

Supplementary material

Optimized isolation procedure for the extraction of bioactive compounds from spent coffee grounds

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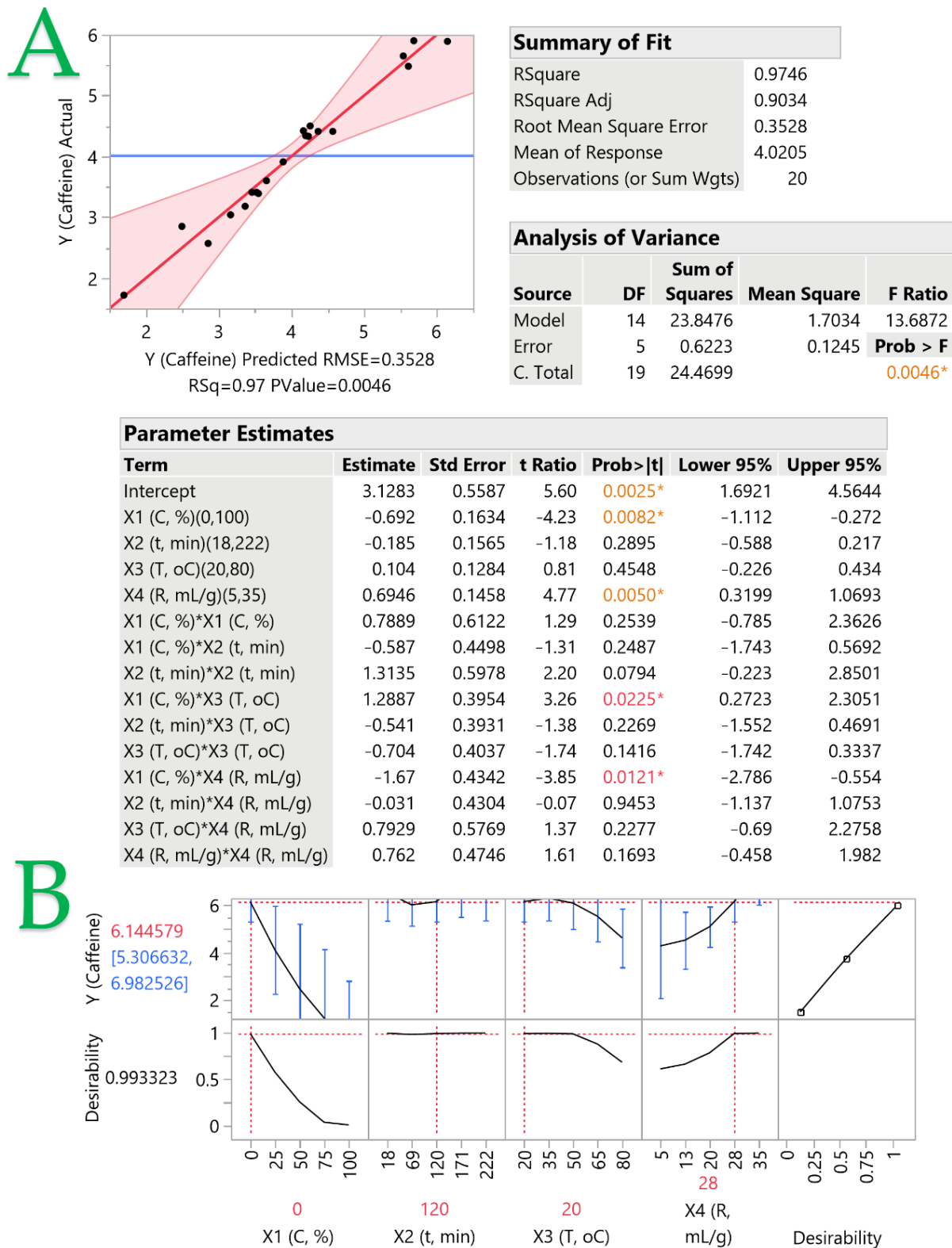


Figure S1. Plot of actual *vs* predicted response (Caffeine, mg/g) (plot A) and desirability function (plot B) for the optimization of extraction of spent coffee grounds performed with hydroethanolic solutions. The inset tables provide statistics related to the evaluation of the resulting model. Values with color and asterisk are statistically significant.

