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Comparative Studies of the Sample Decomposition of Green and Roasted Coffee for Determination of Nutrients and Data Exploratory Analysis

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Table S1. Concentrations of K, N, Ca, Mg (% m/m) and Na (mg kg^{-1}) in 35 coffee samples

S. / Elem.	Na (10-174) *	K (1.3816-3.7400) *	N (1.9000-2.2500) *	Ca (0.0826-0.1310) *	Mg (0.1600-0.3000) *
PG 1	43.5 ± 2.2 (1)	1.5138 ± 0.0516 (1)	1.9855 ± 0.0165 (2)	0.0932 ± 0.0019 (1)	0.2214 ± 0.0029 (1)
	46.3 ± 2.7 (2)	1.5019 ± 0.0354 (2)		0.0822 ± 0.0034 (2)	0.2286 ± 0.0025 (2)
PG 2	57.2 ± 3.7 (1)	1.6350 ± 0.0043 (1)	2.1637 ± 0.0376 (2)	0.1054 ± 0.0004 (1)	0.1914 ± 0.0028 (1)
	60.9 ± 1.0 (2)	1.5775 ± 0.0022 (2)		0.0772 ± 0.0106 (2)	0.1984 ± 0.0035 (2)
PG 3	58.1 ± 3.5 (1)	1.6536 ± 0.0371 (1)	2.0181 ± 0.0488 (2)	0.0995 ± 0.0009 (1)	0.2016 ± 0.0009 (1)
	45.6 ± 2.6 (2)	1.5252 ± 0.0019 (2)		0.0843 ± 0.0037 (2)	0.2017 ± 0.0021 (2)
PG 4	53.0 ± 1.6 (1)	1.5835 ± 0.0141 (1)	2.1897 ± 0.0189 (2)	0.1172 ± 0.0018 (1)	0.1990 ± 0.0012 (1)
	49.6 ± 3.2 (2)	1.5383 ± 0.0054 (2)		0.1034 ± 0.0007 (2)	0.1964 ± 0.0027 (2)
PG 5	42.3 ± 2.0 (1)	1.5246 ± 0.0098 (1)	2.2442 ± 0.0348 (2)	0.1049 ± 0.0003 (1)	0.2085 ± 0.0016 (1)
	47.7 ± 1.7 (2)	1.5199 ± 0.0423 (2)		0.0788 ± 0.0020 (2)	0.2054 ± 0.0010 (2)
PG 6	55.7 ± 3.5 (1)	1.4967 ± 0.0560 (1)	1.9506 ± 0.0132 (2)	0.1102 ± 0.0078 (1)	0.2020 ± 0.0026 (1)
	67.0 ± 2.8 (2)	1.5190 ± 0.0163 (2)		0.0881 ± 0.0021 (2)	0.2008 ± 0.0026 (2)
PG 7	73.9 ± 3.5 (1)	1.4802 ± 0.0413 (1)	1.8236 ± 0.0142 (2)	0.1242 ± 0.0025 (1)	0.1861 ± 0.0031 (1)
	74.7 ± 7.7 (2)	1.4392 ± 0.0507 (2)		0.0973 ± 0.0052 (2)	0.1868 ± 0.0033 (2)
PG 8	70.7 ± 2.1 (1)	2.1448 ± 0.0361 (1)	1.9194 ± 0.0179 (2)	0.1706 ± 0.0043 (1)	0.1609 ± 0.0013 (1)
	75.5 ± 2.6 (2)	2.0984 ± 0.0400 (2)		0.1872 ± 0.0037 (2)	0.1598 ± 0.0011 (2)
PG 9	42.8 ± 2.3 (1)	1.5729 ± 0.0031 (1)	2.2285 ± 0.0281 (2)	0.1108 ± 0.0010 (1)	0.2043 ± 0.0019 (1)
	52.0 ± 1.4 (2)	1.6368 ± 0.0054 (2)		0.1080 ± 0.0007 (2)	0.1935 ± 0.0007 (2)
PG 10	40.0 ± 3.7 (1)	1.5740 ± 0.0037 (1)	2.1680 ± 0.0652 (2)	0.0935 ± 0.0023 (1)	0.2066 ± 0.0005 (1)
