

Electronic Supplementary Material to:

**Food-safe process for high recovery of flavonoids from cocoa beans: antioxidant and
HPLC- DAD-ESI-MS/MS analysis**

Said Toro-Uribe ¹, Elena Ibañez ², Eric A. Decker ³, Arley René Villamizar-Jaimes ⁴, Luis
Javier López-Giraldo ^{1,*}

Table S1. ANOVA for TP, TF, and TF3 through 24 surface design + central points+ start points.

	Total Polyphenols (mgGAE/g)					Total Flavonoids (mgECE/g)					Total Flavan-3-ols (mgECE/g)				
	SS	df	MS	F	p	SS	df	MS	F	p	SS	df	MS	F	p
T	121.89	1	121.892	25.054	0.00002	145.61	1	145.612	25.0688	0.00002	331.817	1	331.817	67.2240	0.00000
T²	24.53	1	24.534	5.043	0.03251	724.60	1	724.600	124.748	0.00000	6.457	1	6.457	1.3082	0.26207
SS	279.34	1	279.342	57.416	0.00000	2281.04	1	2281.037	392.706	0.00000	4.410	1	4.410	0.8934	0.35235
SS²	283.53	1	283.529	58.277	0.00000	113.79	1	113.786	19.5896	0.00012	56.859	1	56.859	11.5193	0.00201
EW	765.38	1	765.383	157.31	0.00000	106.59	1	106.594	18.3514	0.00018	209.481	1	209.481	42.4395	0.00000
EW²	5940.53	1	5940.52	1221.0	0.00000	5591.41	1	5591.412	962.625	0.00000	1710.30	1	1710.30	346.495	0.00000
pH	382.70	1	382.701	78.661	0.00000	134.49	1	134.493	23.1546	0.00004	595.725	1	595.725	120.690	0.00000
pH²	227.97	1	227.967	46.857	0.00000	5.92	1	5.920	1.0193	0.32104	5.672	1	5.672	1.1492	0.29256
T×SS	3.89	1	3.894	0.800	0.37832	43.38	1	43.376	7.4676	0.01058	98.727	1	98.727	20.0015	0.00011
T×EW	28.04	1	28.045	5.764	0.02299	9.23	1	9.226	1.5883	0.21761	282.789	1	282.789	57.2912	0.00000
T×pH	0.03	1	0.026	0.005	0.94216	1.21	1	1.210	0.2084	0.65143	6.530	1	6.530	1.3229	0.25946
SS×EW	4.75	1	4.751	0.977	0.33121	511.66	1	511.657	88.0875	0.00000	46.878	1	46.878	9.4972	0.00448
SS×pH	3.76	1	3.764	0.774	0.38632	1.59	1	1.587	0.2733	0.60510	26.738	1	26.738	5.4170	0.02712
EW×pH	169.72	1	169.718	34.884	0.00000	3.97	1	3.972	0.6839	0.41500	130.251	1	130.251	26.3881	
Error	475.99	39	12.205			585.86	39	15.022			436.821	39	11.201		
Total SS	10988.6	53				12768.3	53				4622.14	53			

where SS is the sum of square, df the degree of freedom, MS the mean square, p is the value of confidence interval, T (temperature), SS (solute/solvent ratio), and EA (ethanol/water ratio). TP is total polyphenol, TF is total flavonoid, and TF3 is total flavan-3ol

Supplementary Equations

Predicted mathematical for TP, TF, and TF3 on cocoa beans, as follows:

Equation S1. Predicted model for total polyphenols content

$$Y_{TPC} = 104.36 + 0.01T - 2063.89 SS + 36443.83 SS^2 + 2.62 EW - 0.02EW^2 \\ - 19.01pH + 2.72 pH^2 - 0.09EW * pH$$

Equation S2. Predicted model for total flavonoids content

$$Y_{TF} = 99.20 - 3.71T + 0.04 T^2 + 23087.14 SS^2 + 1.33 EW - 0.02EW^2 \\ + 19.19 SS * pH$$

Equation S3. Predicted model for a total flavan-3-ol content

$$Y_{TF3} = 16320.24 SS^2 - 0.01 EW^2 - 21.08 T * SS + 0.01 T * EW + 5.81 SS * pH \\ + 0.08 EW * pH$$