

Supplementary Material

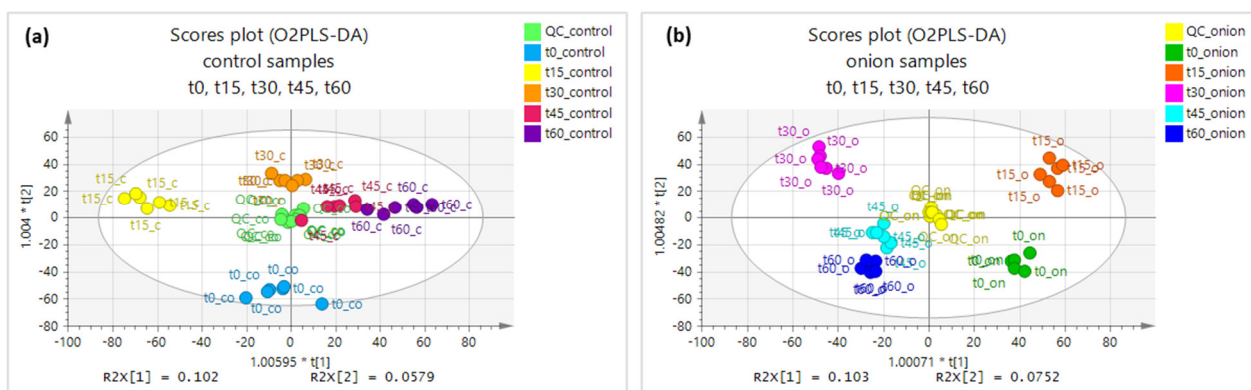


Figure S1: Score plot O2PLS-DA of (a) control samples and (b) onion samples at five time points (t0, t15, t30, t45, t60) with their corresponding QC samples using UV scaling in positive ionization mode.

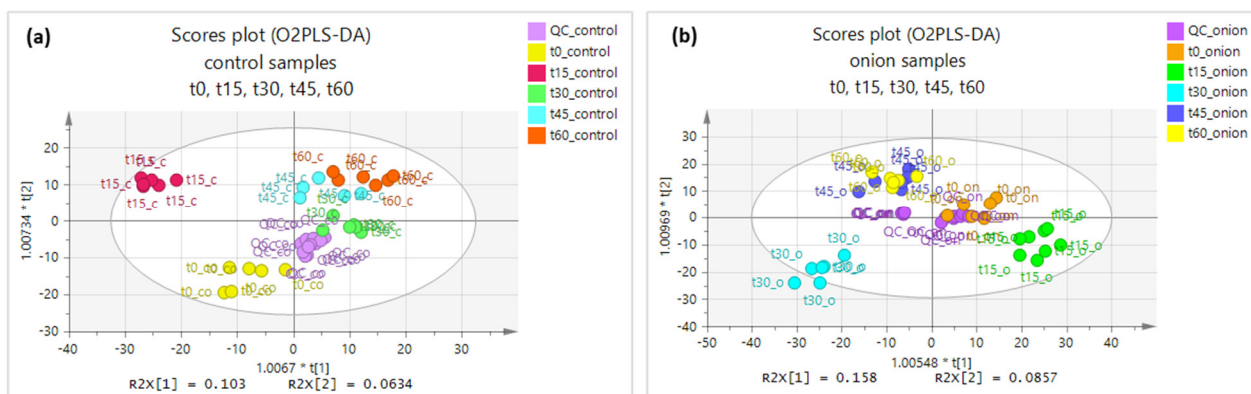


Figure S2: Score plot O2PLS-DA of (a) control samples and (b) onion samples at five timepoints (t0, t15, t30, t45, t60) with their corresponding QC samples using UV scaling in negative ionization mode.