	47.8 ± 4.3 (2)	1.6546 ± 0.0077 (2)		0.0804 ± 0.0010 (2)	0.1913 ± 0.0008 (2)
PG 11	37.3 ± 0.3 (1)	1.6696 ± 0.0102 (1)	2.1315 ± 0.0004 (2)	2.1315 ± 0.0004 (2)	0.1999 ± 0.0021 (1)
	59.5 ± 1.9 (2)	1.8400 ± 0.0215 (2)		0.0885 ± 0.0002 (2)	0.1778 ± 0.0037 (2)
PG 12	53.9 ± 1.1 (1)	1.5277 ± 0.0075 (1)	2.2169 ± 0.0535 (2)	0.1192 ± 0.0004 (1)	0.1957 ± 0.0020 (1)
	61.2 ± 1.0 (2)	1.5497 ± 0.0089 (2)		0.1055 ± 0.0007 (2)	0.1838 ± 0.0004 (2)
PG 13	55.3 ± 3.5 (1)	1.5883 ± 0.0227 (1)	2.0279 ± 0.0134 (2)	0.0969 ± 0.0008 (1)	0.1911 ± 0.0008 (1)
	51.0 ± 0.1 (2)	1.6612 ± 0.0086 (2)		0.0761 ± 0.0007 (2)	0.1798 ± 0.0026 (2)
PG 14	54.1 ± 1.6 (1)	1.5718 ± 0.0071 (1)	2.1244 ± 0.0054 (2)	0.1085 ± 0.0014 (1)	0.1948 ± 0.0018 (1)
	59.3 ± 1.3 (2)	1.5849 ± 0.0091 (2)		0.1079 ± 0.0009 (2)	0.1838 ± 0.0035 (2)
PG 15	41.8 ± 2.4 (1)	1.7110 ± 0.0085 (1)	2.0564 ± 0.0262 (2)	0.0947 ± 0.0009 (1)	0.1905 ± 0.0021 (1)
	46.9 ± 2.7 (2)	1.6960 ± 0.0099 (2)		0.0760 ± 0.0002 (2)	0.1855 ± 0.0073 (2)
PG 16	49.6 ± 3.5 (1)	1.6540 ± 0.0020 (1)	1.6423 ± 0.0419 (2)	0.0885 ± 0.0004 (1)	0.1873 ± 0.0008 (1)
	50.9 ± 2.2 (2)	1.6213 ± 0.0002 (2)		0.0834 ± 0.0005 (2)	0.1804 ± 0.0013 (2)
PG 17	39.3 ± 1.9 (1)	1.5869 ± 0.0025 (1)	2.1942 ± 0.0026 (2)	0.0893 ± 0.0029 (1)	0.1996 ± 0.0014 (1)
	40.2 ± 2.2 (2)	1.6301 ± 0.0023 (2)		0.0732 ± 0.0002 (2)	0.1902 ± 0.0011 (2)
PG 18	36.7 ± 2.5 (1)	1.7604 ± 0.0154 (1)	2.1389 ± 0.0629 (2)	0.1023 ± 0.0009 (1)	0.1751 ± 0.0003 (1)
	38.3 ± 3.6 (2)	1.7776 ± 0.0132 (2)		0.0986 ± 0.0001 (2)	0.1724 ± 0.0013 (2)
PG 19	52.6 ± 0.5 (1)	1.6237 ± 0.0123 (1)	2.0901 ± 0.0580 (2)	0.0928 ± 0.0003 (1)	0.1866 ± 0.0018 (1)
	50.5 ± 1.4 (2)	1.6025 ± 0.0286 (2)		0.0944 ± 0.0002 (2)	0.1818 ± 0.0068 (2)
PG 20	41.9 ± 0.9 (1)	1.5967 ± 0.0211 (1)	2.3508 ± 0.0035 (2)	0.0817 ± 0.0008 (1)	0.2016 ± 0.0010 (1)
	55.5 ± 1.2 (2)	1.5815 ± 0.0248 (2)		0.0728 ± 0.0007 (2)	0.1946 ± 0.0009 (2)
FG 21	52.6 ± 3.2 (1)	1.6275 ± 0.0627 (1)	2.3536 ± 0.0468 (2)	0.0807 ± 0.0008 (1)	0.1794 ± 0.0074 (1)
FG 22	30.4 ± 0.7 (1)	1.5108 ± 0.0858 (1)	2.5731 ± 0.0676 (2)	0.0730 ± 0.0015 (1)	0.1598 ± 0.0087 (1)

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Table S1. cont.

