

# How to perform Outlier Detection Analysis in our platform?

CLOVER MS Data Analysis Software

## What is it?

Sample Name	PCA Reconstruction Test	Spectra Correlation Test	Outlier Level
Pseudomonas_D1_12113966_0_C9_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C9_2	Likely to be Outlier	Outlier	●●●●○
Pseudomonas_D1_12113966_0_C10_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_2	Outlier	Outlier	●●●●●

In Clover Biosoft, the **Outlier Detection** module identifies outliers that are presented in the dataset. An **outlier** is an extreme value in a dataset that lies an abnormal distance from other values (either much larger or much smaller from the overall pattern of the data). Identifying and handling outliers is important in data analysis to ensure that they do not unduly influence statistical measures and model performance.

## 1 First steps

*This guide is the same for MALDI and FTIR spectra*

The screenshot shows the software interface with the 'Bio Analysis' section selected. The 'Outlier Detection' module is highlighted with a green box and a '1' icon. Below the interface, a flowchart shows the steps: 'Go to the Bio Analysis section and click on Outlier Detection' (2), 'Choose a Study' (3), and 'Choose an Experiment' (4).

Go to the **Bio Analysis** section and click on **Outlier Detection** → Choose a **Study** → Choose an **Experiment**

## 2 Outlier Detection Results

**Summary Table.** A list of the potential outliers tested by two different analyses: PCA Reconstruction and Spectra Correlation tests

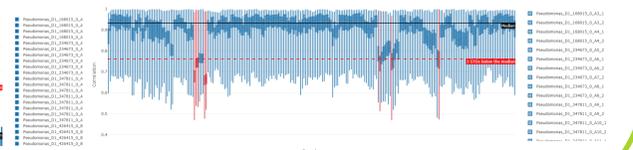
Tip: Select desired spectra on the table and click the "Mark as Outlier" link to persist them as detected outliers in the experiment

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Pseudomonas_D1_12113966_0_C10_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_2	Outlier	Outlier	●●●●●
Pseudomonas_D1_16226119_0_H9_2	Likely to be Outlier	Outlier	●●●●○
Pseudomonas_D1_16239464_0_A2_2	Outlier	Outlier	●●●●○
Pseudomonas_D1_16279539_0_B5_2	Likely to be Outlier	Outlier	●●●●○
Pseudomonas_D1_16279539_0_C10_2	Outlier	Outlier	●●●●○
Pseudomonas_D1_16281818_0_H10_2	Outlier	Outlier	●●●●○

PCA Reconstruction



Spectra Correlation



## 3 Tips for Outlier Detection

- The **eye icon** allows us to visualize the spectra per sample.
- We consider a replicate/sample as an outlier if **both tests (PCA Reconstruction & Spectra Correlation)** detect it as an outlier (in red).
- Select those outliers and **mark them as outliers**.
- Outliers will be **removed** from your experiment. You can check them in the **transformation pipeline** in the experiment view section.

Sample Name	PCA Reconstruction Test	Spectra Correlation Test	Outlier Level
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Pseudomonas_D1_12113966_0_C9_2	Likely to be Outlier	Outlier	●●●●○
Pseudomonas_D1_12113966_0_C10_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_2	Outlier	Outlier	●●●●●
Pseudomonas_D1_16226119_0_H9_2	Likely to be Outlier	Outlier	●●●●○
Pseudomonas_D1_16239464_0_A2_2	Outlier	Outlier	●●●●○
Pseudomonas_D1_16279539_0_B5_2	Outlier	Outlier	●●●●○

Experiment

Study: Pseudomonas aeruginosa Outbreak

Name: Test

Description: -

Created by: Training Clover [training@cloverbiosoft.com] at: 13-02-2024 11:04:51 GMT+1

242 files

Spectra Visualizer

Metadata

Transformation Pipeline

You can chain several actions to transform the spectra included in the experiment. The resulting output spectra will be used in the rest of analysis within this experiment

Input: 242 spectra across 242 files

Outlier Analysis

Output: 238 Spectra

Detail:

- Pseudomonas\_D1\_12113966\_0\_C10\_1
- Pseudomonas\_D1\_12113966\_0\_C12\_1
- Pseudomonas\_D1\_12113966\_0\_C12\_2
- Pseudomonas\_D1\_12113966\_0\_C9\_1



You can perform an Outlier Analysis **before grouping replicates or after that.**



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## What is it?

