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sponsored by metabolites

WebSpecmine: A website for metabolomics data analysis and mining

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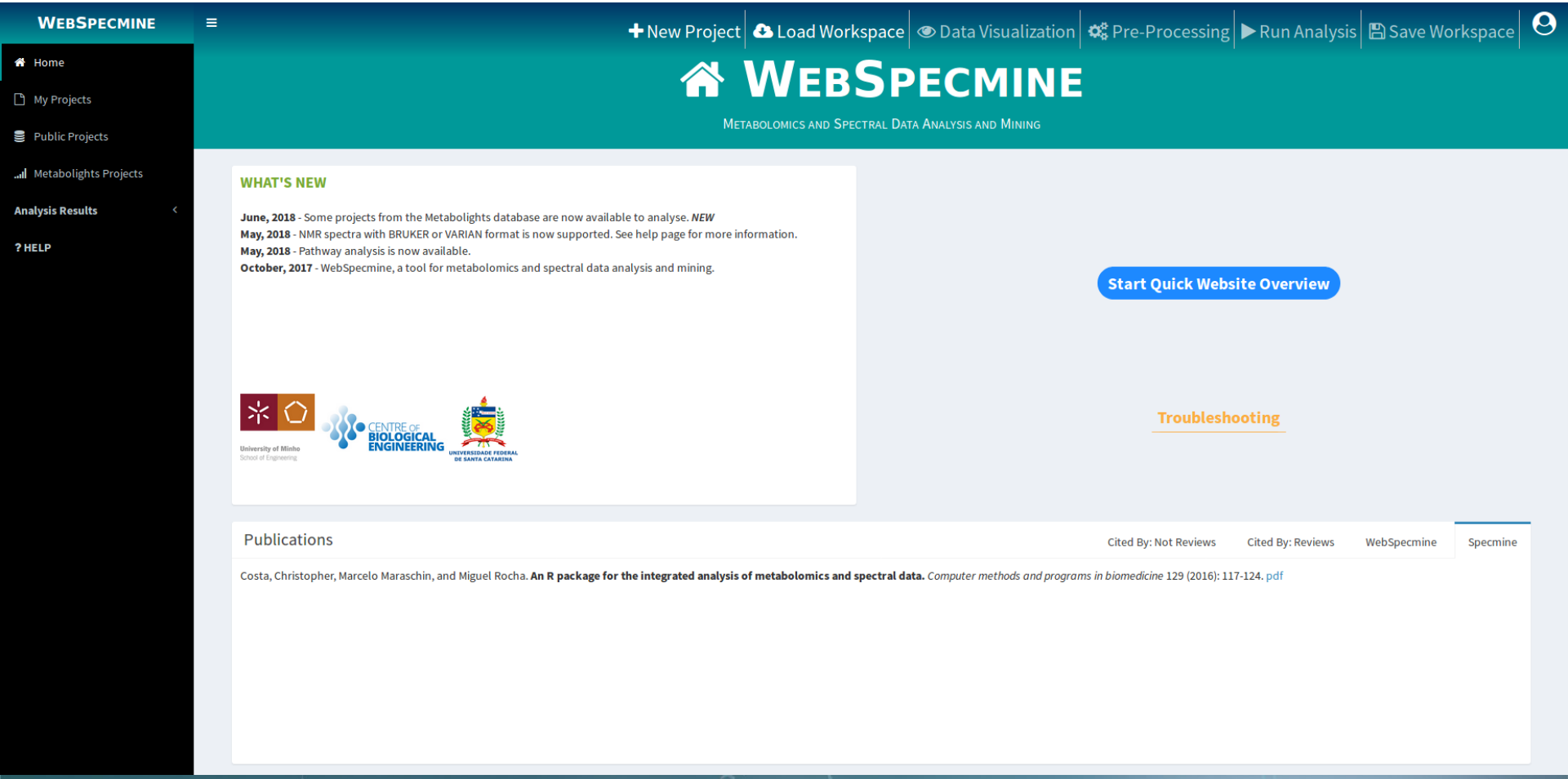
WebSpecmine: A website for metabolomics data analysis and mining



Introduction

Metabolomics

- ✓ Analysing metabolomics data correctly and efficiently is nowadays very important in biological and biomedical research.

However

Most people that want to perform this analysis may not have the programming skills needed

A website to perform metabolomics data analysis is an important asset

Introduction

Some of the Existing Websites

	Covered Techniques	Univariate Analysis	Multivariate Analysis	Other Features
MetaboAnalyst 4.0	LC/GC-MS Raw Spectra LC/GC-MS Peak Lists NMR Peak Lists Metabolites' Concentrations (Quantitative Data)	T-Test; ANOVA; Fold Change	PCA; Clustering; Machine Learning (only PLS-DA); Feature Selection (only Random Forests and SVM)	Correlation Analysis; Metabolite Identification (only for MS); Pathway Analysis
XCMS Online	LC/GC-MS Raw Spectra	T-Test; ANOVA; Non-Parametric Tests;	PCA; Clustering; Machine Learning (only LDA, PLS-DA and Random Forests)	Metabolite Identification; Pathway Analysis; User Account

Introduction

What is missing in the existing websites?

✗ A wide variety of techniques and data formats supported	→ Spectral Data (Raman, UV-Vis and IR) is missing
✗ A wide variety of pre-processing methods	→ Mostly just normalization, scaling, missing values treatment
✗ A wide variety of analysis methods	→ There should be more model options for machine learning, for example
✗ Flexible Pipeline	→ Most of the time, users have to follow a strict pipeline
✗ User Account	→ So that data and results can be stored and shared

What was our main goal, then?

- ✓ Create an easy-to-use and freely available website that provides a wide variety of methods and data types for analysis, and ways to store and share metabolomics data and the results generated.

SOLUTION: WEBSPECMINE

METABOLOMICS AND SPECTRAL DATA ANALYSIS AND MINING

WebSpecmine: overview

Metabolomics data Supported

- ✓ NMR
- ✓ LC/GC-MS
- ✓ Infrared, UV-Visible, and Raman Spectra
- ✓ Concentrations Data (Quantitative Data)

Data Pre-Processing

Metabolomics data Analysis Available

- ✓ Univariate Statistical Analysis
- ✓ Unsupervised Multivariate Statistical Analysis
- ✓ Supervised Multivariate Statistical Analysis
- ✓ Metabolite Identification
- ✓ Pathway Analysis

User Account

- ✓ Store data and results privately
- ✓ Share data across users

Tutorials and User Guide

WebSpecmine: Supported data

LC/GC-MS

Raw Spectra Data Formats

- ✓ .mzData
- ✓ .mzXML
- ✓ .netDF

Peak Lists Data Formats

- ✓ CSV
- ✓ TSV

WebSpecmine: Supported data

NMR

Raw Spectra Data Formats

- ✓ BRUKER
- ✓ VARIAN

Peak Lists Data Formats

- ✓ CSV
- ✓ TSV

WebSpecmine: Supported data

Spectral Data:
Raman, IR and UV-Vis

Spectra Data Formats

- ✓ CSV
- ✓ (J)DX
- ✓ SPC
- ✓ MS EXCEL (.xlsx)

WebSpecmine: Supported data

Concentrations (Quantitative) Data

- ✓ **CSV/TSV File:**

```
Patient ID,1.6-Anhydro-beta-D-glucose,1-Methylnicotinamide,2-Aminobutyrate,2-Hydroxyisobutyrate,2-Oxoglutarate
PIF_178,40.85,65.37,18.73,26.05,71.52
PIF_087,62.18,340.36,24.29,41.68,67.36
PIF_090,270.43,64.72,12.18,65.37,23.81
NETL_005_V1,154.47,52.98,172.43,74.44,1199.91
PIF_115,22.2,73.7,15.64,83.93,33.12
```

Metabolites Names or Identifiers

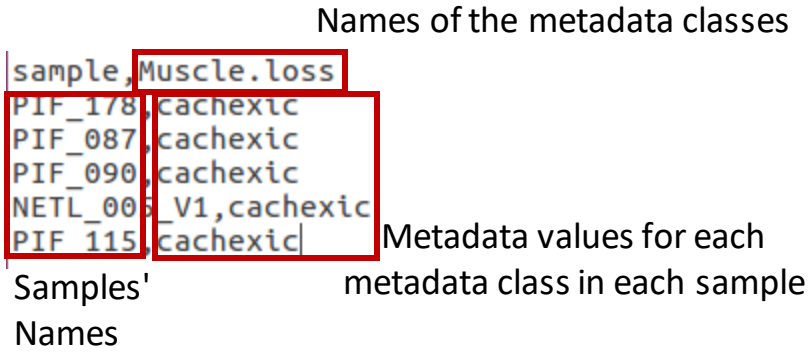
Samples' Names

Concentrations values of each metabolite in each sample

WebSpecmine: Supported data

Metadata

- ✓ **All types of data should have a metadata file associated**
- ✓ **CSV/TSV File:**



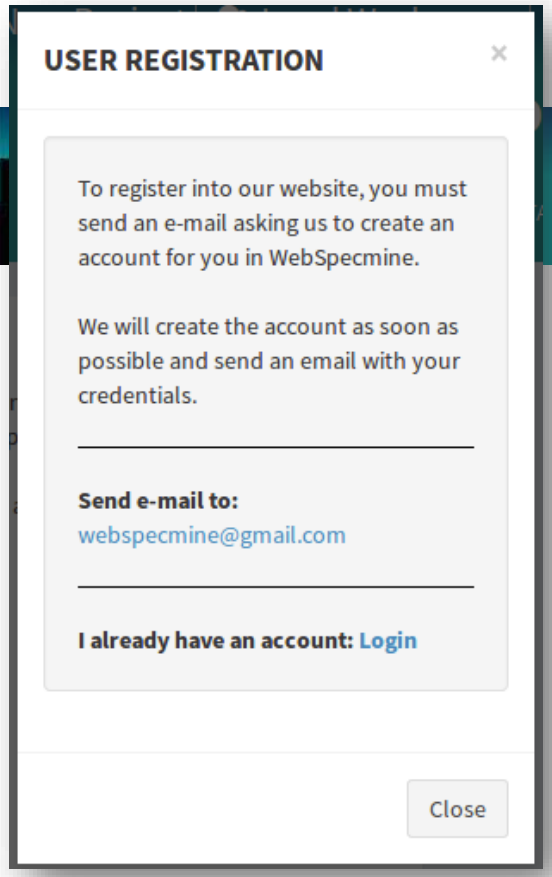
WebSpecmine: User Account

Why a User Account?

- ✓ Main website functionalities are accessible without a user account
- ✓ But you will have to create an account if you want to:
  - Save and Share data and results
  - Leave an analysis in 'stand-by'

WebSpecmine: User Account

Creation of a User Account



To have one, users have to send an email, asking to create an account, and an email with the credentials will be sent as soon as possible.

Email: webspecmine@gmail.com

WebSpecmine: User Account

Data Projects: What is?

A project is a study, or group of studies, which contains the data and metadata for each study, as well as reports from the results obtained

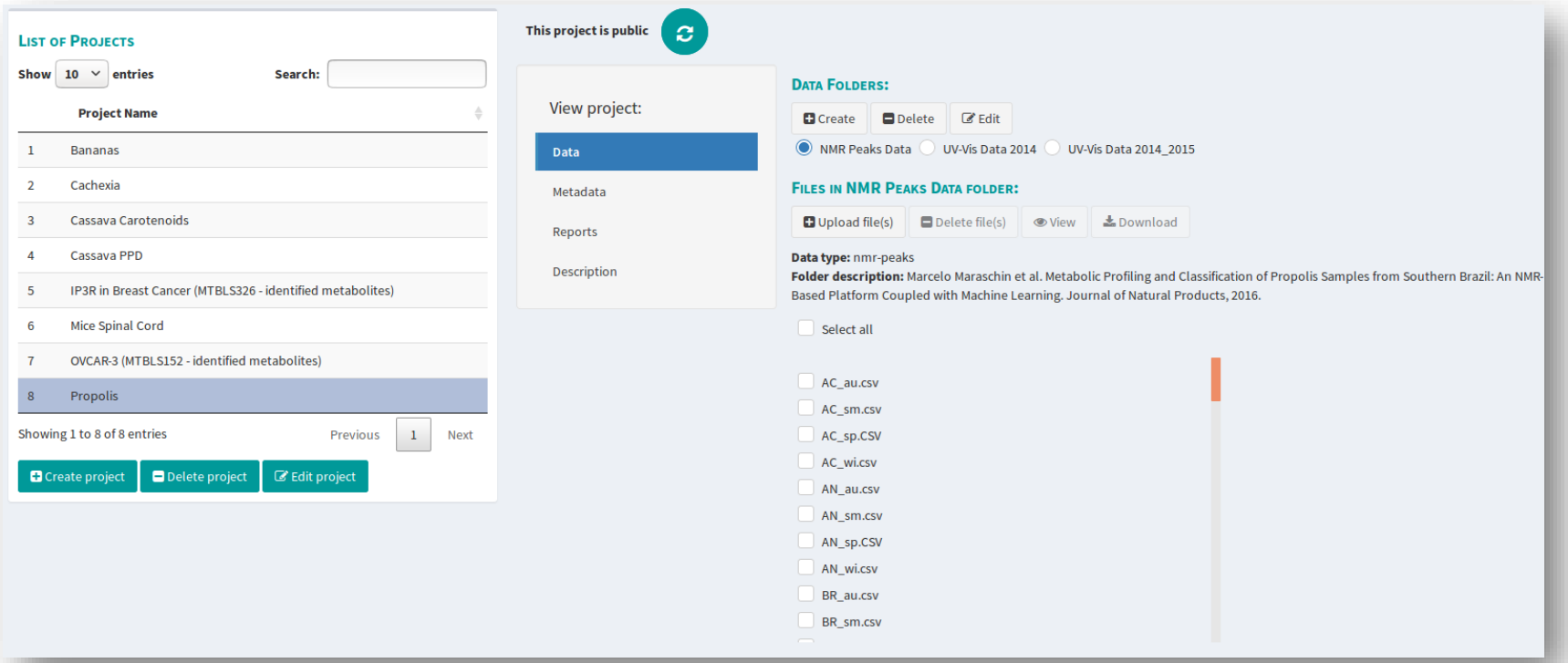
Projects can be:

Private  Public

WebSpecmine: User Account

Your Projects

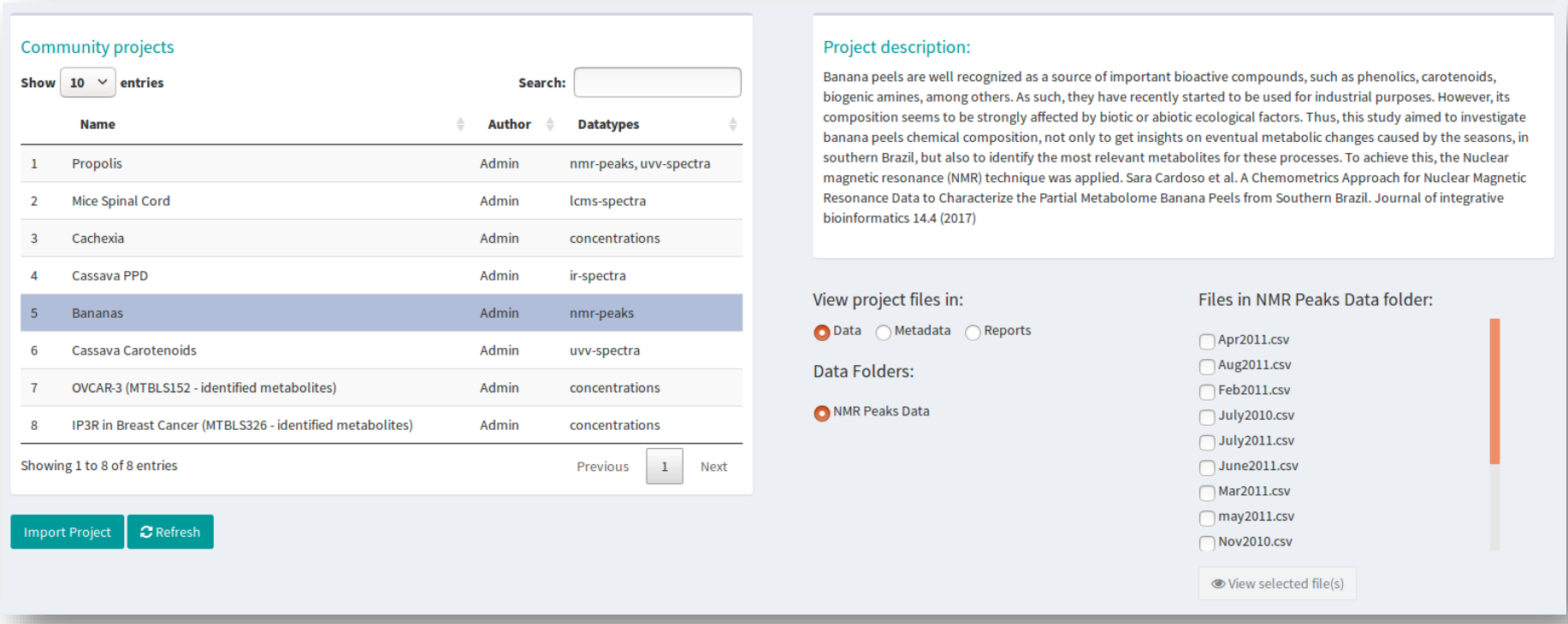
The projects stored in an account are accessible through ***My Projects*** sidebar tab



WebSpecmine: User Account

Public Projects

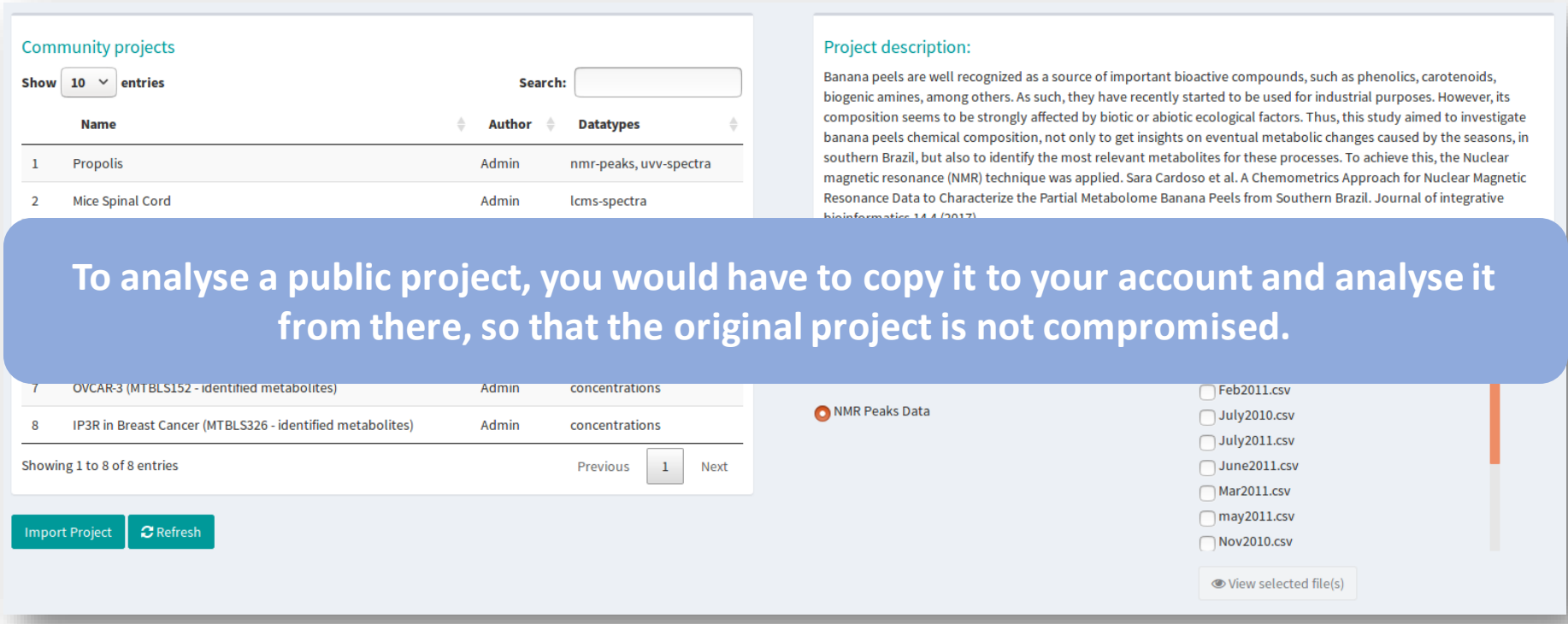
Everyone that accesses the website can see all public projects, at the ***Public Projects*** sidebar tab



WebSpecmine: User Account

Public Projects

Everyone that accesses the website can see all public projects, at ***Public Projects*** sidebar tab

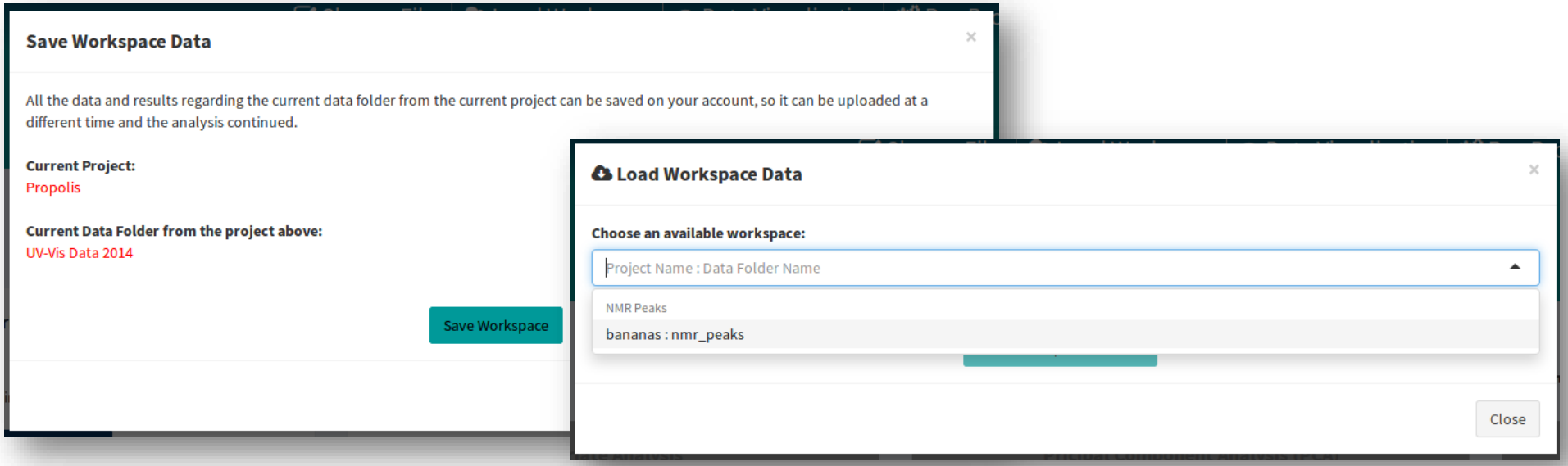


To analyse a public project, you would have to copy it to your account and analyse it from there, so that the original project is not compromised.

