Chemometric study on the effect of cooking on bioactive compounds in tomato pomace enriched sauces

Johana González-Coria[1,2], Camilla Mesirca-Prevedello,[3,4] Julián Lozano-Castellón[2,5,6], Enrico Casadei[3,4], Enrico Valli[3,4], Anallely López-Yerena[2,5], Carolina Jaime-Rodríguez[1,2], Diana Pinto[7], Montse Illan[5], Xavier Torrado[5], Joan Romanyà[1,2,6], Anna Vallverdú-Queralt[2,5,6], Alessandra Bendini[3,4,*], Rosa M. Lamuela-Raventós[2,5,6] , Maria Pérez [2,5,6,*]

[1]Department of Biology, Health, and the Environment, Faculty of Pharmacy and Food Sciences, University of Barcelona, 08028 Barcelona, Spain.

[2]Institute of Nutrition and Food Safety (INSA-UB), University of Barcelona, Barcelona, Spain.

[3]Department of Agricultural and Food Sciences, Alma Mater Studiorum—Università di Bologna, 47521 Cesena, Italy

[4]Interdepartmental Centre for Industrial Agrofood Research, Alma Mater Studiorum—Università di Bologna, 47521 Cesena, Italy

[5]Polyphenol Research Group, Department of Nutrition, Food Science and Gastronomy, Faculty of Pharmacy and Food Sciences, University of Barcelona, 08028 Barcelona, Spain.

[6]CIBER Physiopathology of Obesity and Nutrition (CIBEROBN), Institute of Health Carlos III, 28029 Madrid, Spain.

[7]REQUIMTE/LAQV, Instituto Superior de Engenharia do Porto, Rua Dr. António Bernardino de Almeida, 4249-015 Porto, Portugal.

*Corresponding Authors: E-mail address: alessandra.bendini@unibo.it, mariaperez@ub.edu

Supplementary information 1

Table S1. Characteristics of bioactive compounds detected in tomato sauces.

