### What is it?

	Sample Name 🜲	PCA Reconstruction Test 💠	Spectra Correlation Test 🖕 1	Outlier Level 🛛 🛊
0	Pseudomonas_D1_12113966_0_C9_1	0 Outlier	0 Outlier	•••••
0	Pseudomonas_D1_12113966_0_C9_2	A Likely to be Outlier	0 Outlier	••••
0	Pseudomonas_D1_12113966_0_C10_1	1 Outlier	Outlier	•••••
0	Pseudomonas_D1_12113966_0_C12_1	0 Outlier	0 Outlier	•••••
0	Pseudomonas_D1_12113966_0_C12_2	• Outlier	0 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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This guide is the sam MALDI and FTIR spec	me for ctra	Outlier Detec	tion Results	S	
r [training@cloverbiosoft.com] Premium 🏛 Training Clover BioSoft  🔂	Logout	Summary Table. A analyses: PCA Reco	list of the potenti onstruction and S	al outliers test Spectra Correlo	ed by two differer ation tests
$\odot$		Summary These are the samples detected as outliers by one of the tests or by bot	h of them.		
		<b>Tip:</b> Select desired spectra on the table and click the "Mark as Outlier	" link to persist them as detected outliers in the experiment		×
samples that fall outside the average distribution of a A reconstruction error rate and correlation values		Samula Nama A	DCA Percentruction Test	Sporter Correlation Tast 4	Mark as Outlier
e the metrics used to detect the outliers.		Pseudomonas_D1_12113966_0_C9_1	O Outlier	Outlier	
periment		Pseudomonas_D1_12113966_0_C9_2	▲ Likely to be Outlier	0 Outlier	••••
		Pseudomonas_D1_12113966_0_C10_1	0 Outlier	0 Outlier	•••••
9		Pseudomonas_D1_12113966_0_C12_1	0 Outlier	0 Outlier	•••••
		Pseudomonas_D1_12113966_0_C12_2	0 Outlier	0 Outlier	•••••
		Pseudomonas_D1_16226119_0_H9_2	Likely to be Outlier	0 Outlier	••••O
[training@cloverbiosoft.com] Premium 🏛 Training Clover BioSoft 🕒 Log	ogout	Pseudomonas_D1_16239464_0_A2_2	•	0 Outlier	•••00
		Pseudomonas_D1_16279539_0_B5_2	0	0 Outlier	000
		Pseudomonas_D1_12113966_0_C10_2	▲ Likely to be Outlier	•	0000
ch Q Order by Date V	1 <del>1</del>	Pseudomonas_D1_16226119_0_H10_2	0 Outlier		•••00
Choose an Experiment			Pseudomnas_D1_234673_0_A       0.1         Pseudomnas_D1_234673_0_A       0.1         Pseudomnas_D1_234673_0_A       0.1         Pseudomnas_D1_234673_0_A       0.1         Pseudomnas_D1_234673_0_A       0.1         Pseudomnas_D1_234673_0_A       0.1         Pseudomnas_D1_347811_0_A       0.1         Pseudomnas_D1_426415_0_B       0.1         Pseudomnas_D1_426415_0_B       0.1         Pseudomnas_D1_426415_0_B       0.1         Pseudomnas_D1_426415_0_B       0.1         Pseudomnas_D1_426415_0_B       0.1		Samples
	3 Mark as Outlier				
Spectra Correlation Test 🖵 1	Outlier Level 🟮 🗢				
1) Outlier					
0 Outlier	••••				
Outlier					
Outline					
1 Outlier					
1 Outlier				•	
Outlier					
Outlier	000				

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	Sample Name 🜲	PCA Reconstruction Test 🜲
0	Pseudomonas_D1_12113966_0_C9_1	0 Outlier
0	Pseudomonas_D1_12113966_0_C9_2	🛕 Likely to be Outlier
0	Pseudomonas_D1_12113966_0_C10_1	I Outlier
0	Pseudomonas_D1_12113966_0_C12_1	Outlier
0	Pseudomonas_D1_12113966_0_C12_2	Outlier
	<ul> <li></li> &lt;</ul>	<ul> <li>Sample Name          <ul> <li>Sample Name              <li>Pseudomonas_D1_12113966_0_C9_1</li> <li>Pseudomonas_D1_12113966_0_C9_2</li> <li>Pseudomonas_D1_12113966_0_C10_1</li> <li>Pseudomonas_D1_12113966_0_C12_1</li> <li>Pseudomonas_D1_12113966_0_C12_2</li> </li></ul> </li> </ul>

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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Spectra Correlation Test 🖕 1	Outlier Level ()
Outlier	
Outlier	••••
Outlier	
Outlier	
Outlier	

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### How to perform Outlier Detection Analysis in our platform?

