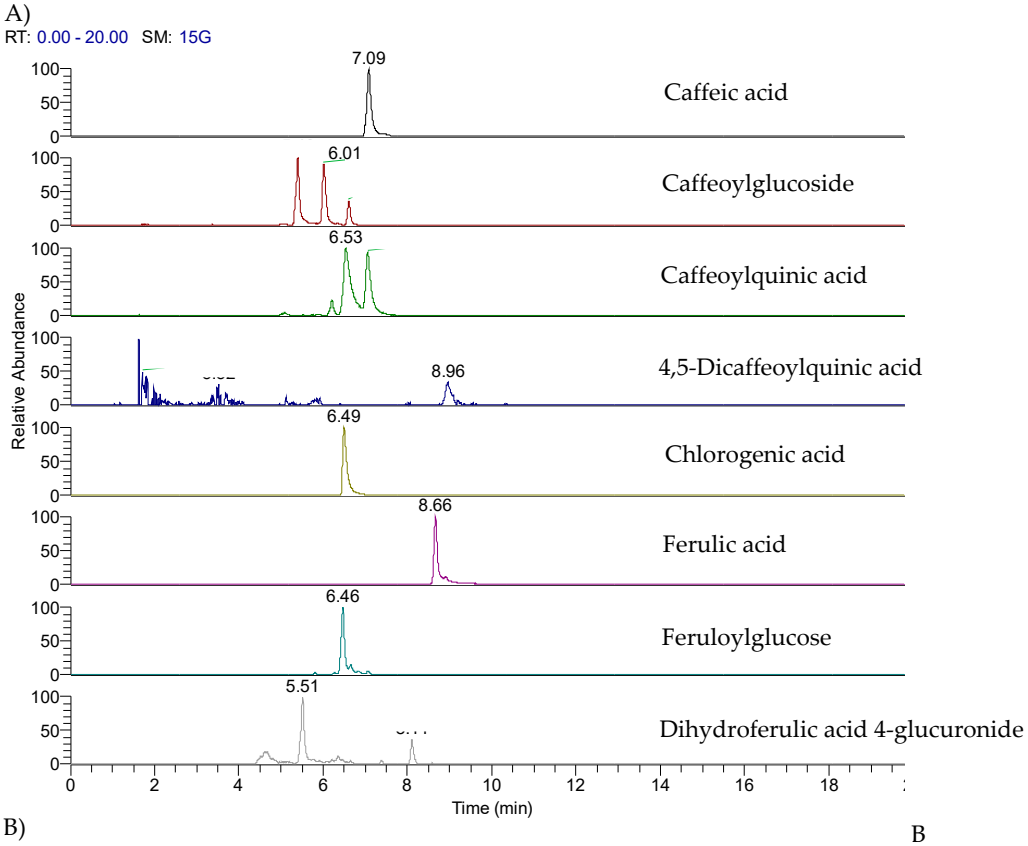
Table S1. LC-HRMS/MS characteristics of phenolic compounds in goji berries samples.

