Supplementary Material

Table S1. Phenolic compound identified in quince peel extracts.

Peak	R*t* (min)	λ_{max} (nm)	[M-H]$^-$ (*m*/*z*)	Tentative identification
1 [A]	4.43	324	353	*cis*-3-*O*-Caffeoylquinic acid
2 [A]	4.39	325	353	*trans*-3-*O*-Caffeoylquinic acid
3 [B]	5.85	292	337	3-*O*-*p*-Coumaroylquinic acid
4 [A]	6.56	326	353	*cis*-5-*O*-Caffeoylquinic acid
5 [A]	7.43	323	353	*trans*-5-*O*-Caffeoylquinic acid
6 [C]	8.63	275	289	(+)-Catechin
7 [*]	10.47	311	337	5-*O*-*p*-Coumaroylquinic acid
8 [C]	11.08	276	865	β-Type (epi)catechin trimer
9 [C]	12.52	272	1153	β-Type (epi)catechin tetramer
10 [*]	13.83	298	577	β-Type (epi)catechin dimer
11 [C]	14.16	280	1153	β-Type (epi)catechin tetramer
12 [*]	14.57	271	865	β-Type (epi)catechin trimer
13 [C]	15.10	275	865	β-Type (epi)catechin trimer
14 [*]	15.76	275	865	β-Type (epi)catechin trimer
15 [D]	16.70	355	609	Quercetin-*O*-deoxyhexosil-hexoside
16 [*]	17.52	268	863	Procyanidin with A-type linkage
17 [D]	19.86	357	593	Kaempferol-*O*-deoxyhexosil-hexoside

R*t*: retention time; λ_{max}: wavelengths of maximum absorption in the UV-vis region; [M-H]$^-$: deprotonated ion. Standards used in quantification: [A] chlorogenic acid; [B] *p*-coumaric acid; [C] catechin; and [D] quercetin-3-*O*-glucoside. [*]Not used in the optimization process.

Table S2. Contents (mg/g BE) of individual phenolic compounds obtained experimentally from quince peel.

Runs	Phenolic compounds											
	1	**2**	**3**	**4**	**5**	**6**	**8**	**9**	**11**	**13**	**15**	**17**
1	0.530	0.733	0.172	1.425	0.400	0.653	1.542	0.931	0.589	0.645	1.233	0.917
2	0.597	0.721	0.213	1.751	0.435	0.693	1.471	0.909	0.490	0.608	1.292	0.812
3	0.549	0.730	0.195	1.517	0.397	0.653	1.459	0.862	0.538	0.563	1.188	0.828
4	0.544	0.825	0.184	1.756	0.432	0.744	1.559	0.947	0.541	0.658	1.262	0.679
5	0.394	0.483	0.112	0.989	0.279	0.421	0.884	0.562	0.365	0.446	1.148	0.777
6	0.433	0.587	0.148	1.259	0.332	0.576	1.165	0.718	0.385	0.536	1.031	0.779
7	0.490	0.524	0.094	0.745	0.347	0.446	0.935	0.638	0.409	0.451	1.049	0.971
8	0.552	0.658	0.173	1.349	0.349	0.555	1.332	0.849	0.504	0.615	1.193	0.767
9	0.385	0.585	0.150	1.424	0.276	0.565	1.402	0.772	0.501	0.621	1.490	0.760
10	0.616	0.752	0.222	1.701	0.422	0.646	1.446	0.890	0.617	0.627	1.339	0.762
11	0.504	0.644	0.182	1.591	0.339	0.612	1.236	0.821	0.471	0.624	1.204	0.646
12	0.501	0.718	0.186	1.677	0.304	0.554	1.292	0.893	0.484	0.605	1.158	0.666
13	0.580	0.915	0.191	1.481	0.397	0.594	1.378	0.879	0.583	0.701	1.213	0.873
14	0.343	0.521	0.107	0.774	0.254	0.412	0.888	0.530	0.380	0.411	1.137	0.740
15	0.475	0.732	0.125	1.251	0.316	0.548	1.269	0.739	0.436	0.511	1.240	0.785
16	0.599	0.642	0.097	0.880	0.395	0.436	1.059	0.667	0.445	0.473	1.045	0.935
17	0.550	0.724	0.102	1.329	0.325	0.512	1.324	0.696	0.420	0.450	1.206	0.847
18	0.550	0.634	0.099	0.937	0.420	0.445	1.025	0.659	0.432	0.509	1.070	0.933
19	0.366	0.644	0.122	1.192	0.315	0.406	1.176	0.684	0.369	0.434	1.336	0.754
20	0.436	0.652	0.122	1.353	0.321	0.486	1.280	0.706	0.390	0.483	1.164	0.781