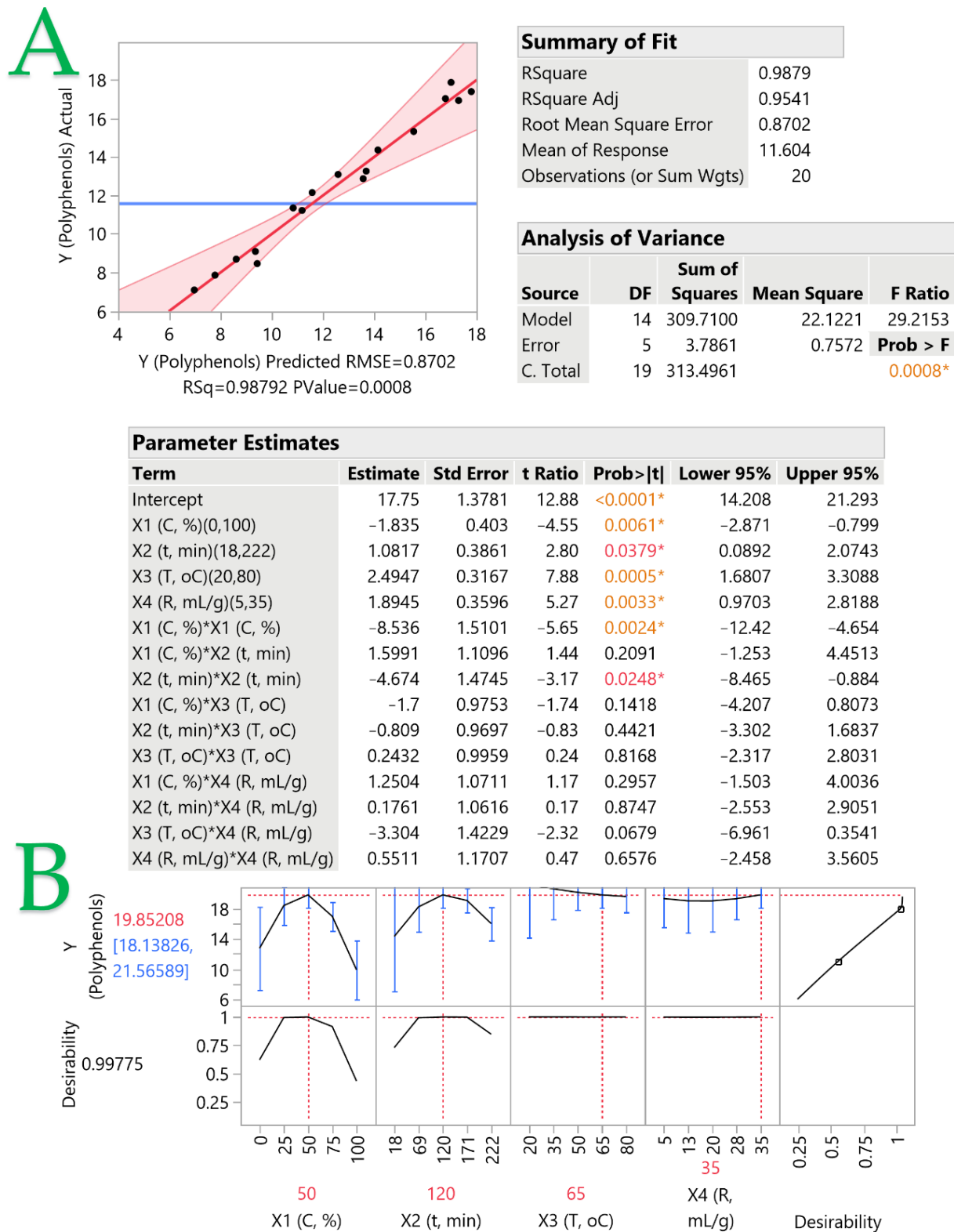
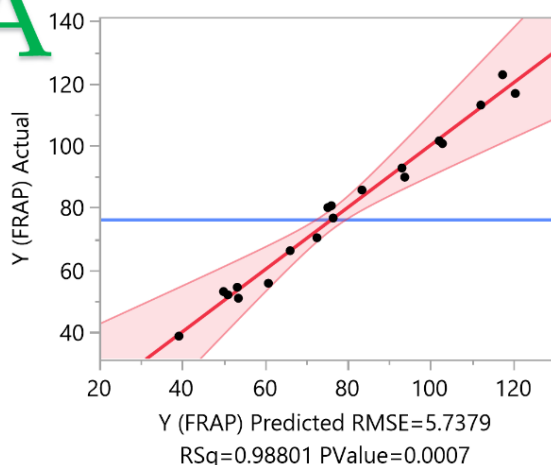