RT	Tentatively identification	Chemical Formula	[m/z] theoretical	[m/z] experimental	δ (ppm)	Product ion	MSI MI level[1]
7.1	Caffeic acid	C9H8O4	179.0349	179.035	6.506	135.0452 / 107.0504 / 90.9243	1
6.0	Caffeoylglucoside	C15H18O9	341.0878	341.0873	1.675	323.0768 / 179.0345 / 161.0239	2
6.2	Caffeoylquinic acid	C16H18O9	353.0878	353.0872	1.449	309.0974 / 179.0345 / 161.0239	2
9.0	4,5-Dicaffeoylquinic acid	C25H24O12	515.1194	515.1193	1.665	191.0563 / 173.0455 / 135.0452	1
6.5	Chlorogenic acid	C16H18O9	353.0878	353.0871	1.024	191.0563 / 135.0452 / 127.0402	1
8.6	Ferulic acid	C10H10O4	193.0506	193.0505	4.894	178.0273 / 149.0972 / 121.0659	1
5.5	Feruloylglucose	C16H20O9	355.1023	355.1024	0.173	193.0502 / 177.0193 / 161.0451	2
5.5	Dihydroferulic acid 4-glucuronide	C16H20O10	371.0983	371.098	2.012	195.0655 / 179.0344 / 59.0135	2
6.3	Dihydroisoferulic acid	C10H12O4	195.0662	195.0661	4.535	136.0531 / 121.0297 / 59.0139	2
8.3	Dihydroferulic acid	C10H12O4	195.0662	195.0661	4.535	136.0531 / 121.0297 / 59.0139	1
8.3	p-coumaric acid	C9H8O3	163.04	163.0399	5.455	121.0522 / 119.0503 / 93.0344	1
6.2	Coumaroylglucoside	C15H18O8	325.0929	325.0928	3.002	197.0271 / 164.0424 / 121.0523	2
6.3	Coumaroyl dihexoside	C21H28O13	487.1457	487.1453	1.443	487.1455 / 164.0424 / 119.0503	2
8.6	Sinapic acid	C11H12O5	223.0611	223.0612	4.923	208.0379 / 193.1045 / 93.0347	1
6.7	Sinapoyl hexoside	C17H22O10	385.114	385.1133	1.004	223.0539 / 205.0494 / 190.0241	2
7.5	Rutin	C27H30O16	609.1461	609.1454	0.622	300.0276 / 271.0246 / 243.0296	1
7.3	Quercetin rutinoside (Rutin isomer)	C27H30O16	609.1461	609.1459	1.525	300.0276 / 271.0246 / 243.0296	2
5.2	Rutin hexoside	C33H40O21	771.1989	771.1993	1.952	301.0335 / 300.0275 / 178.9999	2
7.9	Quercetin 3-glucoside (Isoquercitrin)	C21H20O12	463.0881	463.0878	1.442	300.0275 / 271.0245 / 255.0303	1
8.0	Kaempferol rutinoside	C27H30O15	593.1511	593.1509	1.321	285.0406 / 227.035 / 183.0449	2
8.1	Isorhamnetin rutinoside	C28H32O16	623.1617	623.1617	1.731	315.051 / 299.0197 / 271.0249	2
8.5	Isorhamnetin glucoside	C22H22O12	477.1038	477.1034	1.273	314.0435 / 285.0407 / 199.0409	2
8.7	Taxifolin	C15H12O7	303.051	303.0509	3.402	285.0407 / 175.0408 / 125.0246	1
11.8	Apigenin	C15H10O5	269.0455	269.0455	3.903	57.8443 / 64.8013 / 65.6261	1
8.1	Apigenin rutinoside	C27H30O14	577.1563	577.1558	1.106	269.0451 / 161.0451 / 145.0503	2
12.1	Diosmetin	C16H12O6	299.0561	299.0562	3.797	284.0327 / 133.0295 / 63.0241	1
11.7	Naringenin	C15H12O5	271.0612	271.0612	3.911	177.0195 / 151.0039 / 119.0504	1

9.3	Naringenin 6-glucoside	C21H22O10	433.114	433.1139	2.232	271.0617 / 151.0042 / 119.0504	2
9.0	Narirutin	C27H32O14	579.1719	579.1726	3.07	271.0617 / 151.004 / 119.505	1
6.7	Narirutin glucoside	C33H42O19	741.2247	741.2233	-0.52	433.1145 / 271.0617 / 151.004	2
10.5	Eriodyctiol	C15H12O6	287.0561	287.056	3.433	151.0038 / 135.0453 / 107.0138	1
11.6	Phloretin	C15H14O5	273.0768	273.0769	4.101	167.0352 / 123.0452 / 93.0359	1
9.0	Phloridzin	C21H24O10	435.1296	435.1288	0.475	273.0772 / 167.0352 / 123.0452	1

