Supplementary Material

Improved extraction of rutin from banana peels with organic acids-water mixtures

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Equations

Equation S1:

$$\alpha = (2^k)^{\frac{1}{4}} \qquad (S1)$$

where α is the distance between the axial points and the central point and k is the number of contributing parameters for obtaining the final answer.

Tables

Table S1. 2^3 factorial planning.

	X_1	X_2	X_3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1
9	-1.68	0	0
10	1.68	0	0
11	0	-1.68	0
12	0	1.68	0
13	0	0	-1.68
14	0	0	1.68
15	0	0	0
16	0	0	0
17	0	0	0
18	0	0	0
19	0	0	0
20	0	0	0

Table S2. Coded levels of independents variables used in the factorial planning.

	-1.682	**-1**	**0**	**1**	**1.68**
X_1 - Temperature (*T*, °C)	25	30	38	46	51
X_2 - Extraction time (*t*, min)	10	30	60	90	110
X_3 - Solid-liquid ratio *(S/L Ratio)*	0.02	0.05	0.10	0.15	0.18

Table S3. Influence of the degree of ripeness of banana peels on the rutin content. Extraction conditions: *t* = 60 min; *T* = 25 °C and *S/L ratio* = 1:10 and methanol or a mixture of methanol and water (wt%) as extraction solvent.

Banana	Methanol concentration (wt%)	Rutin content (mg/100 g DW)
Green	100	10.7 ± 0.3
Green	75	11.5 ± 0.8
Green	50	13.5 ± 0.1
Semi-ripe	100	22 ± 1
Semi-ripe	75	17 ± 2
Semi-ripe	50	25.8 ± 0.8
Ripe	100	25.9 ± 0.4
Ripe	75	28.4 ± 0.2
Ripe	50	42 ± 1

Table S4. Relative solubility $\log_{10}(x_{RS})$ and probability of solubility of rutin in different solvents pure and hydrated, at 25°C, predicted by COSMO-RS. Green color: high probability of solubility (60-100%); yellow color: medium probability of solubility (20-60%); red color: low probability of solubility (0-20%).

Solvent	Pure organic acids		Organic acid-water mixtures (75 wt%)	
	$\log_{10}(x_{RS})$	Probability (%)	$\log_{10}(x_{RS})$	Probability (%)
Acetic acid	8.56	22.30	8.57	100.00
Mandelic acid	8.39	15.16	8.52	88.32
Lactic acid	8.30	12.24	8.45	75.21
3-phenyl acetic acid	7.31	1.26	8.43	72.86
5-phenyl valeric acid	7.07	0.71	8.37	63.26
5-phenyl valeric acid	6.57	0.23	8.26	48.97
Benzoic acid	7.54	2.12	8.26	48.28
Levulinic acid	7.62	2.55	8.23	45.74
Butanoic acid	8.17	8.98	8.23	45.49
Propionic acid	8.41	15.90	8.19	41.41
Pentanoic acid	7.81	3.92	8.19	41.06
Benzoic acid	7.46	1.78	8.12	35.35
Tartaric acid	-1.85	0.00	8.06	30.29
Citric acid	9.21	100.00	7.95	23.65
Ricinoleic acid	5.40	0.02	7.82	17.26
Oleic acid	4.77	0.00	7.72	13.92
Malic acid	7.89	4.79	7.49	7.99
Glycolic acid	7.09	0.75	7.13	3.26
Water	6.14	0.08	6.14	0.00

Table S5. Rutin content of extracts from ripe banana peels obtained with pure organic acid or a mixture of organic acid and water (wt%) as extraction solvent. Extraction conditions: *t* = 60 min; *T* = 25 °C and *S/L ratio* = 1:10 and using.