Compound	Neutral molecular formula	RT (min)	Accurate mass	Experimental mass	Error (mmu)	MS^2 ions (m/z)
Phenolic acids						
p-Hydroxybenzaldehyde	$C_7H_6O_2$	5.30	121.0295	121.0294	0.744	66.0682/93.0296
4-hydroxybenzoic acid*	$C_7H_6O_3$	4.13	137.0244	137.0242	-0.227	930.339
2,5-dihydroxybenzoic acid*	$C_7H_6O_4$	4.19	153.0193	153.0190	-0.322	109.0287
2,6-dihydroxybenzoic acid*	$C_7H_6O_4$	5.94	153.0193	153.0187	-0.642	135.0079/109.0287
3,5-dihydroxybenzoic acid*	$C_7H_6O_4$	2.42	153.0193	153.0191	-0.242	109.0289
Dihydroxybenzoic acid-*O*-pentoside	$C_{12}H_{14}O_8$	4.46	285.0615	285.0610	-0.631	153.0182
Protocatechuic acid	$C_7H_6O_4$	2.38	153.0193	153.0190	-0.372	106.0288
Caffeic acid	$C_9H_8O_4$	5.97	179.0339	179.0348	0.9050	135.0444
Gentisic acid*	$C_7H_6O_4$	6.28	153.0193	153.0190	-0.322	109.0288
Caffeoylmalic acid	$C_{13}H_{12}O_8$	8.67	295.0459	295.0450	-0.991	133.0135
Homovanillic acid hexose I	$C_{15}H_{20}O_9$	5.61	343.1034	343.1024	-1.005	137.0600
Homovanillic acid hexose II	$C_{15}H_{20}O_9$	5.93	343.1034	343.1028	-0.675	137.0600
Homovanillic acid hexose III	$C_{15}H_{20}O_9$	6.46	343.1034	343.1026	-0.825	137.0600
p-Coumaric acid*	$C_9H_8O_3$	8.18	163.0400	163.0397	-0.317	119.0495
Coumaric acid-*O*-hexoside (I, II, III)	$C_{15}H_{18}O_8$	6.21	325.0928	325.0919	-0.911	163.0392/ 145.0286
Coumaroylquinic acid I	$C_{16}H_{18}O_8$	7.75	337.0928	337.0920	-0.911	191.0571
Coumaroylquinic acid II	$C_{16}H_{18}O_8$	8.32	337.0928	337.0917	-1.181	191.0571
Ferulic acid*	$C_{10}H_{10}O_4$	9.81	193.0506	193.0499	-0.732	149.0599/178.0261
Isoferulic acid	$C_{10}H_{10}O_4$	14.3	193.0506	193.0503	-0.342	149.0600/121.0652
Caffeoyl-hexose I (caffeic acid hexose)	$C_{15}H_{18}O_9$	4.38	341.0878	341.0873	-0.525	179.0342
Caffeoyl-hexose II (caffeic acid hexose)	$C_{15}H_{18}O_9$	4.6	341.0878	341.0874	-0.375	179.0342
Caffeoyl-hexose III (caffeic acid hexose)	$C_{15}H_{18}O_9$	5.18	341.0878	341.0872	-0.645	179.0342
Caffeoyl-hexose IV (caffeic acid hexose)	$C_{15}H_{18}O_9$	5.71	341.0878	341.0874	-0.375	179.0342
3-(2-Hydroxyphenyl) propanoic acid hexose	$C_{15}H_{20}O_8$	5.59	327.1085	327.1080	-0.571	165.0550
3,4-Dihydroxyhydrocinnamic acid	$C_9H_{10}O_4$	5.55	181.0506	181.0503	-0.312	137.0600
Sinapic acid-*O*-hexoside	$C_{17}H_{22}O_{10}$	6.61	385.1140	385.1130	-1.040	223.0598
1-Caffeoylquinic acid	$C_{16}H_{18}O_9$	5.85	353.0878	353.0870	-0.765	191.0551
3-Caffeoylquinic acid (chlorogenic acid)	$C_{16}H_{18}O_9$	6.59	353.0878	353.0873	-0.495	191.0552/179.0342
5-Caffeoylquinic acid	$C_{16}H_{18}O_9$	7.84	353.0878	353.0868	-0.985	191.0552/179.0342
3-(2-Hydroxy-4-methoxyphenyl) propanoic acid hexose	$C_{16}H_{22}O_9$	6.87	357.1191	357.1184	-0.695	195.0655