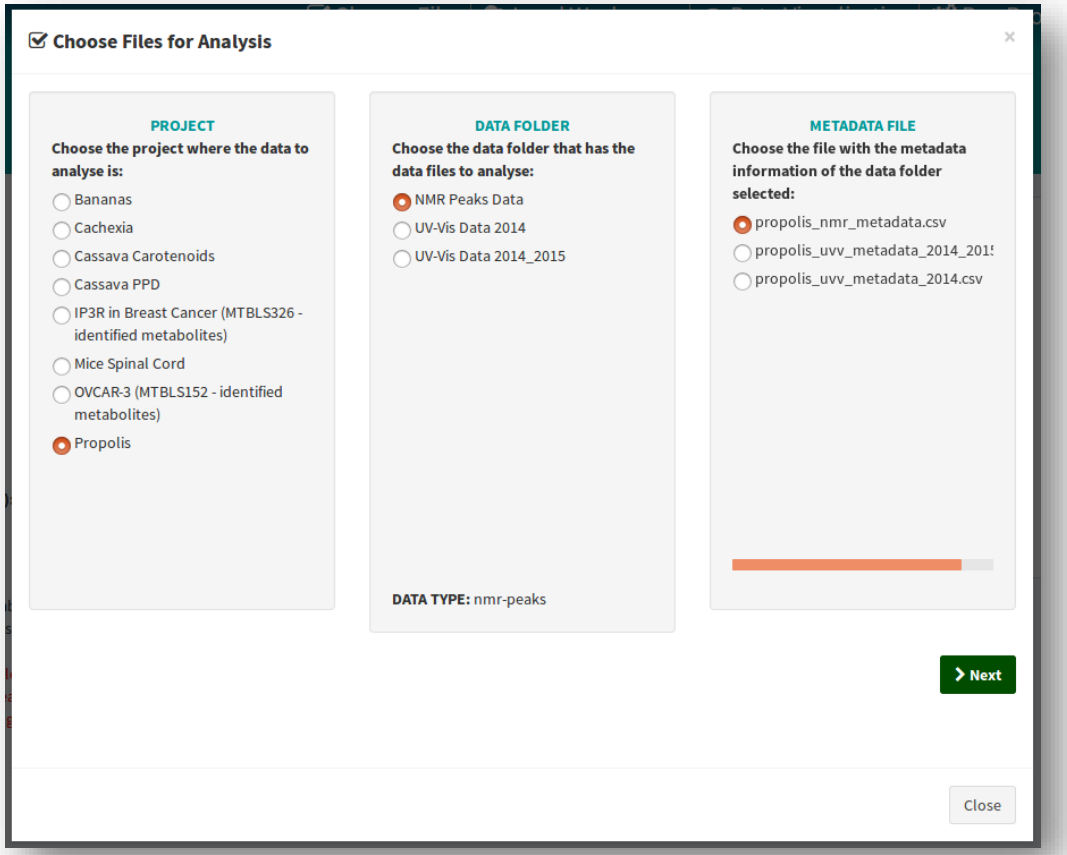
WebSpecmine: User Account

Workspace:
Users can leave their analysis in 'stand-by' and continue later

Users can leave an analysis at any time, by saving the workspace, and continue next time



WebSpecmine: Select Data for Analysis

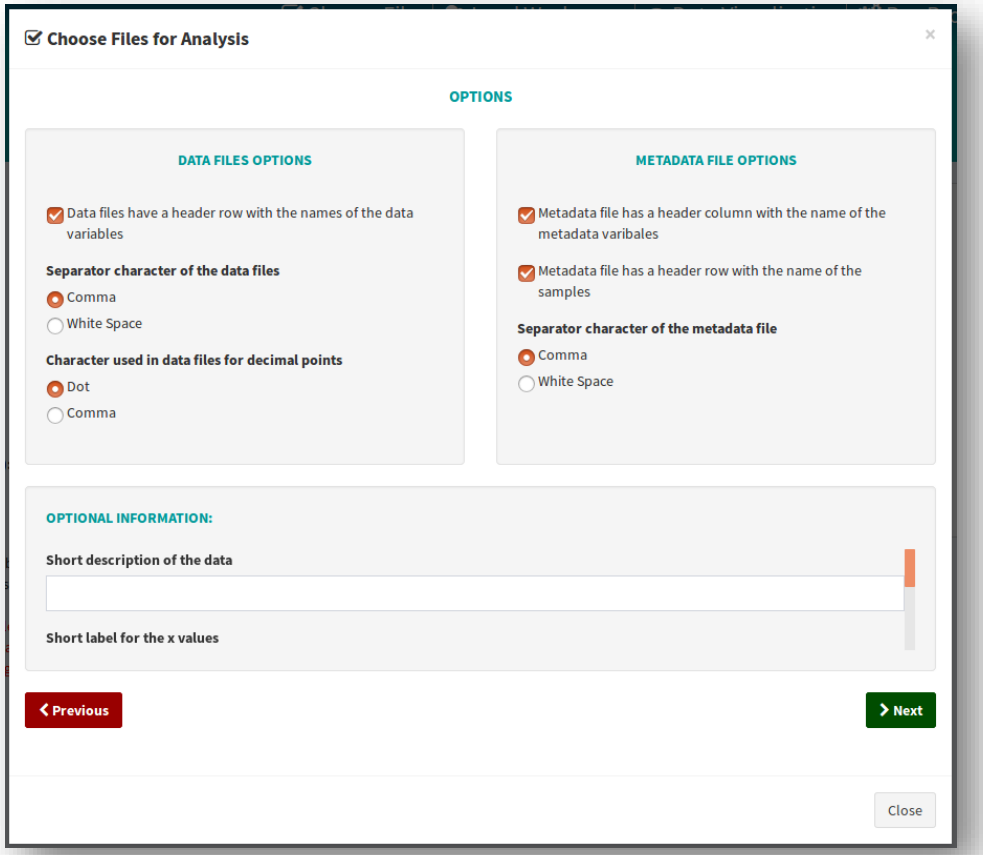


For Logged In Users

1

Select the Project, the data folder from that project where the data to analyse is, and the metadata file from that project that corresponds to the data selected

WebSpecmine: Select Data for Analysis



For Logged In Users

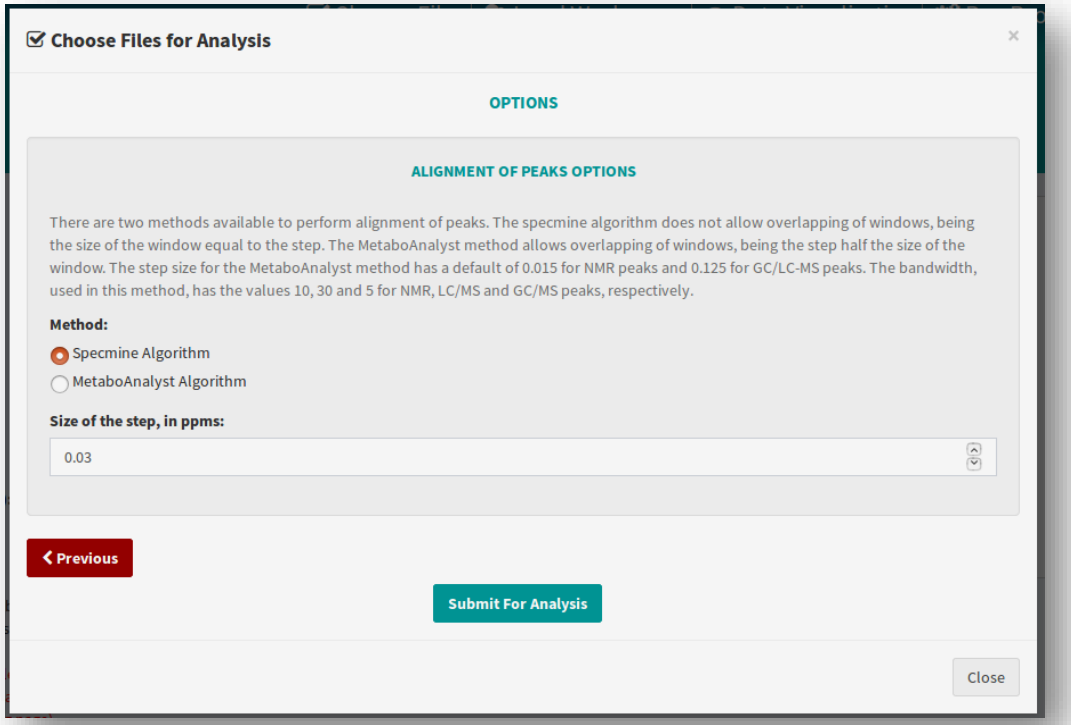
1

2

Set the options required to correctly read the data and metadata files

WebSpecmine: Select Data for Analysis

For Logged In Users



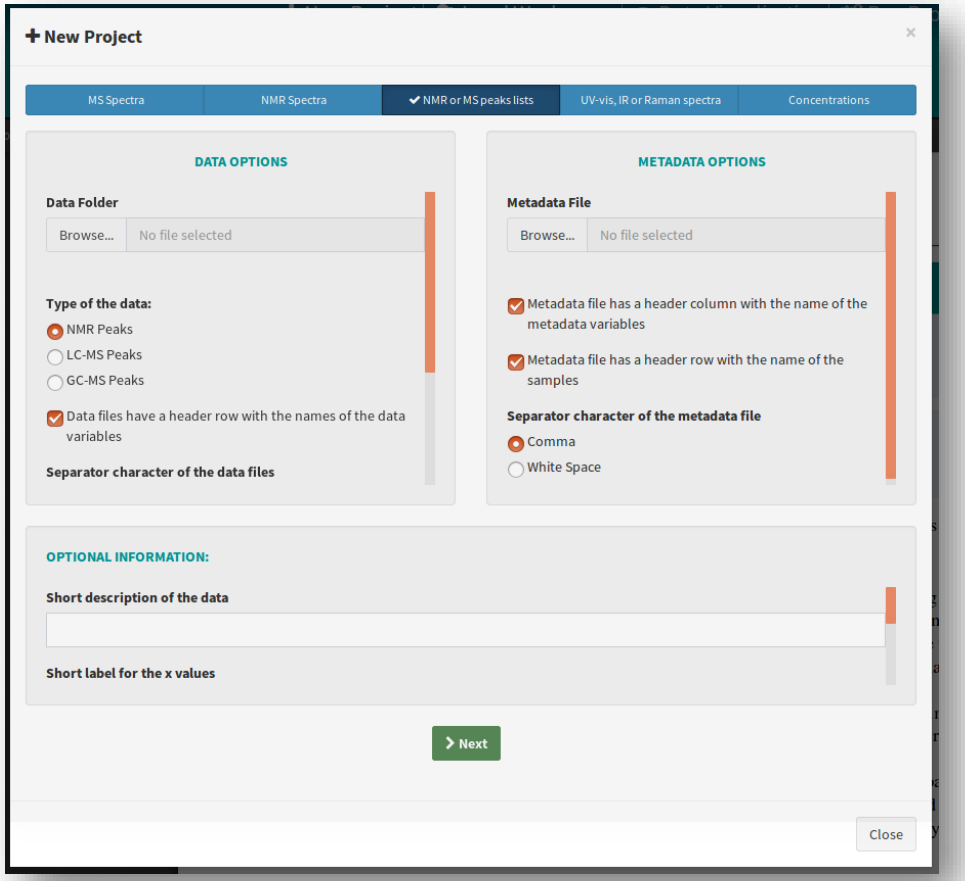
1

2

3

After finishing the setting of data and metadata options, the user can submit the data for analysis

WebSpecmine: Select Data for Analysis



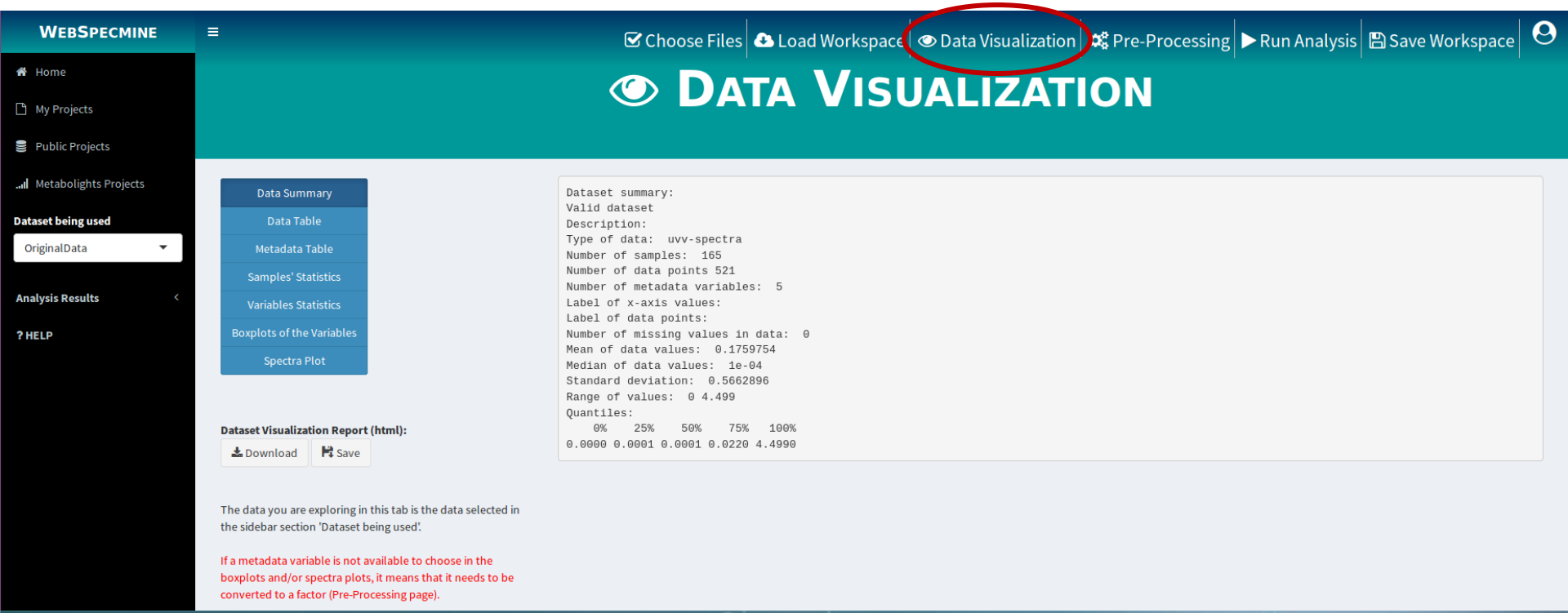
For Logged Out Users

- ✓ The Procedure is similar, but the data files and metadata files have to be submitted, as they are not stored in the website.
- ✓ The data submitted will only be temporarily stored, while the analysis is in action.

Once the user selects the data, the data analysis pages will be accessible

WebSpecmine: Data Visualization

1 The website provides a way to visualize the data



WebSpecmine: Data Visualization

1 2 Data Summary

- Data Summary
- Data Table
- Metadata Table
- Samples' Statistics
- Variables Statistics
- Boxplots of the Variables
- Peaks Plot

Dataset Visualization Report (html):

Download Save

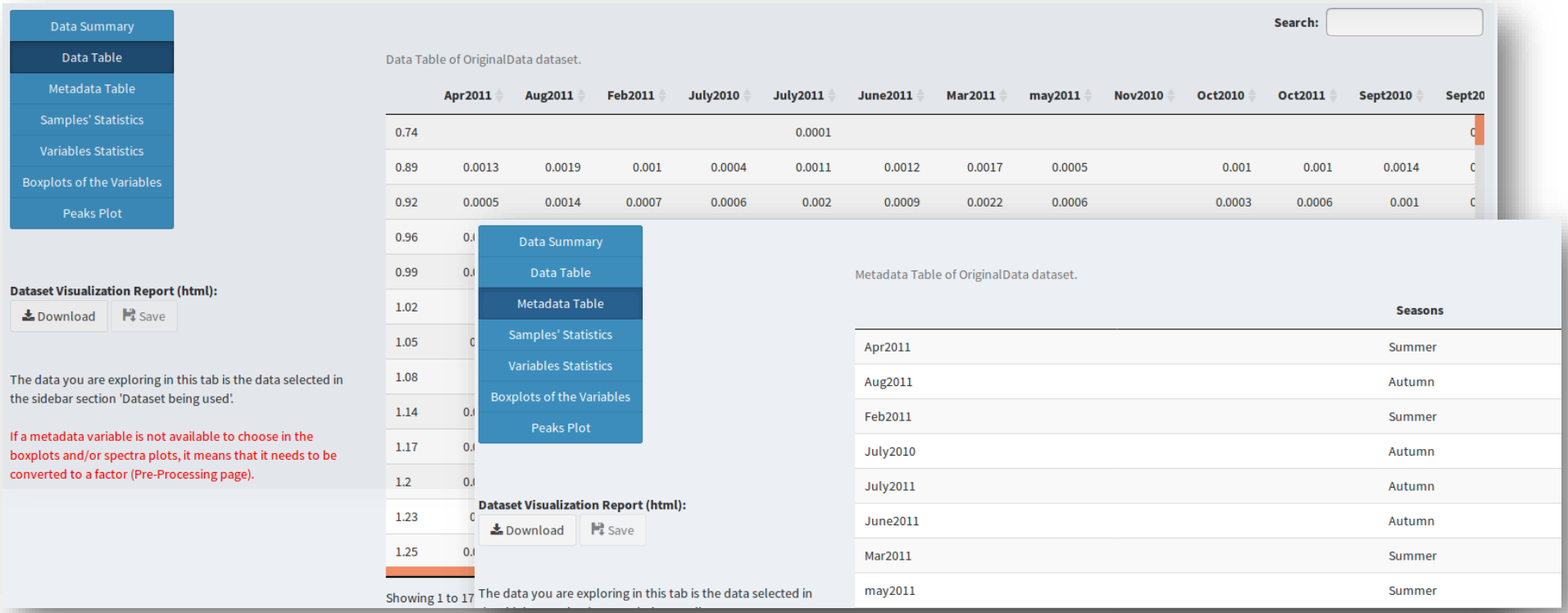
```
Dataset summary:
Valid dataset
Description:
Type of data:  nmr-peaks
Number of samples:  13
Number of data points 173
Number of metadata variables:  1
Label of x-axis values:  ppm
Label of data points:  Intensity
Number of missing values in data:  795
Mean of data values:  0.02179374
Median of data values:  0.0019
Standard deviation:  0.04556014
Range of values:  1e-04 0.3023
Quantiles:
      0%      25%      50%      75%     100%
0.000100 0.000700 0.001900 0.010875 0.302300
```

The data you are exploring in this tab is the data selected in the sidebar section 'Dataset being used'.

If a metadata variable is not available to choose in the boxplots and/or spectra plots, it means that it needs to be converted to a factor (Pre-Processing page).