S. / Elem.	Na (10-174) *	K (1.3816-3.7400) *	N (1.9000-2.2500) *	Ca (0.0826-0.1310) *	Mg (0.1600-0.3000) *
FG 23	47.9 ± 3.4 (1)	1.4333 ± 0.0033 (1)	2.1830 ± 0.0422 (2)	0.0917 ± 0.0007 (1)	0.1797 ± 0.0034 (1)
FG 24	46.8 ± 2.1 (1)	1.4222 ± 0.0582 (1)	2.0046 ± 0.0184 (2)	0.1223 ± 0.0016 (1)	0.2138 ± 0.0030 (1)
FG 25	43.7 ± 2.5 (1)	1.4251 ± 0.0328 (1)	2.1165 ± 0.0729 (2)	0.1086 ± 0.0015 (1)	0.1749 ± 0.0048 (1)
FG 26	54.5 ± 3.1 (1)	1.4055 ± 0.0715 (1)	2.1815 ± 0.0628 (2)	0.1008 ± 0.0032 (1)	0.1855 ± 0.0099 (1)
FG 27	45.6 ± 0.1 (1)	1.5008 ± 0.0953 (1)	2.2488 ± 0.0010 (2)	0.0877 ± 0.0031 (1)	0.1704 ± 0.0059 (1)
FG 28	47.6 ± 3.7 (1)	1.5533 ± 0.0093 (1)	2.3050 ± 0.0177 (2)	0.0871 ± 0.0008 (1)	0.1815 ± 0.0027 (1)
FG 29	51.8 ± 2.8 (1)	1.5313 ± 0.0161 (1)	2.3474 ± 0.0400 (2)	0.1356 ± 0.0137 (1)	0.1806 ± 0.0017 (1)
FG 30	43.5 ± 2.4 (1)	1.2975 ± 0.0411 (1)	2.2208 ± 0.0589 (2)	0.1189 ± 0.0039 (1)	0.1833 ± 0.0072 (1)
FG 31	51.8 ± 2.6 (1)	1.7603 ± 0.0173 (1)	2.1537 ± 0.0121 (2)	0.0967 ± 0.0005 (1)	0.1847 ± 0.0084 (1)
R 1	67.7 ± 3.7 (1)	1.9633 ± 0.0495 (1)	2.5210 ± 0.0400 (2)	0.1121 ± 0.0012 (1)	0.2236 ± 0.0048 (1)
	96.0 ± 8.5 (2)	2.1295 ± 0.0276 (2)		0.1390 ± 0.0023 (2)	0.2194 ± 0.0017 (2)
R 2	85.3 ± 1.5 (1)	2.6675 ± 0.0241 (1)	2.1441 ± 0.0302 (2)	0.1943 ± 0.0031 (1)	0.1913 ± 0.0003 (1)
	90.6 ± 2.8 (2)	2.7930 ± 0.0513 (2)		0.1944 ± 0.0020 (2)	0.1835 ± 0.0021 (2)
R 3	77.3 ± 1.7 (1)	2.1120 ± 0.0358 (1)	2.4487 ± 0.0313 (2)	0.1243 ± 0.0018 (1)	0.2335 ± 0.0004 (1)
	111.9± 3.5 (2)	2.0880 ± 0.0325 (2)		0.1200 ± 0.0009 (2)	0.2283 ± 0.0100 (2)
R 4	80.6 ± 7.1 (1)	2.3151 ± 0.0754 (1)	2.1340 ± 0.0392 (2)	0.1314 ± 0.0054 (1)	0.2356 ± 0.0028 (1)
