

A. Metabolomics PLS-DA by Temperature and Day

This PLS-DA score plot displays the relationship between temperature and day on the first two principal components. The x-axis, 'Component 1: 12% Explained Variance', ranges from -5 to 10. The y-axis, 'Component 2: 12% Explained Variance', ranges from -5 to 5. Samples are categorized by temperature: 15°C (blue), 20°C (red), and 25°C (grey). Within each temperature group, samples are further distinguished by day (indicated by different markers). The plot shows a clear separation along Component 1, with 15°C samples clustered on the left (negative values), 20°C samples in the middle-right (positive values), and 25°C samples clustered on the left (negative values). Component 2 separates samples by day within each temperature group.

Heatmap of Spearman correlation coefficients between ME variables. The color scale ranges from -0.5 (blue) to 0.5 (red). The diagonal is white (1.0). The matrix is symmetric. The variables are ME6, ME7, ME4, ME8, ME5, ME0, ME1, ME3, and ME2. A dendrogram on the left shows the hierarchical clustering of these variables.

	ME6	ME7	ME4	ME8	ME5	ME0	ME1	ME3	ME2
ME6	1.000	0.9	0.7	0.1	0.2	0.8			
ME7	0.002	1.000	0.3	0.01	0.3	0.3			
ME4	0.1	0.6	1.000	0.04	0.07				
ME8	0.2	0.3	0.04	1.000	0.4				
ME5	0.06	0.3	0.07	0.4	1.000				
ME0	0.8	0.3				1.000			
ME1						0.03	1.000		
ME3						0.03	0.001	1.000	
ME2						0.6	0.7	0.1	1.000

A PCA plot showing the relationship between Component 1 (27% Explained Variance) on the x-axis and Component 2 (19% Explained Variance) on the y-axis. The plot displays three distinct clusters of data points, each represented by a different color: black, blue, and red. Each cluster consists of multiple points, and lines connect each point to a central point within its respective cluster. The black cluster is located in the upper-left quadrant, the blue cluster is in the lower-left quadrant, and the red cluster is in the upper-right quadrant. The axes range from -20 to 20 on the x-axis and -20 to 30 on the y-axis.

Heatmap showing Spearman correlation coefficients between 15 MEs (rows) and three sets of variables (columns). The MEs are clustered on the left. The color scale ranges from -1 (blue) to 1 (red).

ME	Variable Set 1	Variable Set 2	Variable Set 3
ME1	0.02	1	0.005
ME7	0.005	0.8	0.003
ME2	0.002	0.9	2e-04
ME12	0.002	0.1	0.08
ME10	2e-04	0.2	0.007
ME4	1e-05	0.8	2e-08
ME5	0.5	0.1	0.007
ME8	0.1	0.1	4e-04
ME9	0.09	0.02	9e-07
ME0	0.3	0.03	0.2
ME11	0.2	0.001	0.03
ME13	0.3	0.3	0.9
ME15	0.5	0.5	0.1
ME14	0.3	0.7	0.09
ME6	0.4	0.1	0.003
ME3	0.8	7e-05	3e-07