ARTICLE

Using a biphasic system and digital imaging analysis with chemometric tools for simultaneous determination of Cu^{2+} and furfural in cachaça

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Supplementary Information

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Table S1: Volumes of all reagents used in the work to set up the partial least squares (PLS) regression.

Sample	Cu^{2+} (µL)	Furfural (µL)	40% Alcohol (µL)	Borate buffer (µL)	CPZ (µL)	Aniline ion (µL)
1	34	43	113	100	100	20
2	36	0	154	100	100	20
3	0	0	190	100	100	20
4	0	86	104	100	100	20
5	68	18	104	100	100	20
6	15	90	85	100	100	20
7	72	45	73	100	100	20
8	38	21	131	100	100	20
9	17	24	149	100	100	20
10	19	59	112	100	100	20
11	48	95	47	100	100	20
12	76	65	49	100	100	20
13	52	48	90	100	100	20
14	40	100	49	100	100	20
15	80	105	4	100	100	20
16	85	0	105	100	100	20
17	0	71	118	100	100	20
18	57	0	133	100	100	20
19	0	50	140	100	100	20
20	42	78	70	100	100	20
21	63	86	42	100	100	20
22	68	27	95	100	100	20
23	22	0	168	100	100	20
24	0	31	159	100	100	20

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25	25	52	113	100	100	20
26	37	46	107	100	100	20
27	9	82	99	100	100	20
28	65	83	42	100	100	20
29	66	47	77	100	100	20
30	38	85	67	100	100	20
31	68	11	111	100	100	20
32	10	12	168	100	100	20
33	10	49	131	100	100	20
34	39	12	139	100	100	20

Table S2. Concentration of the calibration set (Standard) and the values obtained by using the prediction set for the samples used for model validation.

			Cu^{2+} (mg/L)			Furfural (mg/100mL[a])		
	Sample		Calibration value	Predicted value	R.E%	Calibration value	Predicted value	R.E%
01	Standard	Validation	3.6	3.6 ± 0.2	0.0	4.6	3.6 ± 0.4	21.7
02	Standard	Calibration	3.8	4.2 ± 0.3	10.5	0.0	0.5 ± 0.3	-
03	Standard	Calibration	0.0	0.2 ± 0.1	-	0.0	0.2 ± 0.2	-
04	Standard	Calibration	0.0	0.12 ± 0.1	-	9.0	8.9 ± 0.2	1.1
05	Standard	Calibration	7.2	6.72 ± 0.2	-6.9	1.9	2.6 ± 0.3	-36.8
06	Standard	Calibration	1.5	1.42 ± 0.2	-6.7	9.5	9.6 ± 0.1	-1.1
07	Standard	Validation	7.6	7.72 ± 0.3	1.3	4.8	4.7 ± 0.2	2.1
08	Standard	Calibration	4.0	4.02 ± 0.2	0.0	2.2	1.9 ± 0.1	13.6
09	Standard	Calibration	1.8	1.82 ± 0.1	0.0	2.5	3.2 ± 0.3	-28.0
10	Standard	Calibration	2.0	1.72 ± 0.2	-15.0	6.3	5.8 ± 0.2	7.9
11	Standard	Calibration	5.0	4.92 ± 0.2	-2.0	10.0	10.7 ± 0.4	-7.0
12	Standard	Calibration	8.0	7.92 ± 0.3	-1.3	6.9	7.2 ± 0.3	-4.3