Compound **1**: *cis*-3-*O*-caffeoylquinic acid; compound **2**: *trans*-3-*O*-caffeoylquinic acid; compound **3**: 3-*O*-*p*-coumaroylquinic acid; compound **4**: *cis*-5-*O*-caffeoylquinic acid; compound **5**: *trans*-5-*O*-caffeoylquinic acid; compound **6**: (+)-catechin; compound **8**: β-type (epi)catechin trimer; compound **9**: β-type (epi)catechin tetramer; compound **11**: β-type (epi)catechin tetramer; compound **13**: β-type (epi)catechin trimer; compound **15**: quercetin-*O*-deoxyhexosil-hexoside; compound **17**: kaempferol-*O*-deoxyhexosil-hexoside.

Table S3. Contents (g/100 g BE) of quinic acid, total organic acids, fructose, glucose, sucrose, and total soluble sugars obtained experimentally from quince peel.

Run	Experimental domain			Bioactive extract (BE) dependent variables					
	t (min)	*T* (ºC)	*S* (%)	Quinic acid	Total organic acids	Fructose	Glucose	Sucrose	Total soluble sugars
1	25	40	20	0.277	6.71	42.19	13.45	5.30	60.94
2	95	40	20	0.200	4.79	40.98	12.03	5.85	58.86
3	25	80	20	0.480	6.91	41.91	13.46	7.41	62.78
4	95	80	20	0.410	7.04	39.32	11.81	6.30	57.43
5	25	40	80	0.000	0.59	39.43	10.96	6.45	56.84
6	95	40	80	0.000	0.79	36.95	9.89	6.36	53.20
7	25	80	80	0.270	4.59	36.79	9.94	5.78	52.51
8	95	80	80	0.392	6.57	32.92	7.69	3.73	44.34
9	1	60	50	0.240	4.19	38.23	12.81	6.37	57.41
10	119	60	50	0.404	5.47	36.30	10.14	5.50	51.94
11	60	26	50	0.000	2.90	42.17	12.01	5.60	59.78
12	60	94	50	0.413	7.38	40.35	10.99	5.77	57.11
13	60	60	0	0.620	6.68	41.84	11.39	5.92	59.15
14	60	60	100	0.200	1.83	33.99	6.12	5.13	45.24
15	60	60	50	0.139	4.74	39.69	10.91	5.38	55.98
16	60	60	50	0.000	4.72	37.80	9.88	4.72	52.40
17	60	60	50	0.260	5.63	37.30	10.61	4.31	52.22
18	60	60	50	0.070	4.64	36.79	9.24	4.53	50.56
19	60	60	50	0.000	4.75	38.79	11.16	4.40	54.35
20	60	60	50	0.000	5.41	39.08	10.70	5.54	55.32

t: time; *T*: temperature; *S*: solvent (EtOH percentage).

Table S4. Parametric values estimated with the polynomial Equation (1) and statistical data of the models' fitting procedure for sugars and organic acids.