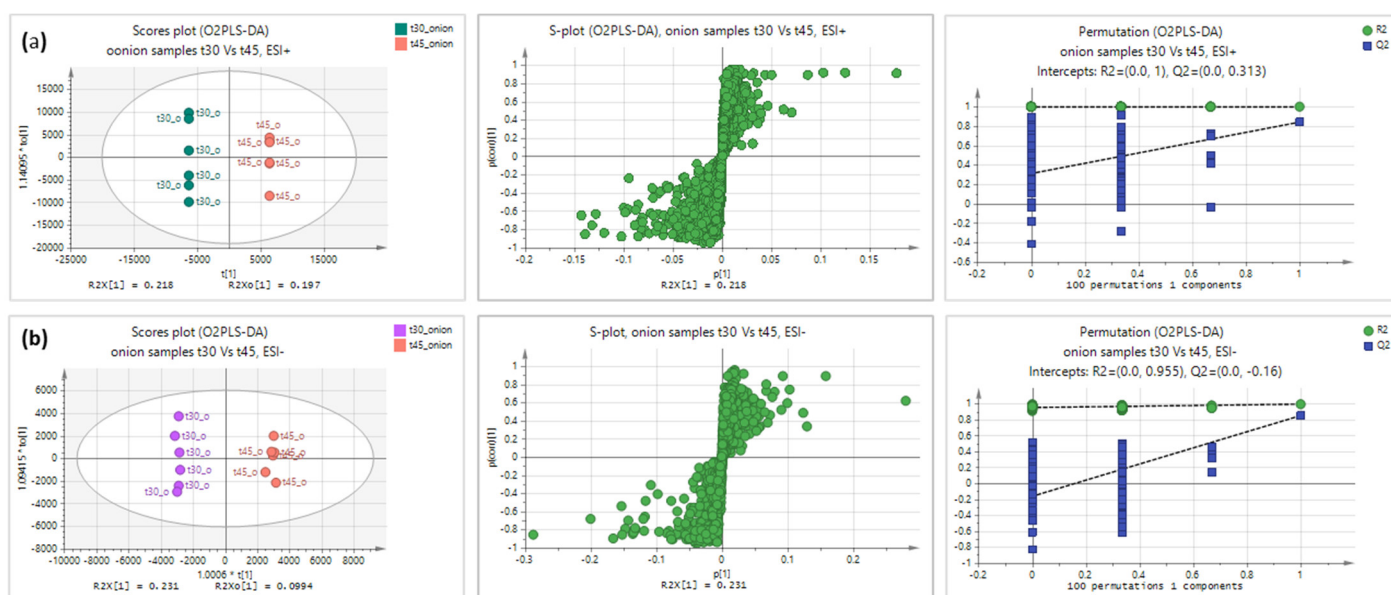


Figure S3: Score plot O2PLS-DA discrimination using pareto scaling, S-Plot, and permutation testing for onion samples at t30 vs. t45 in (a) positive ionization mode and (b) negative ionization mode.