Dicaffeoylquinic acid I	$C_{25}H_{24}O_{12}$	14.68	515.1194	515.1191	-0.359	353.0856
Dicaffeoylquinic acid II	$C_{25}H_{24}O_{12}$	16.52	515.1194	515.1189	-0.599	353.0856
Dicaffeoylquinic acid III	$C_{25}H_{24}O_{12}$	18.59	515.1194	515.1187	-0.849	353.0856
3,4,5-Tricaffeoylquinic acid	$C_{34}H_{30}O_{15}$	18.57	677.1511	677.1505	-0.683	515.1172
Flavonoids						
Naringenin*	$C_{15}H_{12}O_5$	18.77	271.0611	271.0598	-1.357	151.0028
Naringenin chalcone*	$C_{15}H_{12}O_5$	18.95	271.0611	271.0610	-0227	151.0026
Naringenin 7-glucoside*	$C_{21}H_{22}O_{10}$	14.76	433.1140	433.1129	-1.140	271.0596
Naringenin chalcone hexose I	$C_{21}H_{22}O_{10}$	11.34	433.1140	433.1127	-1.320	271.0598
Naringenin chalcone hexose II	$C_{21}H_{22}O_{10}$	12.02	433.1140	433.1133	-0.680	271.0598
Naringenin dihexose I	$C_{27}H_{32}O_{15}$	7.98	595.1668	595.1660	-0.823	355.1008
Naringenin dihexose II	$C_{27}H_{32}O_{15}$	8.09	595.1668	595.1651	-1.743	355.1008
O-acetylprurin	$C_{23}H_{24}O_{11}$	17.72	475.1245	475.1237	-0.835	271.0597
Hesperetin*	$C_{16}H_{14}O_6$	19.1	301.0717	301.0716	-0.171	286.0466/242.0571
Eriodictyol	$C_{15}H_{12}O_6$	17.6	287.0561	287.0558	-0.291	151.0029
Eriodictyol chalcone	$C_{15}H_{12}O_6$	16.18	287.0561	287.0555	-0.571	151.0029
Homoeriodictyol	$C_{16}H_{14}O_6$	18.92	301.0717	301.0718	0.079	151/ 177/165/107/233
Eriodictyol-*O*-hexoside	$C_{21}H_{22}O_{11}$	12.42	449.1089	449.1086	-0.355	287.0547
Kaempferol*	$C_{15}H_{10}O_6$	19	285.0404	285.0400	-0.481	-
Dihydrokaempferol	$C_{15}H_{12}O_6$	18.19	287.0561	287.0558	-0.321	151.0029
Kaempferol-*O*-hexoside	$C_{21}H_{20}O_{11}$	10.54	447.0932	447.0925	-0.785	-
Kaempferol-*O*-rutinoside	$C_{27}H_{30}O_{15}$	14.38	593.1511	593.1512	-0.013	285.0389
Kaempferol-*O*-rutinoside-*O*-pentoside	$C_{32}H_{38}O_{19}$	13.06	725.1934	725.1927	-0.762	593.1485/284.0308
Kaempferol-*O*-rutinoside-hexoside	$C_{33}H_{40}O_{20}$	9.22	755.2040	755.2034	-0.647	593/285
Taxifolin*	$C_{15}H_{12}O_7$	10.94	303.0510	303.0504	-0.576	285.0384
Isorhamnetin 3-sophoroside I	$C_{28}H_{32}O_{17}$	12.2	639.1566	639.1560	-0.663	315.0510
Isorhamnetin 3-sophoroside II	$C_{28}H_{32}O_{17}$	12.83	639.1566	639.1561	-0.603	-
Quercetin *O*-hexoside	$C_{21}H_{20}O_{12}$	12.76	463.0881	463.0880	-0.219	301.0336
Quercetin*	$C_{15}H_{10}O_7$	17.99	301.0353	301.0351	-0.316	178.9981
Quercetin-3-*O*-rutinoside	$C_{27}H_{30}O_{16}$	12.58	609.1461	609.1466	0.502	301.0344/271.0239
Quercetin-*O*-dihexoside	$C_{27}H_{30}O_{17}$	10.41	625.1410	625.1403	-0.702	300.0260/271.0232/ 343.0440/
Quercitrin	$C_{21}H_{20}O_{11}$	14.65	447.0932	447.0929	-0.425	301.0341
Rutin pentoside	$C_{32}H_{38}O_{20}$	11.66	741.1883	741.1890	0.593	300.0268/ 609.1446