Coefficients		Quinic acid	Total organic acids	Fructose	Glucose	Sucrose	Total soluble sugars
Intercept	b_0	0.11 ± 0.03	4.99 ± 0.10	37.89 ± 0.27	10.40 ± 0.24	4.81 ± 0.17	53.64
Linear terms	b_1	0.02 ± 0.02*	0.19 ± 0.09*	-0.98 ± 0.26	-0.80 ± 0.16	-0.30 ± 0.11	-2.08 ± 0.48
	b_2	0.13 ± 0.02	1.45 ± 0.09	-0.85 ± 0.26	-0.38 ± 0.16	-0.03 ± 0.11*	-1.26 ± 0.48
	b_3	-0.10 ± 0.02	-1.54 ± 0.09	-2.31 ± 0.26	-1.55 ± 0.16	-0.28 ± 0.11	-4.14 ± 0.48
Quadratic terms	b_{11}	0.07 ± 0.02	ns	ns	0.49 ± 0.15	0.42 ± 0.11	ns
	b_{22}	ns	ns	1.10 ± 0.25	0.50 ± 0.15	0.34 ± 0.11	1.87 ± 0.63
	b_{33}	0.10 ± 0.02	-0.25 ± 0.09	ns	-0.47 ± 0.15	0.28 ± 0.11	ns
Interaction terms	b_{12}	ns	0.48 ± 0.13	ns	ns	-0.45 ± 0.14	ns
	b_{13}	ns	0.50 ± 0.13	ns	ns	ns	ns
	b_{23}	ns	0.93 ± 0.13	-0.59 ± 0.33	ns	-0.73 ± 0.14	-1.70 ± 0.63
Modeling statistics							
Model F-value		13.41	78.28	26.02	23.56	9.51	24.81
Model *p*-value		<0.0001	<0.0001	<0.0001	<0.0001	0.0006	<0.0001
Lack-of-Fit		0.7304	0.7700	0.7938	0.8672	0.9139	0.7804
R^2		0.8273	0.9786	0.9028	0.9322	0.8737	0.8986
Adj R^2		0.7656	0.9661	0.8681	0.8923	0.7819	0.8624
Adequate precision		13.26	29.44	16.47	18.53	12.89	16.32
C.V. (%)		42.25	7.58	2.45	5.39	7.43	3.23

In each term, parametric subscripts 1, 2, and 3 stand for the independent variables time (*t*), temperature (*T*), and solvent (*S*), respectively. R^2: coefficient of determination; R^2_{ajd}: adjusted coefficient of determination; C.V.: coefficient of variation (%). *Not significant but necessary for model hierarchy.

Table S5. Optimal conditions for extraction of quince peel constituents and respective response values.

Responses	Optimal processing conditions			Response optimum
	X_1: ***t*** (min)	X_2: ***T*** (°C)	X_3: ***S*** (%, *v*/*v*)	Model-predicted values
BE yield	66.4	26.7	33.4	69 ± 2% (*w*/*w*)
Phenolic compounds	64.2	88.0	0.0	10.6 ± 0.2 mg/g
Phenolic compounds [#]	8.5	34.9	39.5	9.6 ± 0.2 mg/g
Phenolic acids	114.3	82.8	36.3	4.1 ± 0.1 mg/g
Flavan-3-ols	40.4	85.9	0.0	4.7 ± 0.2 mg/g
Flavonols	10.6	52.8	0.0	2.31 ± 0.03 mg/g
Malic acid	87.7	92.7	54.4	7.9 ± 0.3 g/100 g
Malic acid [#]	10.0	44.4	26.5	6.1 ± 0.3 g/100 g
Quinic acid	96.7	91.8	8.5	0.74 ± 0.07 g/100 g
Organic acids	89.2	92.5	56.2	8.2 ± 0.3 g/100 g
Fructose	1.0	69.2	0.0	43.7 ± 0.7 g/100 g
Glucose	7.4	36.5	34.1	14.3 ± 0.5 g/100 g
Sucrose	18.4	76.7	16.8	7.8 ± 0.3 g/100 g
Soluble sugars	5.01	70.7	0.0	65 ± 1 g/100 g
FC yield	69.1	61.3	99.9	64 ± 2% (*w*/*w*)
Dietary fiber	-	92.2	35.5	67 ± 1 g/100 g
Lightness (*L**)	-	65.9	99.2	71 ± 1 (0–100)

t: time; *T*: temperature; *S*: solvent (EtOH percentage). The standard error was kept "in range" in all cases.
[#] Extraction conditions obtained by minimizing the time and temperature values.
- The variable was not significant ($p < 0.05$).