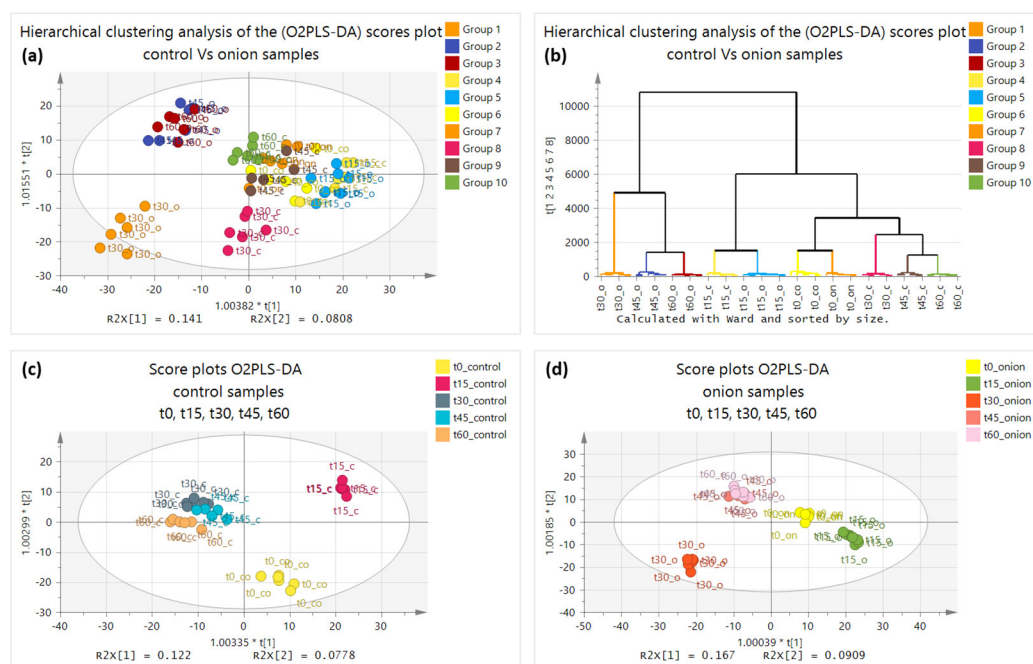


Figure S4: Plots of O2PLS-DA and hierarchical clustering analysis: (a) score plots of control and onion samples (b) hierarchical clustering analysis O2PLS-DA of control and onion samples; score plot O2PLS-DA discrimination between (c) control samples and (d) onion samples at five timepoints (t0, t15, t30, t45, t60) using UV scaling in negative ionization mode.

