Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Information

A high-throughput method for the element determination in green coffee bean using diluted nitric acid and ultrasound energy

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Table S1. Summary of the obtained models for the experimental design of all analytes.

Analyte	Parameter	Estimate	Std. Error	t value	Pr(>|t|)
Ba	(Intercept)	0.316	0.111	2.858	0.008**
	A	-0.027	0.068	-0.394	0.696
	B	0.425	0.068	6.278	0.000***
	A^2	0.091	0.081	1.130	0.268
	B^2	-0.619	0.081	-7.672	0.000***
	A:B	-0.144	0.096	-1.502	0.145
	Residual standard error: 0.3319 on 27 degrees of freedom, Multiple R^2: 0.8075, Adjusted R^2: 0.7718, F-statistic: 22.65 on 5 and 27 DF, p-value: 6.943e-09				
Ca	(Intercept)	0.132	0.083	1.596	0.122
	A	0.038	0.051	0.755	0.457
	B	0.208	0.051	4.119	0.000***
	A^2	0.030	0.060	0.490	0.628
	B^2	-0.502	0.060	-8.335	0.000***
	A:B	-0.154	0.072	-2.151	0.041*
	Residual standard error: 0.2479 on 27 degrees of freedom, Multiple R^2: 0.7892, Adjusted R^2: 0.7502, F-statistic: 20.22 on 5 and 27 DF, p-value: 2.283e-08				
Cu	(Intercept)	1.449	0.121	11.961	0.000***
	A	0.169	0.074	2.283	0.031*
	B	0.552	0.074	7.445	0.000***
	A^2	-0.069	0.088	-0.784	0.440
	B^2	-1.190	0.088	-13.476	0.000***
	A:B	-0.108	0.105	-1.025	0.314
	Residual standard error: 0.3634 on 27 degrees of freedom, Multiple R^2: 0.904, Adjusted R^2: 0.8863, F-statistic: 50.87 on 5 and 27 DF, p-value: 6.716e-13				
Fe	(Intercept)	0.881	0.101	8.711	0.000***
	A	0.077	0.062	1.236	0.227
	B	0.856	0.062	13.824	0.000***
	A^2	-0.331	0.074	-4.486	0.000***
	B^2	-0.803	0.074	-10.891	0.000***
	A:B	0.413	0.088	4.712	0.000***
	Residual standard error: 0.3034 on 27 degrees of freedom, Multiple R^2: 0.9255, Adjusted R^2: 0.9117, F-statistic: 67.05 on 5 and 27 DF, p-value: 2.287e-14				
K	(Intercept)	1.226	0.106	11.540	0.000***
	A	0.179	0.065	2.747	0.011*
	B	0.169	0.065	2.590	0.015*
	A^2	-0.072	0.077	-0.927	0.362
	B^2	-0.862	0.077	-11.133	0.000***
	A:B	-0.162	0.092	-1.758	0.090
	Residual standard error: 0.3188 on 27 degrees of freedom, Multiple R^2: 0.8451,				