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13	Standard	Calibration	5.5	6.02 ± 0.3	9.1	5.0	5.1 ± 0.1	-2.0
14	Standard	Validation	4.2	3.9 ± 0.2	-7.1	10.6	10.0 ± 0.4	5.7
15	Standard	Calibration	8.4	8.7 ± 0.4	3.6	11.1	11.1 ± 0.2	0.0
16	Standard	Calibration	8.9	8.9 ± 0.3	0.0	0.0	-0.2 ± 0.2	-
17	Standard	Calibration	0.0	0.1 ± 0.1	-	7.5	7.3 ± 0.1	2.7
18	Standard	Calibration	6.0	6.0 ± 0.2	0.0	0.0	-0.1 ± 0.1	-
19	Standard	Calibration	0.0	0.0 ± 0.1	-	5.3	5.2 ± 0.2	1.9
20	Standard	Calibration	4.4	4.5 ± 0.1	2.3	8.3	8.2 ± 0.2	1.2
21	Standard	Calibration	6.6	6.4 ± 0.3	-3.0	9.0	8.8 ± 0.3	2.2
22	Standard	Calibration	7.2	7.0 ± 0.2	-2.8	2.9	2.6 ± 0.3	10.3
23	Standard	Validation	2.3	2.4 ± 0.2	4.3	0.0	0.1 ± 0.1	-
24	Standard	Calibration	0.0	-0.1 ± 0.1	-	3.3	2.8 ± 0.1	15.2
25	Standard	Calibration	2.6	2.4 ± 0.2	-7.7	5.5	5.7 ± 0.2	-3.6
26	Standard	Calibration	3.9	3.9 ± 0.2	0.0	4.9	4.7 ± 0.2	4.1
27	Standard	Calibration	1.0	1.0 ± 0.2	0.0	8.6	7.9 ± 0.4	8.1
28	Standard	Validation	6.9	7.8 ± 0.4	13.0	8.8	6.7 ± 0.2	23.9
29	Standard	Calibration	7.0	7.2 ± 0.3	2.9	5.0	4.6 ± 0.3	8.0
30	Standard	Validation	4.0	4.4 ± 0.2	10.0	8.9	8.2 ± 0.4	7.9
31	Standard	Calibration	7.1	7.1 ± 0.1	0.0	1.2	1.0 ± 0.2	16.7
32	Standard	Calibration	1.0	0.9 ± 0.3	-10.0	1.3	1.0 ± 0.2	23.1
33	Standard	Calibration	1.0	1.2 ± 0.2	20.0	5.2	5.3 ± 0.1	-1.9
34	Standard	Validation	4.1	4.6 ± 0.2	12.2	1.3	1.4 ± 0.2	-7.7
35	Cachaça	Calibration	2.8	2.8 ± 0.1	0.0	0.0	-0.2 ± 0.2	-
36	Cachaça	Calibration	2.6	2.5 ± 0.1	-3.8	4.9	5.0 ± 0.2	-2
37	Cachaça	Validation	6.8	6.7 ± 0.1	-1.5	1.9	2.1 ± 0.1	-10.5
38	Cachaça	Validation	0.0	0.4 ± 0.2	-	0.1	0.8 ± 0.4	-700.0
39	Cachaça	Calibration	5.4	5.4 ± 0.1	0.0	2.6	2.5 ± 0.2	3.8
40	Cachaça	Calibration	0.4	0.6 ± 0.2	50.0	0.0	0.2 ± 0.2	-
41	Cachaça	Validation	8.2	7.3 ± 0.3	-11.0	0.3	0.9 ± 0.2	-200.0

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42	Cachaça	Calibration	3.2	3.0 ± 0.2	-6.3	0.0	0.2 ± 0.3	-
43	Cachaça	Calibration	3.5	3.4 ± 0.2	-2.9	1.2	1.2 ± 0.1	0.0

[a]Concentration in mg/100 mL of anhydrous ethanol. R.E% = relative error.

