

TABLES SUPPLEMENTARY MATERIAL

Table S1. The ICP analysis standard concentration range.

Elem.	m/z	Certified concentrations	Concentrations range of standard dilutions	ISTD m/z	ISTD concentration
Be	9	20 µg/l	0.018-17.82 µg/l	Sc 45	90.9 µg/l
B	11	102 µg/l	0.091-90.87 µg/l	Sc 45	90.9 µg/l
Na	23	7271 µg/l	6.478-6478 µg/l	Sc 45	90.9 µg/l
Mg	24	14946 µg/l	13.32-13300 µg/l	Sc 45	90.9 µg/l
Al	27	1000 mg/l	9.145-9145 µg/l	Sc 45	90.9 µg/l
K	39	2703 µg/l	2.408-2408 µg/l	Sc 45	90.9 µg/l
Ca	43	35381 µg/l	31.52-31500 µg/l	Sc 45	90.9 µg/l
V	51	50.6 µg/l	0.045-45.08 µg/l	Sc 45	90.9 µg/l
Cr	53	20.3 µg/l	0.018-18.09 µg/l	Sc 45	90.9 µg/l
Mn	55	30.2 µg/l	0.027-26.91 µg/l	Sc 45	90.9 µg/l
Fe	56	100 µg/l	0.089-89.09 µg/l	Sc 45	90.9 µg/l
Co	59	25 µg/l	0.022-22.27 µg/l	Sc 45	90.9 µg/l
Ni	60	50.3 µg/l	0.045-44.81 µg/l	Sc 45	90.9 µg/l
Cu	63	20.5 µg/l	0.018-18.26 µg/l	Sc 45	90.9 µg/l
Zn	66	49 µg/l	0.044-43.66 µg/l	Sc 45	90.9 µg/l
As	75	50.6 µg/l	0.045-45.08 µg/l	Y 89	90.9 µg/l
Se	82	10.4 µg/l	0.009-9.265 µg/l	Y 89	90.9 µg/l
Sr	88	106 µg/l	0.094-94.44 µg/l	Y 89	90.9 µg/l
Mo	95	104 µg/l	0.093-92.66 µg/l	Y 89	90.9 µg/l
Ag	107	---	---	Y 89	90.9 µg/l
Cd	111	19.8 µg/l	0.018-17.64 µg/l	Y 89	90.9 µg/l
Ba	137	50.6 µg/l	0.045-45.08 µg/l	Re 185	90.9 µg/l
Au	197	---	---	Re 185	90.9 µg/l
Hg	202	10 mg/l	0.091-90.91 µg/l	Re 185	90.9 µg/l
Tl	205	10.4 µg/l	0.009-9.265 µg/l	Re 185	90.9 µg/l
Pb	208	25.5 µg/l	0.023-22.72 µg/l	Re 185	90.9 µg/l
Bi	209	10.5 µg/l	0.009-9.355 µg/l	Re 185	90.9 µg/l
U	238	---	---	Re 185	90.9 µg/l
Cu*	63	8.658 µg/l	49.15-7864 µg/l	Sc 45	90.9 µg/l
Zn*	66	58.600 µg/l	333-53300 µg/l	Sc 45	90.9 µg/l

* For Cu and Zn, it was necessary to make three standards to higher concentrations using salts of Zinc sulfate 7-hydrate and Copper sulfate pentahydrate PANREAC® (Spain).

Table S2. Upper outlier values (μg) using the quartiles* technique.