	Adjusted R^2: 0.8164, F-statistic: 29.46 on 5 and 27 DF, p-value: 3.919e-10				
Mg	(Intercept)	0.503	0.117	4.309	0.000***
	A	0.141	0.071	1.974	0.059
	B	0.150	0.071	2.103	0.045*
	A^2	0.063	0.085	0.736	0.468
	B^2	-0.636	0.085	-7.483	0.000***
	A:B	-0.128	0.101	-1.265	0.217
	Residual standard error: 0.3501 on 27 degrees of freedom, Multiple R^2: 0.7362, Adjusted R^2: 0.6874, F-statistic: 15.07 on 5 and 27 DF, p-value: 4.296e-07				
Mn	(Intercept)	-0.121	0.102	-1.186	0.246
	A	0.047	0.062	0.758	0.455
	B	0.100	0.062	1.607	0.120
	A^2	0.081	0.074	1.088	0.286
	B^2	-0.353	0.074	-4.745	0.000***
	A:B	-0.081	0.088	-0.921	0.365
	Residual standard error: 0.3058 on 27 degrees of freedom, Multiple R^2: 0.5521, Adjusted R^2: 0.4691, F-statistic: 6.656 on 5 and 27 DF, p-value: 0.0003712				
P	(Intercept)	0.581	0.172	3.382	0.002**
	A	-0.117	0.105	-1.113	0.275
	B	0.722	0.105	6.863	0.000***
	A^2	-0.107	0.125	-0.856	0.400
	B^2	-0.661	0.125	-5.273	0.000***
	A:B	0.364	0.149	2.445	0.021*
	Residual standard error: 0.5156 on 27 degrees of freedom, Multiple R^2: 0.7538, Adjusted R^2: 0.7082, F-statistic: 16.53 on 5 and 27 DF, p-value: 1.75e-07				
Sr	(Intercept)	0.266	0.104	2.562	0.016*
	A	-0.005	0.063	-0.081	0.936
	B	0.405	0.063	6.379	0.000***
	A^2	0.090	0.076	1.188	0.245
	B^2	-0.622	0.076	-8.231	0.000***
	A:B	-0.112	0.090	-1.246	0.223
	Residual standard error: 0.311 on 27 degrees of freedom, Multiple R^2: 0.8215, Adjusted R^2: 0.7884, F-statistic: 24.85 on 5 and 27 DF, p-value: 2.56e-09				
Zn	(Intercept)	0.989	0.197	5.028	0.000***
	A	-0.082	0.120	-0.678	0.503
	B	0.266	0.120	2.206	0.036*
	A^2	-0.559	0.143	-3.902	0.001***
	B^2	-0.803	0.143	-5.603	0.000***
	A:B	-0.363	0.170	-2.129	0.043*
	Residual standard error: 0.5902 on 27 degrees of freedom, Multiple R^2: 0.6342, Adjusted R^2: 0.5664, F-statistic: 9.362 on 5 and 27 DF, p-value: 2.899e-05				

Significance codes: 0 '***' 0.001 '**' 0.01 '*'; A (time in minutes); B (HNO_3 concentration in mol/L); DF (degrees of freedom)

Table S2. The total concentration of elements, in μg g^{-1}, in various coffee bean samples determined by ICP-OES after UAE (results expressed as a mean ± interval with 95% of confidence level).