Table S6. Pearson's correlation coefficients (*R*) of extract constituents with antioxidant activity.

		TBARS	OxHLIA	
			Δ*t* 60	**Δ*t* 120**
Phenolics compounds	*R*	0.654	-0.207	0.0117
	Sig.	0.056	0.593	0.763
Phenolics acids	*R*	**-0.754***	**-0.566**	**-0.720***
	Sig.	0.019	0.112	0.029
Flavan-3-ols	*R*	0.864**	0.103	0.427
	Sig.	0.003	0.792	0.252
Flavonols	*R*	0.777*	-0.109	0.236
	Sig.	0.014	0.780	0.542
Malic acid	*R*	**-0.964****	**-0.660**	**-0.875****
	Sig.	0.000	0.053	0.002

Very strong correlation: ≥ 0.9 (■); Strong correlation: 0.7–0.9 (■); Moderate correlation: 0.5–0.7 (■).
*Significant at $p \leq 0.05$. **Significant at $p \leq 0.01$.

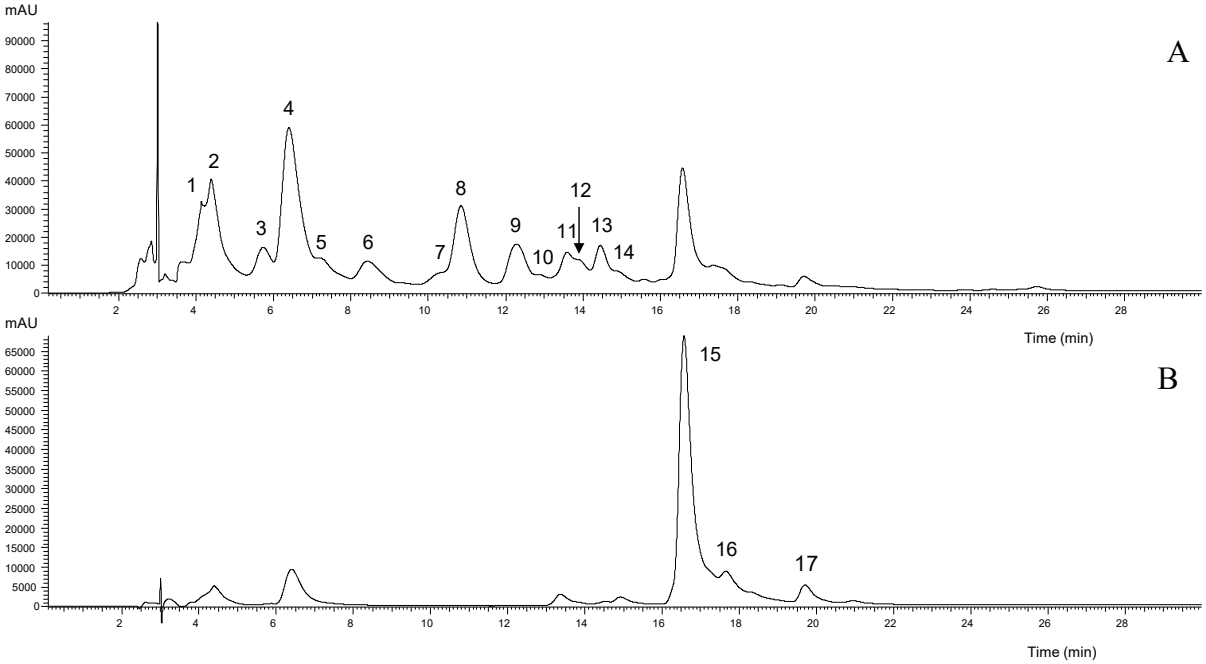


Figure S1: Representative chromatogram of the phenolic profile of the quince peel extract obtained with the 19th run of the design matrix recorded at 280 nm (a) and 370 nm (b). Peak identification is shown in Table S1.

