

Table 1S. Repeatability and intermediate precision over three months of validation of a group of target coffee analytes and thujone's solution (ESTD).

	Week 1		Week 2		Week 3		Week 1-3	
Compounds	aver. norm. area (<i>n</i> =5)	RSD%	aver. norm. area (<i>n</i> =5)	RSD%	aver. norm. area (<i>n</i> =5)	RSD%	aver. norm. area (<i>n</i> =15)	RSD%
pyridine	71.3	10.1	67.7	2.6	71.1	4.2	70.0	2.9
2,6-dimethylpyrazine	53.5	5.1	55.0	3.2	54.6	2.6	54.4	1.3
furfural	61.4	4.3	62.5	5.7	51.7	4.2	58.5	10.1
acetoxy acetone	40.5	4.5	46.4	4.1	47.1	1.4	44.7	8.2
furfuryl acetate	94.6	3.5	96.4	2.3	101.7	1.4	97.6	3.8
furfuryl alcohol	230.9	3.8	244.6	4.1	250.2	2.4	241.9	4.1
	aver. absol. area (<i>n</i> =5)	RSD%	aver. absol. area (<i>n</i> =5)	RSD%	aver. absol. area (<i>n</i> =5)	RSD%	aver. absol. area (<i>n</i> =15)	RSD%
α -thujone	267971286	1.2	217343616	0.8	249706653	1.4	249706653	11.3
β -thujone	35081728	1.8	28748286	0.8	32524366	1.9	32524366	10.3

Table 2S. Correlation equations and coefficients of the indices of roasting identified for Arabica, Robusta and Blend 50/50 obtained *versus* the average colors of the training set samples.

N°	Index	Arabica		Robusta		Blend 50/50	
		equation	r ²	equation	r ²	equation	r ²
1	pyridine/5-methyl furfural	y = -166x + 10762	0.9301	y = -91x + 6244	0.9635	y = -164x + 10586	0.9635
2	pyridine/furfural	y = -268x + 16959	0.9446	y = -118x + 8147	0.9812	y = -240x + 15441	0.9548
3	2-methyl furan/2,3-pentandione	y = -245x + 15741	0.9434	y = -311x + 21064	0.9767	y = -267x + 17648	0.9707
4	2,5-dimetil furan/2,3-pentandione	y = -41x + 2648	0.9613	y = -46x + 3194	0.9930	y = -45x + 3007	0.9816
5	2-methyl furan/furfural	y = -28x + 1705	0.9315	-----	-----	-----	-----
6	5-methyl furfural/2-acetyl furan	y = 107x - 2743	0.9998	y = 96x - 2217	0.9951	y = 99x - 2394	0.9981
7	2,3-pentandione/2,3-butandione	y = 38x - 936	0.9973	-----	-----	-----	-----
8	guaiacol/2-ethyl-3,6-dimethylpyrazine	-----	-----	y = -53x + 3701	0.9892	y = -38x + 2625	0.9851
9	pyridine/methylpyrazine	y = -44x + 3511	0.9861	y = -22x + 1841	0.9956	y = -39x + 3114	0.9822
10	pyridine/2,6-dimethylpyrazine	y = -111x + 8318	0.9812	y = -47x + 3785	0.9934	y = -90x + 68398	0.9789
11	pyridine/2,5-dimethylpyrazine	y = -133x + 9785	0.9822	y = -58x + 4511	0.9908	y = -109x + 8090	0.9800
12	furfuryl acetate/2-ethyl-3,6-dimethylpyrazine	y = -129x + 10143	1.0000	y = -67x + 5796	0.9969	y = -96x + 8018	1.0000
13	pyridine/ethylpyrazine	y = -230x + 17604	0.9842	y = -89x + 7238	0.9938	y = -181x + 13921	0.9785
14	pyridine/2-ethyl-6-methylpyrazine	y = -214x + 15780	0.9858	y = -79x + 6215	0.9926	y = -163x + 12189	0.9790
	Index	Unique correlation equation for Arabica, Robusta and Blend 50/50					
		equation			r ²		
6	5-methyl furfural/2-acetyl furan	y = 101x - 2451			0.9989		