

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

Experiment	% MeOH	Temperature (°C)	Amplitude (%)	Cycle	pH	Ratio (mL)	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	40	30	0.45	2	10	4.19	4.30	2.68	9.57	9.77	2.12
X ₂	50	40	70	0.45	2	10	4.42	4.51	1.99	10.49	10.62	1.20
X ₃	50	40	30	0.45	7	10	4.32	4.02	6.95	11.31	11.48	1.55
X ₄	50	40	70	0.45	7	10	4.37	4.31	1.41	10.39	10.67	2.65
X ₅	50	40	30	0.45	2	20	4.25	4.67	9.82	9.05	9.05	0.00
X ₆	50	40	70	0.45	2	20	4.19	4.02	3.99	10.36	8.89	14.22
X ₇	50	40	30	0.45	7	20	3.74	4.02	7.39	9.42	9.17	2.64
X ₈	50	40	70	0.45	7	20	4.37	4.27	2.34	9.19	9.14	0.54
X ₉	50	10	50	0.2	2	15	3.99	4.50	12.69	7.33	7.43	1.35
X ₁₀	50	70	50	0.2	2	15	4.07	4.10	0.82	8.36	8.82	5.54
X ₁₁	50	10	50	0.7	2	15	4.34	4.63	6.78	8.59	8.76	1.93
X ₁₂	50	70	50	0.7	2	15	4.64	4.46	3.93	10.11	10.25	1.35
X ₁₃	50	10	50	0.2	7	15	3.65	4.03	10.55	7.20	8.29	15.17
X ₁₄	50	70	50	0.2	7	15	3.78	4.12	9.00	7.80	8.57	9.98
X ₁₅	50	10	50	0.7	7	15	4.27	4.32	1.06	9.32	10.06	7.99
X ₁₆	50	70	50	0.7	7	15	4.79	4.89	2.14	9.12	10.06	10.34
X ₁₇	25	40	30	0.2	4.5	15	3.20	3.52	10.08	9.35	10.16	8.67
X ₁₈	75	40	30	0.2	4.5	15	2.40	2.35	2.02	9.19	9.34	1.62
X ₁₉	25	40	70	0.2	4.5	15	2.62	2.76	5.29	7.53	8.94	18.68
X ₂₀	75	40	70	0.2	4.5	15	2.43	2.63	8.20	8.69	9.02	3.81

Experiment	% MeOH	Temperature (°C)	Amplitude (%)	Cycle	pH	Ratio (mL)	mg anthocyanins measured /g Açaí	mg anthocyanins predicted /g Açaí	Relative error of prediction (%)	mg total phenolics measured /g Açaí	mg total phenolics predicted /g Açaí	Relative error of prediction (%)
X ₂₁	25	40	30	0.7	4.5	15	3.13	3.54	12.93	9.47	10.87	14.86
X ₂₂	75	40	30	0.7	4.5	15	2.00	2.12	5.87	7.37	7.58	2.90
X ₂₃	25	40	70	0.7	4.5	15	2.90	2.98	2.78	9.12	10.48	14.88
X ₂₄	75	40	70	0.7	4.5	15	2.58	2.85	10.30	9.70	9.75	0.51
X ₂₅	50	10	30	0.45	4.5	10	4.46	4.78	7.23	10.30	9.78	4.98
X ₂₆	50	70	30	0.45	4.5	10	3.96	4.03	1.84	8.43	8.64	2.55
X ₂₇	50	10	70	0.45	4.5	10	4.39	4.52	3.05	9.52	8.81	7.48
X ₂₈	50	70	70	0.45	4.5	10	3.72	3.98	6.89	7.00	8.46	20.80
X ₂₉	50	10	30	0.45	4.5	20	4.03	4.15	2.88	7.00	7.05	0.68
X ₃₀	50	70	30	0.45	4.5	20	4.42	4.61	4.23	8.86	9.19	3.74
X ₃₁	50	10	70	0.45	4.5	20	4.18	4.16	0.45	9.62	8.86	7.92
X ₃₂	50	70	70	0.45	4.5	20	4.30	4.26	0.97	8.54	9.96	16.66
X ₃₃	25	10	50	0.45	2	15	2.59	2.49	3.79	6.64	6.75	1.69
X ₃₄	75	10	50	0.45	2	15	2.10	2.05	2.19	7.00	6.93	1.03
X ₃₅	25	70	50	0.45	2	15	2.53	2.35	7.20	6.95	7.02	0.97
X ₃₆	75	70	50	0.45	2	15	2.44	2.56	4.71	6.77	6.98	3.10
X ₃₇	25	10	50	0.45	7	15	2.38	2.43	2.27	5.33	5.53	3.74
X ₃₈	75	10	50	0.45	7	15	2.37	2.34	1.08	7.42	7.58	2.21
X ₃₉	25	70	50	0.45	7	15	2.95	2.59	12.18	8.03	8.01	0.23
X ₄₀	75	70	50	0.45	7	15	2.40	2.43	1.12	8.66	8.23	4.93
X ₄₁	25	40	50	0.2	4.5	10	2.96	3.12	5.33	7.60	8.01	5.42

Experiment	% MeOH	Temperature (°C)	Amplitude (%)	Cycle	pH	Ratio (mL)	mg anthocyanins measured /g Açaí	mg anthocyanins predicted /g Açaí	Relative error of prediction (%)	mg total phenolics measured /g Açaí	mg total phenolics predicted /g Açaí	Relative error of prediction (%)
X ₄₂	75	40	50	0.2	4.5	10	2.52	2.63	4.43	8.41	9.25	10.00
X ₄₃	25	40	50	0.7	4.5	10	2.72	2.76	1.41	7.53	7.63	1.31
X ₄₄	75	40	50	0.7	4.5	10	2.84	2.88	1.52	6.95	7.58	9.03
X ₄₅	25	40	50	0.2	4.5	20	3.59	3.65	1.74	9.00	9.23	2.50
X ₄₆	75	40	50	0.2	4.5	20	2.45	2.52	3.01	8.91	9.12	2.41
X ₄₇	25	40	50	0.7	4.5	20	2.65	2.87	8.43	7.55	8.05	6.65
X ₄₈	75	40	50	0.7	4.5	20	2.33	2.35	0.80	9.52	9.10	4.39
R ₁	50	40	50	0.45	4.5	15	4.08	4.53	11.04	9.27	10.06	8.57
R ₂	50	40	50	0.45	4.5	15	4.11	4.53	10.15	9.22	10.06	9.15
R ₃	50	40	50	0.45	4.5	15	4.59	4.53	1.28	10.33	10.06	2.56
R ₄	50	40	50	0.45	4.5	15	4.57	4.53	0.97	9.50	10.06	5.92
R ₅	50	40	50	0.45	4.5	15	4.61	4.53	1.69	9.17	10.06	9.75
R ₆	50	40	50	0.45	4.5	15	4.84	4.53	6.42	9.34	10.06	7.80