TargetedMetaCorePeakTable\_wo\_peakid\_Analysis\_1

# MetaboAnalyst 網頁狀態回饋:

Data Integrity Check:  
Checking sample names - spaces will replaced with underscore, and special characters will be removed;  
Checking the class labels - at least three replicates are required in each class.  
The data (except class labels) must not contain non-numeric values.  
If the samples are paired, the pair labels must conform to the specified format.  
The presence of missing values or features with constant values (i.e. all zeros).  
Data processing information:  
Checking data content ...passed.  
Samples are in columns and features in rows.  
The uploaded file is in comma separated values (.csv) format.  
The uploaded data file contains 6 (samples) by 82 (peaks(mz/rt)) data matrix.  
Samples are not paired.  
2 groups were detected in samples.  
Only English letters, numbers, underscore, hyphen and forward slash (/) are allowed.  
Other special characters or punctuations (if any) will be stripped off.  
All data values are numeric.  
No missing values were detected. Click the Proceed button to the next step.  
Data processing information:  
Checking data content ...passed.  
Samples are in columns and features in rows.  
The uploaded file is in comma separated values (.csv) format.  
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No missing values were detected. Click the Proceed button to the next step.  
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Other special characters or punctuations (if any) will be stripped off.  
All data values are numeric.  
  
No missing values were detected. Click the Proceed button to the next step.  
Edit Groups  
Proceed  
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Proceed

# LLM檢測分析之結果:

Okay, I'm ready to analyze the MetaboAnalyst output you've provided. Here's a report explaining the data, focusing on the volcano plot and the concepts behind it, presented in a numbered bullet-point format.  
  
\*\*Metabolomics Data Analysis Report – Volcano Plot Interpretation\*\*  
  
1. \*\*Overview of the Volcano Plot:\*\* The image you sent is a volcano plot. This is a common visualization tool in metabolomics (and other 'omics fields) used to display the results of differential metabolite analysis. It simultaneously shows both the \*statistical significance\* and the \*magnitude of change\* (fold change) between two or more groups.  
  
2. \*\*Axes Explanation:\*\*  
 \* \*\*X-axis (Features):\*\* Represents the individual metabolites (or 'features') identified in your experiment. Each dot corresponds to one metabolite. They are numbered sequentially, from 1 to 85 in this case.  
 \* \*\*Y-axis (-log10(raw P-value)):\*\* This represents the statistical significance of the difference in abundance for each metabolite. The negative logarithm (base 10) of the p-value is used because p-values are often very small numbers, making them difficult to visualize on a standard linear scale. A higher value on this axis indicates a more statistically significant difference.  
  
3. \*\*Understanding P-values:\*\*  
 \* A \*\*p-value\*\* is the probability of observing the results you obtained (or more extreme results) \*if there is actually no real difference\* between the groups being compared. In simpler terms, it tells you how likely it is that your observed differences are due to random chance.  
 \* A small p-value suggests that the observed differences are unlikely to be due to chance, and therefore there is evidence of a real effect.  
 \* The standard threshold for statistical significance is \*\*p < 0.05\*\*. This means there is less than a 5% probability that the observed results are due to random chance.  
  
4. \*\*Significance Threshold & -log10(P-value):\*\*  
 \* When we use -log10(p-value), a p-value of 0.05 corresponds to -log10(0.05) ≈ 1.3. Therefore, metabolites with a -log10(p-value) \*greater than 1.3\* are generally considered statistically significant at the 0.05 level.  
 \* More stringent thresholds (e.g., p < 0.01, corresponding to -log10(0.01) ≈ 2.0) are often used to reduce the risk of false positives.  
  
5. \*\*Fold Change (Not Directly Shown, but Implied):\*\* While the plot doesn't \*directly\* show fold change, the position of the dots along the x-axis \*implies\* the magnitude of the change. Metabolites further to the right (positive x-values) are more increased in abundance in the group being compared, while those further to the left (negative x-values) are more decreased. The further from the center (x=0), the larger the fold change. MetaboAnalyst typically uses fold change calculations alongside the p-values.  
  
6. \*\*Interpreting the Plot – Significant Metabolites:\*\*  
 \* \*\*Purple Dots:\*\* These represent metabolites that are considered \*statistically significant\* (based on the p-value threshold). In your plot, these are the metabolites with a -log10(p-value) above approximately 1.3. There are 4 metabolites identified as significant.  
 \* \*\*Gray Dots:\*\* These represent metabolites that are \*not statistically significant\* (p-value > 0.05).  
  
7. \*\*Focusing on Significant Metabolites:\*\* The most important metabolites to investigate further are those in the upper right and upper left quadrants of the plot.  
 \* \*\*Upper Right:\*\* Metabolites that are significantly \*increased\* in abundance.  
 \* \*\*Upper Left:\*\* Metabolites that are significantly \*decreased\* in abundance.  
  
8. \*\*Multiple Testing Correction:\*\* The plot shows "raw P-value". In metabolomics, we often analyze many metabolites simultaneously. This increases the chance of finding false positives (Type I error). Therefore, it's crucial to apply \*multiple testing correction\* methods (like Benjamini-Hochberg FDR correction, often used in MetaboAnalyst) to adjust the p-values and control for this. The plot shows the corrected p-value.  
  
9. \*\*Next Steps:\*\* Based on this volcano plot, you should:  
 \* Identify the specific metabolites corresponding to the significant purple dots.  
 \* Determine the fold change for each of these metabolites to understand the magnitude of the difference.  
 \* Investigate the biological pathways these metabolites are involved in to gain insights into the underlying mechanisms driving the observed changes.  
  
  
  
Let me know if you'd like me to elaborate on any of these points, or if you have additional data from MetaboAnalyst (e.g., pathway analysis results) that you'd like me to analyze.

# 圖片結果顯示:









