	Mn (KED)	6 (4 runs)	2.12±0.10	2.26±0.18	7	8
0.21-1.35	Cu (KED)	12 (7 runs)	24.0±1.8	30.5±0.95	27	3
0.17-1.65	As (KED)		0.57±0.08	Below LOQ	---	---

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

Offset could be explained by a matrix effect (no salt matrix added to SLRS-6).

Table 9: Replicate analyses of MESS-3 reference material during ICP-MS measurements (n=24 measurements, 10 digested samples, 7 ICP-MS runs)

LOQ [#] [mg/kg]	Element	MESS-3 reference [mg/kg]	MESS-3 measured [mg/kg]	Accuracy (%)	Method precision (%RSD)
0.03-0.36	Co	14.4±2	14.1±0.1	-2	1
0.10-2.18	Ni	46.9±2.2	48.1±1.1	3	2
0.07-2.78	Mo	2.78±0.07	2.69±0.09	-3	3
0.05-4.93	Pb	21.1±0.7	19.6±5.2	-8	26

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run

Table 10: Replicate analyses of BHVO-2 reference material during ICP-MS measurements (n=71 measurements, 11 digested samples, 8 ICP-MS runs)

LOQ [#] [mg/kg]	Element	BHVO-2 reference [mg/kg]	BHVO-2 measured [mg/kg]	Accuracy (%)	Method precision (%RSD)
0.03-0.36	Co	45±3	46±2	3	3
0.10-2.18	Ni	119±7	126±4	6	3

[#] LOQ: limit of quantification; 10*standard deviation of acid blanks for each run