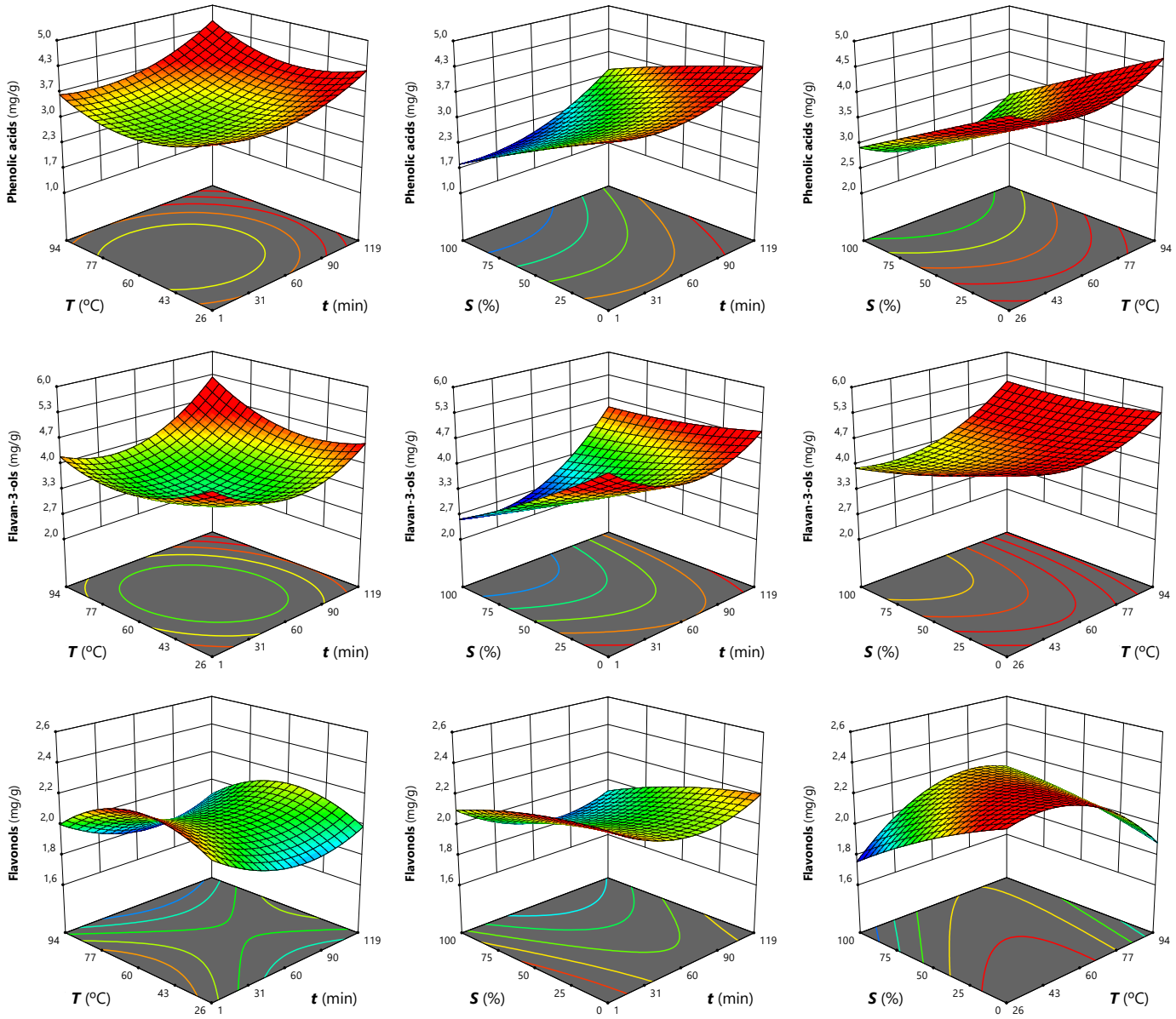


Figure S2. Response surface plots illustrating the effects of the independent variables on the extraction of phenolic acids, flavan-3-ols, flavonols from quince peel. In each 3D plot, the unplotted independent variable was kept constant at its optimal value in Table S4.