Solvent	Concentration (wt%)	Rutin content (mg/100 g DW)
Methanol	100	25.9 ± 0.4
Methanol	75	28.4 ± 0.2
Methanol	50	42 ± 1
Methanol	25	6.4 ± 0.6
Ethanol	100	14.6 ± 0.4
Ethanol	75	25.6 ± 0.4
Ethanol	50	21.3 ± 0.6
Ethanol	25	12.4 ± 0.1
Lactic Acid	100	68 ± 2
Lactic Acid	75	83.0 ± 0.9
Lactic Acid	50	61 ± 2
Lactic Acid	25	40 ± 2
Glycolic Acid	75	56 ± 2
Glycolic Acid	50	56 ± 2
Glycolic Acid	25	38 ± 1
Citric Acid	75	67 ± 2
Citric Acid	25	42 ± 2
Acetic Acid	100	40 ± 1
Acetic Acid	80	177 ± 12
Acetic Acid	75	182 ± 3
Acetic Acid	60	192 ± 1
Acetic Acid	50	158 ± 3
Acetic Acid	25	35 ± 2
Water	100	6 ± 2
Acidified water (pH = 3)	100	6.3 ± 0.4

Table S6. Regression coefficients of the predicted second-order polynomial model for the rutin content obtained from the RSM, $R^2 = 0.956$ and $R_{adj}^2 = 0.916$.

	Regression coefficients	**Standard deviation**	**t-student (10)**	**p-value**
Interceção	164.57	54.1929	3.03676	0.028857
(1) *T* (°C)	3.28	2.2986	1.42529	0.008925
***T*² (°C)**	-0.11	0.0280	-3.98320	0.010497
(2) *t* (min)	1.99	0.4801	4.14832	0.213392
***t*² (min)**	0.00	0.0020	-1.45592	0.205186
(3) *S/ L ratio*	-1051.09	288.0617	-3.64885	0.014766
razão S/L²	-4235.58	715.5413	-5.91941	0.001961
1L by 2L	-0.03	0.0100	-3.37742	0.019730
1L by 3L	51.68	5.9981	8.61602	0.000348
2L by 3L	-2.76	1.5995	-1.72617	0.144905

Table S7. ANOVA data for the extraction of rutin obtained from the RSM.

	SS	**DF**	**Mean square**	**F**	**p-value**
Regression	10319.58	9	1146.62	23.93	0.000013
Residual	479.09	10	47.91		
Total	10798.67				

Table S8. Experimental data and response surface predicted values of the factorial planning.

T (ºC)	*t* (min)	*S/L ratio*	Experimental (mg TE/100 g DW)	Predicted (mg TE/ 100g DW)	Relative deviation (%)
30	30	0.05	200.60	199.65	0.47
46	30	0.05	147.21	141.82	3.66
30	90	0.05	236.46	229.25	3.05
46	90	0.05	135.14	139.02	-2.87
30	30	0.15	163.66	156.58	4.32
46	30	0.15	177.43	181.45	-2.26
30	90	0.15	167.43	169.62	-1.31
46	90	0.15	164.32	162.07	1.37
25	60	0.10	193.87	200.08	-3.20
51	60	0.10	146.88	145.18	1.15
38	10	0.10	177.04	181.08	-2.28
38	110	0.10	189.22	189.70	-0.25
38	60	0.02	167.00	171.21	-2.52
38	60	0.18	154.15	154.46	-0.20
38	60	0.10	191.96	192.75	-0.41
38	60	0.10	189.33	192.75	-1.81
38	60	0.10	204.86	192.75	5.91
38	60	0.10	189.24	192.75	-1.86
38	60	0.10	185.82	192.75	-3.73
38	60	0.10	196.07	192.75	1.69

Table S9. Rutin content obtained using the optimal operating conditions and applying different extraction times.

t (min)	Experimental Rutin Content (mg/100 g DW)	Predicted Rutin Content (mg/100 g DW)	Relative deviation (%)
110	242 ± 3	240	0.96
80	241 ± 2	229	4.73
50	210 ± 4	214	-1.89

Table S10. Rutin content obtained during the biomass recyclability studies.

Cycle	Rutin content (mg/100g DW)
1	241 ± 2
2	0.94 ± 0.09

Table S11. Rutin content and concentration obtained during the solvent recyclability studies.