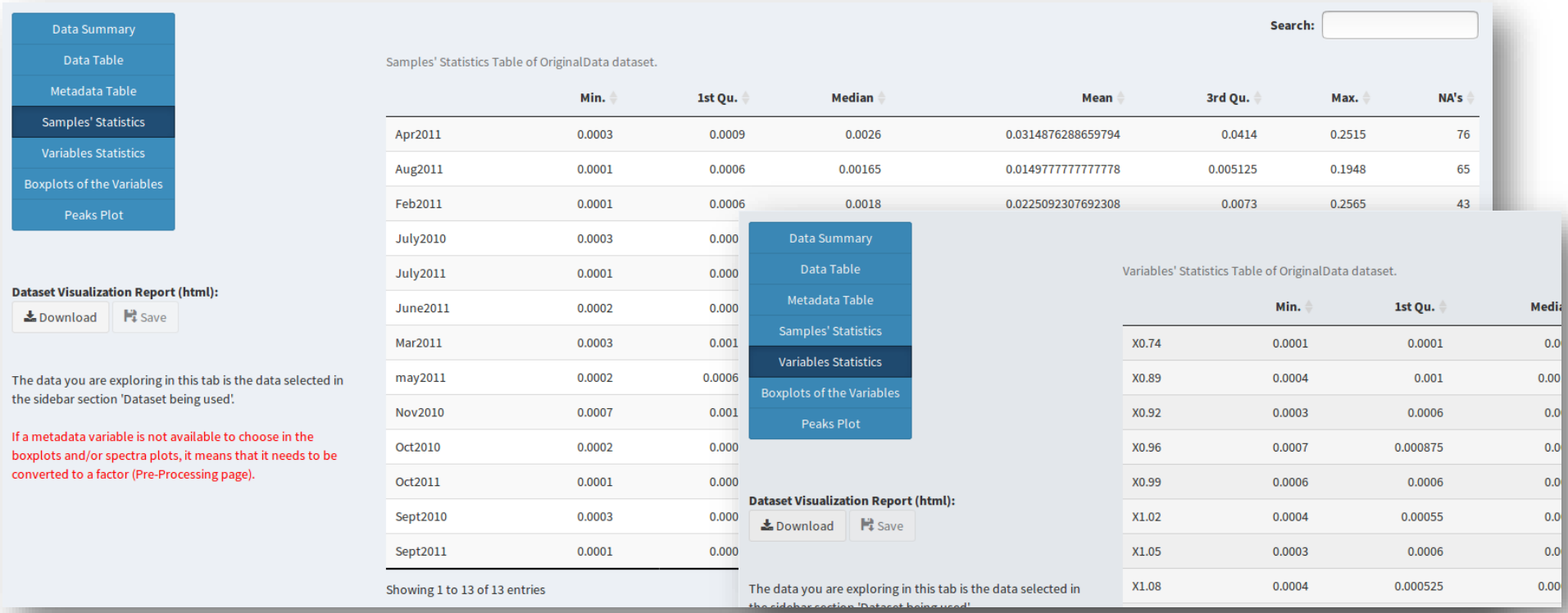
WebSpecmine: Data Visualization

1 2 3 Data and Metadata Tables



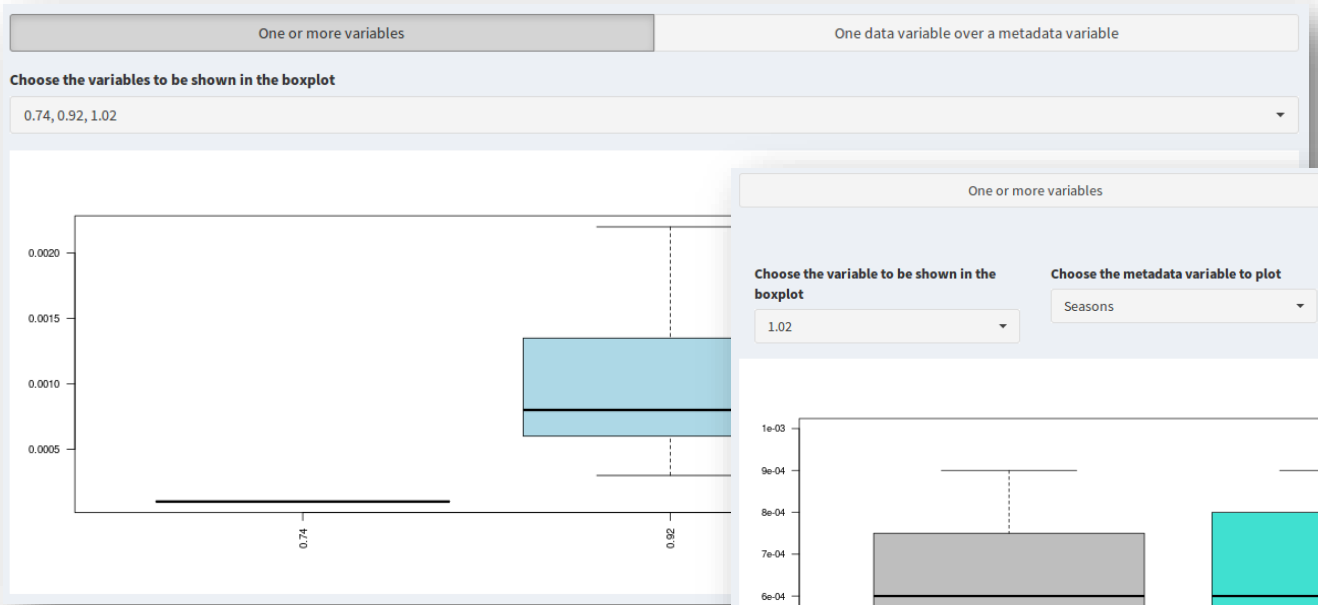
WebSpecmine: Data Visualization

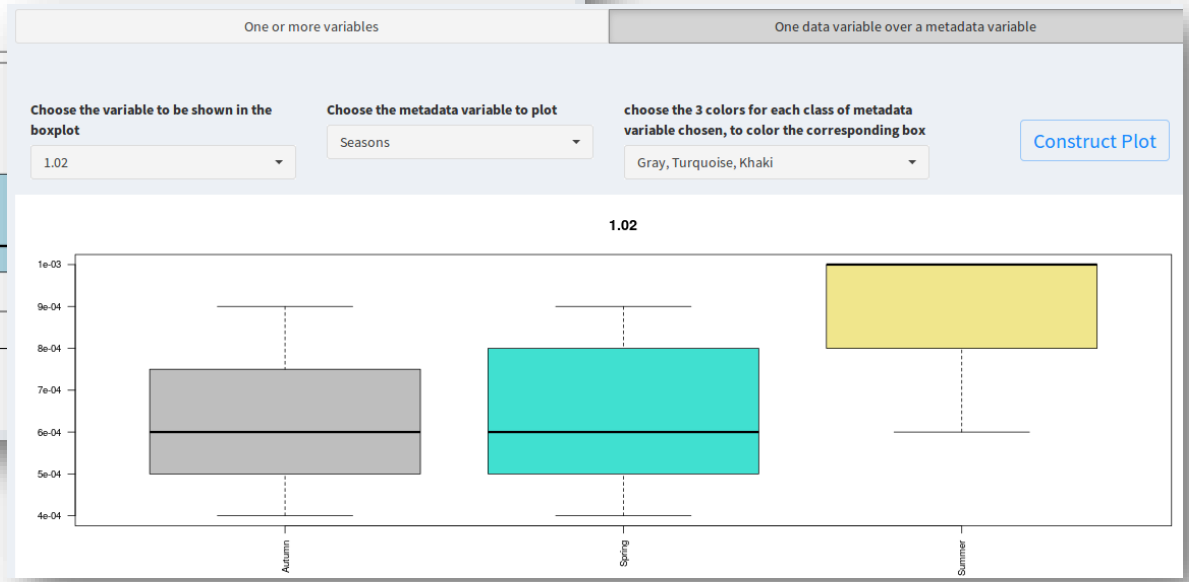
1 2 3 4 Samples' and Variables' Statistics



WebSpecmine: Data Visualization

1 2 3 4 5 Boxplots of the Variables





WebSpecmine: Data Visualization

1 2 3 4 5 **6** Plot for Peaks Data

- Data Summary
- Data Table
- Metadata Table
- Samples' Statistics
- Variables Statistics
- Boxplots of the Variables
- Peaks Plot

Metadata variable to color the plot: Seasons

Select samples to appear on the plot: Show all samples.

Show axis range 0 2.6 5.4 10

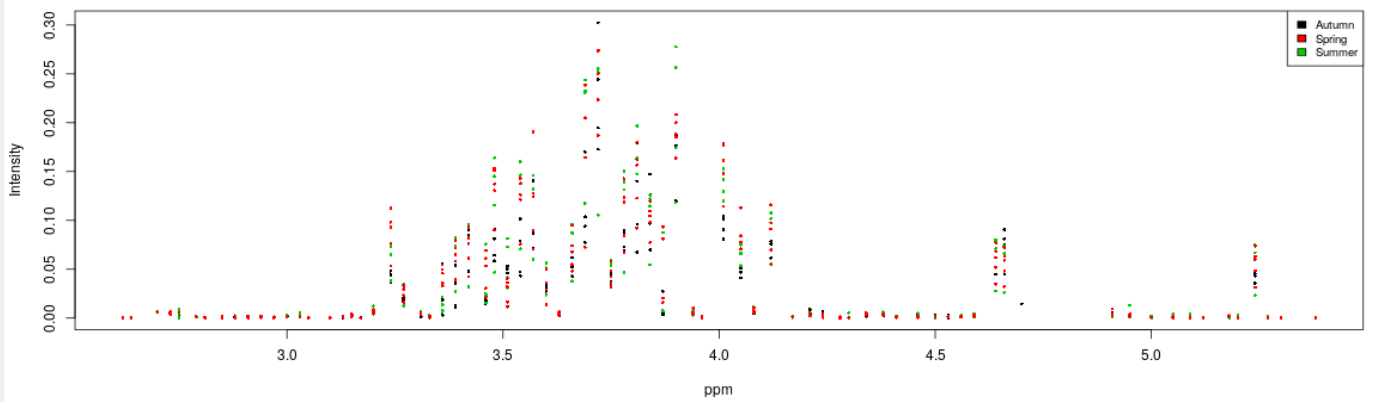
Reverse x-axis

Dataset Visualization Report (html):

Download Save

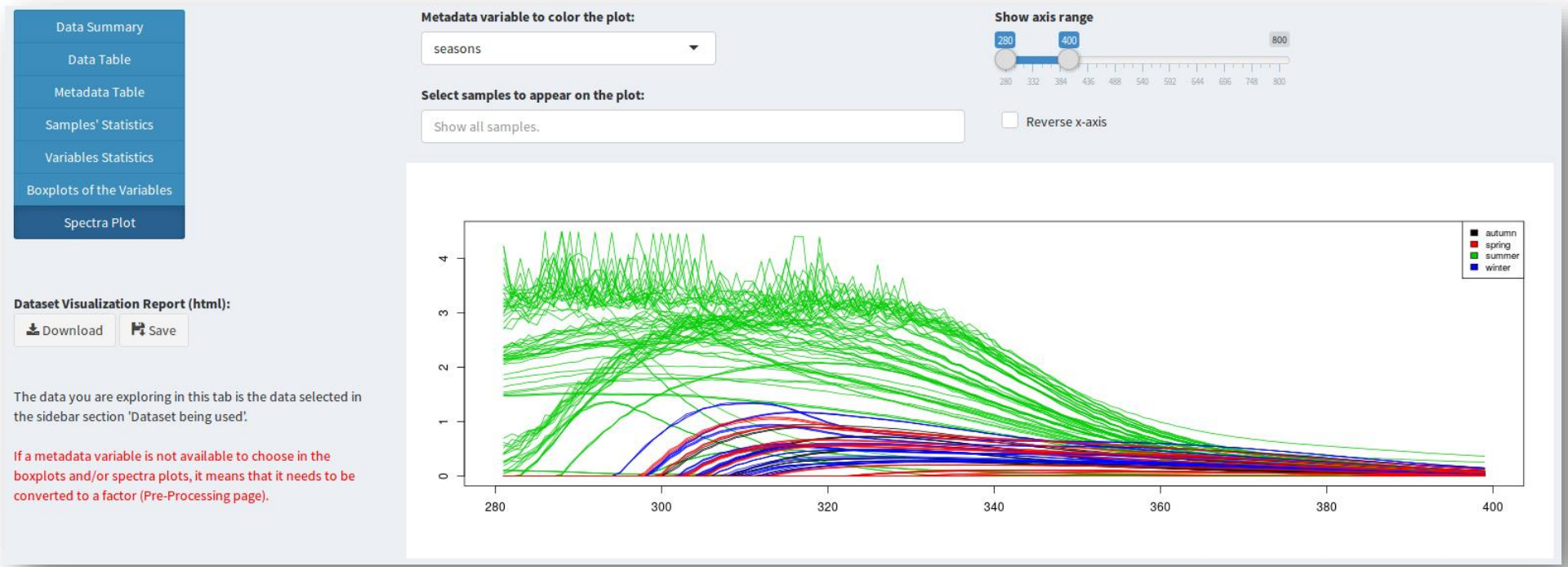
The data you are exploring in this tab is the data selected in the sidebar section 'Dataset being used'.

If a metadata variable is not available to choose in the boxplots and/or spectra plots, it means that it needs to be converted to a factor (Pre-Processing page).