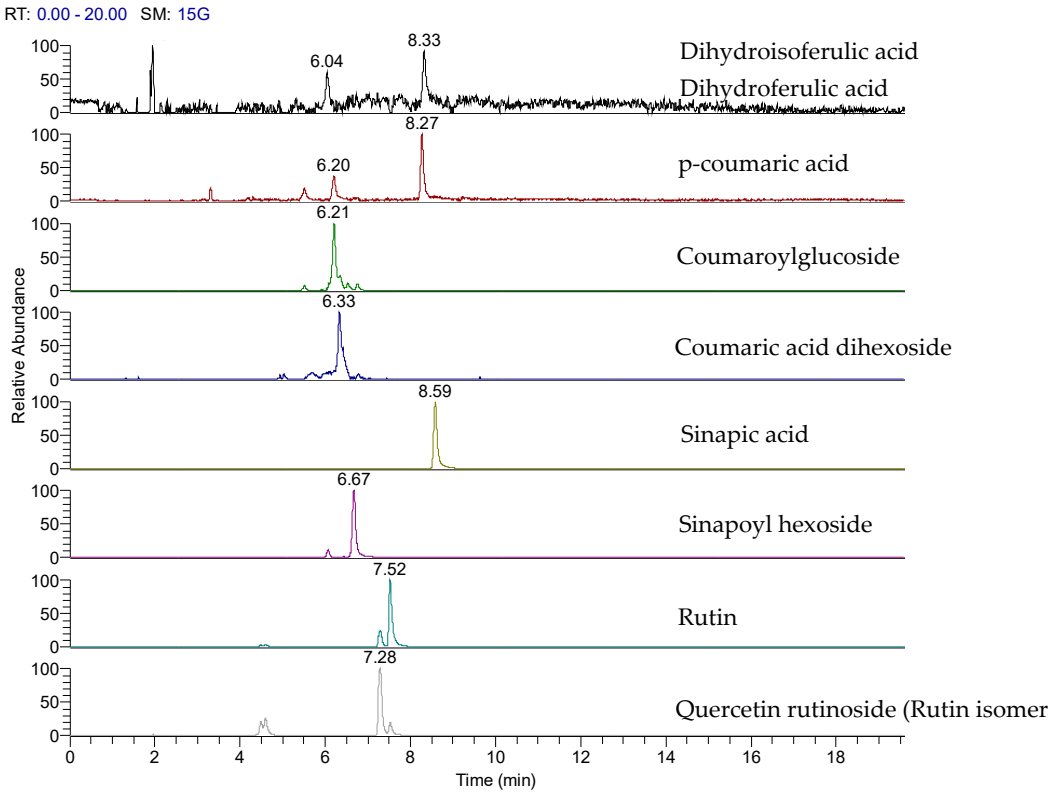
RT: Retention time. **δ**: Mass error. [1]Metabolite Standards Initiative metabolite identification (MSIMI) levels. Reference compounds were available for all compounds identified at MSIMI level 1. Compounds at MSIMSI level 2 were tentatively identified.

A)


RT: 0.00 - 20.00 SM: 15G
Relative Abundance
Time (min)
7.09
Caffeic acid
6.01
Caffeoylglucoside
6.53
Caffeoylquinic acid
8.96
4,5-Dicaffeoylquinic acid
6.49
Chlorogenic acid
8.66
Ferulic acid
6.46
Feruloylglucose
5.51
Dihydroferulic acid 4-glucuronide

B)

B


RT: 0.00 - 20.00 SM: 15G
Relative Abundance
Time (min)
8.33
6.04
Dihydroisoferulic acid
Dihydroferulic acid
8.27
6.20
p-coumaric acid
6.21
Coumaroylglucoside
6.33
Coumaric acid dihexoside
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Sinapic acid
6.67
Sinapoyl hexoside
7.52
Rutin
7.28
Quercetin rutinoside (Rutin isomer