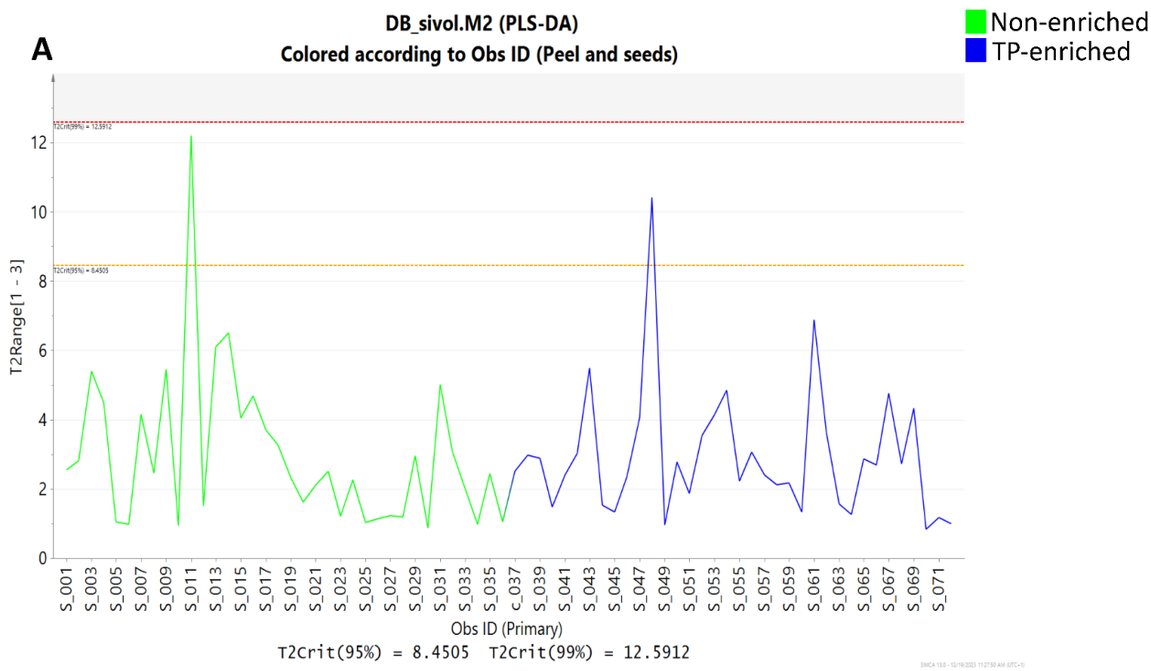
Quercetin-*O*-rutinoside-*O*-hexoside	$C_{33}H_{40}O_{21}$	7.87	771.1989	771.1985	-0.441	609.1445
Rutin*	$C_{27}H_{30}O_{16}$	12.56	609.1461	609.1466	0.502	301.0335
Luteolincat	$C_{15}H_{10}O_6$	18.07	285.0394	285.0394	-0.423	241.0491
Apigenin	$C_{15}H_{10}O_5$	18.86	269.0444	269.0453	0.322	225.0547
2-Methyl-6-methylene-2-octene-1,8-diol-8-*O*-(2,6-diacetyl-glucopyranoside)	$C_{20}H_{32}O_9$	13.8	415.1963	415.1969	0.601	-
Apigenin acetylhexoside	$C_{21}H_{30}O_{12}$	14.95	473.1654	473.1660	0.597	431.1520
Phloridzin-*C*-diglycoside	$C_{33}H_{44}O_{20}$	11.06	759.2353	759.2341	-1.247	-
Phloretin-*C*-dihexoside	$C_{27}H_{34}O_{15}$	13.93	597.1813	597.1829	1.463	357.0962/387.1068/477.1386