	84.5 ± 6.0 (2)	2.2698 ± 0.0527 (2)		0.1440 ± 0.0048 (2)	0.2276 ± 0.0040 (2)
R 5	70.2 ± 4.6 (1)	2.0433 ± 0.0233 (1)	2.3406 ± 0.0177 (2)	0.1219 ± 0.0019 (1)	0.2222 ± 0.0039 (1)
	100.1± 4.2 (2)	2.0474 ± 0.0486 (2)		0.1335 ± 0.0010 (2)	0.2165 ± 0.0117 (2)

* found concentration values in literature; S. / Elem. – Sample / Element ;PG – Patrocínio/Minas Gerais green coffee; FG – Franca/São Paulo green coffee; R – Commercial soluble / roasted coffee; (1) microwave oven procedure; (2) digester heating block procedure.

Table S2. Concentration of Fe, Mn, Zn and Cu (mg kg^{-1}) in 35 coffee samples

S. / Elem.	Fe (25.0-140.0) *	Mn (14.0-60.0) *	Zn (1.00-10.00) *	Cu (1.0-33.0) *
PG 1	33.5 ± 0.7 (1)	33.2 ± 0.2 (1)	6.58 ± 0.06 (1)	14.2 ± 0.2 (1)
	31.6 ± 0.9 (2)	33.1 ± 0.4 (2)	6.61 ± 0.10 (2)	14.6 ± 0.3 (2)
PG 2	30.7 ± 0.7 (1)	18.4 ± 0.1 (1)	9.80 ± 0.52 (1)	15.5 ± 0.4 (1)
	28.2 ± 0.2 (2)	18.4 ± 0.2 (2)	9.77 ± 0.30 (2)	15.2 ± 0.2 (2)
PG 3	30.2 ± 0.4 (1)	13.7 ± 0.1 (1)	10.45 ± 0.13 (1)	13.9 ± 0.1 (1)
	28.2 ± 0.5 (2)	13.8 ± 0.1 (2)	10.73 ± 0.17 (2)	13.1 ± 0.4 (2)
PG 4	33.7 ± 0.2 (1)	28.2 ± 0.2 (1)	7.48 ± 0.56 (1)	15.5 ± 0.2 (1)
	28.3 ± 0.6 (2)	28.1 ± 0.2 (2)	10.35 ± 0.19 (2)	15.7 ± 0.3 (2)
PG 5	37.0 ± 0.8 (1)	31.0± 0.4 (1)	6.17 ± 0.07 (1)	14.3 ± 0.3 (1)
	32.4 ± 0.7 (2)	31.2 ± 0.1 (2)	9.34 ± 0.10 (2)	14.9 ± 0.3 (2)
PG 6	42.2 ± 1.1 (1)	14.7 ± 0.1 (1)	6.73 ± 0.90 (1)	14.5 ± 0.3 (1)
	41.4 ± 1.0 (2)	14.4 ± 0.2 (2)	16.81 ± 0.22 (2)	14.0 ± 0.2 (2)
PG 7	107.5± 4.7 (1)	13.4 ± 0.3 (1)	7.81 ± 0.37 (1)	14.3 ± 0.6 (1)
	97.9 ± 5.2 (2)	16.2 ± 0.2 (2)	9.67 ± 0.24 (2)	14.0 ± 0.7 (2)
PG 8	107.0± 3.4 (1)	23.6 ± 0.1 (1)	5.89 ± 0.41 (1)	16.7 ± 0.4 (1)