Element	Q1	Q2	Q3	IQR	1st grade	2nd grade**
Be	0	0	0.001	0.001	0.003	0.004
B	1.17	2.33	3.59	2.42	7.22	10.85
Na	44.2	97.7	189.3	145.1	406.9	624.5
Mg	8.6	18.7	39.9	31.3	86.9	133.9
Al	0.9	5.98	11.94	11.04	28.5	45.06
K	7.3	21	45.3	38	102.4	159.4
Ca	127.4	278.9	567	439.6	1226.5	1885.9
V	0.032	0.077	0.151	0.119	0.33	0.508
Cr	0.024	0.135	0.199	0.175	0.462	0.724
Mn	0.067	0.119	0.211	0.144	0.427	0.643
Fe	5.4	8.78	12.72	7.32	23.69	34.67
Co	0.00	0.006	0.016	0.016	0.04	0.064
Ni	0.062	0.216	0.365	0.303	0.82	1.274
Cu	16.2	67.2	142.2	126	331.2	520.1
Zn	285.9	485.5	634.6	348.7	1157.6	1680.7
As	0.011	0.02	0.033	0.022	0.066	0.099
Se	0.36	0.48	0.56	0.2	0.87	1.17
Sr	1.24	3.14	7	5.77	15.65	24.3
Mo	0.02	0.039	0.063	0.043	0.128	0.192
Cd	0.013	0.025	0.049	0.036	0.103	0.157
Ba	0.12	0.289	0.499	0.379	1.068	1.636
Hg	0.742	2.087	4.671	3.929	10.565	16.458
Tl	0.00	0.00	0.00	0.00	0.00	0.00
Pb	0.5	1.167	2.537	2.037	5.593	8.648
Bi	0.002	0.005	0.012	0.01	0.027	0.042
Ag	0.00	0.00	0.001	0.001	0.003	0.004
Au	0.00	0.00	0.00	0.00	0.00	0.00
U	0.00	0.00	0.00	0.00	0.00	0.00

* Values are expressed as $\mu\text{g/g}$

** Upper outlier of the first grade = $Q3 + (\text{IQR} \times 1.5)$; upper outlier of the second grade: $Q3 + (\text{IQR} \times 3)$.
IQR= $Q3-Q1$

Table S3. General statistics after eliminating values below the LOD and outlier excess of the second degree *

Elem.	N**	LOD	Min-Max.	\bar{X}_G	$\bar{X}_A \pm SD$	CI 95% (\bar{X}_A)	Me	γ_1	γ_2	K-S (<i>p</i>)
B	376	0.08	0.08-9.46	1.96	2.71±1.72	3.08-3.37	2.46	1	1	<0.01
Na	409	2.8	3-623	83	137±127	125-149	98	1.5	2	<0.01
Mg	360	0.1	0.1-43.4	5.3	8.9±7.7	8.1-9.7	7.2	1	1.6	<0.01
Al	348	0.4	0.4-43.4	5.9	9.2±7.7	8.4-10	7.5	1	1.6	<0.01
K	384	0.56	0.6-155	19	32±30	29-35	22	1.5	2	<0.01
Ca	403	0.8	9-1465	254	384±318	352-415	285	1	1	<0.01
V	409	0.0004	0.001-0.46	0.06	0.10±0.09	0.09-0.11	0.07	1	1.5	<0.01
Cr	350	0.005	0.006-0.59	0.12	0.16±0.107	0.15-0.17	0.155	1	2	<0.01
Mn	400	0.004	0.004-0.64	0.11	0.16±0.124	0.15-0.17	0.124	1	1.4	<0.01
Fe	375	1.2	1.1-32.7	8.3	10.0±5.5	09-11	9.2	0.9	1.3	<0.01
Co	280	0.001	0.001-0.063	0.01	0.014±0.011	0.013-0.015	0.012	1.4	2	<0.01
Ni	385	0.005	0.01-1.26	0.16	0.26±0.21	0.24-0.28	0.22	1	3	<0.01
Cu	414	0.05	0.7-515	47	98±105	88-108	66	1.7	3	<0.01
Zn	417	0.13	10-1422	358	477±277	450-504	484	0.4	0	<0.05
As	376	0.003	0.003- 0.099	0.019	0.024±0.017	0.022-0.026	0.02	1.4	2	<0.01
Se	377	0.05	0.05-1.12	0.42	0.46±0.17	0.45-0.48	0.49	-0.3	1	<0.01
Sr	415	0.02	0.04-19.6	2.7	4.5±4.0	4.2-4.9	3.1	1	0.4	<0.01
Mo	394	0.001	0.002-0.162	0.032	0.045±0.031	0.041-0.048	0.04	0.9	0.9	<0.01
Cd	389	0.002	0.002-0.157	0.024	0.036±0.033	0.033-0.039	0.025	1.6	2	<0.01
Ba	413	0.002	0.004-1.59	0.22	0.35±0.28	0.32-0.37	0.29	1.3	2	<0.01
Hg	411	0.003	0.014-15.66	1.56	3.12±3.16	2.84-3.45	2.04	1	2	<0.01
Pb	405	0.004	0.032-8.588	0.947	1.692±1.708	1.525-1.859	1.138	2	3	<0.01
Bi	341	0.0002	0.001-0.040	0.005	0.008±0.008	0.007-0.009	0.005	2	4	<0.01