*Comparison with standard.

Supplementary information 2

Table S2. Model validation parameters.

Model type	Factor	R2X (cum)	R2Y (cum)	Q2 (cum)	*p*-value CV-ANOVA
PCA					
PLS-DA	TP-enrichment	0.638	0.993	0.988	0.000
OPLS-DA	Cooking technique	0.756	0.869	0.746	1.64E-30
OPLS-DA	Temperature	0.790	0.963	0.870	1.04E-18
OPLS-DA	Time	0.796	0.887	0.643	1.61E-07



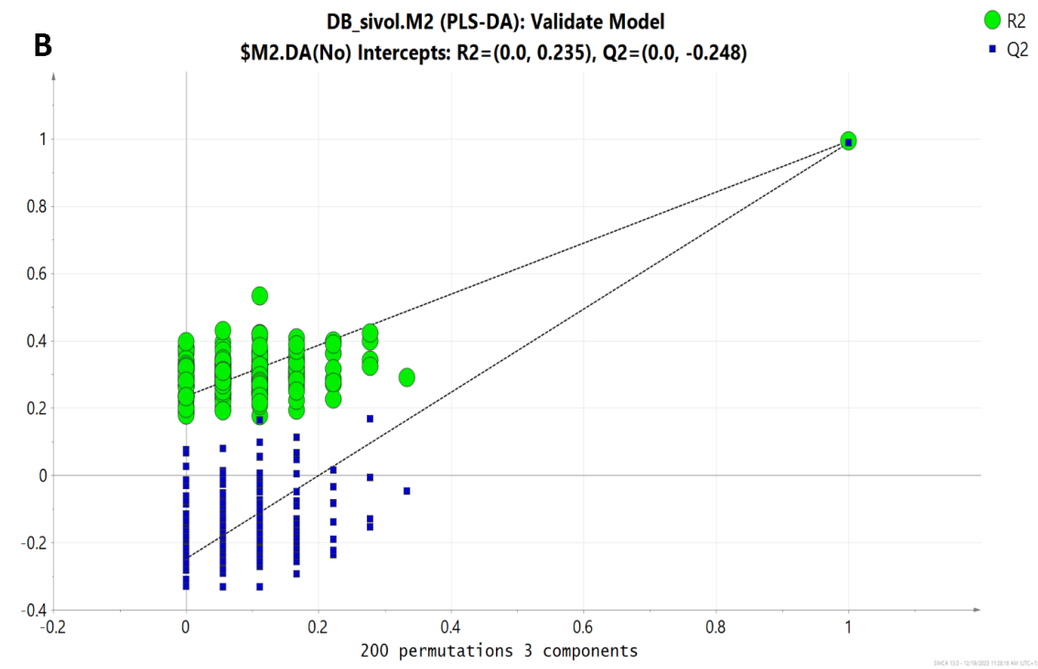


Figure S1. PLS-DA model using TP-enrichment as a factor A) Hotelling's T2, B) Residuals N-plot.