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First steps

Biomarker Analysis	
Intended to search characteristics for identifying groups of samples. Results are mainly shown in the form of a peak table showing the appearance, coefficient of variation and mean of each selected group and also ROC curve can be visualized.	
Analysis runs on one experiment	
% %	
Reproducibility	
Intended to analyse the reproducibility of the spectra so reliable and comparable data are used in subsequent analysis, then increasing the	
are	
on Analysis - Select Study <b>2</b>	
are	=
on Analysis - Select Experiment 🔸 🛛 3	
osa Outbreak periment you want to run the analysis on:	
o to the Bio Analysis ection and click on Outlier Detection	ose a Study



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Phone: +34 958 991 543 email: info@cloverbiosoft.com <u>support@cloverbiosoft.co</u>m



### **Outlier Detection Results**

### Summary

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

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

				Mark as Outlie
	Sample Name 🗢	PCA Reconstruction Test 🜲	Spectra Correlation Test 🖕 1	Outlier Level 🚺 🛊
0	Pseudomonas_D1_12113966_0_C9_1	Outlier	Outlier	•••••
0	Pseudomonas_D1_12113966_0_C9_2	🛕 Likely to be Outlier	<ul> <li>Outlier</li> </ul>	●●●●○
0	Pseudomonas_D1_12113966_0_C10_1	Outlier	0 Outlier	•••••
0	Pseudomonas_D1_12113966_0_C12_1	<ul> <li>Outlier</li> </ul>	0 Outlier	•••••
0	Pseudomonas_D1_12113966_0_C12_2	<ul> <li>Outlier</li> </ul>	<ul> <li>Outlier</li> </ul>	•••••
0	Pseudomonas_D1_16226119_0_H9_2	🛕 Likely to be Outlier	<ul> <li>Outlier</li> </ul>	
0	Pseudomonas_D1_16239464_0_A2_2		<ul><li>Outlier</li></ul>	000
0	Pseudomonas_D1_16279539_0_B5_2		0 Outlier	000
0	Pseudomonas_D1_12113966_0_C10_2	🛕 Likely to be Outlier		0000
0	Pseudomonas_D1_16226119_0_H10_2	<ul> <li>Outlier</li> </ul>		000

### **PCA Reconstruction**



## How to perform Outlier Detection Analysis in our platform?

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	Pseudomonas_D1_168015_0_A3_1
	Pseudomonas_D1_168015_0_A3_2
	Pseudomonas_D1_168015_0_A4_1
	Pseudomonas_D1_168015_0_A4_2
	Pseudomonas_D1_234673_0_A5_2
	Pseudomonas_D1_234673_0_A6_1
	Pseudomonas_D1_234673_0_A6_2
	Pseudomonas_D1_234673_0_A7_2
	Pseudomonas_D1_234673_0_A8_1
	Pseudomonas D1 234673 0 A8 2
	Pseudomonas_D1_347811_0_A9_1
	Pseudomonas D1 347811 0 A9 2
	Pseudomonas D1 347811 0 A10 1
	Pseudomonas D1 347811 0 A10 2
	Pseudomonas D1 347811 0 A11 1
	Pseudomonas D1 347811 0 A11 2
	Pseudomonas D1 347811 0 A12 1
i	Pseudomonas D1 347811 0 A12 2
	Pseudomonas D1 426415 0 B2 1
i	Pseudomonas D1 426415 0 B2 2
i.	Pseudomonas D1 426415 0 B3 1
i	Pseudomonas D1 426415 0 B3 2





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

### **Spectra Correlation**

Pseudomonas\_D1\_168015\_0\_A3\_1 Pseudomonas\_D1\_168015\_0\_A3\_2 Pseudomonas\_D1\_168015\_0\_A4\_1 Pseudomonas\_D1\_168015\_0\_A4\_2 Pseudomonas\_D1\_234673\_0\_A5\_2 Pseudomonas\_D1\_234673\_0\_A6\_1 Pseudomonas\_D1\_234673\_0\_A6\_2 Pseudomonas\_D1\_234673\_0\_A7\_2 Pseudomonas\_D1\_234673\_0\_A8\_1 Pseudomonas\_D1\_234673\_0\_A8\_2 Pseudomonas\_D1\_347811\_0\_A9\_1 Pseudomonas\_D1\_347811\_0\_A9\_2 Pseudomonas\_D1\_347811\_0\_A10\_1 Pseudomonas\_D1\_347811\_0\_A10\_2 Decudementer D1 347011 0 411

Samples

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3

## **Tips for Outlier Detection**

1. The eye icon allows us to visualiz the spectra per sample.

2. We consider a replicate/sampl as an outlier if both tests (PC Reconstruction & Spect Correlation) detect it as an outlie (in red).