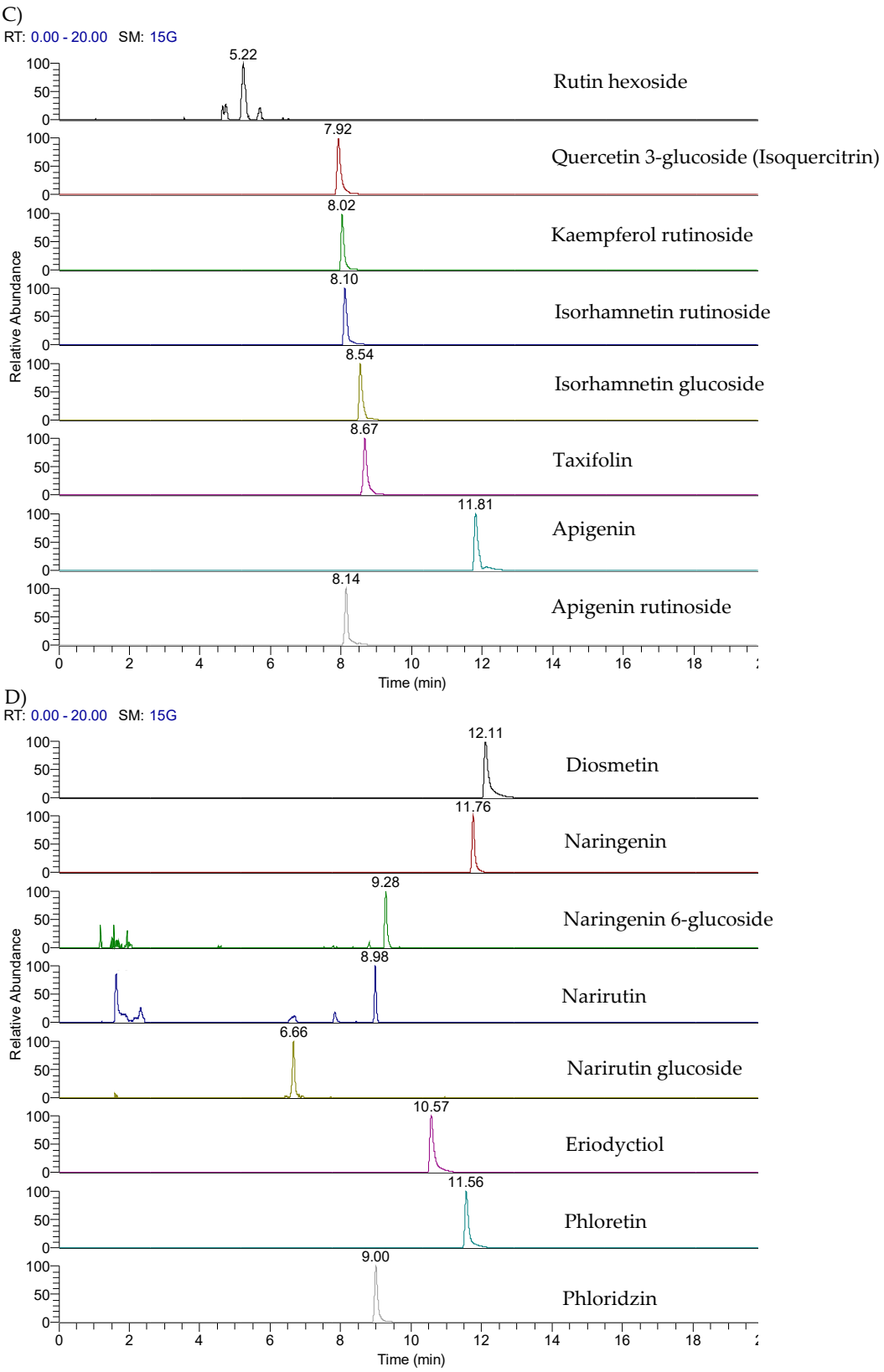

Figure S1 A-D. HPLC-HRMS/MS chromatograms of the phenolic compounds.