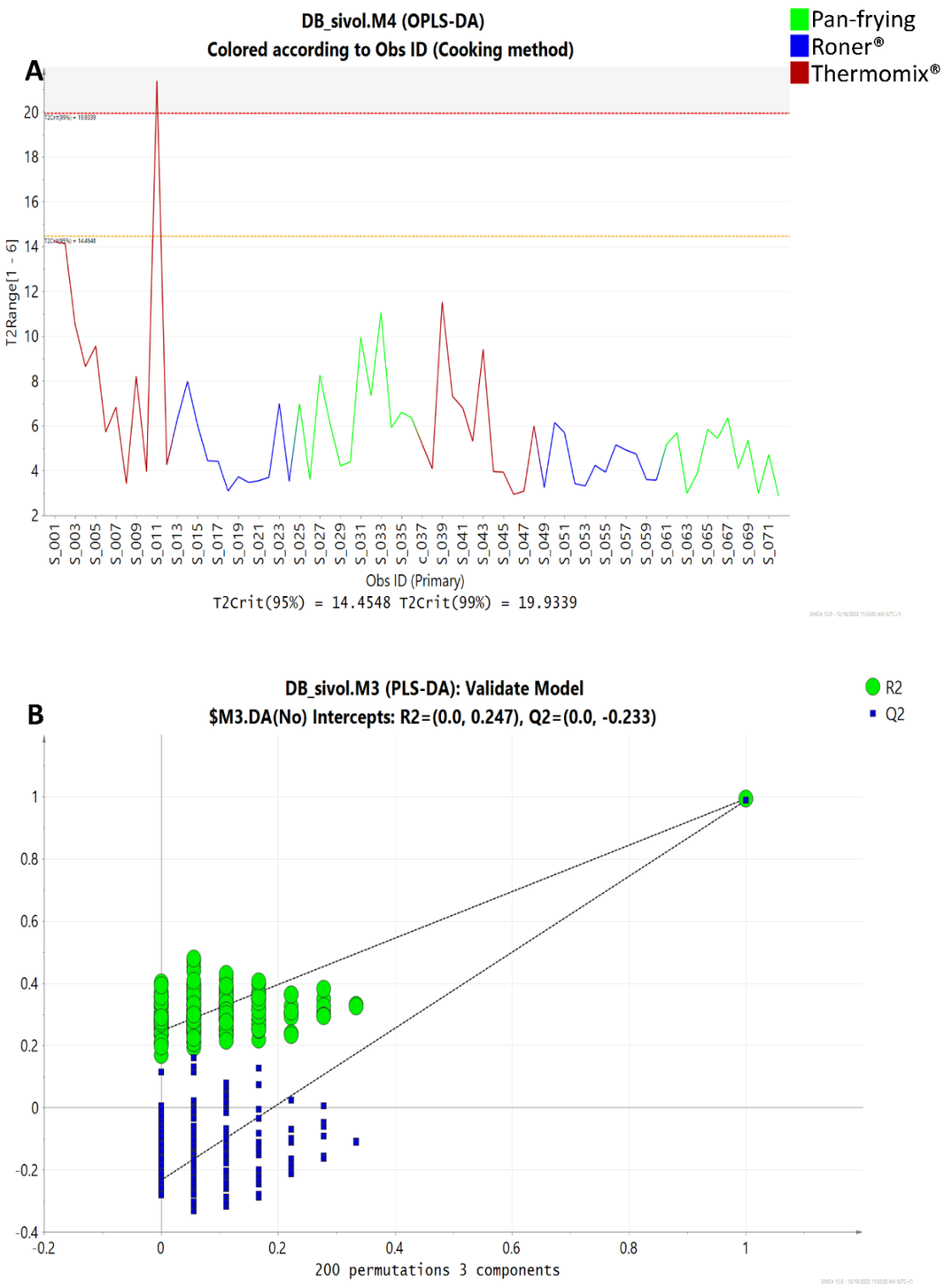
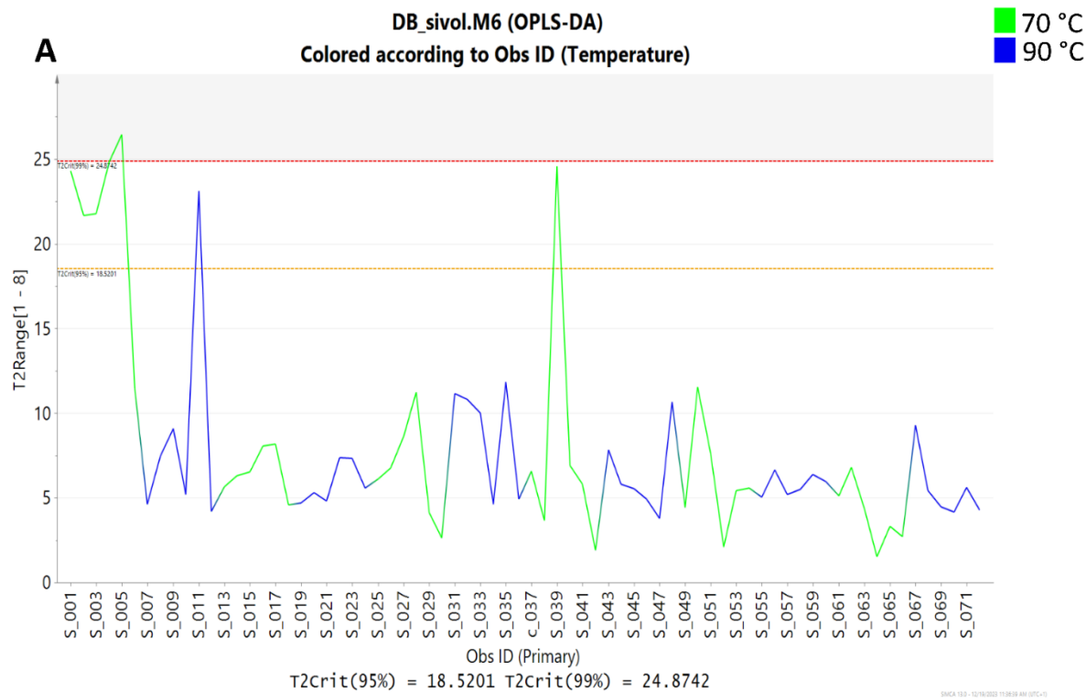


Figure S2. OPLS-DA model using cooking technique as a factor A) Hotelling's T2, B) Residuals N-plot.