3. Select those outliers and mar them as outliers.

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



You can perform an Ou before grouping replicates

## How to perform Outlier Detection Analysis in our platform?

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Sample Name :       PCA Reconstruction Test         Image: Preudomonat_D1_12113966_0_0_0_1       Outlier         Image: Preudomonat_D1_12113966_0_0_0_2       Image: Preudomonat_D1_12113966_0_0_0_2         Image: Preudomonat_D1_12113966_0_0_0_2       Image: Preudomonat_D1_12113966_0_0_0_2         Image: Preudomonat_D1_12113966_0_0_0_2       Image: Preudomonat_D1_16226119_0_149_2         Image: Preudomonat_D1_16226119_0_149_2       Image: Preudomonat_D1_16226119_0_0_120_2         Image: Preudomonat_D1_16226119_0_149_2       Image: Preudomonat_D1_16226119_0_0_0_0_0_0_0_0_0_0_0_0_0_0_0_0_0_0_	
Image: Preudomonas_D1_12113966_0_0_5_2       Image: D1_12113966_0_0_5_2         Image: Preudomonas_D1_12113966_0_0_12_2       Image: D1_12113966_0_0_12_2         Image: Preudomonas_D1_12213966_0_0_12_2       Image: D1_12213966_0_0_12_2         Image: Preudomonas_D1_16226119_0_19_2       Image: D1_16229396_0_0_12_2         Image: Preudomonas_D1_16229396_0_0_12_2       Image: D1_16219396_0_0_12_2         Image: Preudomonas_D1_16229396_0_0_12_2       Image: D1_16219396_0_0_12_2         Image: Preudomonas_D1_16229396_0_0_12_2       Image: D1_16219396_0_0_12_2         Image: Preudomonas_D1_16229396_0_0_12_2       Image: D1_12113966_0_0_12_2         Image: Preudomonas_D1_16219396_0_0_12_2       Image: D1_12113966_0_0_12_2         Image: Preudomonas_D1_12113966_0_0_12_2       Image: D1_12113966_0_0_12_2         Image: Preudomonas_D1_12113966_0_0_12_2       Image: D1_12113966_0_0_12_2         Image: Preudomonas_D1_12113966_0_0_12_2       Image: D1_12113966_0_0_12_2         Image: Preudomonas_D1_12113966_0_0_12_2       Image: D1_12113966_0_0_12_2         Image: Preudomonas_D1_1211396	¢
Preudomonas_D1_12113966_0_C12_1 Preudomonas_D1_12113966_0_C12_1 Preudomonas_D1_12113966_0_C12_2 Outlier Preudomonas_D1_16223119_0_H9_2 Preudomonas_D1_1622319_0_H9_2 Preudomonas_D1_162319_0_H9_2 Preudomonas_D1_12113966_0_C10_1 Preudomonas_D1_12113966_0_	
Image: Preudomonas_D1_12113966_0_C12_1       Image: Outline Preudomonas_D1_12113966_0_C12_2         Image: Preudomonas_D1_16226119_0_H9_3       Image: Utker         Image: Preudomonas_D1_1622619_0_H9_3       Image: Utker         Image: Preudomonas_D1_16276539_0_B5_2       Image: Utker         Image: Test       Description: -         Image: Created by: Training Clover [training@cloverbiosoft.com] = at: 13-02-202-2242 files         Image: Preudomonas_D1_12113966_0_C10_1	
Image: Preudomonas, D1, 12113966, 0, C12, 2       Image: O cutter         Image: Preudomonas, D1, 12113966, 0, C12, 2       Image: O cutter         Image: Preudomonas, D1, 16229119, 0, Hg, 2       Image: Italian (transmitted of the cutter)         Image: Preudomonas, D1, 1622939, 0, B5, 2       Image: Italian (transmitted of the cutter)         Image: Preudomonas, D1, 16279339, 0, B5, 2       Image: Italian (transmitted of the cutter)         Image: Preudomonas, D1, 16279539, 0, B5, 2       Image: Italian (transmitted of the cutter)         Image: Preudomonas, D1, 16279539, 0, B5, 2       Image: Italian (transmitted of the cutter)         Image: Preudomonas, D1, 16279539, 0, B5, 2       Image: Italian (transmitted of the cutter)         Image: Italian (transmitted of the cutter)       Image: Italian (transmitted of the cutter)         Image: Italian (transmitted of the cutter)       Image: Italian (transmitted of the cutter)         Image: Italian (transmitted of the cutter)       Image: Italian (transmitted of the cutter)         Image: Italian (transmitted of the cutter)       Image: Italian (transmitter)         Image: Italian (transmitter)	