	Sample Name	PCA Reconstruction Test	Spectra Correlation Test	Outlier Level
<input type="checkbox"/>	Pseudomonas_D1_12113966_0_C9_1	Outlier	Outlier	●●●●●
<input type="checkbox"/>	Pseudomonas_D1_12113966_0_C9_2	Likely to be Outlier	Outlier	●●●●○
<input checked="" type="checkbox"/>	Pseudomonas_D1_12113966_0_C10_1	Outlier	Outlier	●●●●●
<input type="checkbox"/>	Pseudomonas_D1_12113966_0_C12_1	Outlier	Outlier	●●●●●
<input type="checkbox"/>	Pseudomonas_D1_12113966_0_C12_2	Outlier	Outlier	●●●●●

In Clover Biosoft, the **Outlier Detection** module identifies outliers that are presented in the dataset. An **outlier** is an extreme value in a dataset that lies an abnormal distance from other values (either much larger or much smaller from the overall pattern of the data). Identifying and handling outliers is important in data analysis to ensure that they do not unduly influence statistical measures and model performance.



# How to perform Outlier Detection Analysis in our platform?

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1

## First steps



This guide is the same for MALDI and FTIR spectra

The screenshots illustrate the navigation process:

- Step 1:** The main dashboard under 'Bio Analysis' features four cards: Biomarker Analysis, Outlier Detection, Reproducibility, and FTIR Quality Control. The Outlier Detection card is highlighted with a green box and a '1' in a square, with an arrow pointing to its description: 'Intended to identify the samples that fall outside the average distribution of a given set of spectra. PCA reconstruction error rate and correlation values between the samples are the metrics used to detect the outliers. Analysis runs on one experiment.'
- Step 2:** The 'Outlier Detection Analysis - Select Study' screen prompts the user to 'Please, select one of your studies:'.
- Step 3:** The 'Outlier Detection Analysis - Select Experiment' screen prompts the user to 'Please, click on the experiment you want to run the analysis on:' and shows a list of experiments, with 'Pseudomonas aeruginosa Outbreak' selected.

Go to the **Bio Analysis** section and click on **Outlier Detection**

Choose a **Study**

Choose an **Experiment**



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## 2

## Outlier Detection Results

### Summary

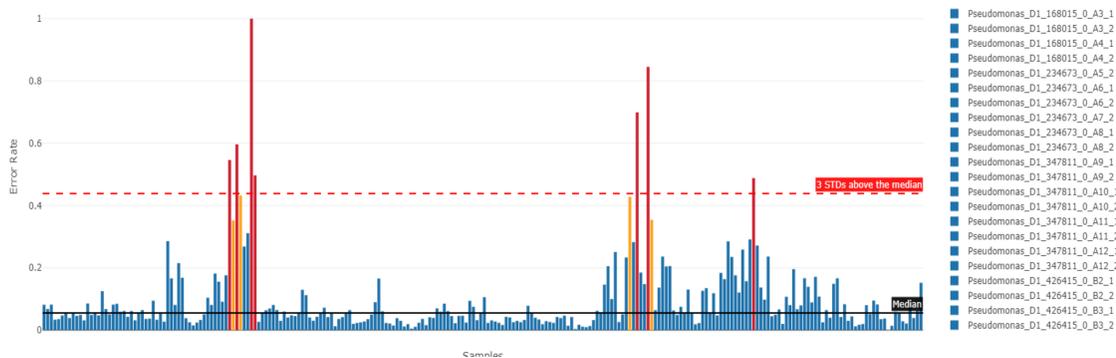
These are the samples detected as outliers by one of the tests or by both of them.