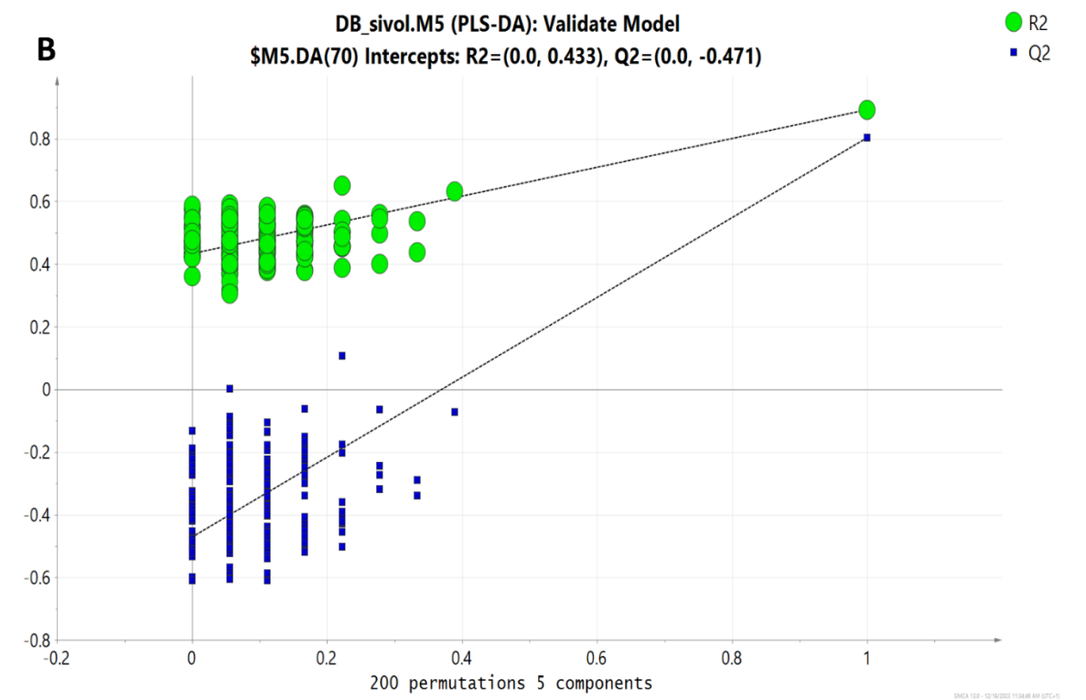


Figure S3. OPLS-DA model using temperature as a factor A) Hotelling's T2, B) Residuals N-plot.

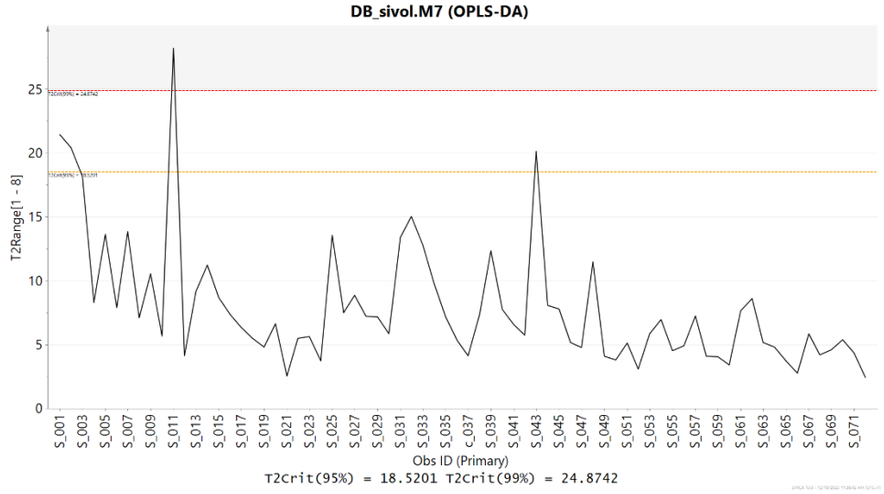


Figure S4. Hotelling's of the OPLS-DA model using time as a factor