Figure S2. Plot of actual *vs* predicted response (Polyphenols, mg GAE/g) (plot A) and desirability function (plot B) for the optimization of extraction of spent coffee grounds performed with hydroethanolic solutions. The inset tables provide statistics related to the evaluation of the resulting model. Values with color and asterisk are statistically significant.

A



Summary of Fit

RSquare	0.988
RSquare Adj	0.9545
Root Mean Square Error	5.7379
Mean of Response	76.326
Observations (or Sum Wgts)	20

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	14	13,568.516	969.180	29.4377
Error	5	164.615	32.923	Prob > F
C. Total	19	13,733.131		0.0007*

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob> t	Lower 95%	Upper 95%
Intercept	112.72	9.0869	12.40	<0.0001*	89.362	136.08
X1 (C, %)(0,100)	-15.49	2.6574	-5.83	0.0021*	-22.32	-8.661
X2 (t, min)(18,222)	6.9922	2.546	2.75	0.0405*	0.4476	13.537
X3 (T, °C)(20,80)	16.335	2.0882	7.82	0.0005*	10.968	21.703
X4 (R, mL/g)(5,35)	13.165	2.3709	5.55	0.0026*	7.0702	19.259
X1 (C, %)*X1 (C, %)	-52.08	9.9575	-5.23	0.0034*	-77.67	-26.48
X1 (C, %)*X2 (t, min)	16.819	7.3165	2.30	0.0699	-1.988	35.627
X2 (t, min)*X2 (t, min)	-32.65	9.7226	-3.36	0.0201*	-57.65	-7.661
X1 (C, %)*X3 (T, °C)	-8.965	6.4309	-1.39	0.2221	-25.5	7.5667
X2 (t, min)*X3 (T, °C)	-12.96	6.3941	-2.03	0.0984	-29.4	3.4734
X3 (T, °C)*X3 (T, °C)	0.5467	6.5666	0.08	0.9369	-16.33	17.427
X1 (C, %)*X4 (R, mL/g)	7.9628	7.0624	1.13	0.3107	-10.19	26.117
X2 (t, min)*X4 (R, mL/g)	-8.744	7	-1.25	0.2669	-26.74	9.2498
X3 (T, °C)*X4 (R, mL/g)	-16.74	9.3824	-1.78	0.1345	-40.85	7.3825
X4 (R, mL/g)*X4 (R, mL/g)	10.66	7.7195	1.38	0.2258	-9.183	30.504