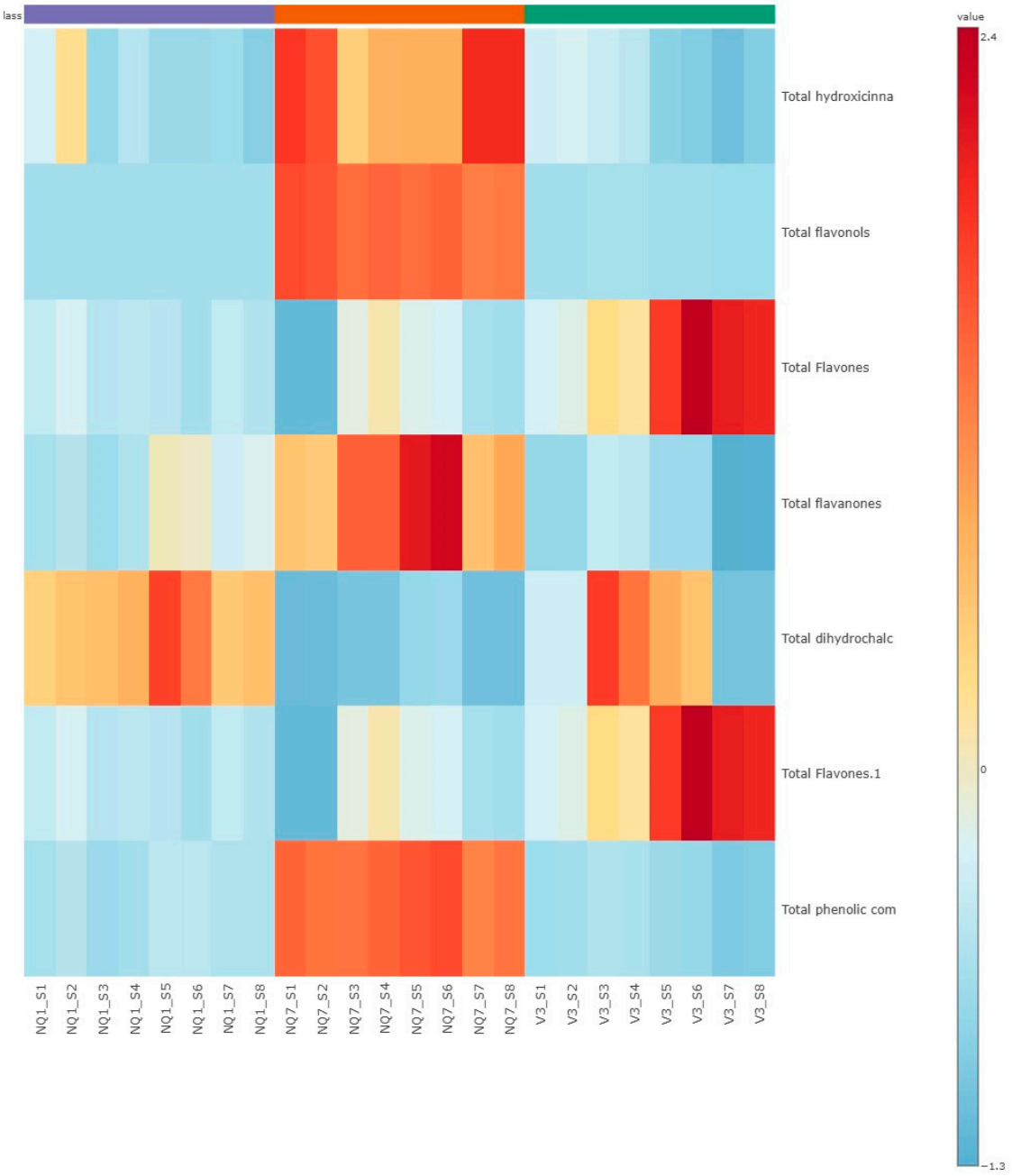

Figure S2. Heatmap showing the concentration of phenolic compounds families from goji berry samples.

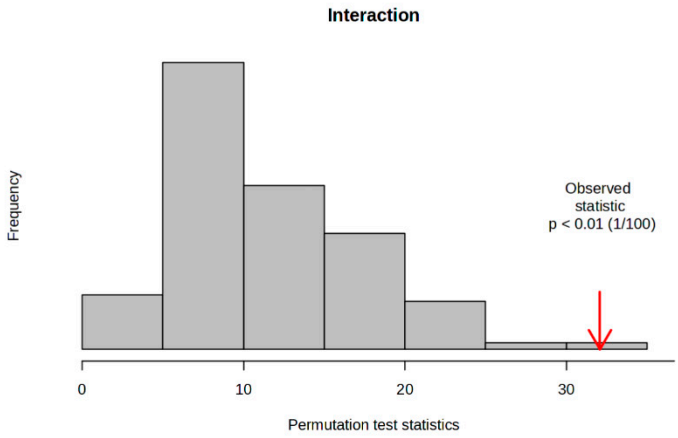

Figure S3. Permutation test (100 iterations) for the ASCA interaction model.

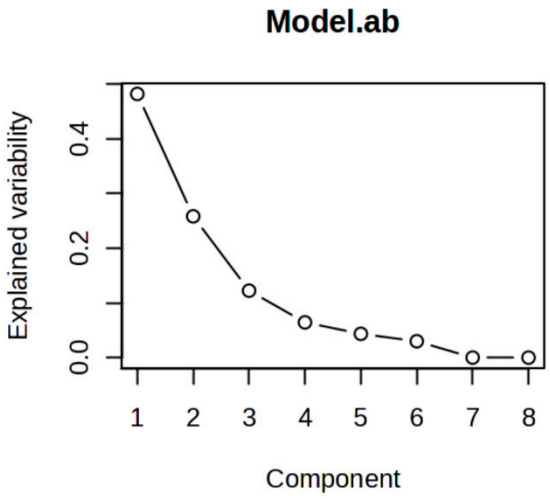

Figure S4. Scree plot of the ASCA interaction model.