	78.7 ± 4.8 (2)	23.5 ± 1.0 (2)	13.64 ± 0.55 (2)	16.0 ± 0.4 (2)
PG 9	28.6 ± 0.4 (1)	40.3 ± 0.5 (1)	4.29 ± 0.07 (1)	15.8 ± 0.6 (1)
	28.3 ± 0.3 (2)	41.1 ± 0.2 (2)	6.9 ± 0.1 (2)	15.4 ± 0.2 (2)
PG 10	28.0 ± 0.6 (1)	24.6 ± 0,1 (1)	5.99 ± 0.05 (1)	15.5 ± 0.1 (1)
	28.7 ± 0.4 (2)	25.6 ± 0,1 (2)	5.13 ± 0.01 (2)	15.4 ± 0.2 (2)
PG 11	26.8 ± 0.7 (1)	24.0 ± 0.4 (1)	4.24 ± 0.06 (1)	13.1 ± 0.1 (1)
	25.8 ± 0.5 (2)	24.1 ± 0.2 (2)	4.55 ± 0.03 (2)	12.7 ± 0.2 (2)
PG 12	30.2 ± 0.4 (1)	21.6 ± 0.4 (1)	6.2 ± 0.5 (1)	15.5 ± 0.6 (1)
	28.4 ± 0.4 (2)	24.1 ± 0.1 (2)	5.5 ± 0.1 (2)	13.5 ± 0.3 (2)
PG 13	35.8 ± 0.7 (1)	24.8 ± 0.6 (1)	7.2 ± 0.4 (1)	14.6 ± 0.4 (1)
	34.4 ± 0.4 (2)	27.6 ± 0.3 (2)	6.12 ± 0.08 (2)	13.6 ± 0.1 (2)
PG 14	26.7 ± 0.6 (1)	19.2 ± 0.3 (1)	6.2 ± 0.1 (1)	15.1 ± 0.1 (1)
	24.0 ± 0.5 (2)	19.7 ± 0.2 (2)	6.28 ± 0.08 (2)	13.5 ± 0.1 (2)
PG 15	31.7 ± 0.7 (1)	19.6 ± 0.2 (1)	6.45 ± 0.3 (1)	16.6 ± 0.1 (1)
	31.6 ± 0.5 (2)	19.8 ± 0.3 (2)	5.53 ± 0.03 (2)	16.2 ± 0.1 (2)
PG 16	20.0 ± 1.7 (1)	19.9 ± 0.1 (1)	5.5 ± 0.2 (1)	14.9 ± 0.1 (1)
	25.7 ± 1.1 (2)	20.4 ± 0.1 (2)	4.2 ± 0.1 (2)	14.5 ± 0.1 (2)
PG 17	31.7 ± 0.3 (1)	18.5 ± 0.2 (1)	4.01 ± 0.5 (1)	16.6 ± 0.2 (1)
	36.1 ± 0.3 (2)	18.6 ± 0.2 (2)	4.68 ± 0.07 (2)	15.4 ± 0.1 (2)
PG 18	32.9 ± 0.5 (1)	22.1 ± 0.1 (1)	4.64 ± 0.06 (1)	14.5 ± 0.1 (1)
	34.5 ± 0.5 (2)	22.6 ± 0.1 (2)	5.78 ± 0.03 (2)	14.6 ± 0.2 (2)
PG 19	28.3 ± 0.8 (1)	20.2 ± 0.1 (1)	6.2 ± 0.3 (1)	14.8 ± 0.6 (1)
	30.1 ± 0.5 (2)	20.8 ± 0.2 (2)	12.6 ± 0.1 (2)	13.6 ± 0.3 (2)
PG 20	33.7 ± 2.8 (1)	20.8 ± 0.3 (1)	6.2 ± 0.3 (1)	16.1 ± 0.1 (1)
	28.0 ± 0.3 (2)	21.3 ± 0.1 (2)	7.8 ± 0.2 (2)	14.5 ± 0.3 (2)