B

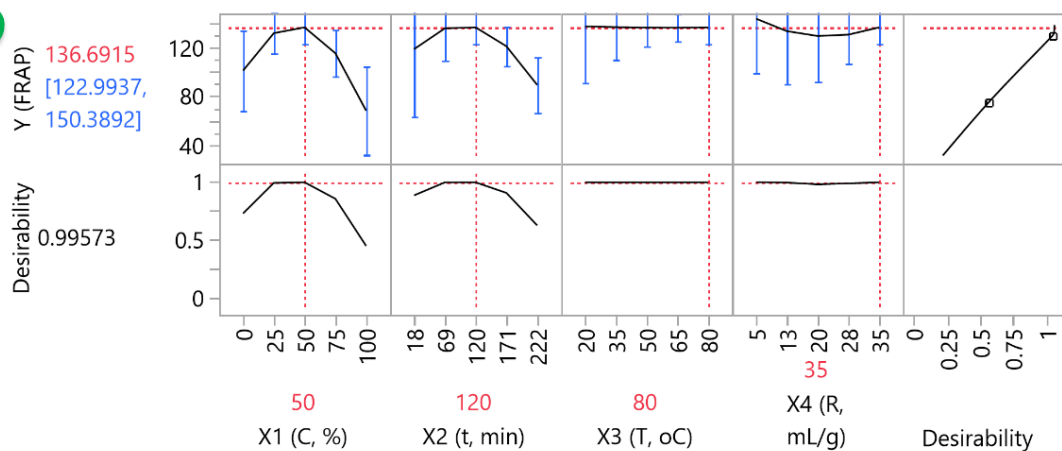


Figure S3. Plot of actual *vs* predicted response (FRAP, $\mu\text{mol AAE/g}$) (plot A) and desirability function (plot B) for the optimization of extraction of spent coffee grounds performed with hydroethanolic solutions. The inset tables provide statistics related to the evaluation of the resulting model. Values with color and asterisk are statistically significant.