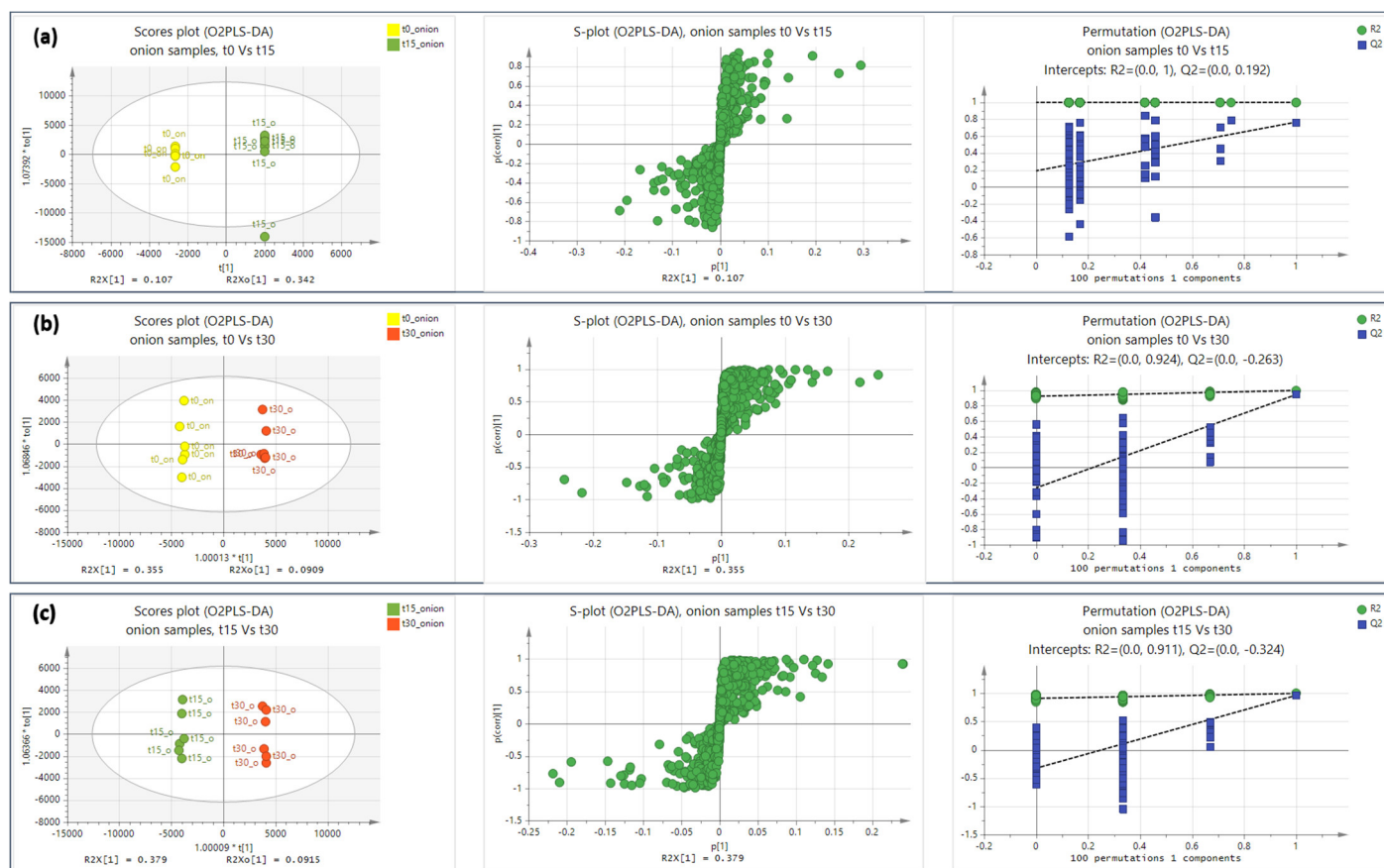


Figure S5: Score plot O2PLS-DA discrimination using pareto scaling, S-Plot, and permutation testing for onion samples at (a) t0 vs. t15, (b) t0 vs. t30, and (c) t15 vs. t30 in negative ionization mode.

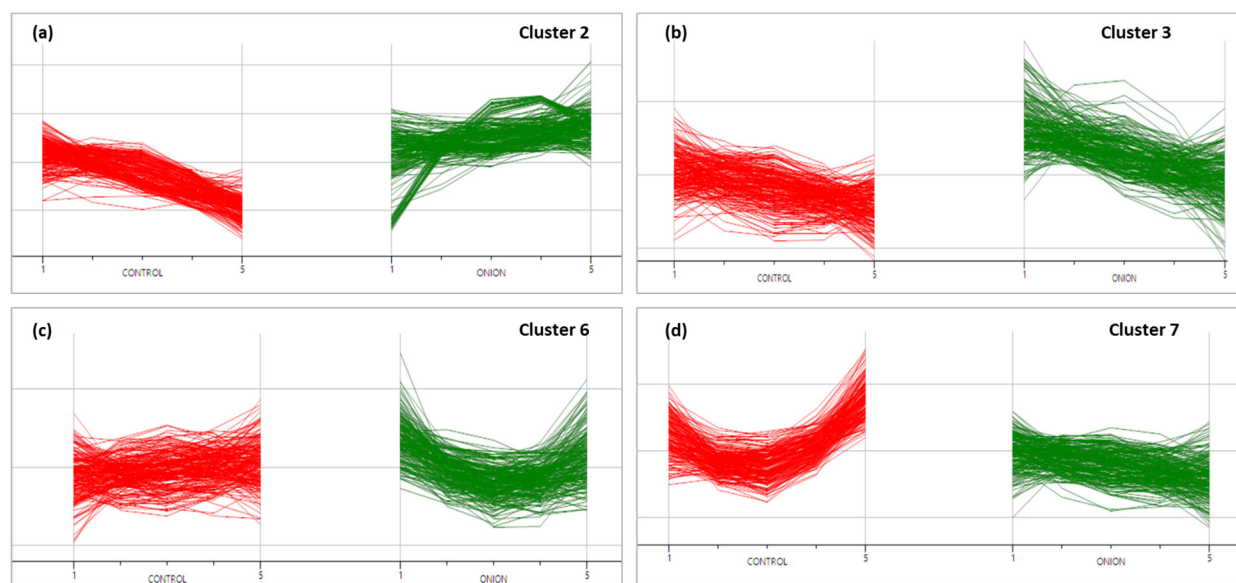


Figure S6: Examples of compound clustering between control (in red) and onion samples (in green) in positive ionization mode using MetaboClust: (a) Cluster 2, (b) Cluster 3, (c) Cluster 6, and (d) Cluster 7.