**Tip:** Select desired spectra on the table and click the "Mark as Outlier" link to persist them as detected outliers in the experiment

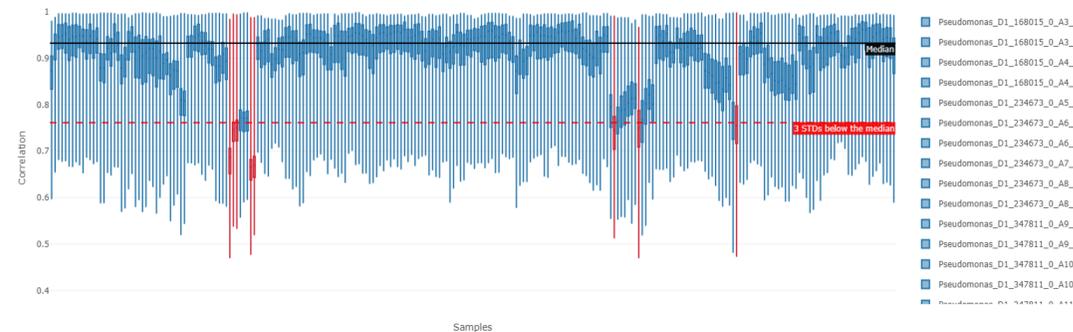
Sample Name	PCA Reconstruction Test	Spectra Correlation Test	Outlier Level
Pseudomonas_D1_12113966_0_C9_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C9_2	Likely to be Outlier	Outlier	●●●●○
Pseudomonas_D1_12113966_0_C10_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_1	Outlier	Outlier	●●●●●
Pseudomonas_D1_12113966_0_C12_2	Outlier	Outlier	●●●●●
Pseudomonas_D1_16226119_0_H9_2	Likely to be Outlier	Outlier	●●●●○
Pseudomonas_D1_16239464_0_A2_2	✓	Outlier	●●●●○
Pseudomonas_D1_16279539_0_B5_2	✓	Outlier	●●●●○
Pseudomonas_D1_12113966_0_C10_2	Likely to be Outlier	✓	●○○○○
Pseudomonas_D1_16226119_0_H10_2	Outlier	✓	●●●○○

**Summary Table.** A list of the potential outliers tested by two different analyses: PCA Reconstruction and Spectra Correlation tests

### PCA Reconstruction



### Spectra Correlation



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2. We consider a replicate/sample as an outlier if **both tests** (PCA Reconstruction & Spectra Correlation) detect it as an outlier (in red).

3. Select those outliers and **mark them as outliers**.

4. Outliers will be **removed** from your experiment. You can check them in the **transformation pipeline** in the experiment view section.



You can perform an Outlier Analysis **before grouping replicates or after that.**

The screenshot displays the software interface for outlier detection. At the top, a table lists samples with columns for 'Sample Name', 'PCA Reconstruction Test', 'Spectra Correlation Test', and 'Outlier Level'. A 'Mark as Outlier' button is visible. Below the table, the 'Experiment' section shows details for 'Study Pseudomonas aeruginosa Outbreak' and 'Experiment Test', including the number of files (242) and available visualizers (Spectra Visualizer, Metadata). The 'Transformation Pipeline' section shows a flow from 'Input: 242 spectra across 242 files' through an 'Outlier Analysis' step to 'Output: 238 Spectra'. A 'Detail' view of the outlier analysis shows a list of samples with red dots indicating they are outliers. Numbered callouts (1-4) highlight key features: 1. Eye icon for visualization, 2. Red dots for both tests, 3. Mark as Outlier button, and 4. Detail view of outliers.

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