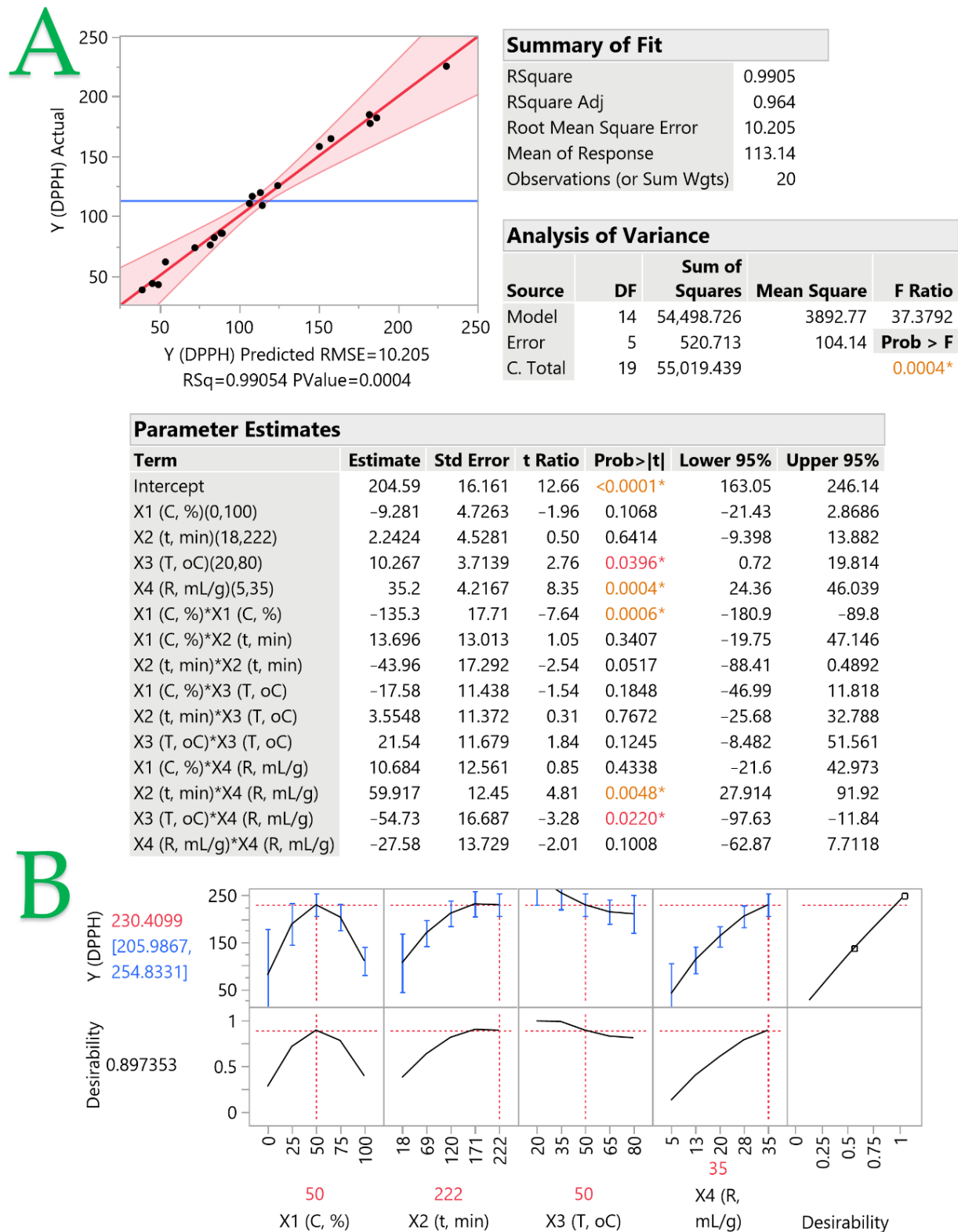


Figure S4. Plot of actual *vs* predicted response (DPPH, $\mu\text{mol DPPH/g}$) (plot A) and desirability function (plot B) for the optimization of extraction of spent coffee grounds performed with hydroethanolic solutions. The inset tables provide statistics related to the evaluation of the resulting model. Values with color and asterisk are statistically significant.