Cycle	Rutin content (mg/100g DW)	[Rutin] (g/L)
1	241 ± 2	0.13 ± 0.01
2	239 ± 3	0.13 ± 0.02
3	28 ± 2	0.016 ± 0.009
4	0.0 ± ---	0.000 ± ---

Figures

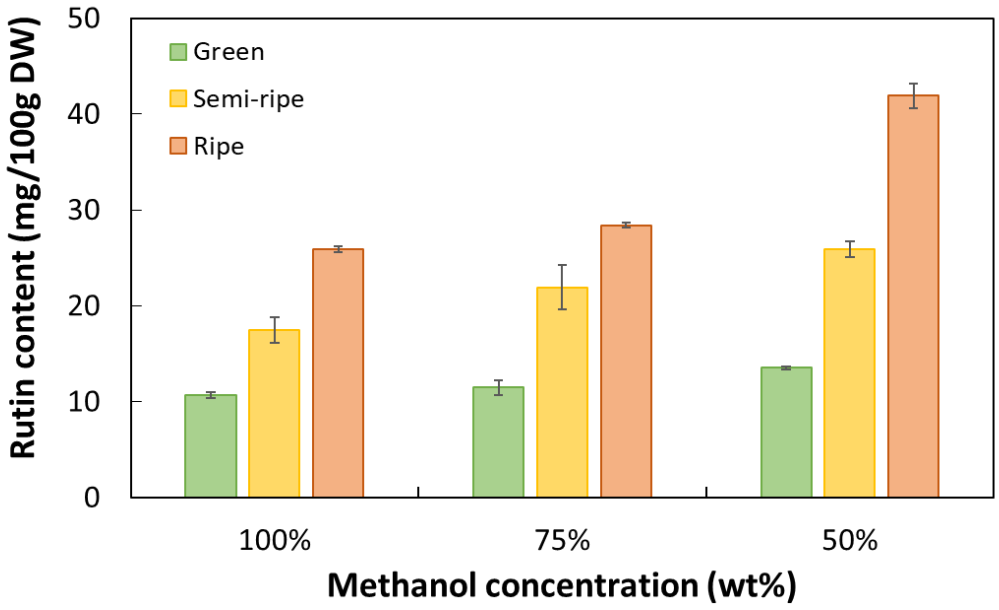

Figure S1. Influence of the degree of ripeness of banana peels on rutin content. Extraction conditions: *t* = 60 min; *T* = 25 °C and *S/L ratio* = 1:10, and ethanol or a mixture of methanol and water (wt%) as extraction solvent.

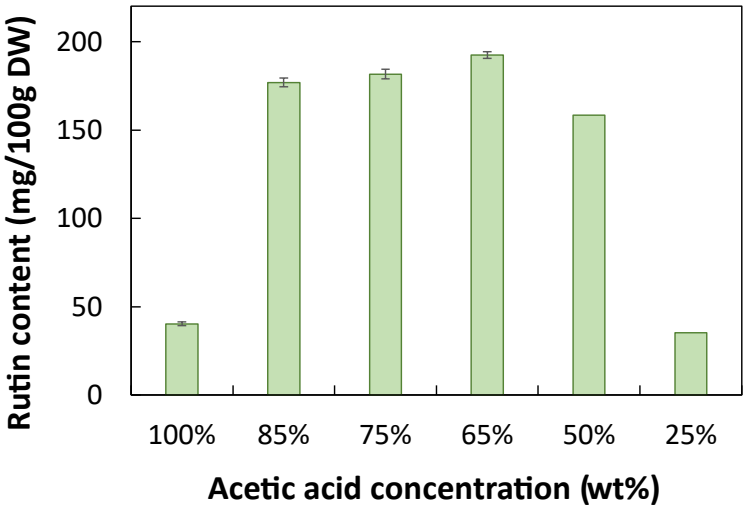

Figure S2. Rutin content of extracts using different concentrations of acetic acid as solvent (wt%). Extraction conditions: *t* = 60 min; *T* = 25 °C and *S/L ratio* = 1:10.