Pseudomonas_D1_12113966_0_C12_2   Outler   Pseudomonas_D1_16226119_0_H9_2   Pseudomonas_D1_16226119_0_H9_2   Pseudomonas_D1_162279539_0_B5_2   Experiment   Study Pseudomonas_D1_16279539_0_B5_2   Experiment   Study Pseudomonas_D1_16279539_0_B5_2   Interpret Pseudomonas_D1_16279539_0_B5_2   Pseudomonas_D1_16279539_0_B5_2   Study Pseudomonas seruginose Outbreak   Study Pseudomonas_D1_16279539_0_B5_2   Interpret Pseudomonas_D1_16279539_0_B5_2   Pseudomonas_D1_16279539_0_B5_2   Interpret Pseudomonas_D1_12113966_0_C10_1 Pseudomonas_D1_12113966_0_C10_1 Pseudomonas_D1_12113966_0_C10_1 Pseudomonas_D1_12113966_0_C10_1 Pseudomonas_D1_12113966_0_C10_1 Pseudomonas_D1_12113966_0_C10_1	
□       ●       Pseudomonas_D1_16228119_0_H9_2       ▲       ↓	
Image: Preudomonas_D1_16239464_0_A2_3       ●         Image: Preudomonas_D1_1623938_0_85_2       ●         Image: Preudomonas_D1_1623936_0_85_2       ●         Image: Preudomonas_D1_1623936_0_85_2       ●         Image: Preudomonas_D1_16239464_0_A2_3       ●         Image: Preudomonas_D1_16239464_0_A2_3       ●         Image: Preudomonas_D1_2023       ●         Image: Preudomonas_	
er evedomonas_D1_16279539_0_85_2 Experiment Study Pseudomonas aeruginosa Outbreak Experiment Test Name: Test Description: - Created by: Training Clover [training@cloverbiosoft.com] at: 13-02-2024 242 files □	
Experiment         Study Pseudomonas aeruginosa Outbreak       Experiment Test         Name: Test       Description: -         Created by: Training Clover [training@cloverbiosoft.com] at: 13-02-2024         242 files       •         Imput       •         You can chain several actions to transform the spectra included in the experiment         Poput       •         242 files       •         Imput       •         Outlier Analysis       •         Petail       Pseudomonas_D1_12113966_0_C10_1         Pseudomonas_D1_12113966_0_C12_1       •	
Study Pseudomonas aeruginosa Outbreak       Experiment Test         Name: Test       Description: -         Created by: Training Clover [training@cloverbiosoft.com] at: 13-02-2024         242 files       •         • Metadata       •         Transformation Pipeline       You can chain several actions to transform the spectra included in the experiment of the spectra across 242 files         • Nput       •         • Labor       •         • Detail       Pseudomonas_D1_12113966_0_C10_1         • • • • • •       •         • • • • • •       •	
Image: Spectra Visualizer         Image: Metadata         Image: Construction Problem         You can chain several actions to transform the spectra included in the expectra included in the expectra across 242 files         Imput         242 spectra across 242 files         Detail         Pseudomonas_D1_12113966_0_C10_1         Pseudomonas_D1_12113966_0_C12_1	11:04:
In In In In Input 242 spectra across 242 files → Detail Pseudomonas_D1_12113966_0_C10_1 → Pseudomonas_D1_12113966_0_C12_1	
in Pe Input 242 spectra across 242 files → Detail Pseudomonas_D1_12113966_0_C10_1 → Pseudomonas_D1_12113966_0_C12_1	
You can chain several actions to transform the spectra included in the example Input 242 spectra across 242 files → Outlier Analysis Detail Pseudomonas_D1_12113966_0_C10_1 → Pseudomonas_D1_12113966_0_C12_1 → Outlier Analysis	
Input       Outlier Analysis         242 spectra across       242 files         242 files       Outlier Analysis         Detail       Pseudomonas_D1_12113966_0_C10_1         ●●●●●       ●●●●●	perime
Detail Pseudomonas_D1_12113966_0_C10_1 Pseudomonas_D1_12113966_0_C12_1 ••••••	238
utlier Analysis eeeee es or after that. Pseudomonas_D1_12113966_0_C12_2 Pseudomonas_D1_12113966_0_C9_1	

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2		3
	Spectra Correlation Test 🖕 1	Outlier Level
	① Outlier	•••••
	<ul><li>Outlier</li></ul>	●●●●○
	🖢 Outlier	•••••
	1) Outlier	•••••
	1) Outlier	•••••
	<ul> <li>Outlier</li> </ul>	
	Outlier	•••00
	<ul> <li>Outlier</li> </ul>	•••00

:51 GMT+1

ent. The resulting output spectra will be used in the rest of analysis within this experiment



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