

Supplemental Table Aa Average concentrations and variances of analytical data for three sub-samples in 10 bottles sampled randomly from 500 bottles

Bottle No.	Na		Mg		Al		K		Ca		Ti	
	Average	Variance	Average	Variance	Average	Variance	Average	Variance	Average	Variance	Average	Variance
	%	%	%	%	%	%	%	%	%	%	%	%
1	0.859	0.00093	1.57	0.00216	7.57	0.00153	2.13	0.000112	4.22	0.000389	0.441	0.0000108
2	0.854	0.00034	1.56	0.00061	7.57	0.00014	2.13	0.000041	4.24	0.000250	0.444	0.0000081
3	0.840	0.00004	1.54	0.00081	7.53	0.00555	2.12	0.000471	4.20	0.001410	0.438	0.0000135
4	0.847	0.00007	1.54	0.00001	7.56	0.00158	2.13	0.000164	4.22	0.000375	0.439	0.0000173
5	0.844	0.00026	1.54	0.00019	7.58	0.00103	2.14	0.000040	4.22	0.000048	0.440	0.0000135
6	0.849	0.00013	1.55	0.00001	7.57	0.00001	2.13	0.000002	4.22	0.000002	0.438	0.0000005
7	0.848	0.00028	1.53	0.00005	7.57	0.00009	2.13	0.000006	4.23	0.000051	0.439	0.0000015
8	0.842	0.00029	1.53	0.00009	7.56	0.00018	2.13	0.000025	4.22	0.000015	0.439	0.0000044
9	0.831	0.00007	1.52	0.00018	7.55	0.00007	2.13	0.000021	4.22	0.000023	0.439	0.0000032
10	0.834	0.00004	1.51	0.00003	7.56	0.00035	2.13	0.000048	4.22	0.000079	0.441	0.0000005

Bottle No.	Fe		Mn		Zn		Sr		Ba	
	Average	Variance	Average	Variance	Average	Variance	Average	Variance	Average	Variance
	%	%	mg kg ⁻¹	mg kg ⁻¹	mg kg ⁻¹	mg kg ⁻¹	mg kg ⁻¹	mg kg ⁻¹	mg kg ⁻¹	mg kg ⁻¹
1	3.92	0.0000144	773	22.7	105	1.3	257	7.2	561	3195
2	3.94	0.0012546	780	121.4	105	22.2	258	3.1	556	2789
3	3.91	0.0004772	768	186.4	102	3.0	255	4.5	561	2494
4	3.92	0.0001528	775	56.9	101	0.0	258	0.4	565	3492
5	3.93	0.0002518	773	22.7	103	7.0	258	2.3	572	1262
6	3.94	0.0000357	775	0.8	110	67.3	259	0.3	580	442
7	3.94	0.0000025	775	0.8	105	64.6	258	3.0	572	32
8	3.94	0.0000004	778	19.7	106	11.5	258	4.3	573	426
9	3.94	0.0000876	771	21.5	105	14.4	259	2.3	583	106
10	3.94	0.0000917	775	0.8	103	9.9	258	1.1	571	644

Supplemental Table Ab ANOVA table for between-bottle homogeneity test

Element	Source of variation	SS	Degrees of freedom	MS	Variance(Sbb^2) Standard deviation(Sr)
Na	Between bottles	0.00194	9	0.00022	-0.00001 (Sbb^2)
	Within bottles	0.00492	20	0.00025	0.0157 (Sr)
	Total	0.00686	29		
Mg	Between bottles	0.00856	9	0.00095	0.00018 (Sbb^2)
	Within bottles	0.00827	20	0.00041	0.0203 (Sr)
	Total	0.01682	29		
Al	Between bottles	0.00479	9	0.00053	-0.00017 (Sbb^2)
	Within bottles	0.02105	20	0.00105	0.0324 (Sr)
	Total	0.02584	29		
Ca	Between bottles	0.00186	9	0.00021	-0.00002 (Sbb^2)
	Within bottles	0.00528	20	0.00026	0.0163 (Sr)
	Total	0.00714	29		
K	Between bottles	0.00076	9	0.00008	-0.000003 (Sbb^2)
	Within bottles	0.00186	20	0.00009	0.0096 (Sr)
	Total	0.00261	29		
Fe	Between bottles	0.00380	9	0.00042	0.00006 (Sbb^2)
	Within bottles	0.00474	20	0.00024	0.0154 (Sr)
	Total	0.00854	29		
Ti	Between bottles	0.00010	9	0.00001	0.000001 (Sbb^2)
	Within bottles	0.00015	20	0.00001	0.0027 (Sr)
	Total	0.00025	29		
Mn	Between bottles	308	9	34.2	-3.7 (Sbb^2)
	Within bottles	907	20	45.4	6.7 (Sr)
	Total	1215	29		
Zn	Between bottles	147	9	16.3	-1.3 (Sbb^2)
	Within bottles	402	20	20.1	4.5 (Sr)
	Total	549	29		
Sr	Between bottles	28	9	3.1	0.076 (Sbb^2)
	Within bottles	57	20	2.8	1.7 (Sr)
	Total	84	29		
Ba	Between bottles	1942	9	216	-424.1 (Sbb^2)
	Within bottles	29763	20	1488	38.6 (Sr)
	Total	31705	29		

SS: sum of squares (ANOVA), MS: mean square (ANOVA), Sbb : between-bottle homogeneity standard deviation, Sr: repeatability standard deviation

Supplemental Table B Robust statistical data for each element

Element	Total Lab. Number	Unit	Average	Median	NIQR	Limit value		Discarded Lab. number
						Lower	Upper	
Na	10	%	0.920	0.928	0.067	0.793	1.063	1
Mg	12	%	1.50	1.50	0.10	1.29	1.70	2
Al	13	%	7.63	7.58	0.27	7.04	8.13	1
K	11	%	2.10	2.14	0.09	1.96	2.32	1
Ca	13	%	4.21	4.23	0.22	3.78	4.68	1
Ti	11	%	0.431	0.421	0.025	0.372	0.470	1
Fe	13	%	3.84	3.91	0.17	3.57	4.25	0
Mn	12	mg kg ⁻¹	780	761	57	647	875	1
Zn	9	mg kg ⁻¹	93.1	93.9	4.2	85.4	102.3	0
Sr	10	mg kg ⁻¹	256	256	10	236	275	0
Ba	9	mg kg ⁻¹	542	537	24	488	586	1

The limit values of upper and lower of each element were calculated using absolute Z score of 2. NIQR: normalized interquartile range.