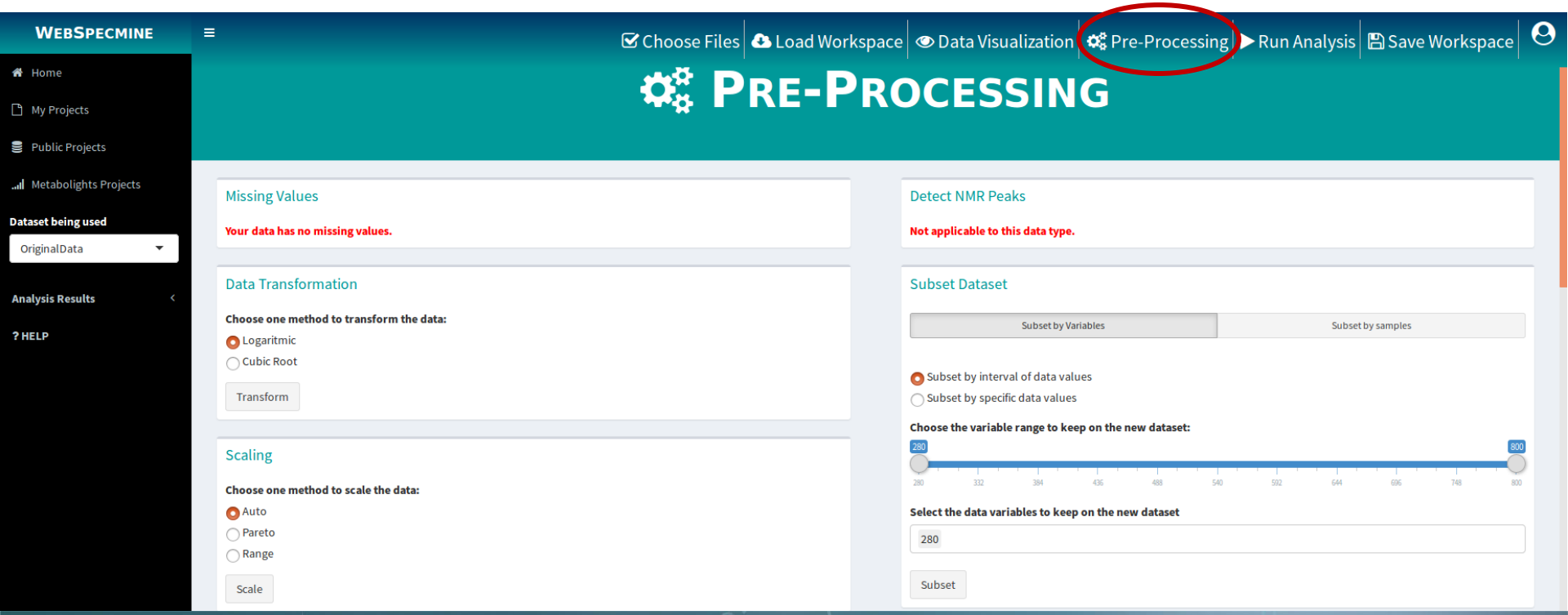
WebSpecmine: Data Visualization

1 2 3 4 5 **6** Plot for Spectra



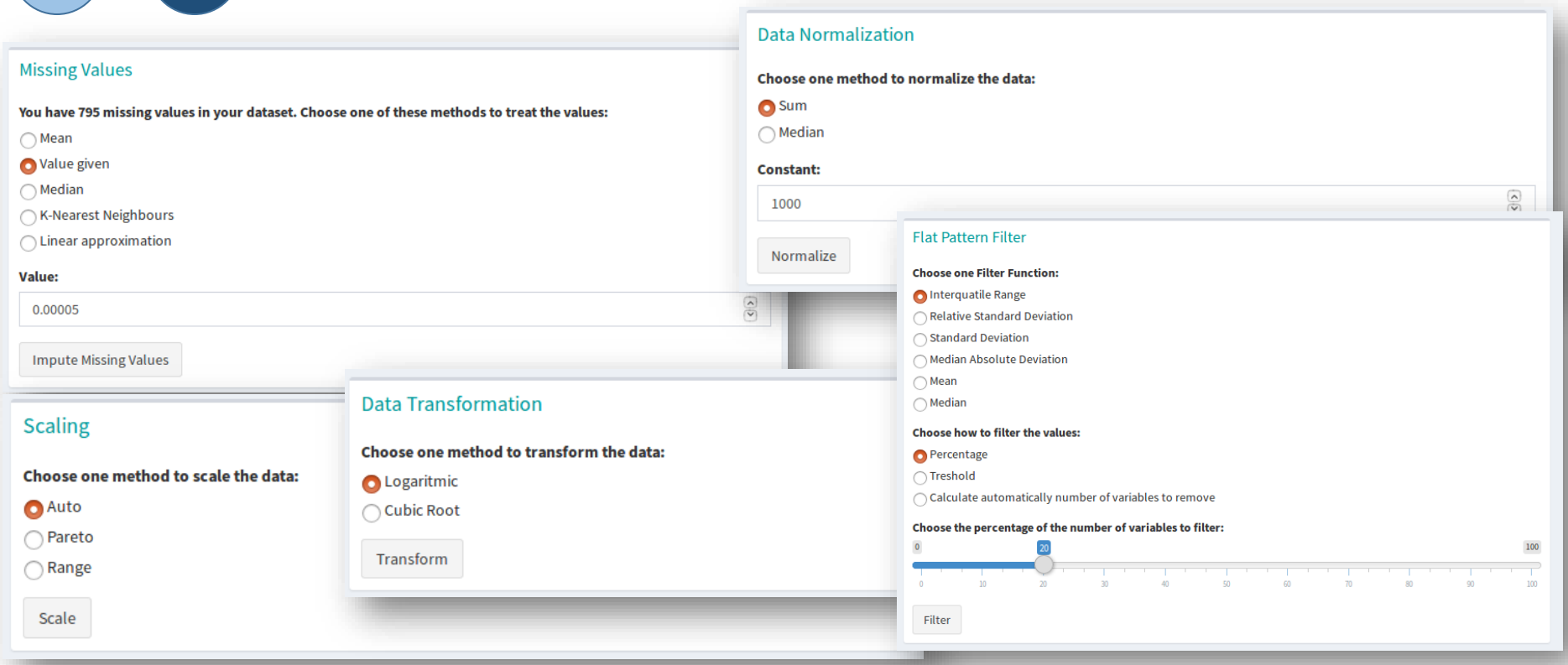
WebSpecmine: Pre-Processing

1 The website provides a wide variety of pre-processing methods, that can be performed in the desired order



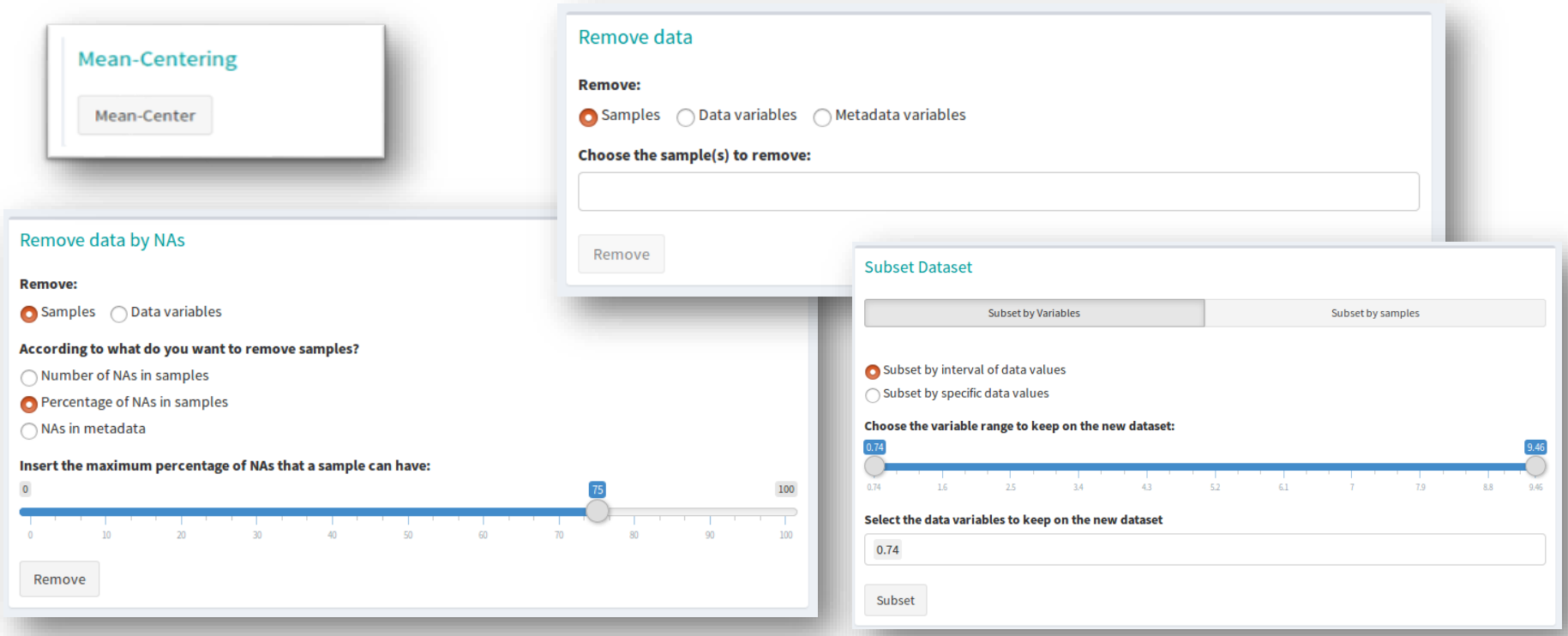
WebSpecmine: Pre-Processing

1 2 Methods that are available for all types of data



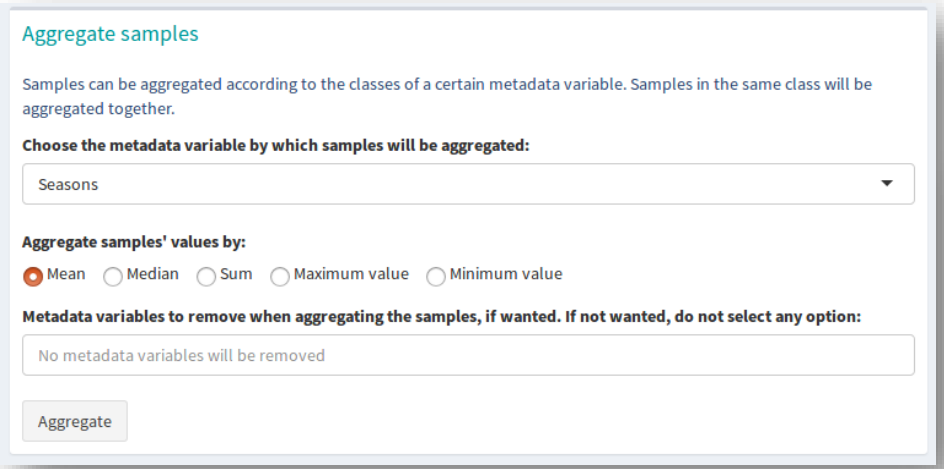
WebSpecmine: Pre-Processing

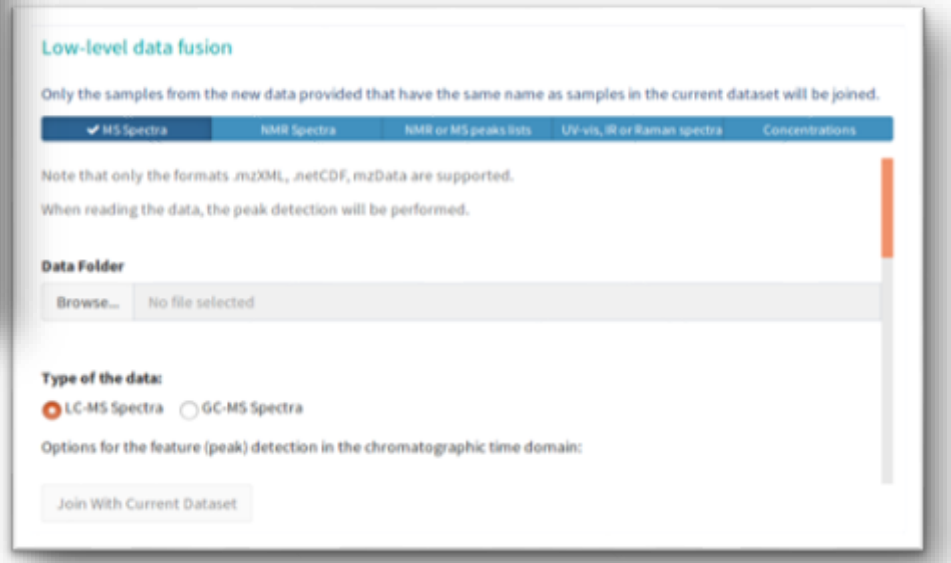
1 2 Methods that are available for all types of data



WebSpecmine: Pre-Processing

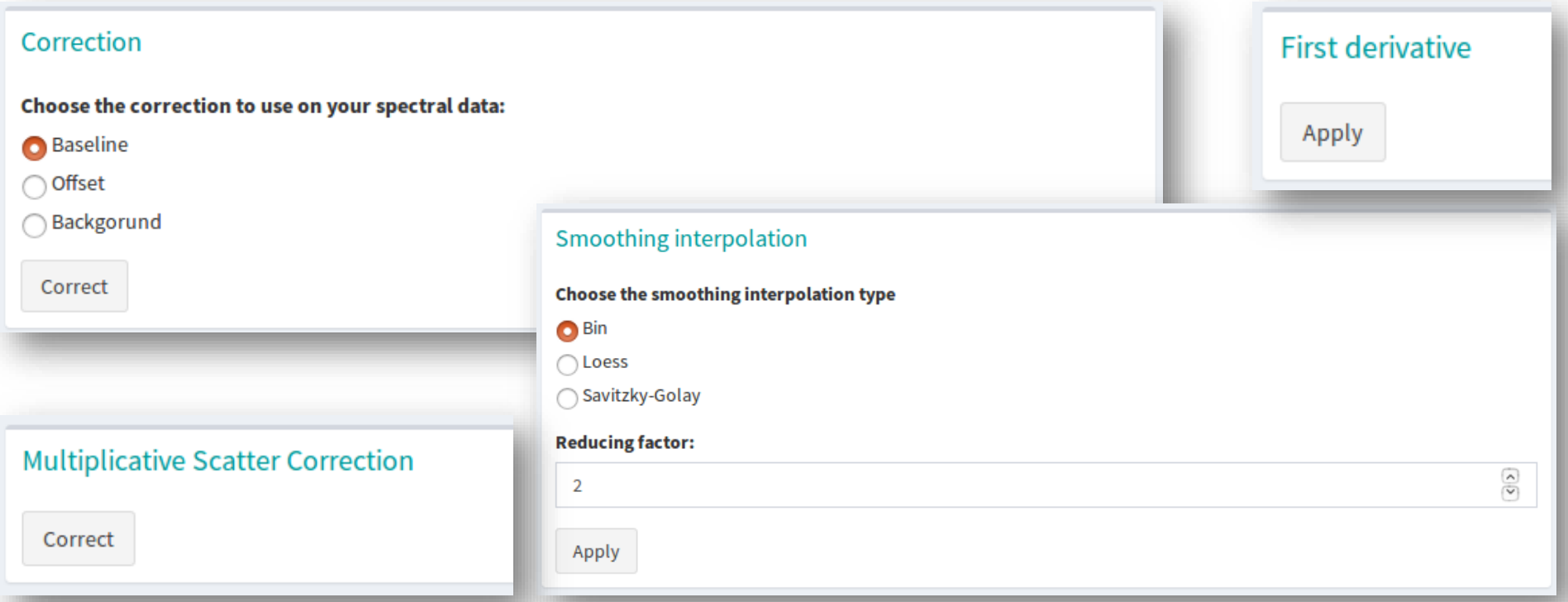
1 2 Methods that are available for all types of data





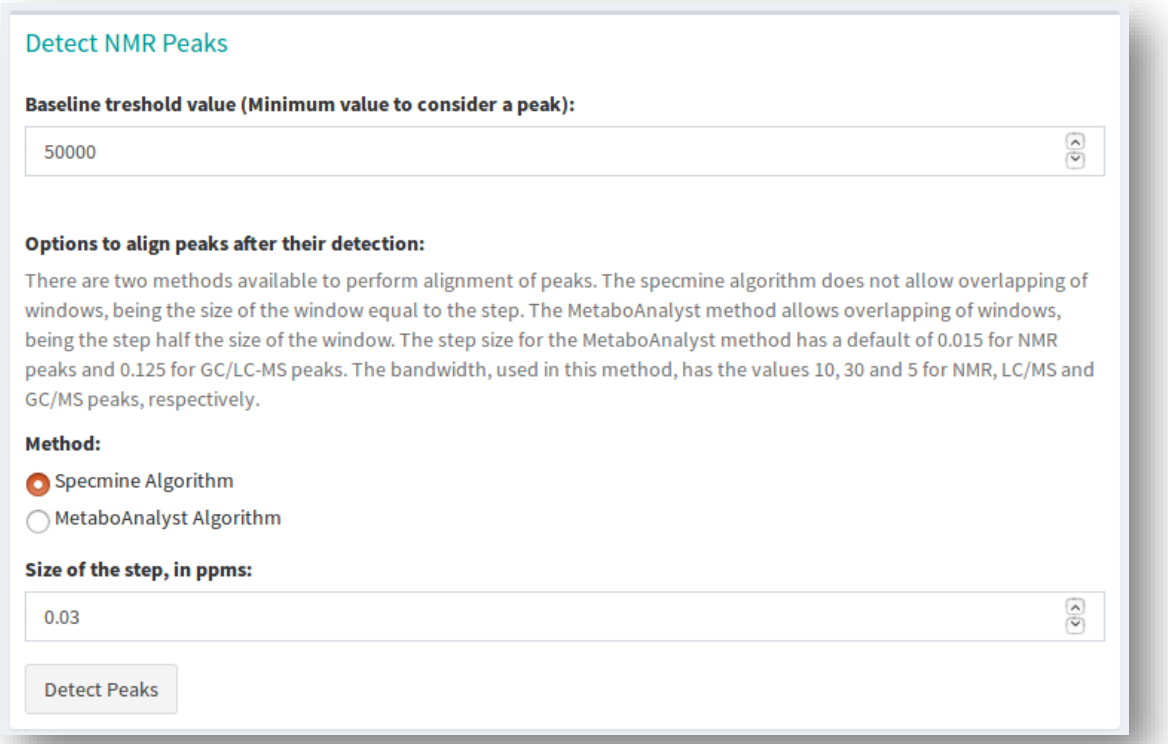
WebSpecmine: Pre-Processing

1 2 3 Methods only for spectral data



WebSpecmine: Pre-Processing

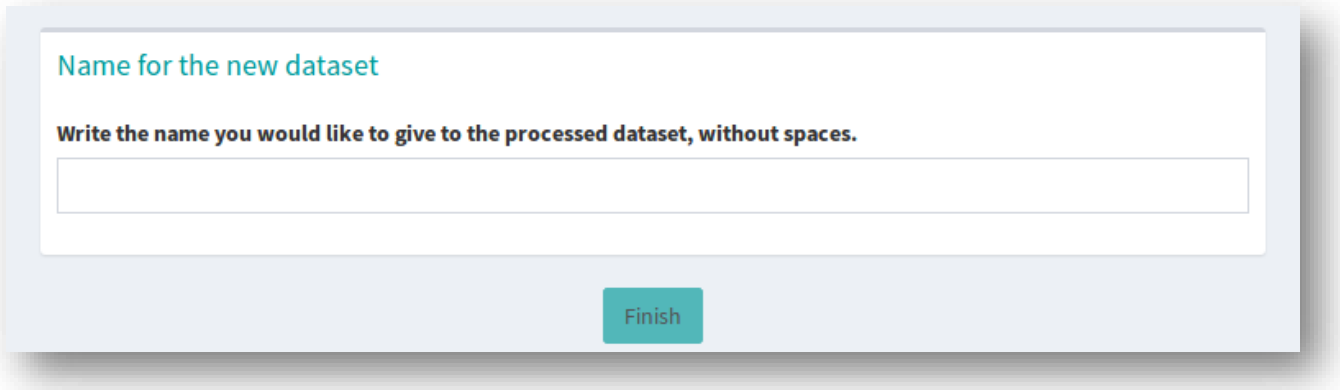
1 2 3 4 Method only for NMR Spectra



WebSpecmine: Pre-Processing

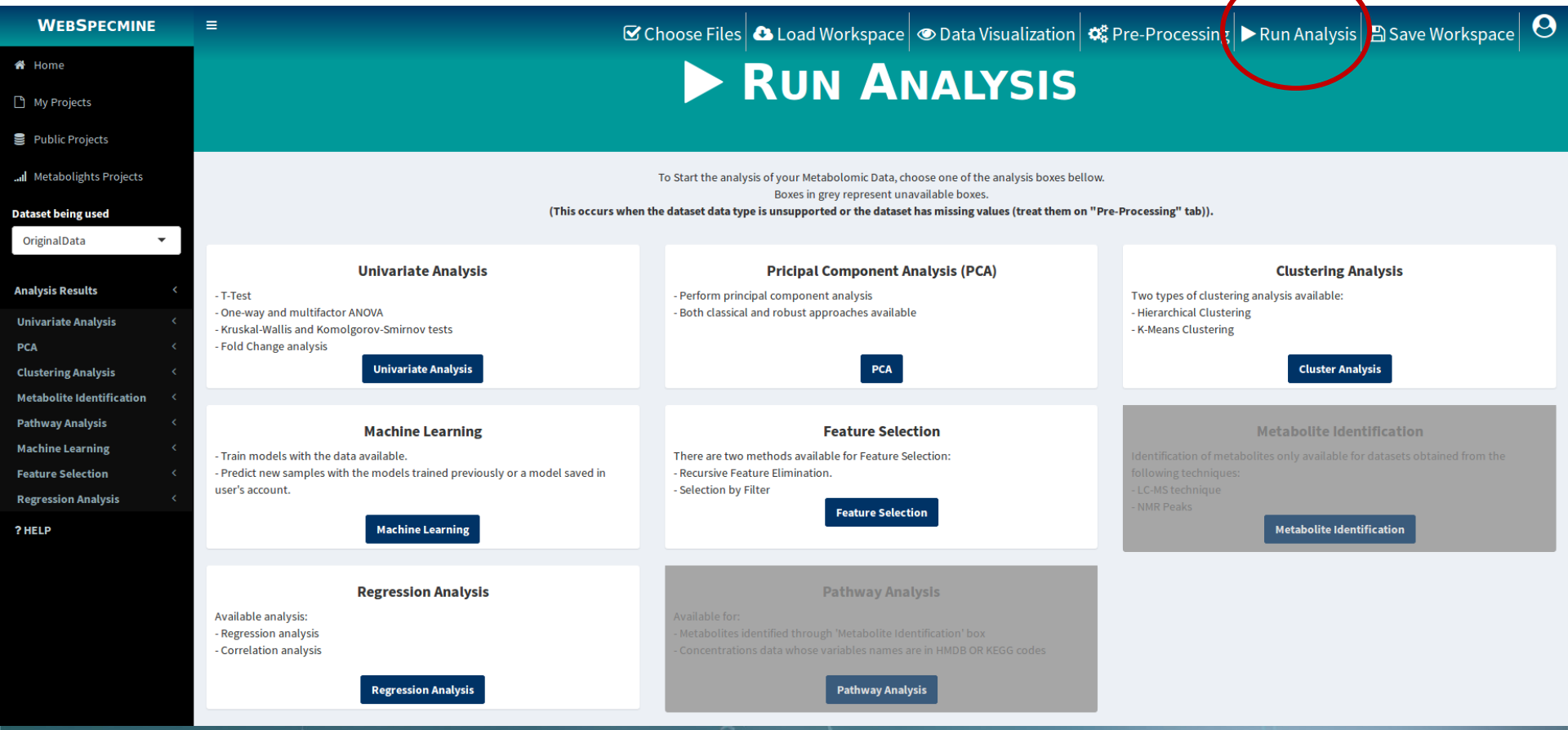
1 — 2 — 3 — 4 — **5**

After processing the data, a name to the new dataset has to be given



ⓘ To perform an analysis on the new dataset, the user will have to choose it on the sidebar panel