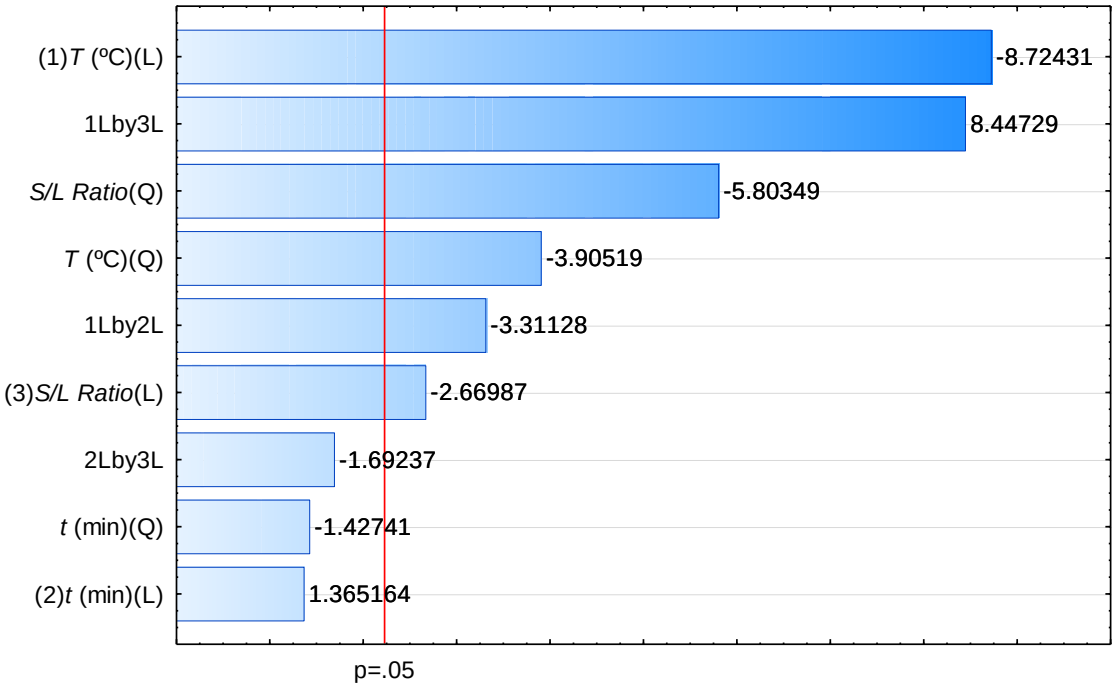

Figure S3. Pareto chart for the standardized main effects in RSM for the Rutin content. The vertical line indicates the statistical significance of the effects.

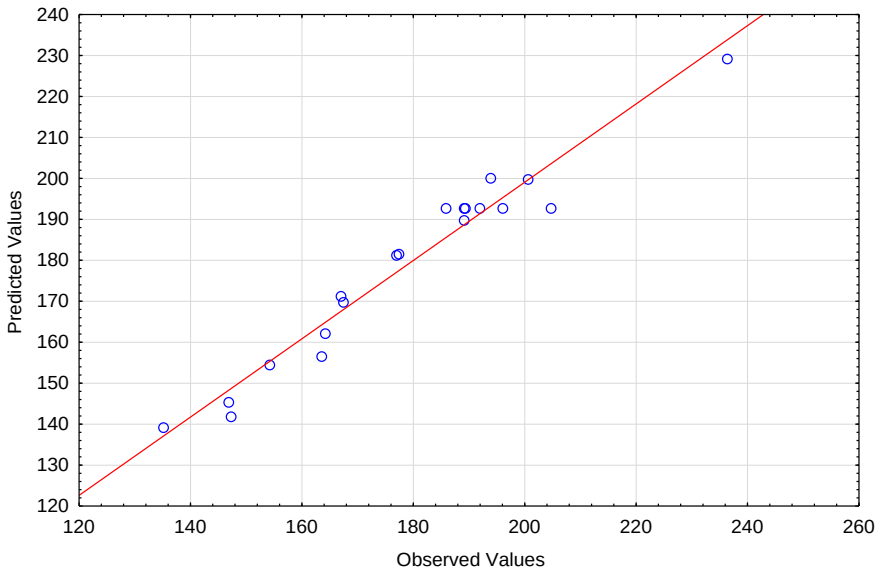

Figure S4. Observed values vs Predicted values.