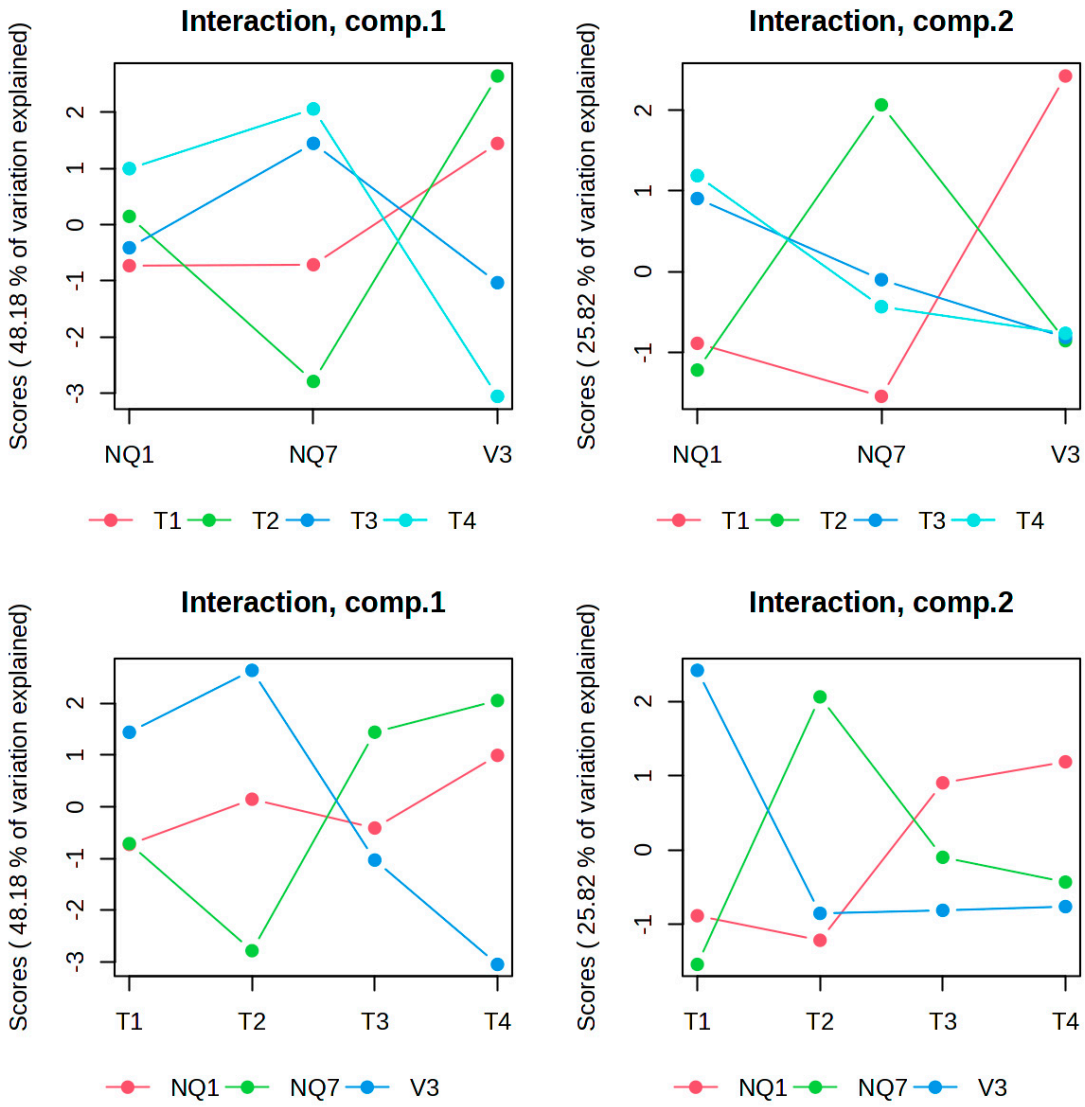

Figure S5. Major interaction patterns from the ASCA model.