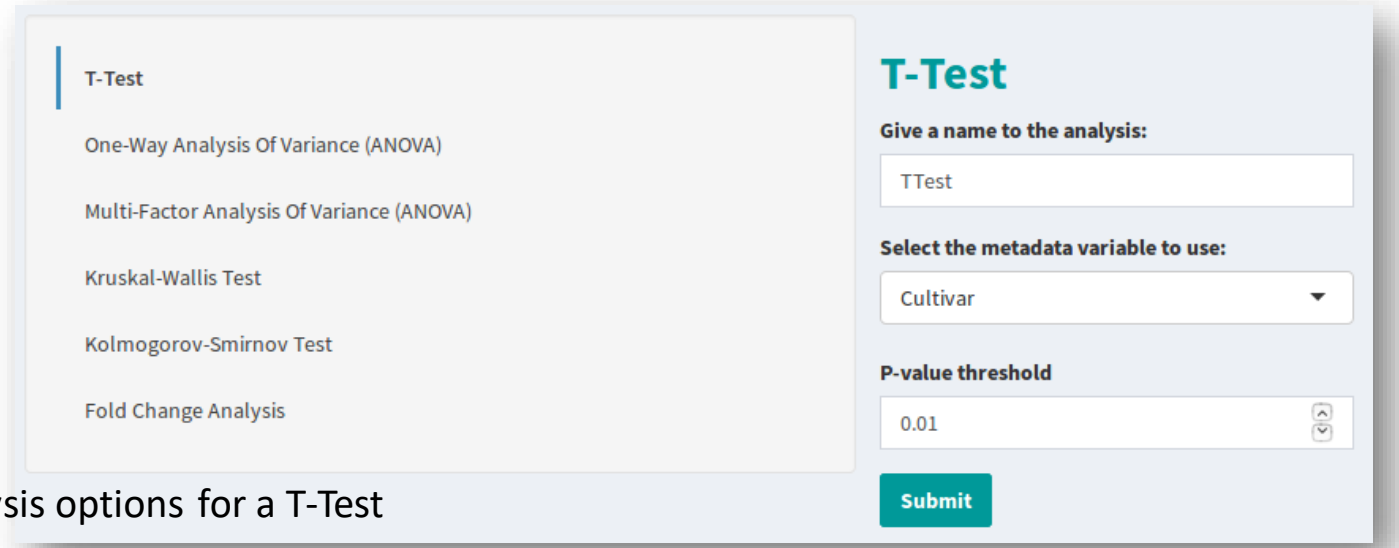
WebSpecmine: Data Analysis



WebSpecmine: Data Analysis

Univariate Analysis

Example for T-Test

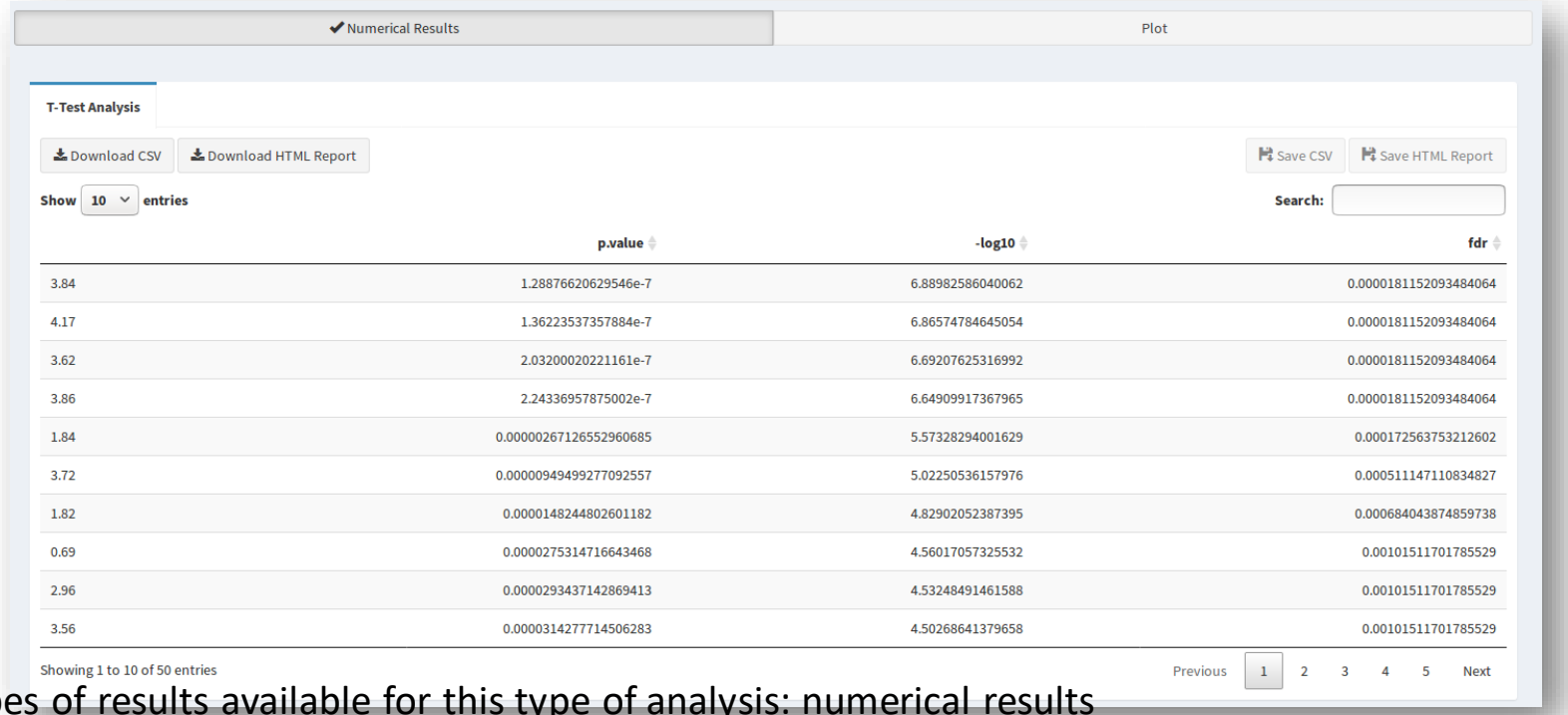


ⓘ Analysis options for a T-Test

WebSpecmine: Data Analysis

Univariate Analysis

Example for T-Test

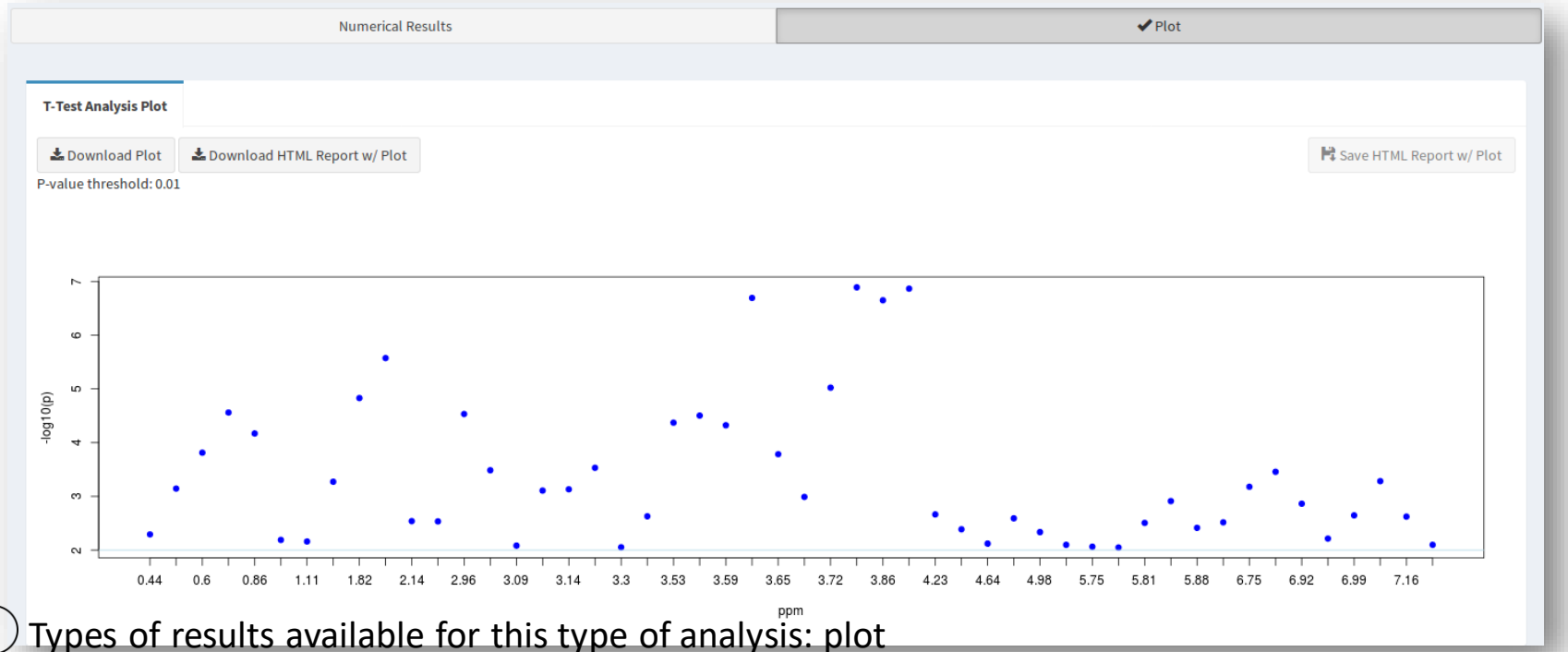


ⓘ Types of results available for this type of analysis: numerical results

WebSpecmine: Data Analysis

Univariate Analysis

Example for T-Test

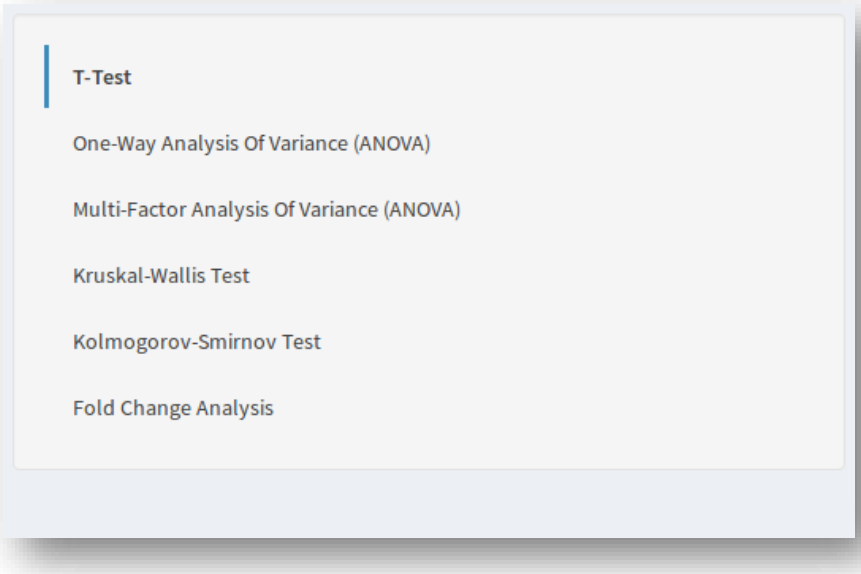


ⓘ Types of results available for this type of analysis: plot

WebSpecmine: Data Analysis

Univariate Analysis

Other Analysis

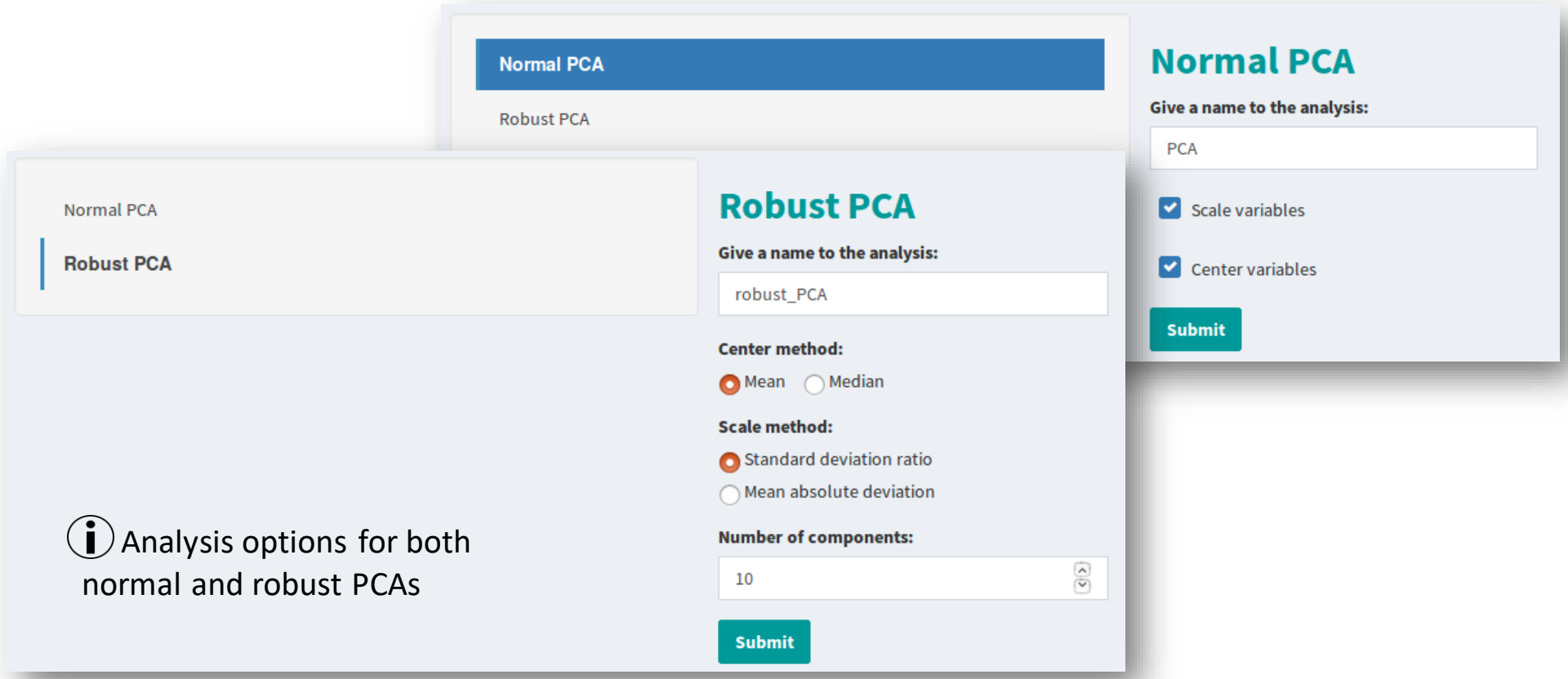


ⓘ There are other Univariate Analysis methods available

ⓘ The types of results available for each analysis is similar to those showed for T-Test

WebSpecmine: Data Analysis

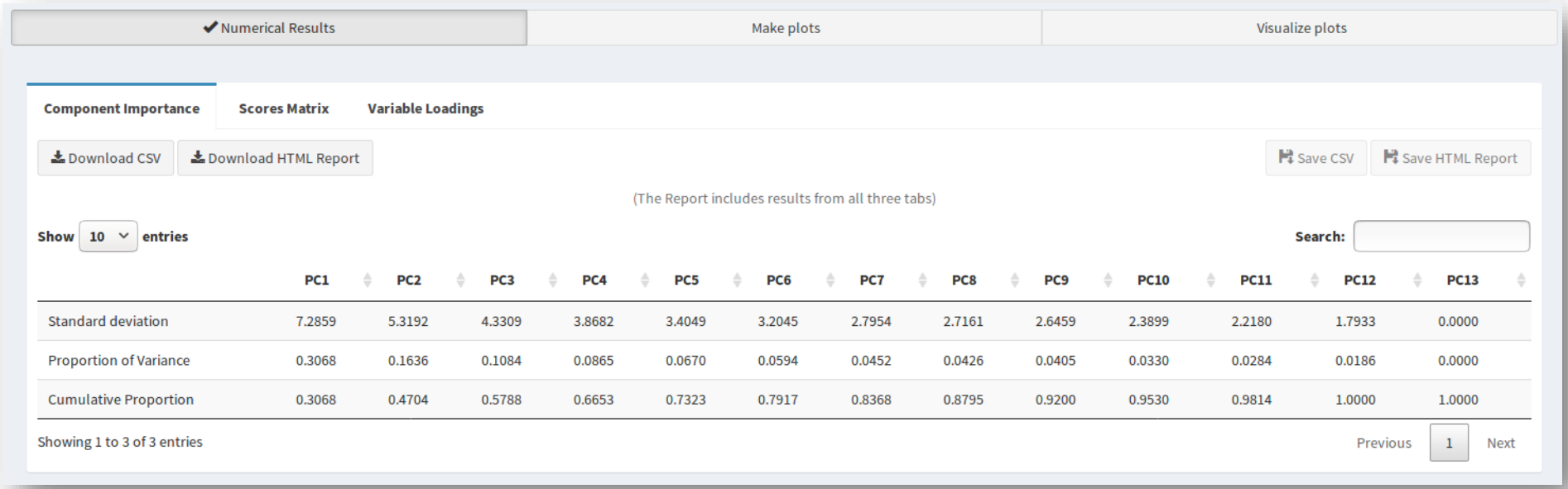
Principal Components Analysis (PCA)



ⓘ Analysis options for both normal and robust PCAs

WebSpecmine: Data Analysis

Principal Components Analysis (PCA)



✔ Numerical Results | Make plots | Visualize plots

Component Importance | **Scores Matrix** | **Variable Loadings**

Download CSV | Download HTML Report | Save CSV | Save HTML Report

(The Report includes results from all three tabs)

Show 10 entries | Search:

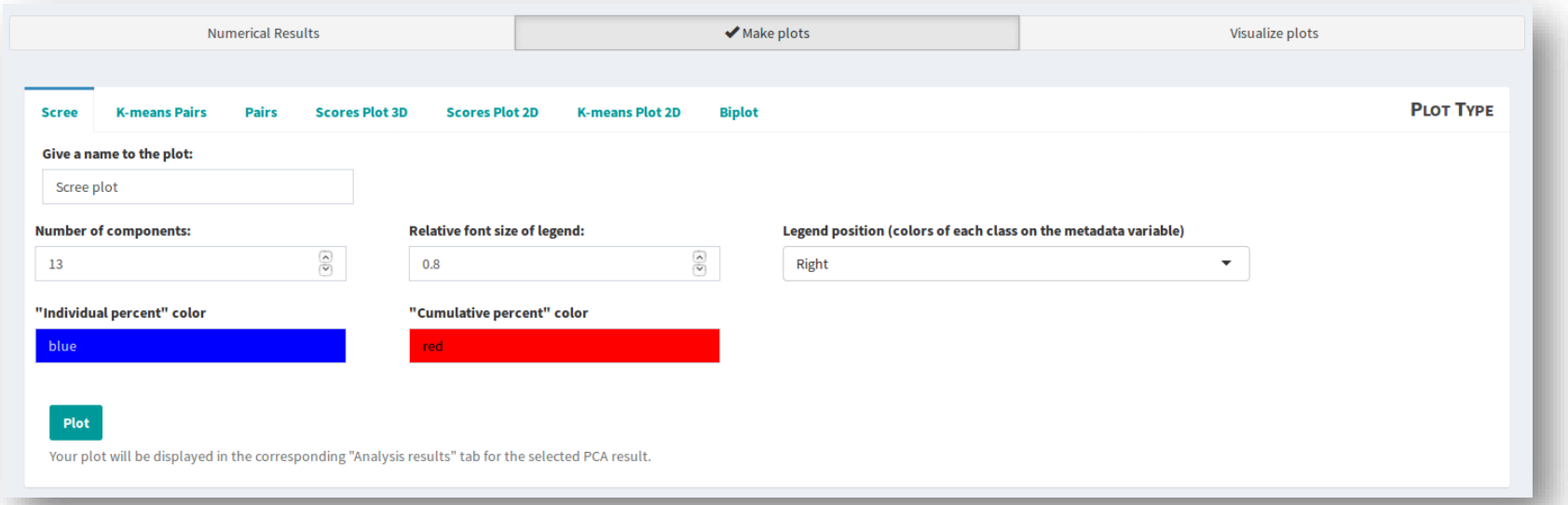
	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9	PC10	PC11	PC12	PC13
Standard deviation	7.2859	5.3192	4.3309	3.8682	3.4049	3.2045	2.7954	2.7161	2.6459	2.3899	2.2180	1.7933	0.0000
Proportion of Variance	0.3068	0.1636	0.1084	0.0865	0.0670	0.0594	0.0452	0.0426	0.0405	0.0330	0.0284	0.0186	0.0000
Cumulative Proportion	0.3068	0.4704	0.5788	0.6653	0.7323	0.7917	0.8368	0.8795	0.9200	0.9530	0.9814	1.0000	1.0000

Showing 1 to 3 of 3 entries | Previous | 1 | Next

ⓘ Types of results available for this type of analysis: numerical results

WebSpecmine: Data Analysis

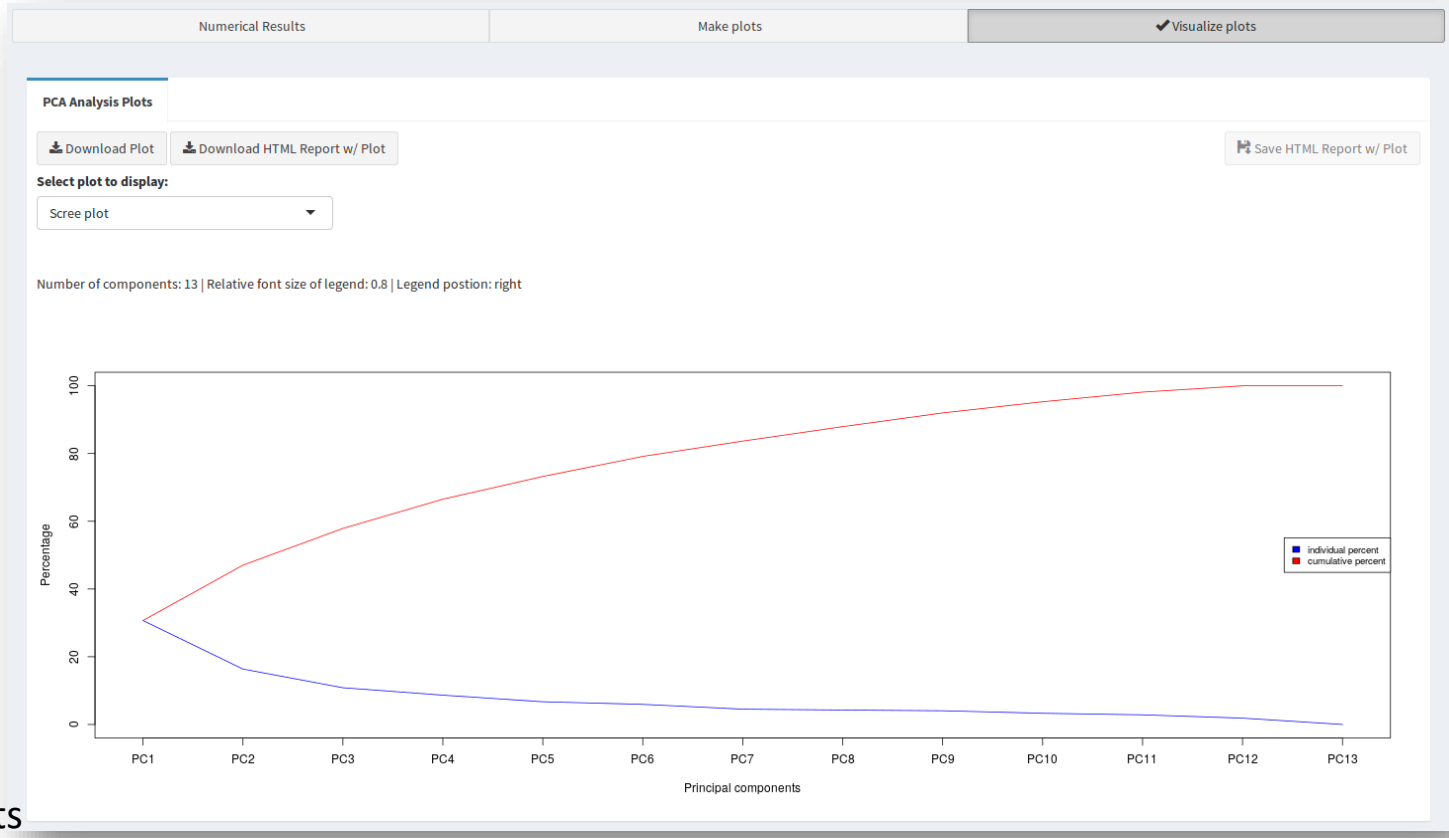
Principal Components Analysis (PCA)



ⓘ Types of results available for this type of analysis: plot results

WebSpecmine: Data Analysis

Principal Components Analysis (PCA)

