

Validation Rules for Input Data

1. Missing Metabolite Names

Validation Rule: If any row in the first column (the "Metabolite name" field) is empty or contains a null value, it will be considered an "invalid data row."

Action:

Display a warning message (e.g., "Row X is missing a metabolite name and will appear as 'empty name' in MetaboAnalyst"). Users are advised to either fill in the missing name or delete the blank row.

2. Incorrect Group Order Affecting Fold Change Calculation

Validation Rule: If the dataset includes two groups (e.g., Control vs. GeneKO), and the expected comparison direction is GeneKO / Control, but alphabetical sorting causes the actual comparison to be Control / GeneKO, this is treated as an "incorrect group order."

Action:

If the user specifies that fold change should be used, then verify whether the group order is correct. If not specified, skip this validation.

3. No Apparent Issues

If no issues are detected during the validation, output "Pass".