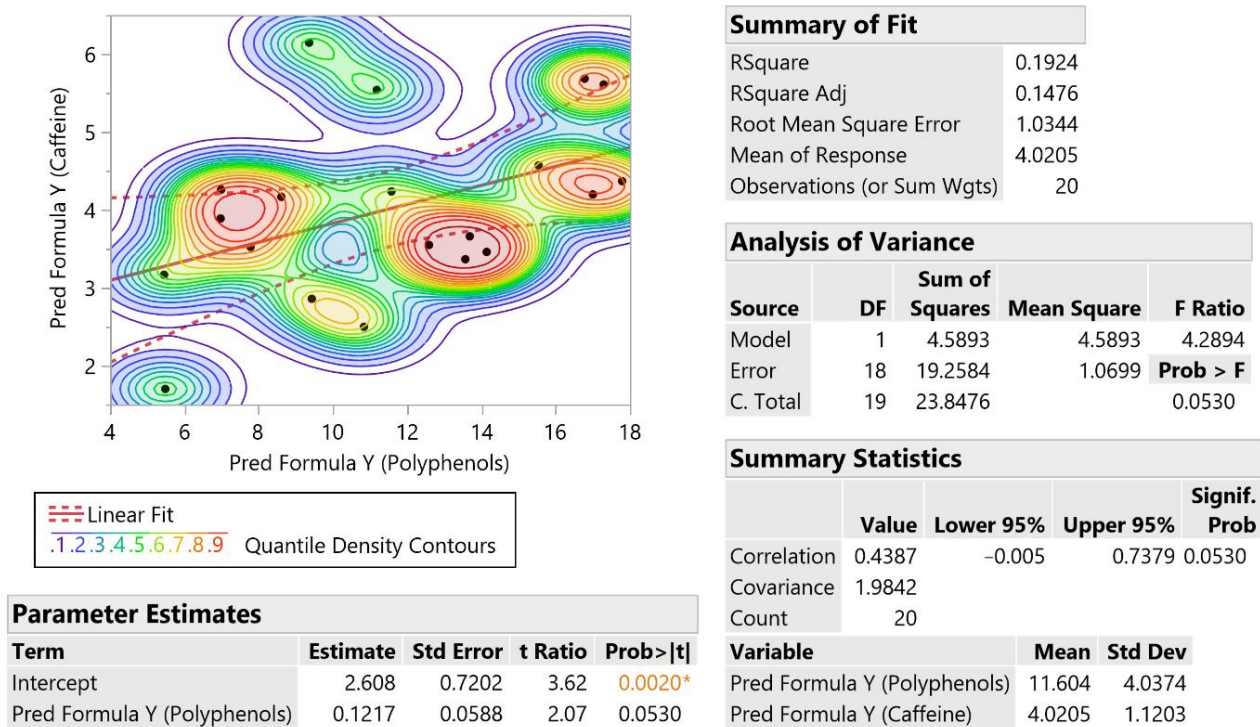


Figure S5. Bivariate response fitting plot (Caffeine *vs* Polyphenols) for the optimization of spent coffee grounds extraction performed with hydroethanolic solutions. The inset tables provide statistics related to the evaluation of the resulting model. Values with color and asterisk are statistically significant.

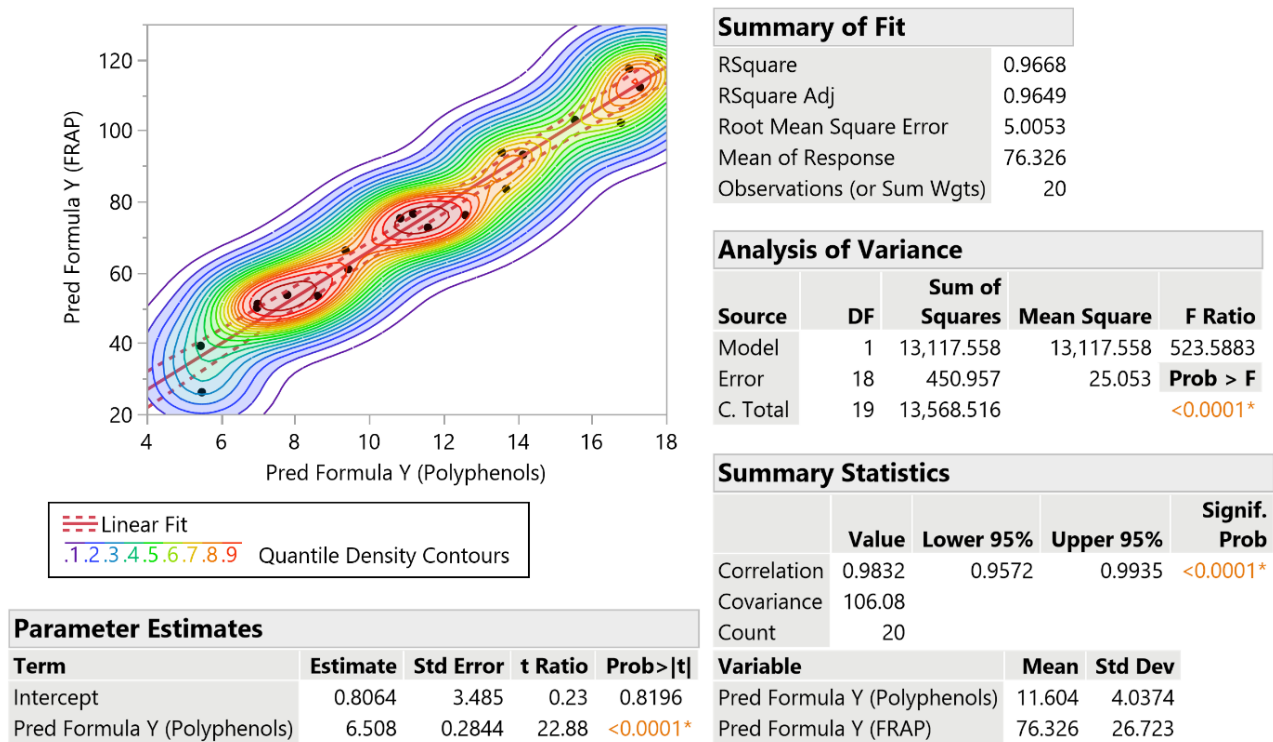


Figure S6. Bivariate response fitting plot (FRAP *vs* Polyphenols) for the optimization of spent coffee grounds extraction performed with hydroethanolic solutions. The inset tables provide statistics related to the evaluation of the resulting model. Values with color and asterisk are statistically significant.