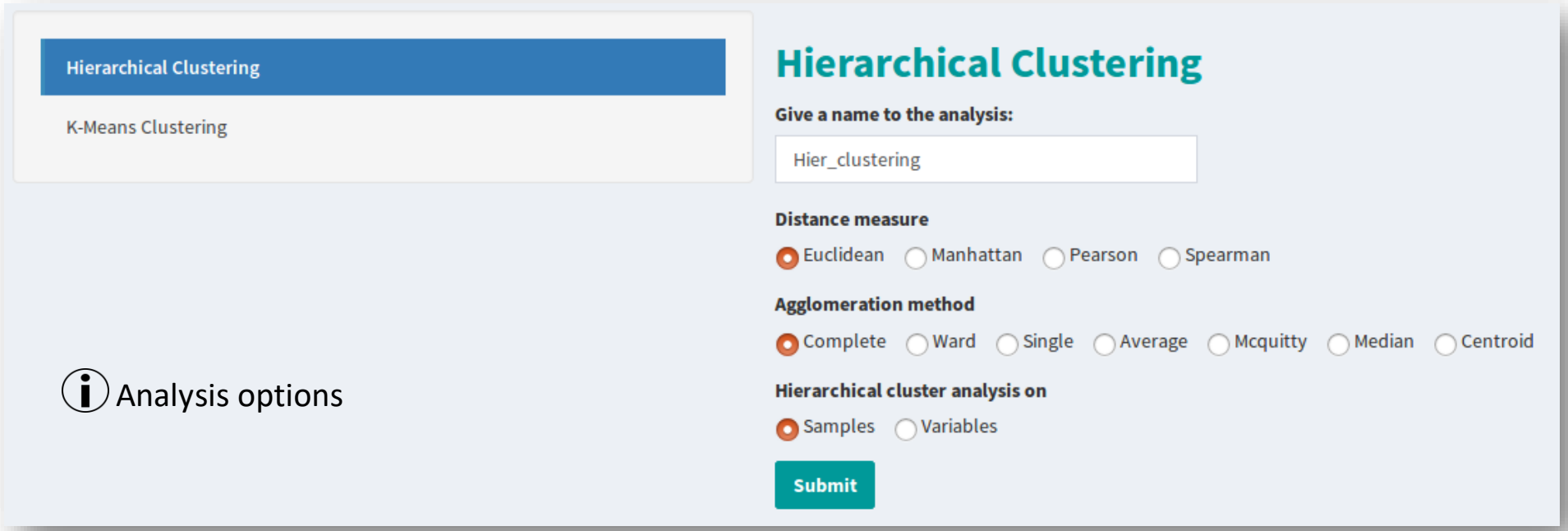


ⓘ Types of results available for this type of analysis: plot results

WebSpecmine: Data Analysis

Clustering Analysis

Hierarchical Clustering

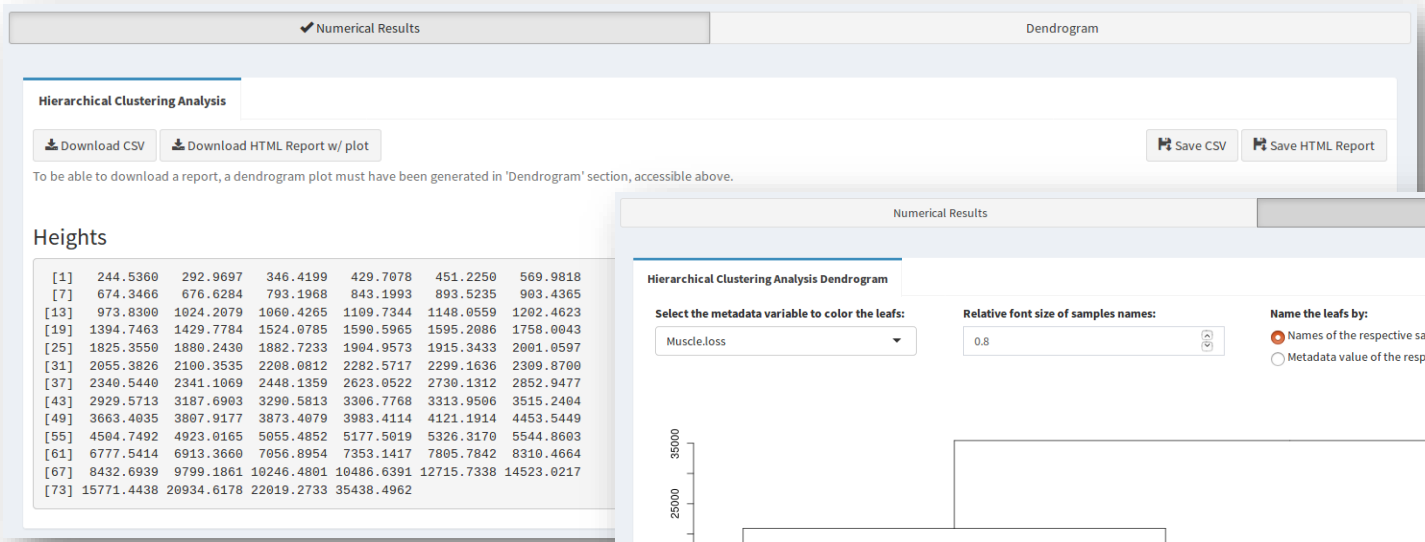


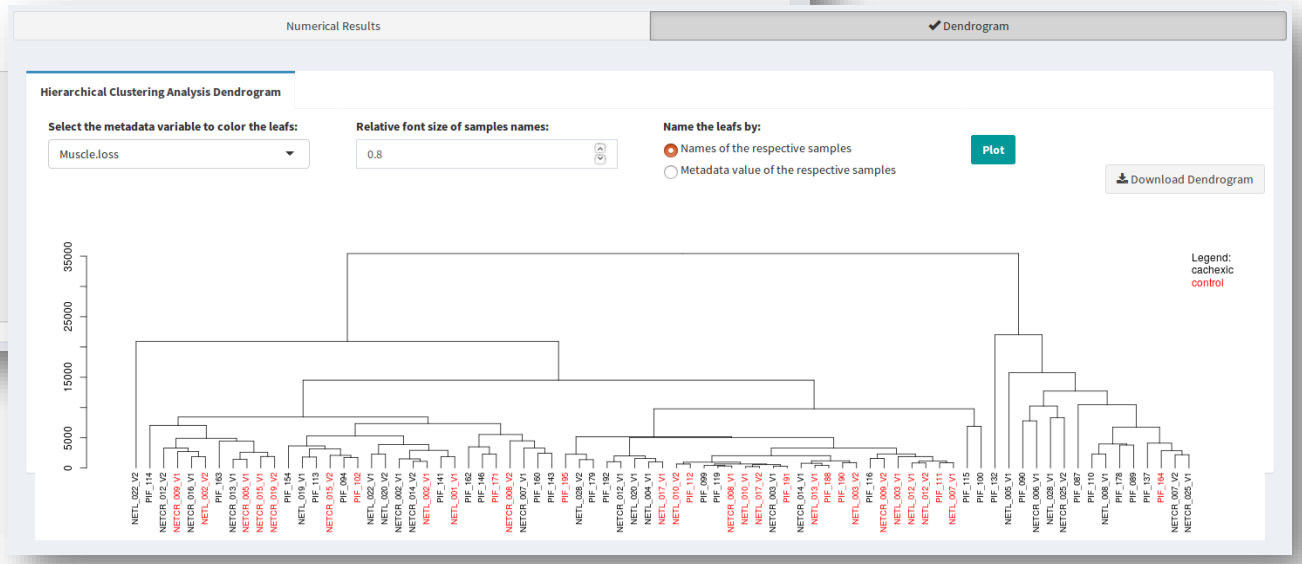
ⓘ Analysis options

WebSpecmine: Data Analysis

Clustering Analysis

Hierarchical Clustering



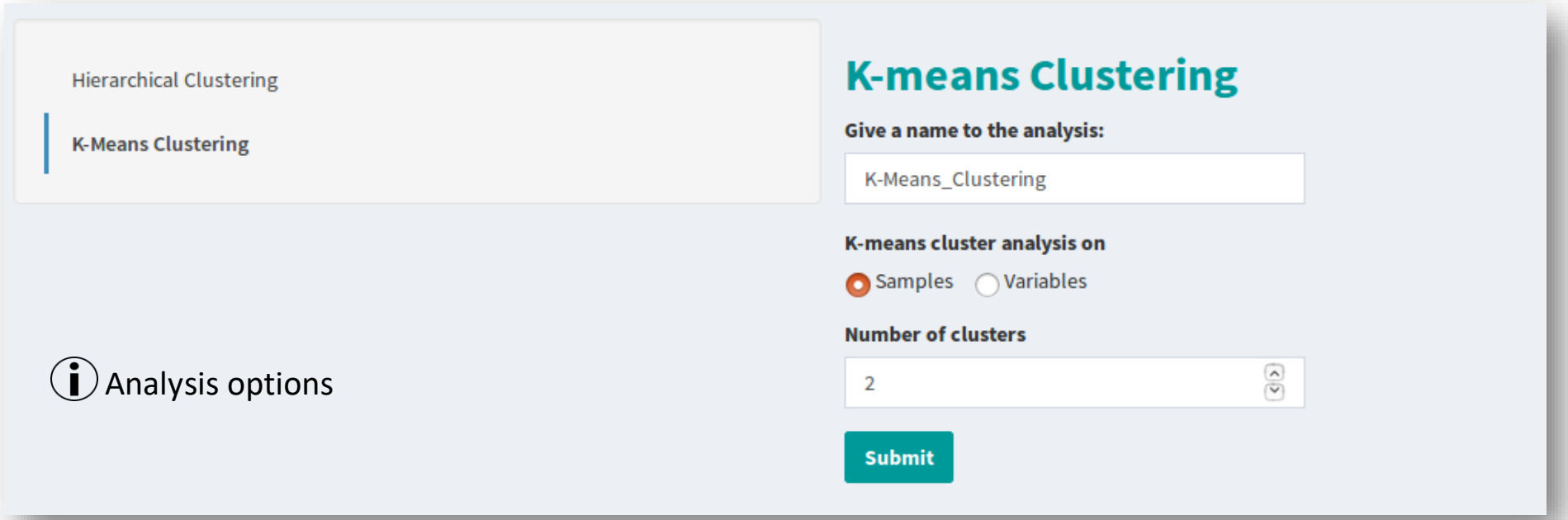


ⓘ Types of results available for this type of analysis

WebSpecmine: Data Analysis

Clustering Analysis

K-Means Clustering

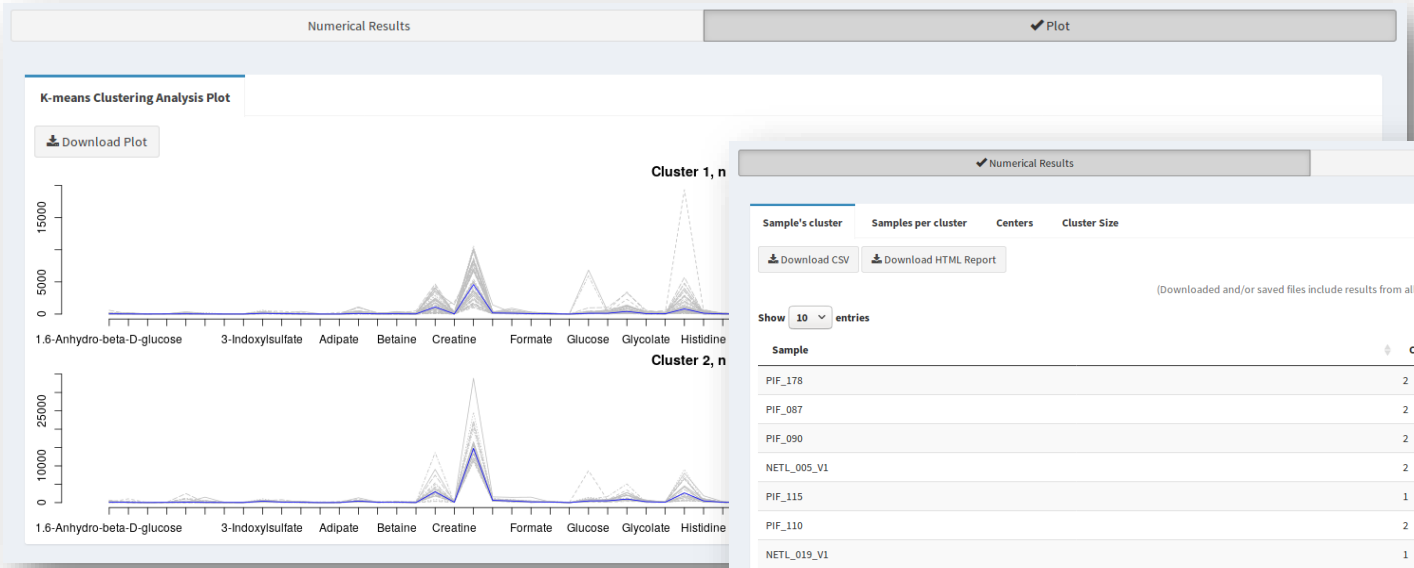


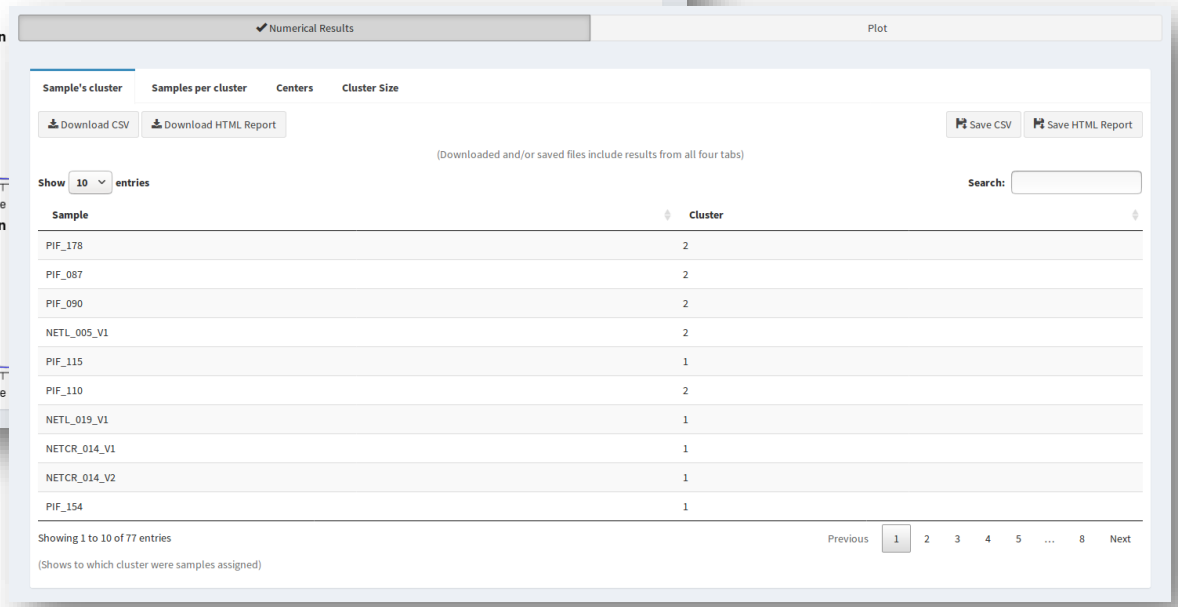
ⓘ Analysis options

WebSpecmine: Data Analysis

Clustering Analysis

K-Means Clustering



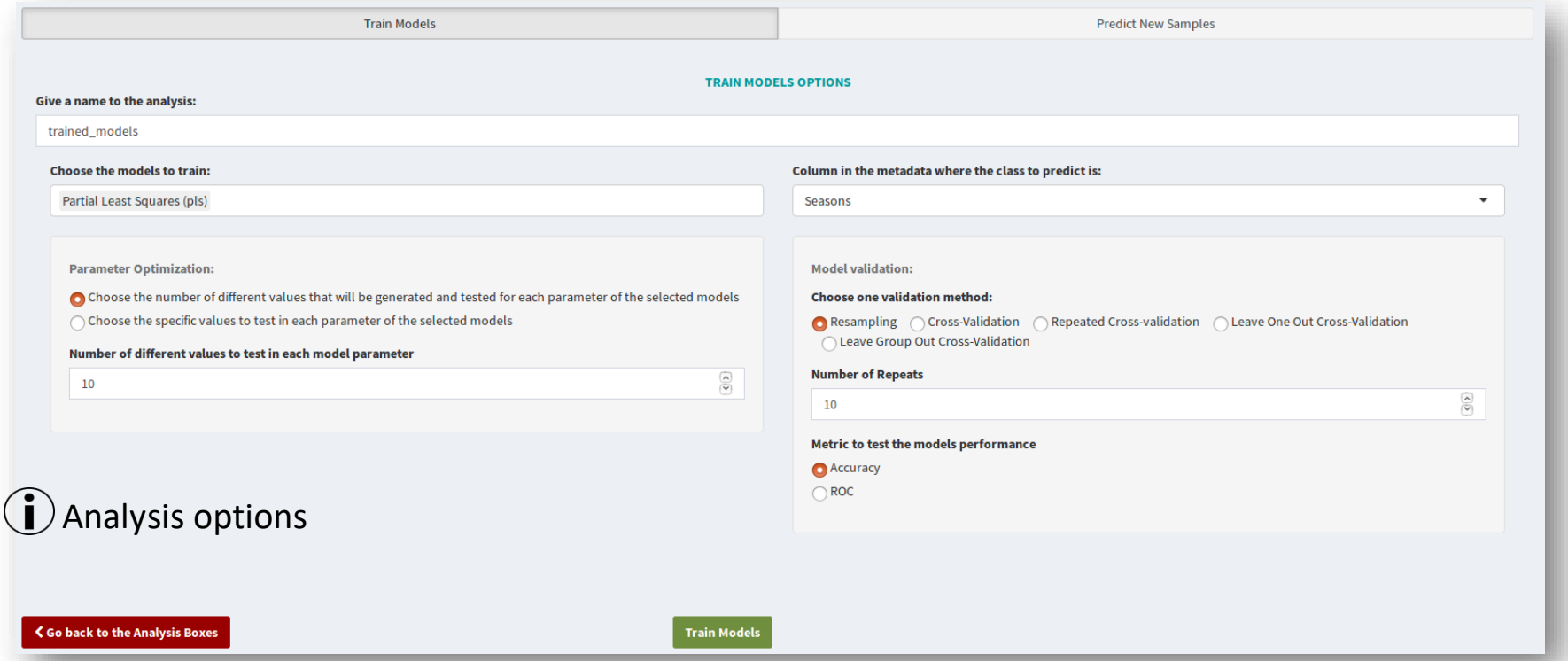


ⓘ Types of results available for this type of analysis

WebSpecmine: Data Analysis

Machine Learning

Train Models

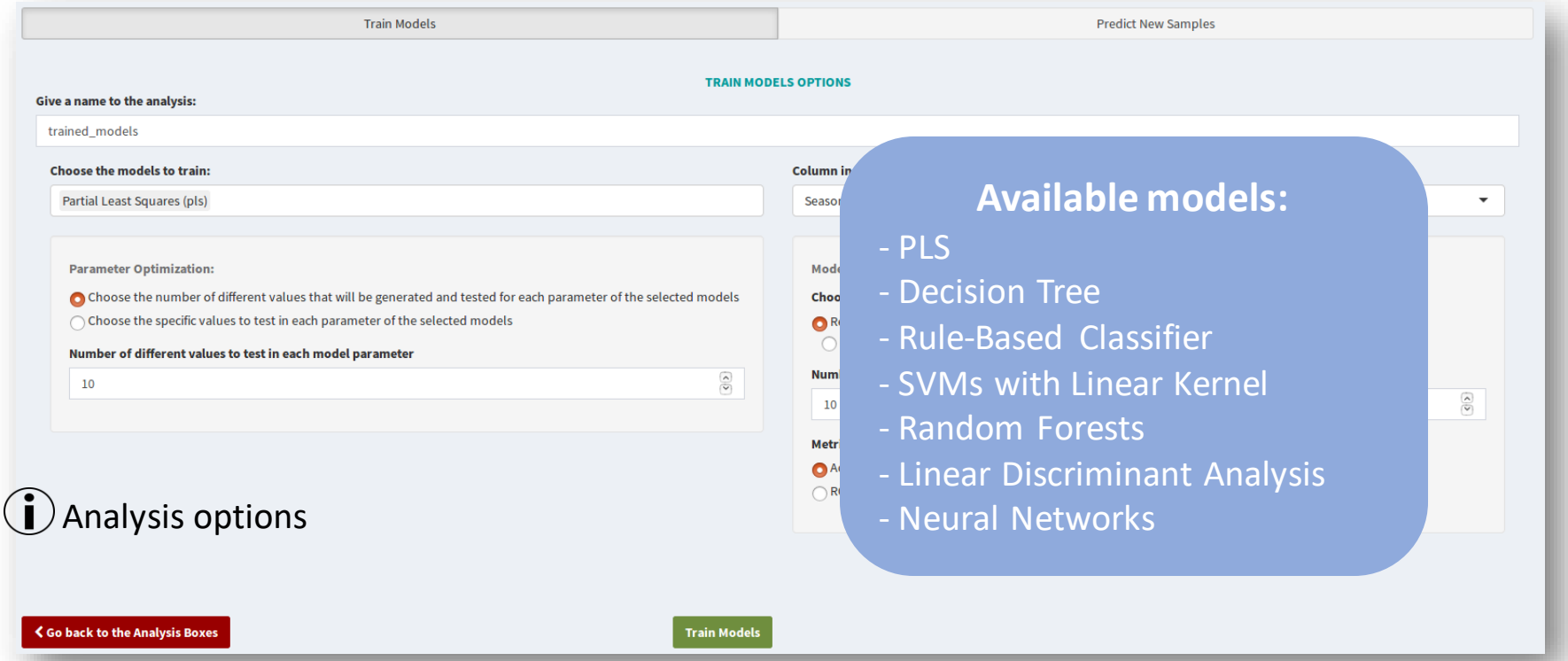


ⓘ Analysis options

WebSpecmine: Data Analysis

Machine Learning

Train Models



Available models:

