

Table S1. Box-Behnken design matrix with the values of the four variables for each experiment and measured and predicted responses ($n = 2$).

Experiment	% MeOH	pH	Temperature (°C)	Ratio	mg anthocyanins measured /g Açaí	mg anthocyanins predicted /g Açaí	Relative error of prediction (%)	mg tot.al phenolics measured /g Açaí	mg total phenolics predicted /g Açaí	Relative error of prediction (%)
X ₁	50	4.5	75	20	4.01	3.97	1.04	9.77	9.54	2.33
X ₂	50	4.5	75	15	4.19	4.19	0.00	9.75	10.05	3.11
X ₃	50	4.5	75	10	4.28	4.15	3.15	9.34	8.65	7.41
X ₄	50	7	75	15	4.22	4.29	1.64	9.87	9.24	6.37
X ₅	50	2	50	15	4.31	4.35	0.87	10.69	9.60	10.21
X ₆	25	2	100	15	4.16	4.17	0.32	9.45	9.88	4.52
X ₇	50	2	50	15	4.17	4.19	0.38	7.15	8.50	18.86
X ₈	25	7	100	15	3.99	4.08	2.26	9.16	8.96	2.17
X ₉	50	4.5	75	20	3.97	4.16	4.66	8.49	9.44	11.16
X ₁₀	50	7	75	10	3.84	3.97	3.49	8.93	8.68	2.81
X ₁₁	50	2	75	10	4.56	4.53	0.60	9.98	9.57	4.15
X ₁₂	50	4.5	75	10	4.27	4.36	2.15	9.93	10.41	4.86

X ₁₃	25	4.5	75	15	4.38	4.24	3.18	10.13	9.12	9.98
X ₁₄	50	7	50	20	3.98	4.14	4.08	10.00	9.44	5.61
X ₁₅	75	4.5	50	15	4.00	3.92	1.94	10.10	9.87	2.27
X ₁₆	75	2	100	15	4.23	4.19	0.95	8.76	9.21	5.18
X ₁₇	50	2	100	20	3.86	3.88	0.54	9.45	8.73	7.66
X ₁₈	50	7	75	15	4.07	4.05	0.55	7.87	8.68	10.31
X ₁₉	25	4.5	75	15	4.17	4.11	1.38	10.28	10.53	2.47
X ₂₀	75	4.5	75	15	4.48	4.45	0.58	10.08	10.12	0.36
X ₂₁	75	7	75	15	4.05	4.09	0.91	10.13	9.96	1.70
X ₂₂	75	4.5	75	20	4.11	4.95	20.50	9.95	10.33	3.80
X ₂₃	50	4.5	50	15	4.18	4.19	0.24	10.53	10.05	4.53
X ₂₄	75	4.5	50	10	4.34	4.20	3.13	9.32	9.85	5.72
X ₂₅	50	4.5	100	15	4.20	4.19	0.24	9.88	10.05	1.75
X ₂₆	25	4.5	100	20	4.05	4.00	1.21	9.46	8.65	8.60
X ₂₇	25	4.5	75	10	4.26	4.13	2.99	9.86	10.20	3.47