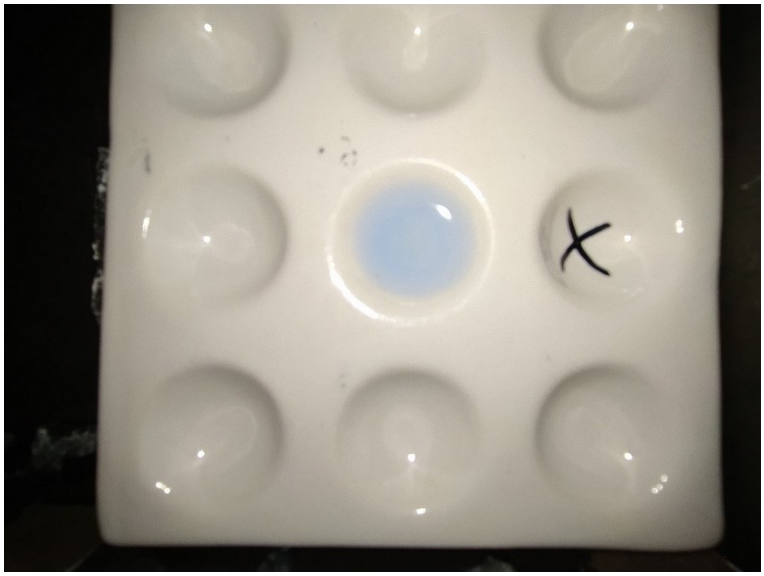

Fig. S1. Original image (2448 x 3264 pixels) acquired using the closed chamber.

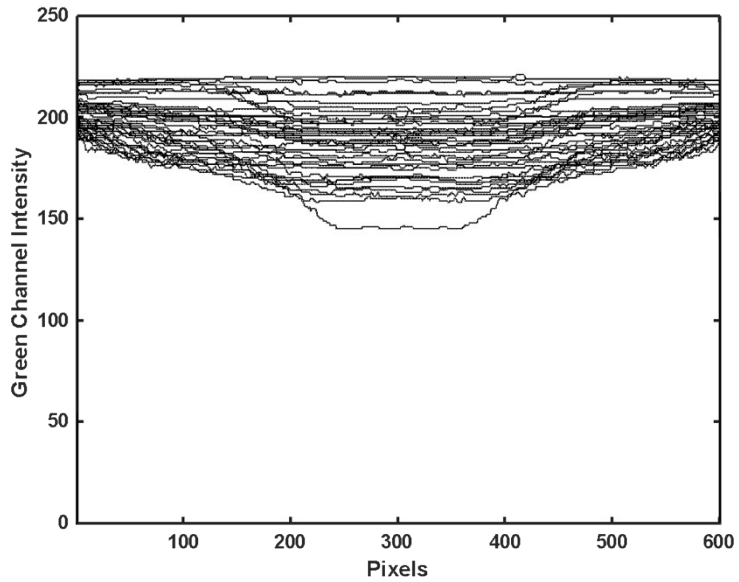

Fig. S2. Intensity of the middle horizontal line of the green channel for each sample.

Table S3: Modelling parameters for Cu^{2+} and furfural determination for all channels evaluated.

Property	Channel	Method	Variables	RMSEC	Rc	RMSEP	Rp	LV
Cu^{2+}	B	PLS	601	1.93	0.72	2.53	0.18	3
		PLS-OPS	50	1.51	0.84	1.62	0.77	3
	G	**PLS**	**601**	**0.38**	**0.99**	**1.42**	**0.83**	**6**
		PLS-OPS	**50**	**0.20**	**1.00**	**0.49**	**0.98**	**6**
	R	PLS	601	1.09	0.92	1.25	0.86	3
		PLS-OPS	50	1.01	0.93	0.85	0.94	3
	RGB	PLS	1803	1.03	0.93	0.93	0.93	3
		PLS-OPS	130	0.86	0.95	0.76	0.95	3
Furfural	B	PLS	601	1.74	0.86	3.15	0.63	2
		PLS-OPS	50	1.56	0.89	2.62	0.75	2
	G	**PLS**	**601**	**0.54**	**0.99**	**1.86**	**0.90**	**5**
		PLS-OPS	**49**	**0.33**	**1.00**	**0.82**	**0.99**	**5**
	R	PLS	601	2.27	0.75	3.31	0.57	3
		PLS-OPS	49	2.11	0.79	2.26	0.81	2
	RGB	PLS	1803	0.79	0.97	1.63	0.94	4
		PLS-OPS	50	0.61	0.98	1.32	0.96	4