FG 21	31.3 ± 0.5 (1)	34.5 ± 0.1 (1)	8.48 ± 0.11 (1)	16.4 ± 0.2 (1)
FG 22	442.0 ± 3.5 (1)	29.2 ± 0.2 (1)	4.64 ± 0.09 (1)	14.0 ± 0.2 (1)
FG 23	29.3 ± 0.9 (1)	22.6 ± 0.1 (1)	7.56 ± 0.11 (1)	16.5 ± 0.5 (1)
FG 24	56.6 ± 0.4 (1)	22.8 ± 0.1 (1)	2.85 ± 0.09 (1)	14.2 ± 0.2 (1)
FG 25	27.6 ± 0.2 (1)	18.8 ± 0.4 (1)	5.84 ± 0.19 (1)	14.2 ± 0.2 (1)
FG 26	27.5 ± 0.6 (1)	28.5 ± 0.1 (1)	3.79 ± 0.02 (1)	14.1 ± 0.3 (1)
FG 27	36.7 ± 0.2 (1)	27.8 ± 0.1 (1)	6.41 ± 0.08 (1)	15.3 ± 0.1 (1)
FG 28	32.6 ± 0.3 (1)	21.5 ± 0.1 (1)	6.67 ± 0.20 (1)	14.0 ± 0.1 (1)
FG 29	39.7 ± 0.4 (1)	30.1 ± 0.1 (1)	7.46 ± 0.14 (1)	18.6 ± 0.1 (1)
FG 30	36.0 ± 1.0 (1)	31.8 ± 0.1 (1)	8.61 ± 0.07 (1)	15.3 ± 0.2 (1)
FG 31	29.2 ± 0.4 (1)	18.6 ± 0.3 (1)	6.96 ± 0.11 (1)	14.1 ± 0.2 (1)
R 1	61.0 ± 0.2 (1)	22.0 ± 1.0 (1)	7.14 ± 0.33 (1)	12.5 ± 0.5 (1)
	51.4 ± 2.1 (2)	19.8 ± 0.9 (2)	10.81 ± 0.22 (2)	13.3 ± 0.2 (2)
R 2	282.3 ± 15.2 (1)	27.4 ± 0.1 (1)	7.08 ± 0.34 (1)	18.7 ± 0.3 (1)
	192.0 ± 5.2 (2)	26.4 ± 0.4 (2)	12.76 ± 0.51 (2)	18.8 ± 0.3 (2)
R 3	69.5 ± 1.6 (1)	27.9 ± 0.1 (1)	4.65 ± 0.42 (1)	14.8 ± 0.4 (1)
	51.7 ± 1.7 (2)	26.2 ± 1.3 (2)	5.23 ± 0.44 (2)	14.5 ± 0.3 (2)
R 4	233.7 ± 2.2 (1)	36.0 ± 0.6 (1)	6.17 ± 0.02 (1)	17.1 ± 0.3 (1)
	154.2 ± 5.6 (2)	31.7 ± 1.6 (2)	15.48 ± 0.27 (2)	18.1 ± 0.2 (2)
R 5	85.0 ± 8.5 (1)	24.5 ± 0.5 (1)	5.31 ± 0.37 (1)	13.7 ± 0.3 (1)
	66.7 ± 1.8 (2)	23.9 ± 0.2 (2)	4.80 ± 0.32 (2)	14.7 ± 0.2 (2)

* found concentration values in literature; S. / Elem. – Sample / Element ;PG – Patrocínio/Minas Gerais green coffee; FG – Franca/São Paulo green coffee; R – Commercial soluble / roasted coffee; (1) microwave oven procedure; (2) digester heating block procedure.