Sample	Ba	Ca	Cu	Fe	K	Mg	Mn	Sr	P	Zn
A-MG14	2.3 ± 1.6	2387 ± 1418	27 ± 18	28 ± 3	55741 ± 33555	3216 ± 1664	33.7 ± 16.0	5.8 ± 3.6	1614 ± 561	6 ± 1
C20-15-MG16	1.1 ± 0.1	1785 ± 107	16 ± 1	27 ± 3	32513 ± 1796	2260 ± 111	28.0 ± 1.6	2.9 ± 0.1	1181 ± 113	12 ± 1
C24-137-MG16	0.2 ± 0.1	1548 ± 224	13 ± 3	24 ± 1	34944 ± 4705	2661 ± 371	32.7 ± 4.1	2.0 ± 0.3	1453 ± 148	6 ± 1
C2-SL-MG14	1.8 ± 0.2	2209 ± 210	19 ± 3	29 ± 3	38943 ± 6118	2762 ± 636	30.8 ± 6.8	3.4 ± 0.4	1581 ± 414	8 ± 1
C36-6-MG16	0.8 ± 0.1	1817 ± 104	18 ± 1	25 ± 2	36341 ± 1467	2355 ± 176	37.9 ± 2.4	2.9 ± 0.1	1451 ± 208	6 ± 1
CA-ES15	1.5 ± 0.2	2387 ± 173	13 ± 1	27 ± 1	35809 ± 5763	2769 ± 167	50.2 ± 3.5	5.2 ± 0.5	1817 ± 217	5 ± 1
CA-ES16	0.3 ± 0.1	1589 ± 95	11 ± 1	28 ± 2	30771 ± 1553	2149 ± 99	27.2 ± 1.6	4.0 ± 0.2	1328 ± 122	6 ± 1
CA-MG14	<LOD	1784 ± 244	10 ± 1	23 ± 4	36617 ± 4255	2854 ± 240	12.1 ± 0.9	1.0 ± 0.2	1413 ± 242	5 ± 1
CA-SP14	3.6 ± 0.9	1808 ± 417	15 ± 4	25 ± 2	40825 ± 9012	2419 ± 478	55.2 ± 12.4	5.6 ± 1.3	1495 ± 350	6 ± 1
CR-MG-16	1.0 ± 0.3	1615 ± 302	15 ± 4	27 ± 1	35238 ± 7044	2424 ± 475	33.8 ± 6.8	2.8 ± 0.6	1520 ± 228	6 ± 1
CV-MG14	<LOD	1894 ± 227	11 ± 2	24 ± 2	38254 ± 4337	3327 ± 394	16.6 ± 3.0	1.1 ± 0.2	2429 ± 643	5 ± 1
IAC-144-MG14	4.1 ± 0.9	2379 ± 455	19 ± 4	24 ± 4	43396 ± 7630	3016 ± 546	54.3 ± 10.3	6.4 ± 1.3	1740 ± 253	7 ± 2
IAC-144-SP14	2.7 ± 0.3	1841 ± 160	16 ± 2	26 ± 2	32942 ± 2638	2424 ± 416	26.5 ± 4.9	6.3 ± 0.5	1700 ± 462	5 ± 1
IAC-44-ES12	1.2 ± 0.3	2067 ± 449	30 ± 6	32 ± 2	45585 ± 9714	2717 ± 214	26.2 ± 2.2	5.2 ± 1.0	1665 ± 317	7 ± 2
IAC-44-ES13	1.3 ± 0.4	2145 ± 355	23 ± 7	22 ± 2	44818 ± 11224	2421 ± 124	20.4 ± 1.6	5.4 ± 1.2	1434 ± 416	4 ± 1
IAC-44-ES14	1.1 ± 0.2	1867 ± 191	21 ± 2	26 ± 2	38585 ± 1843	2998 ± 201	29.8 ± 2.0	4.8 ± 0.5	2061 ± 347	5 ± 1
IAC-44-ES16	1.0 ± 0.1	1752 ± 149	19 ± 2	29 ± 3	41843 ± 2526	3163 ± 212	21.4 ± 1.7	3.3 ± 0.3	2766 ± 106	10 ± 2
IAC-62-SP14	4.3 ± 0.7	1943 ± 314	15 ± 2	29 ± 6	36042 ± 4557	2452 ± 257	148.8 ± 19.9	6.8 ± 1.1	1597 ± 169	6 ± 1
IP59-ES12	<LOD	1853 ± 582	13 ± 5	26 ± 2	33682 ± 11120	2841 ± 965	28.9 ± 9.7	2.7 ± 1.0	2097 ± 768	9 ± 1
IP59-ES13	0.6 ± 0.1	1759 ± 198	14 ± 2	35 ± 4	36346 ± 3168	2970 ± 262	35.8 ± 3.5	2.7 ± 0.3	1977 ± 470	4 ± 1
IP59-ES14	<LOD	1924 ± 117	12 ± 1	32 ± 2	38281 ± 4978	2813 ± 568	26.9 ± 5.1	2.4 ± 0.2	1611 ± 318	5 ± 1
IP59-ES15	0.5 ± 0.2	1952 ± 629	14 ± 4	28 ± 3	38263 ± 7246	2463 ± 331	23.4 ± 5.2	3.9 ± 0.9	1792 ± 932	6 ± 1
IP59-ES16a	0.5 ± 0.2	1795 ± 277	5 ± 1	31 ± 2	33385 ± 5020	2508 ± 397	32.0 ± 5.4	6.0 ± 1.0	1506 ± 279	5 ± 1
IP59-ES16b	<LOD	1784 ± 185	15 ± 2	38 ± 5	35325 ± 2948	2482 ± 338	22.5 ± 3.5	2.8 ± 0.3	1548 ± 370	4 ± 1

MN-376-4-MG14	2.0 ± 0.4	2391 ± 448	23 ± 4	30 ± 3	46646 ± 7799	2848 ± 367	20.3 ± 2.1	5.2 ± 0.9	1506 ± 313	7 ± 1
MN-376-4-MG16	4.3 ± 1.7	2110 ± 739	17 ± 6	30 ± 2	37476 ± 14041	2376 ± 667	28.2 ± 8.8	4.7 ± 0.2	1105 ± 371	6 ± 1
MN-474-19-MG14	2.7 ± 0.4	2576 ± 452	23 ± 6	44 ± 3	48181 ± 6973	2695 ± 506	29.2 ± 4.8	7.6 ± 0.8	1344 ± 481	6 ± 1
MN-474-19-MG16	1.7 ± 0.5	2256 ± 448	21 ± 4	32 ± 3	41990 ± 7278	3132 ± 648	45.6 ± 7.9	3.7 ± 0.9	1954 ± 602	5 ± 1
MN-479-19-MG16	1.4 ± 0.2	1832 ± 117	20 ± 1	27 ± 2	43416 ± 2581	3172 ± 226	32.6 ± 2.1	3.0 ± 0.2	2082 ± 226	6 ± 1