- PLS
- Decision Tree
- Rule-Based Classifier
- SVMs with Linear Kernel
- Random Forests
- Linear Discriminant Analysis
- Neural Networks

ⓘ Analysis options

WebSpecmine: Data Analysis

Machine Learning

Train Models

Partial Least Squares

Best Model Results | Full Results | Variables' Importance | 3D PCA Plot | Loadings Plot | Loadings Table

Download Plot Image

Save Plot Image

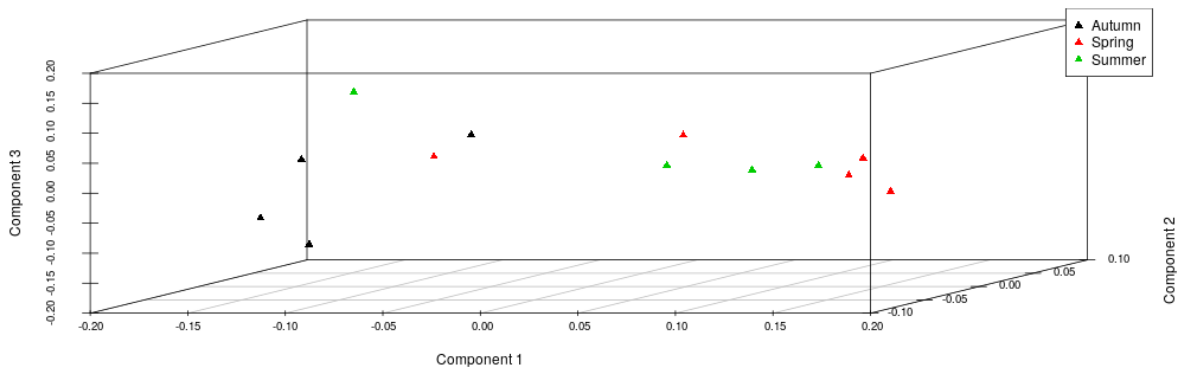
Choose the 3 Principal Comonents (PCs) to show in the plot:

1 2 3

Where to place the legend on the plot:

Top Right

Plot

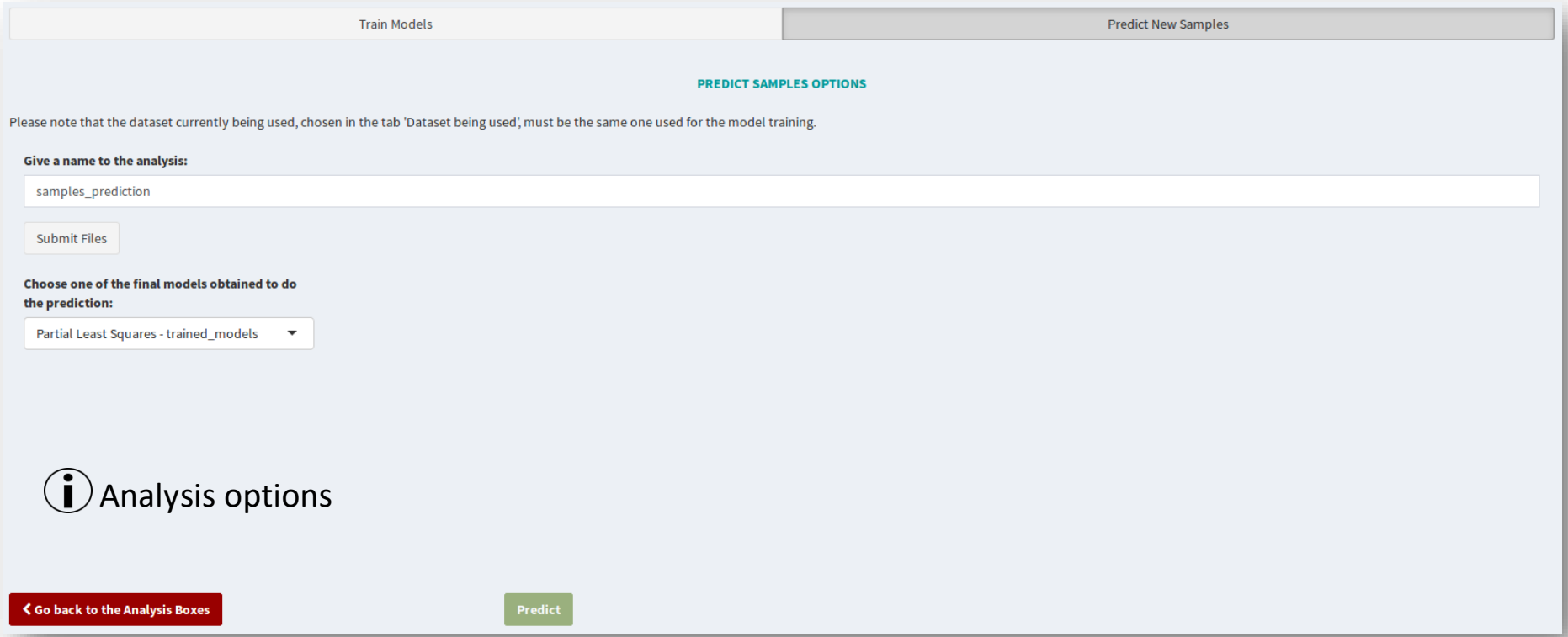


Types of results available for this type of analysis

WebSpecmine: Data Analysis

Machine Learning

Predict New Samples



WebSpecmine: Data Analysis

Machine Learning

Predict New Samples

Predicted samples report (html):

Download | Save

ⓘ Types of results available for this type of analysis

Search:

Samples' Names	Predicted Class
Apr2011	Summer
Aug2011	Autumn
Feb2011	Summer
July2010	Summer
July2011	Autumn
June2011	Autumn
Mar2011	Summer
may2011	Summer
Nov2010	Spring
Oct2010	Spring

Showing 1 to 13 of 13 entries

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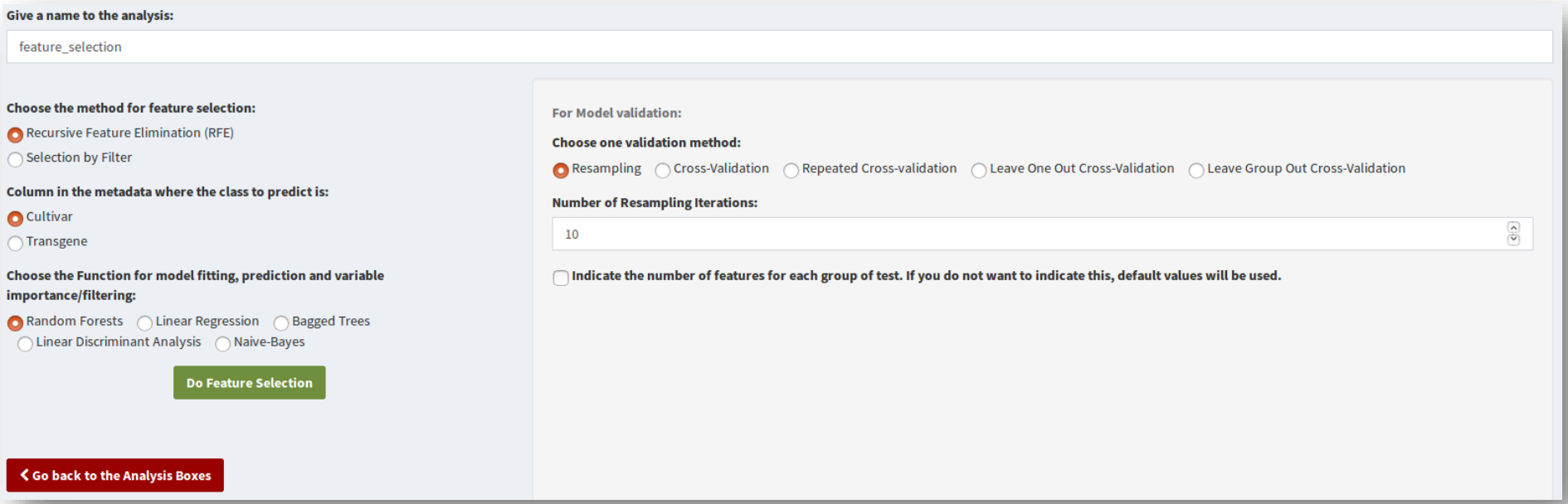
WebSpecmine: Data Analysis