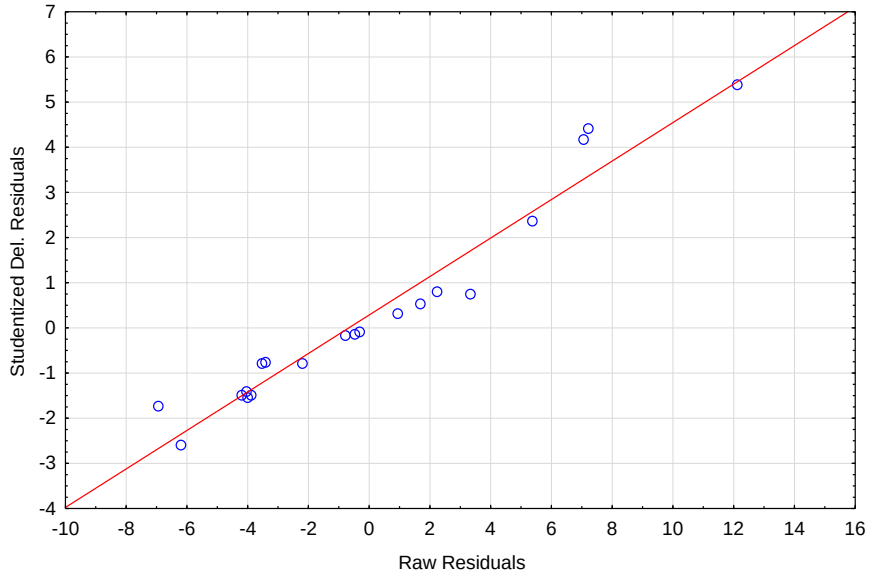

Figure S5. Distribution of residuals.

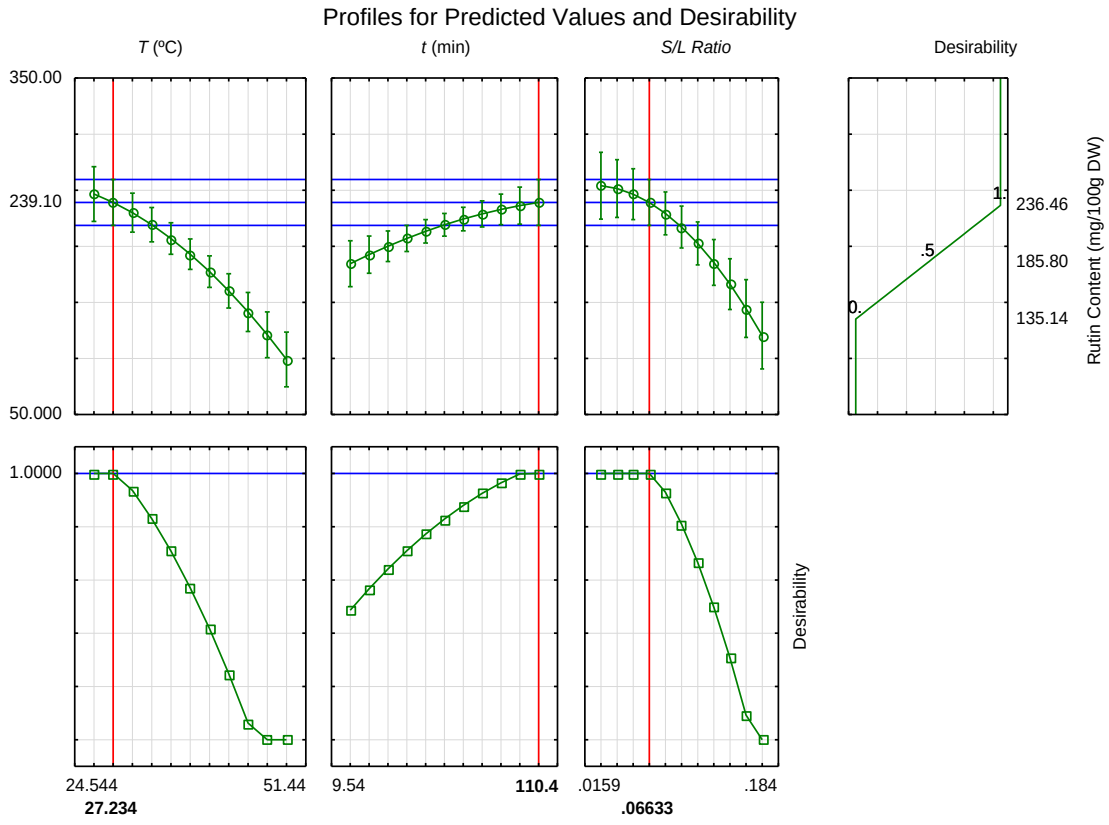

Figure S6. Profiles for predicted values and desirability function for the rutin content from the factorial planning. Red lines indicate optimized values for each variable.