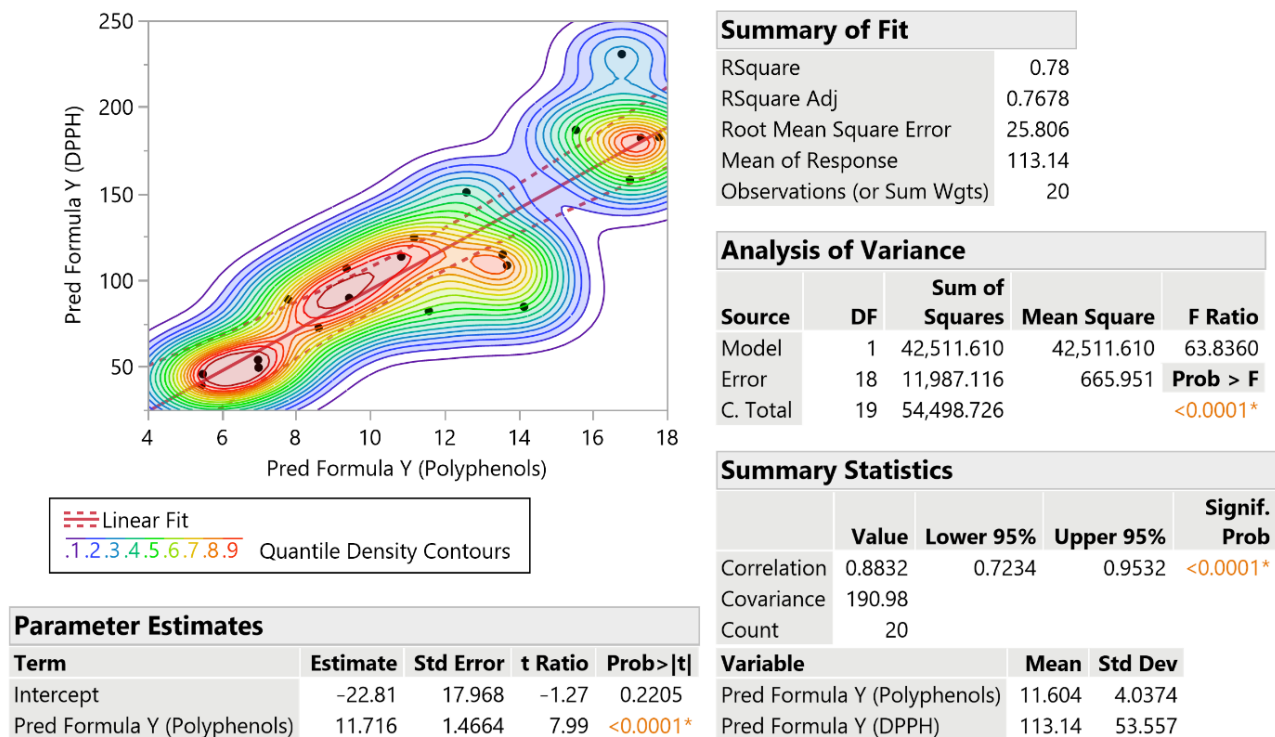


Figure S7. Bivariate response fitting plot (DPPH *vs* Polyphenols) for the optimization of spent coffee grounds extraction performed with hydroethanolic solutions. The inset tables provide statistics related to the evaluation of the resulting model. Values with color and asterisk are statistically significant.