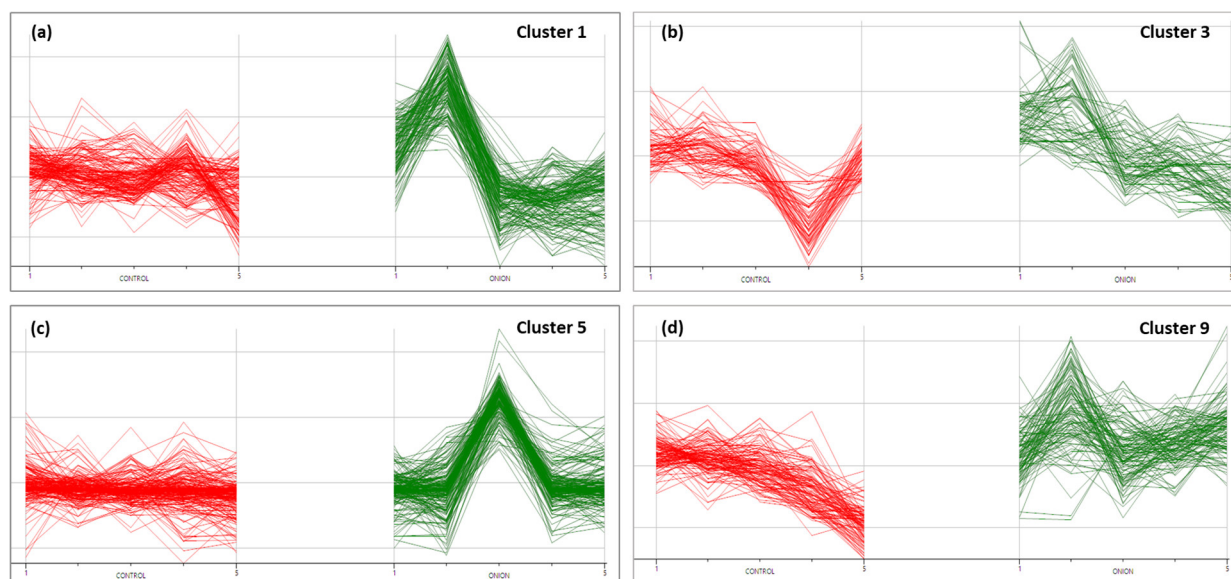


Figure S7: Examples of compound clustering between control (in red) and onion samples (in green) using MetaboClust: (a) Cluster 1, (b) Cluster 3, (c) Cluster 5, and (d) Cluster 9 in negative ionization mode.

Table S1. Performance characteristics of each classification model in **positive** ionization mode

Investigated samples	R ² (Y)	Q ²	p-values	Permutation values		Fisher's probabilities
				R ²	Q ²	
Controls and Onions: t0, t15, t30, t45, t60	0.532	0.391	1.97 ×10 ⁻⁵	0.349	-0.207	0
Controls: t0, t15, t30, t45, t60	0.973	0.572	1.46 ×10 ⁻⁴	0.909	-0.179	8.8×10 ⁻¹⁷
Onions: t0, t15, t30, t45, t60	0.985	0.671	1.28 ×10 ⁻⁶	0.925	-0.231	8.8×10 ⁻¹⁷
t0 onion, t15 onion	1	0.897	1.54 ×10 ⁻¹	1	0.37	0.0022
t0 onion, t30 onion	0.997	0.948	5.52 ×10 ⁻⁴	0.909	-0.285	0.0022
t15 onion, t30 onion	0.999	0.938	1.48 ×10 ⁻³	0.991	-0.135	0.0011

Table S2. Performance characteristics of each classification model in **negative** ionization mode

Investigated samples	R ² (Y)	Q ²	p-values	Permutation values		Fisher's probabilities
				R ²	Q ²	
Controls and Onions: t0, t15, t30, t45, t60	0.791	0.458	2.27 ×10 ⁻³	0.514	-0.319	0
Controls: t0, t15, t30, t45, t60	0.971	0.655	5.27 ×10 ⁻⁴	0.877	-0.239	6.1 ×10 ⁻¹⁶
Onions: t0, t15, t30, t45, t60	0.973	0.755	4.70×10 ⁻¹⁰	0.889	-0.265	9.9 ×10 ⁻¹⁹
t0 onion, t15 onion	1	0.767	3.79 ×10 ⁻¹	1	0.192	0.00033
t0 onion, t30 onion	0.998	0.946	1.60 ×10 ⁻⁴	0.924	-0.263	0.0011
t15 onion, t30 onion	0.999	0.964	3.82×10 ⁻⁵	0.911	-0.324	0.0023