Supplementary Information

Development of a Simple and Fast Procedure Based on Acid Dilution for Determination of Macro and Microelements in Guarana-Based Beverages by ICP OES

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Table S1. Intensities obtained for each analyte in the Box-Behnken design

Exp	Emission intensity / (count s^{-1})								
	Cu	Fe	Mn	Zn	Ca	K	Mg	P	S
1	303.03	1543.74	3006.92	464.34	57979.00	1930592	129065	247.74	3141.30
2	147.31	1561.27	2955.64	440.32	56001.40	1806640	124719	234.04	3108.62
3	200.01	1421.17	2958.91	181.76	54810.87	1891562	122808	244.17	3212.55
4	223.74	1353.86	2742.02	202.96	50549.37	1709437	114932	241.70	3040.53
5	153.81	1383.45	2771.80	220.65	51468.64	1974849	121053	222.66	2940.89
6	188.15	1291.90	2570.10	206.47	46720.52	1805711	112665	196.84	2759.40
7	320.78	1783.67	3980.02	350.35	64570.96	1896710	130919	282.10	3442.78
8	283.98	1544.63	3069.00	229.03	59587.99	1720611	122255	245.88	3292.77
9	230.76	1430.13	2861.06	219.91	52039.20	1983852	124333	236.07	2928.36
10	142.04	1295.61	2601.45	191.38	47299.62	1880025	113344	203.19	2877.63
11	357.60	1640.98	3169.12	297.57	65570.80	1850736	132085	272.15	3324.94
12	192.61	1571.03	2863.97	243.26	60119.75	1735037	121038	257.27	3297.79
13	273.41	1437.87	2967.73	227.64	54698.64	1863122	124155	246.59	3164.21
14	224.82	1467.09	2994.09	234.76	54811.21	1862399	124250	249.10	3165.42
15	216.12	1525.11	3038.26	228.11	55863.65	1870653	124847	229.84	3202.52

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Table S2. Statistical comparison between the analytical curves obtained from external calibration and standard addition method (n =3)

Element	Aqueous curve 2% (v v^{-1}) HNO_3		Standard addition curve		$F_{calculated}$	$t_{calculated}$
	α	R^2	α	R^2		
Cu	14317 ± 297	0.9999	12733 ± 143	0.9999	4.27	2.17
Fe	19519 ± 223	0.9998	19797 ± 241	0.9999	0.85	1.32
Mn	106202 ± 1489	0.9999	101778 ± 670	0.9999	4.93	2.05
Zn	9191 ± 75	0.9998	9907 ± 90	1.0000	0.70	2.20
K	44453 ± 1189	0.9995	38475 ± 76	0.9992	4.35	2.17
Ca	3458 ± 65	0.9999	3568 ± 29	0.9999	4.77	1.78
S	50 ± 0.7	0.9998	54 ± 0.8	0.9993	0.47	2.05
P	136 ± 1.5	0.9993	157 ± 0.4	0.9995	0.71	2.23
Mg	170095.3 ± 5159	0.9991	167337 ± 5865	0.9996	5.26	0.87

α: slope; R^2: determination coefficient; $F_{calculated}$: calculated value for F ($F_{critical}$ = 19.16); $t_{calculated}$: calculated value for t (t critical = 2.78).

Table S3. Background equivalent concentration (BEC), limits of detection and quantification (LOD and LOQ), relative standard deviation (RSD, n = 7), and working linear range for the proposed procedure

Analyte	BEC / (mg L^{-1})	LOD / (mg L^{-1})	LOQ / (mg L^{-1})	RSD / %	Working linear range / (mg L^{-1})
Cu	0.005	0.003	0.010	9.9	0.01-2.0
Fe	0.001	0.0006	0.002	9.3	0.002-2.0
Mn	0.0004	0.0002	0.0006	1.3	0.0006-2.0
Zn	0.010	0.0018	0.006	9.5	0.006-2.0
K	0.030	0.020	0.066	1.1	0.06-80
Ca	0.16	0.019	0.065	4.6	0.065-80
S	0.13	0.070	0.235	1.8	0.235-40
P	0.01	0.011	0.040	6.5	0.04-20
Mg	0.006	0.005	0.020	1.5	0.02-20

Table S4. Comparison between the found values by applying the proposed method and the certified values in the SRM NIST 1643f Trace elements in water (mean ± standard deviation, n = 3)

Element	Concentration / (μg L^{-1})		Student's *t*-test		Recovery / %
	Certified	Found	$t_{tabulated}$	$t_{calculated}$	
Ca	29430 ± 330	30550 ± 101		2.44	104
Cu	21.66 ± 0.71	20.43 ± 0.69		1.80	94
Fe	93.44 ± 0.78	50.02 ± 0.72		37.0	54
Mn	37.14 ± 0.60	35.54 ± 0.36		2.30	96
Mg	7454 ± 60	7589 ± 25	4.30	2.34	102
K	19324 ± 9	18444 ± 7		2.45	75
Zn	74.4 ± 1.7	73.2 ± 8.7		0.47	98
S	nc	130 ± 5			
P	nc	< 40.0			

nc: no certified; $t_{tabulated}$: *t*-value at 95% of confidence level; $t_{calculated}$: calculated value for *t*.

Table S5. Spike addition and recovery test for the proposed method (mean ± standard deviation, n = 3)

Analyte	$C_{initial}$ / (mg L^{-1})	Addition 1 / (mg L^{-1})	Rec / %	Addition 2 / (mg L^{-1})	Rec / %	Addition 3 / (mg L^{-1})	Rec / %
Cu	0.010 ± 0.001	0.17 ± 0.01	82 ± 1	0.33 ± 0.01	82 ± 1	0.50 ± 0.01	82 ± 2
Fe	0.020 ± 0.001	0.21 ± 0.01	103 ± 4	0.41 ± 0.01	100 ± 5	0.59 ± 0.01	96 ± 2
Mn	0.020 ± 0.001	0.20 ± 0.01	98 ± 4	0.38 ± 0.01	94 ± 3	0.56 ± 0.008	90 ± 1
Zn	< 0.006	0.21 ± 0.01	105 ± 2	0.42 ± 0.07	105 ± 2	0.61 ± 0.04	98 ± 7
Ca	11.02 ± 0.4	16.1 ± 0.41	116 ± 1	19.0 ± 0.5	97 ± 7	24.09 ± 0.83	107 ± 7
K	23.83 ± 0.89	27.8 ± 0.77	110 ± 1	31.3 ± 1.0	100 ± 1	35.54 ± 0.25	97 ± 2
P	0.14 ± 0.2	1.30 ± 0.03	116 ± 4	2.42 ± 0.08	114 ± 4	3.65 ± 0.04	117 ± 1
S	57.27 ± 2.5	60.9 ± 0.15	111 ± 7	62.8 ± 0.31	102 ± 7	65.3 ± 0.08	110 ± 1
Mg	1.99 ± 0.08	6.24 ± 0.09	106 ± 2	9.96 ± 0.15	99 ± 2	13.9 ± 0.15	99 ± 1

$C_{initial}$: initial concentration; Rec: recovery value.