* All values as µg/g; LOD: limit of detection; \bar{X}_A : arithmetic mean; \bar{X}_G : geometric mean; SD: standard deviations; Me: median; γ_1 : asymmetry; γ_2 : kurtosis; KS: Kolmogorov-Smirnov test.

** “N” the number of individuals remaining after removing the cases with values below the LOD and outliers excess for 2nd degree)

Table S4. Percentiles after eliminating values below the LOD and outliers excess of second grade*.

	N**	LOD	5	10	15	25	50	65	75	80	85	90	95
B	376	0.08	0.17	0.31	0.87	1.70	2.46	3.05	3.73	4.03	4.41	4.93	6.12
Na	409	2.8	8.5	13.9	25.8	45.5	97.9	146.2	189.1	215.4	246.8	320.7	428.7
Mg	360	0.1	0.4	0.7	1.3	3.2	7.2	10.4	12.8	13.9	15.9	20.4	25.8
Al	348	0.4	0.6	0.9	1.5	3.3	7.5	10.7	13.0	14.1	16.0	20.8	25.9
K	384	0.56	1.8	3.6	4.9	9.8	22.0	33.3	44.5	55.0	63.4	76.4	92.3
Ca	403	0.8	35	56	83	139	285	422	563	642	709	854	1095
V	409	0.0004	0.007	0.015	0.021	0.032	0.074	0.117	0.143	0.162	0.186	0.220	0.275
Cr	350	0.005	0.012	0.020	0.037	0.101	0.155	0.185	0.212	0.229	0.248	0.284	0.352
Mn	400	0.004	0.011	0.025	0.043	0.075	0.124	0.166	0.213	0.251	0.291	0.336	0.432
Fe	375	1.2	1.7	3.0	4.9	6.2	9.2	11.4	12.9	14.0	15.2	16.9	20.9
Co	280	0.001	0.001	0.002	0.003	0.006	0.012	0.016	0.019	0.022	0.026	0.030	0.038
Ni	385	0.005	0.020	0.020	0.040	0.090	0.220	0.290	0.365	0.400	0.451	0.540	0.647
Cu	414	0.05	3.3	5.4	7.7	15.6	65.7	97.9	138.0	159.6	196.9	250.7	333.0
Zn	417	0.13	39	77	131	285	484	567	633	675	754	849	969
As	376	0.003	0.005	0.007	0.010	0.012	0.020	0.026	0.032	0.036	0.040	0.048	0.058
Se	377	0.05	0.11	0.17	0.27	0.41	0.49	0.53	0.56	0.58	0.60	0.65	0.71
Sr	415	0.02	0.31	0.53	0.70	1.26	3.14	5.28	6.99	8.01	8.96	10.89	13.21
Mo	394	0.001	0.004	0.006	0.01	0.02	0.04	0.05	0.06	0.07	0.08	0.09	0.10
Cd	389	0.002	0.003	0.006	0.008	0.014	0.025	0.036	0.046	0.056	0.069	0.082	0.113
Ba	413	0.002	0.02	0.04	0.06	0.12	0.29	0.41	0.50	0.57	0.64	0.71	0.86
Hg	411	0.003	0.08	0.19	0.30	0.72	2.05	3.34	4.44	5.42	6.70	7.95	9.42
Pb	405	0.004	0.09	0.14	0.21	0.49	1.14	1.79	2.38	2.83	3.36	3.86	5.24
Bi	341	0.0002	0.001	0.001	0.002	0.002	0.005	0.007	0.010	0.012	0.015	0.018	0.024

* All values as µg/g.

** Column "N" shows the number of individuals remaining after removing the cases with values below the LOD and outliers (excess for 2nd degree).