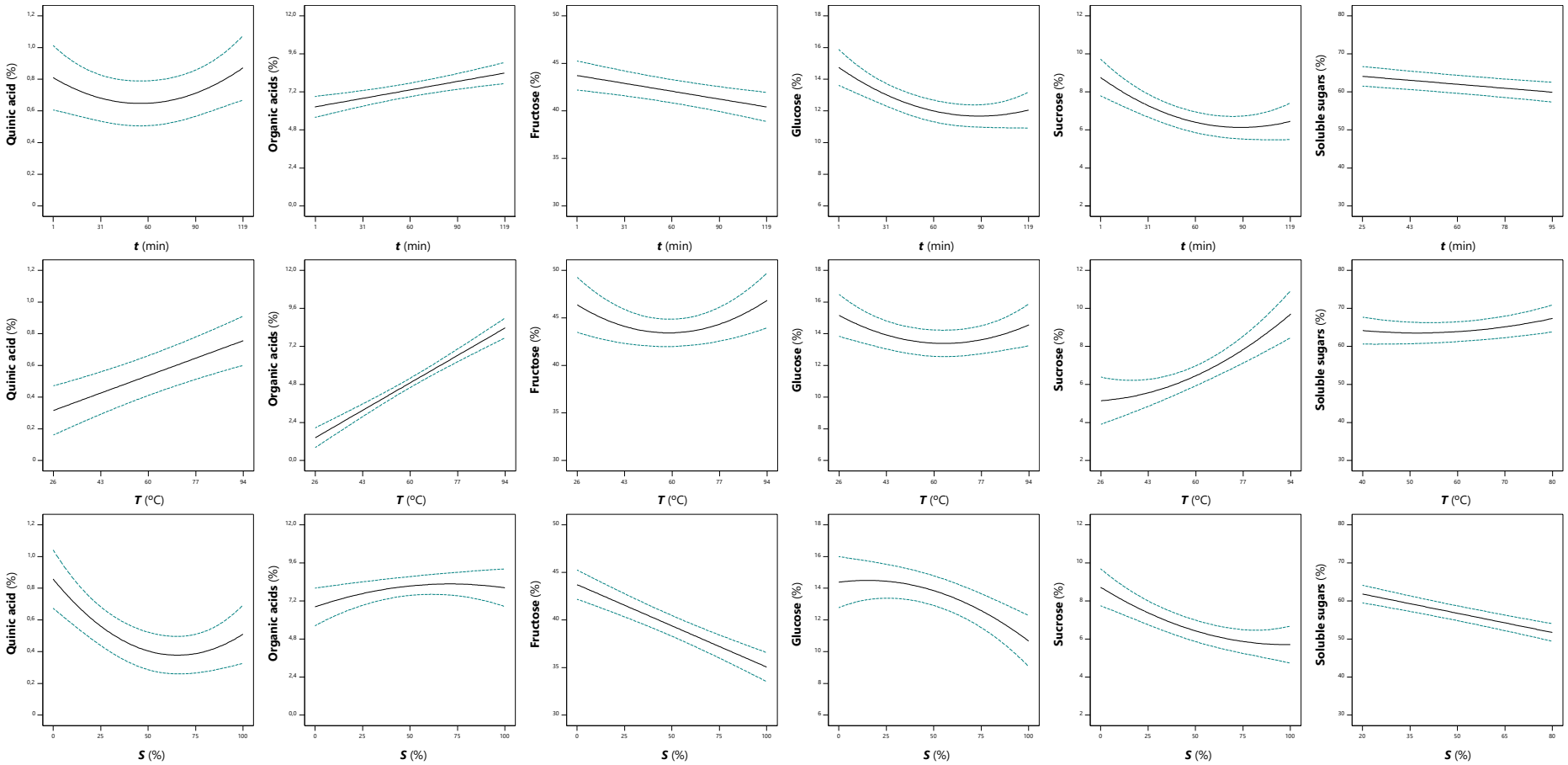


Figure S3. Response plots for the effects of each independent variable on the extraction of organic acids and soluble sugars from quince peel. In each 2D plot, the unplotted independent variable were kept constant at their optimal value in Table S4.