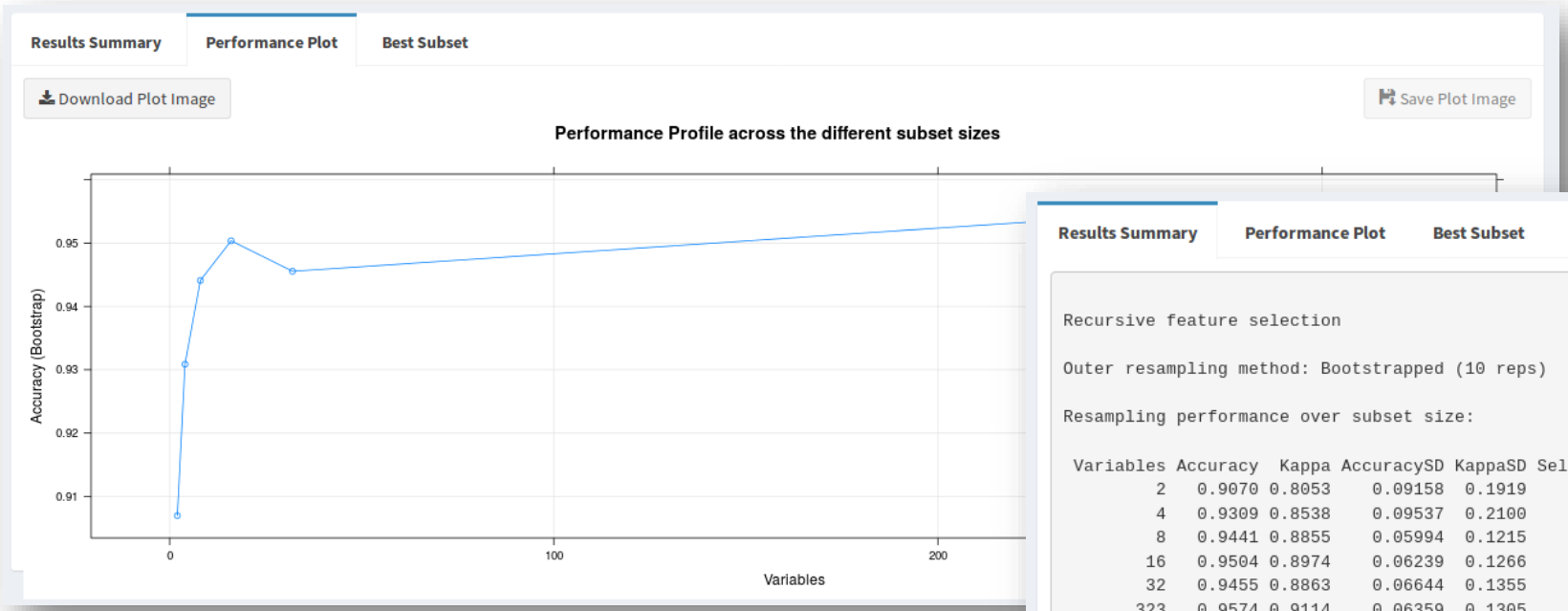
Feature Selection



ⓘ Analysis options

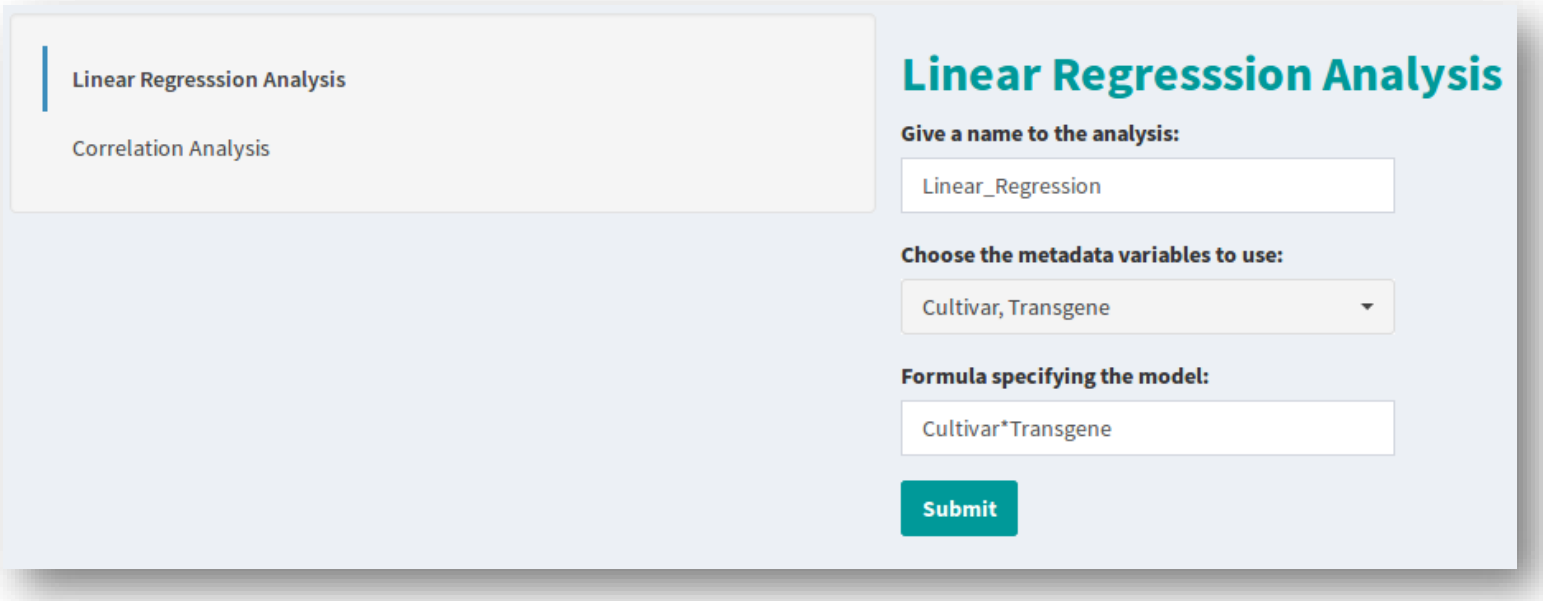
WebSpecmine: Data Analysis

Feature Selection



ⓘ Types of results available for this type of analysis

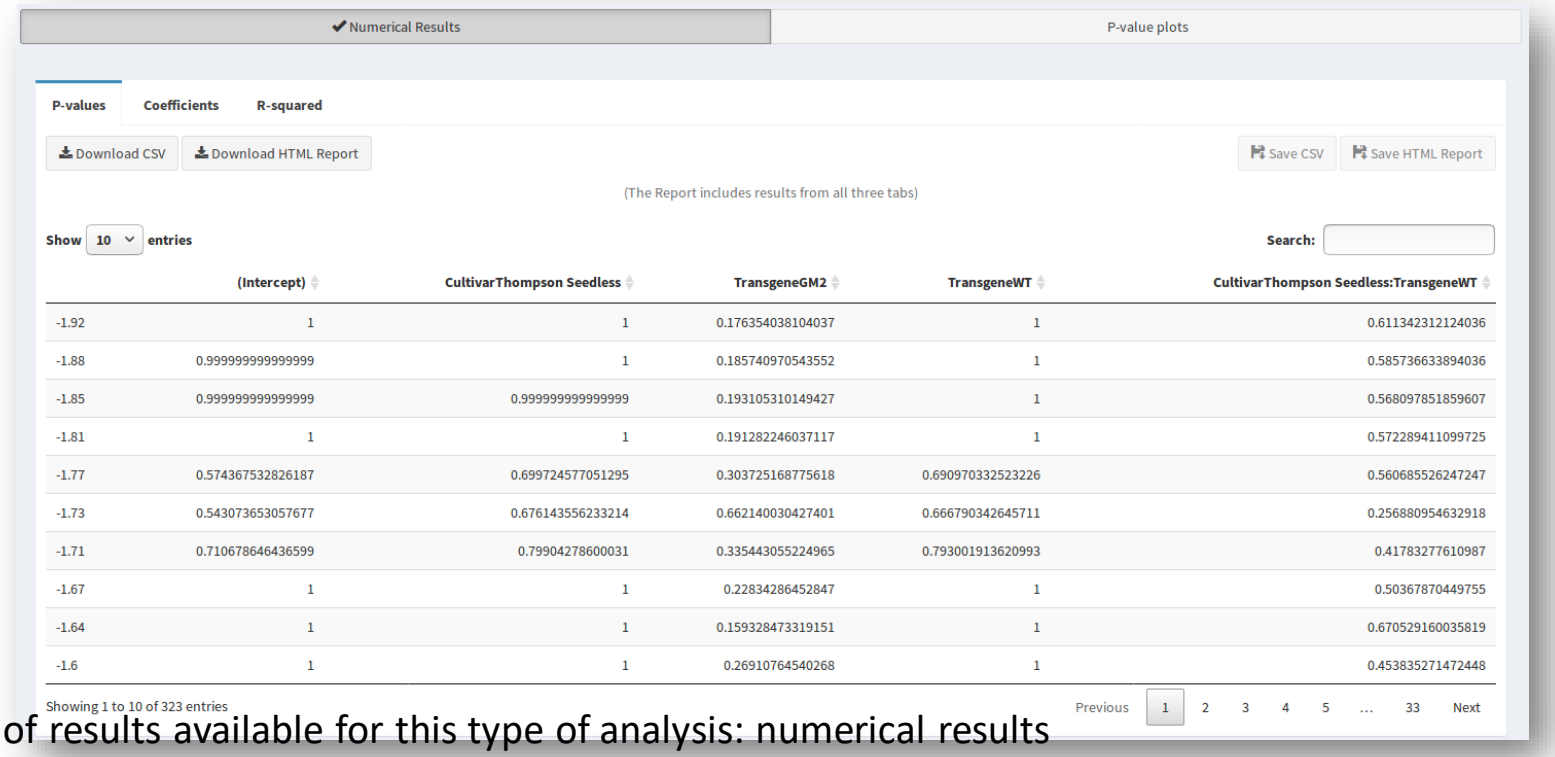
WebSpecmine: Data Analysis



ⓘ Analysis options

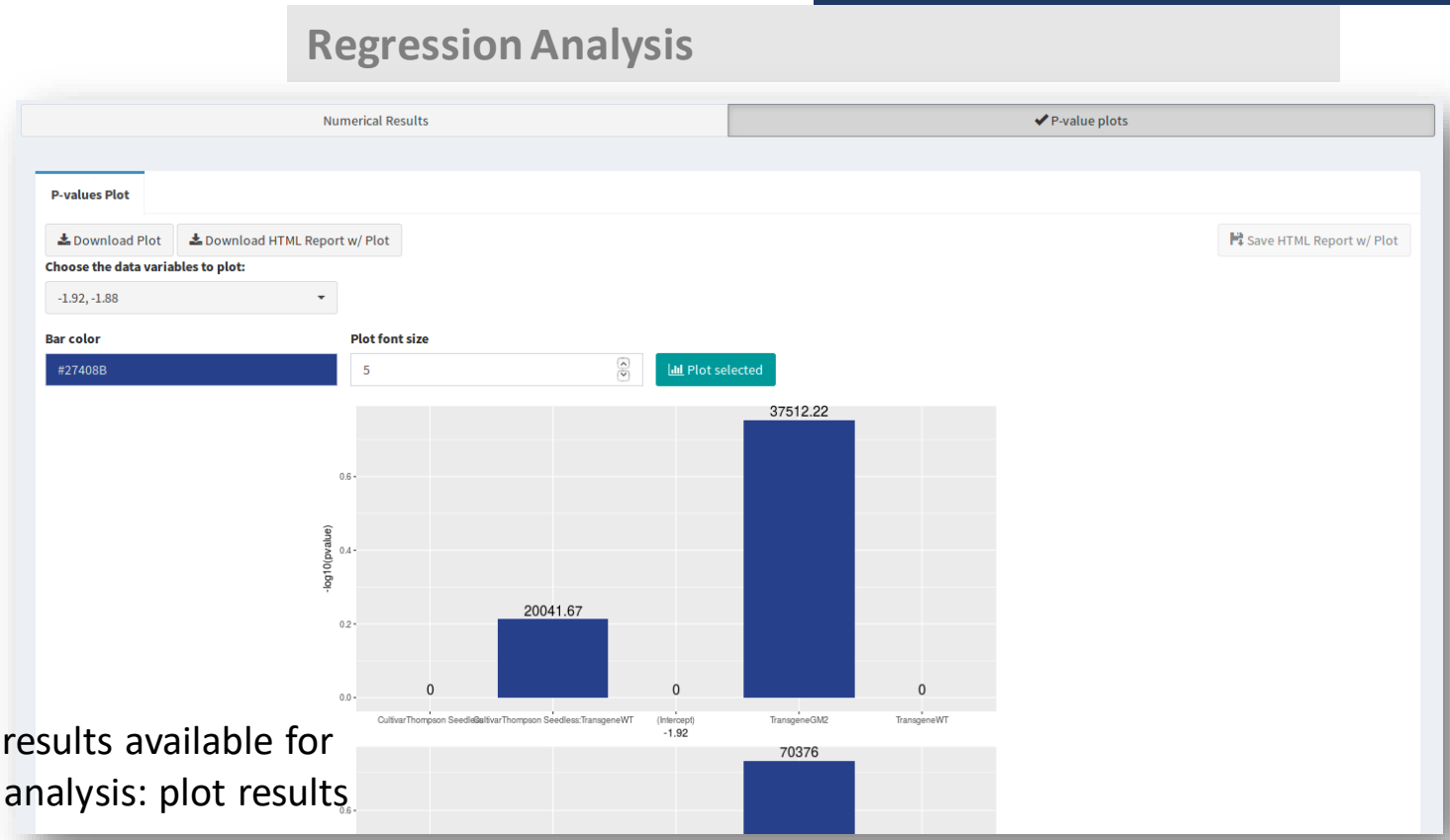
WebSpecmine: Data Analysis

Regression Analysis



ⓘ Types of results available for this type of analysis: numerical results

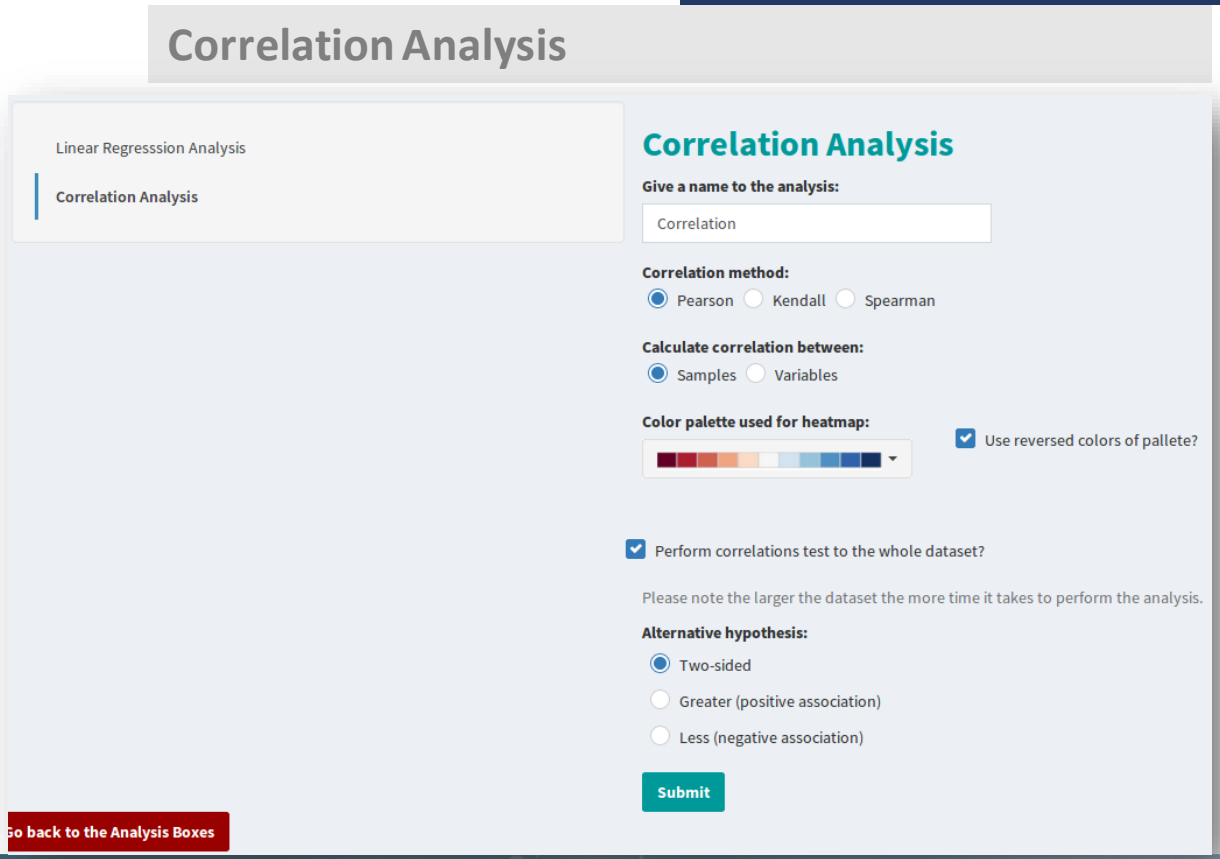
WebSpecmine: Data Analysis



ⓘ Types of results available for this type of analysis: plot results

WebSpecmine: Data Analysis

Regression Analysis

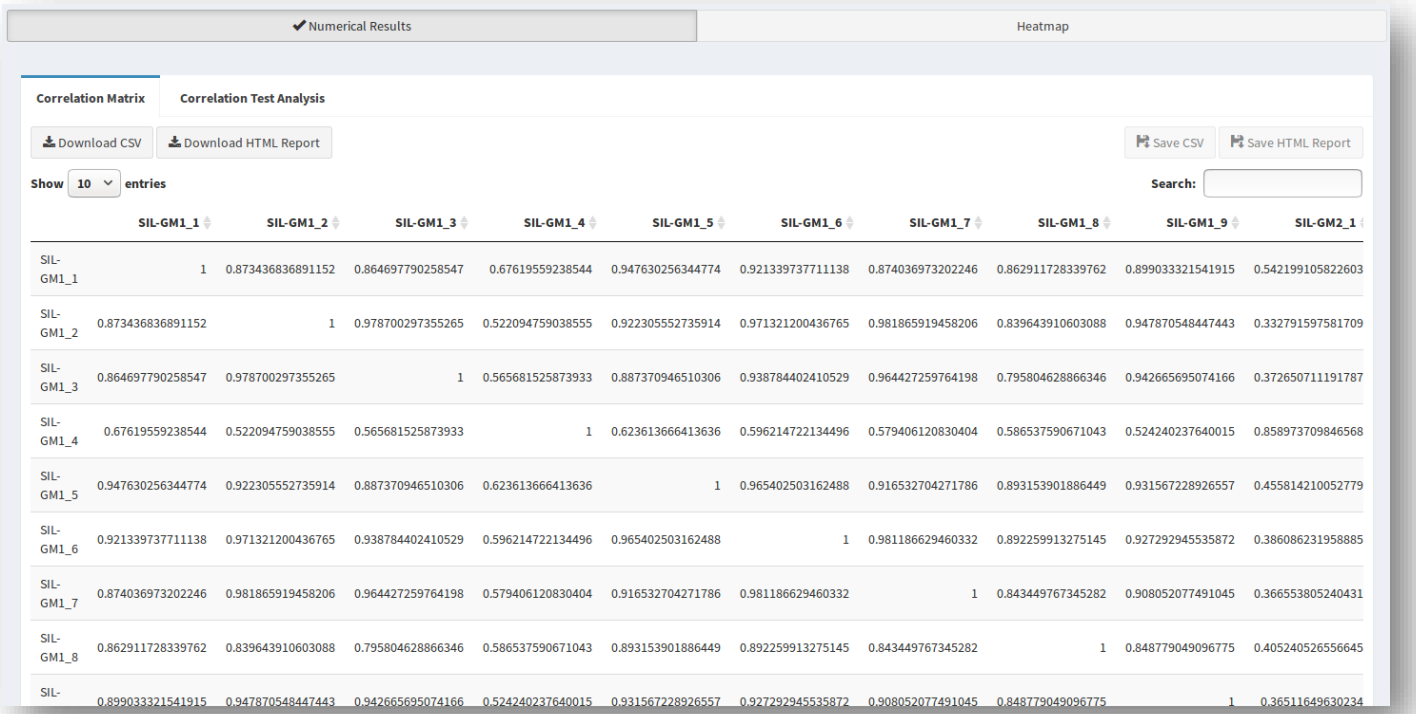


ⓘ Analysis options

WebSpecmine: Data Analysis

Regression Analysis

Correlation Analysis



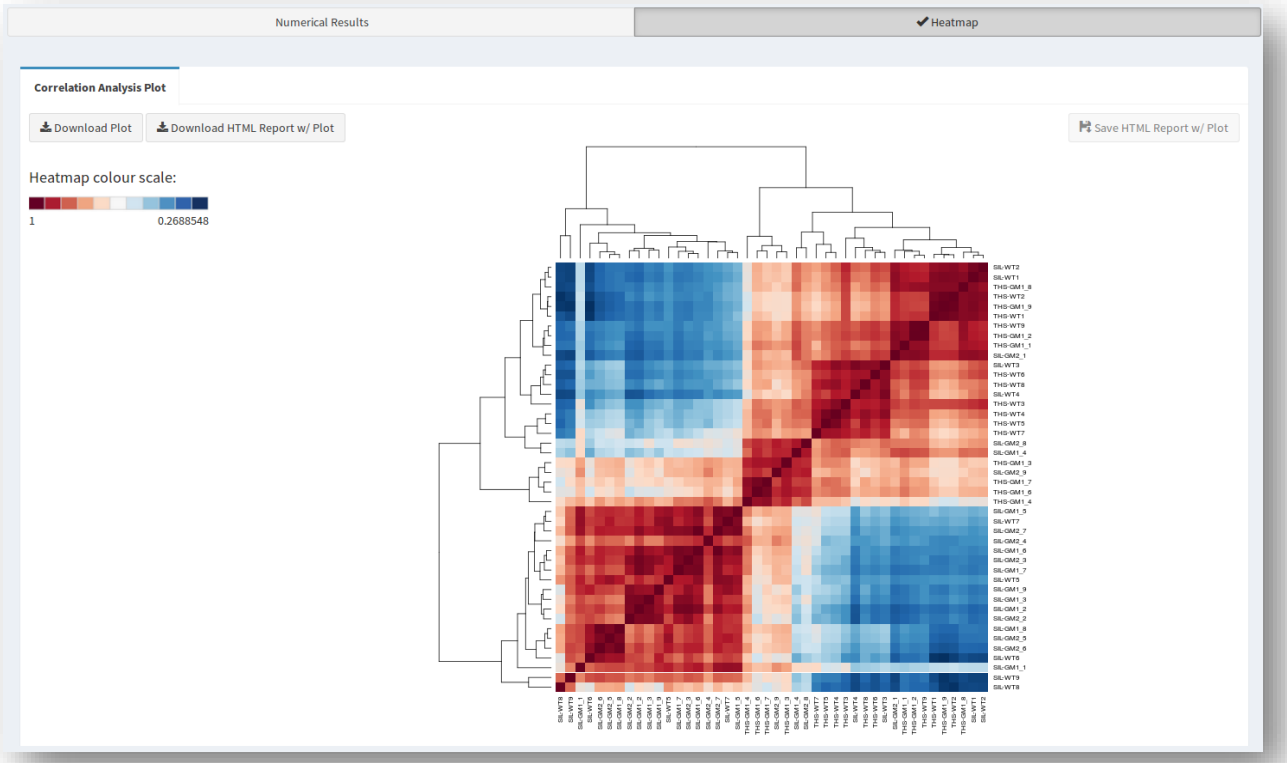
	SIL-GM1_1	SIL-GM1_2	SIL-GM1_3	SIL-GM1_4	SIL-GM1_5	SIL-GM1_6	SIL-GM1_7	SIL-GM1_8	SIL-GM1_9	SIL-GM2_1
SIL-GM1_1	1	0.873436836891152	0.864697790258547	0.67619559238544	0.947630256344774	0.921339737711138	0.874036973202246	0.862911728339762	0.899033321541915	0.542199105822603
SIL-GM1_2	0.873436836891152	1	0.978700297355265	0.522094759038555	0.922305552735914	0.971321200436765	0.981865919458206	0.839643910603088	0.947870548447443	0.332791597581709
SIL-GM1_3	0.864697790258547	0.978700297355265	1	0.565681525873933	0.887370946510306	0.938784402410529	0.964427259764198	0.795804628866346	0.942665695074166	0.372650711191787
SIL-GM1_4	0.67619559238544	0.522094759038555	0.565681525873933	1	0.623613666413636	0.596214722134496	0.579406120830404	0.586537590671043	0.524240237640015	0.858973709846568
SIL-GM1_5	0.947630256344774	0.922305552735914	0.887370946510306	0.623613666413636	1	0.965402503162488	0.916532704271786	0.893153901886449	0.931567228926557	0.455814210052779
SIL-GM1_6	0.921339737711138	0.971321200436765	0.938784402410529	0.596214722134496	0.965402503162488	1	0.981186629460332	0.892259913275145	0.927292945535872	0.386086231958885
SIL-GM1_7	0.874036973202246	0.981865919458206	0.964427259764198	0.579406120830404	0.916532704271786	0.981186629460332	1	0.843449767345282	0.908052077491045	0.366553805240431
SIL-GM1_8	0.862911728339762	0.839643910603088	0.795804628866346	0.586537590671043	0.893153901886449	0.892259913275145	0.843449767345282	1	0.848779049096775	0.405240526556645
SIL-	0.899033321541915	0.947870548447443	0.942665695074166	0.524240237640015	0.931567228926557	0.927292945535872	0.908052077491045	0.848779049096775	1	0.36511649630234

ⓘ Types of results available for this type of analysis: numerical results

WebSpecmine: Data Analysis

Regression Analysis

Correlation Analysis

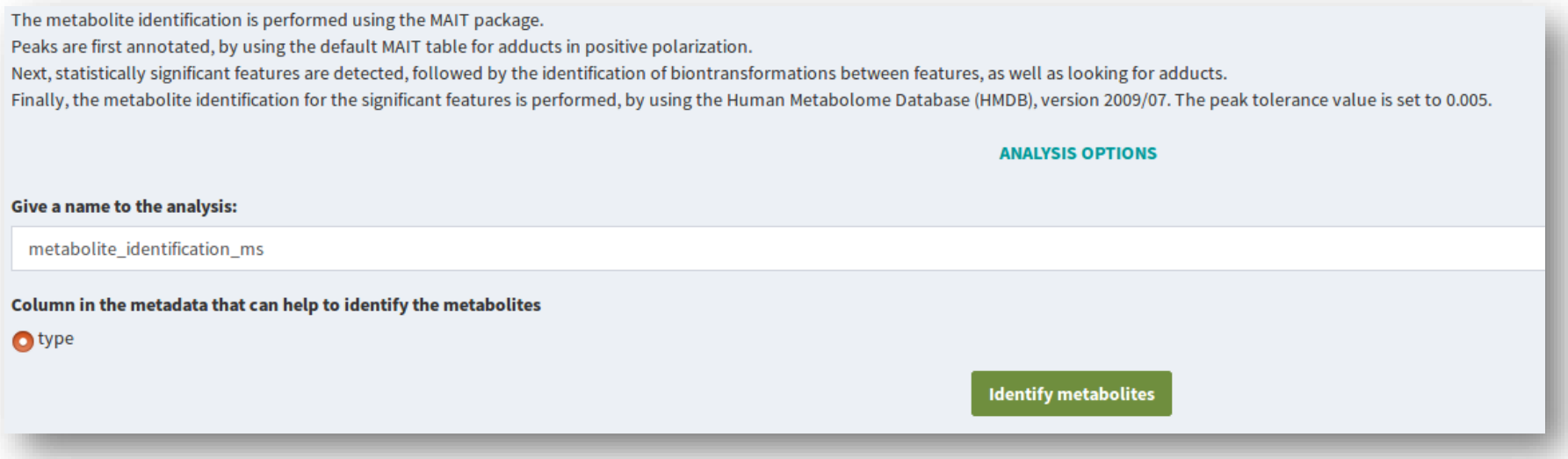


ⓘ Types of results available for this type of analysis: plot results

WebSpecmine: Data Analysis

Metabolite Identification

LC-MS Data

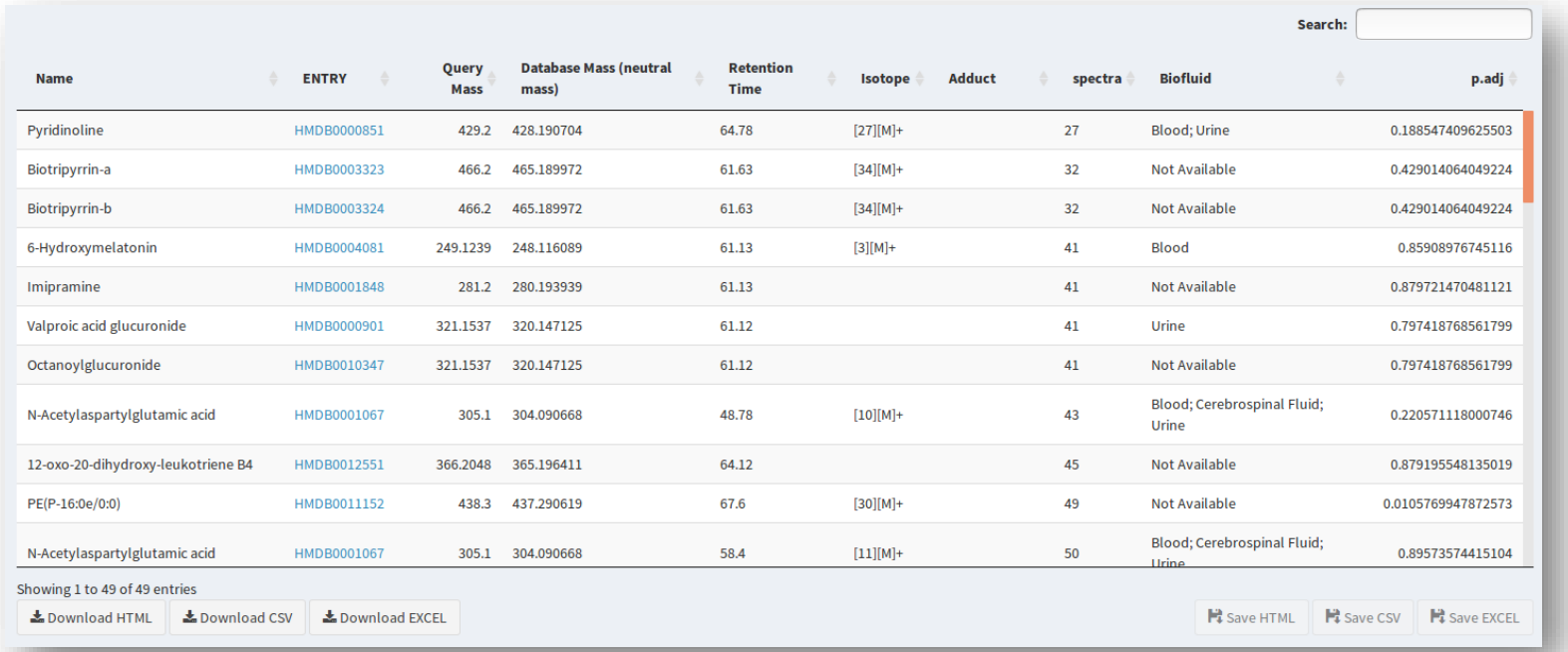


ⓘ Analysis options

WebSpecmine: Data Analysis

Metabolite Identification

LC-MS Data



Search:

Name	ENTRY	Query Mass	Database Mass (neutral mass)	Retention Time	Isotope	Adduct	spectra	Biofluid	p.adj
Pyridinoline	HMDB0000851	429.2	428.190704	64.78	[27][M]+		27	Blood; Urine	0.188547409625503
Biotripyrrin-a	HMDB0003323	466.2	465.189972	61.63	[34][M]+		32	Not Available	0.429014064049224
Biotripyrrin-b	HMDB0003324	466.2	465.189972	61.63	[34][M]+		32	Not Available	0.429014064049224
6-Hydroxymelatonin	HMDB0004081	249.1239	248.116089	61.13	[3][M]+		41	Blood	0.85908976745116
Imipramine	HMDB0001848	281.2	280.193939	61.13			41	Not Available	0.879721470481121
Valproic acid glucuronide	HMDB0000901	321.1537	320.147125	61.12			41	Urine	0.797418768561799
Octanoylglucuronide	HMDB0010347	321.1537	320.147125	61.12			41	Not Available	0.797418768561799
N-Acetylaspartylglutamic acid	HMDB0001067	305.1	304.090668	48.78	[10][M]+		43	Blood; Cerebrospinal Fluid; Urine	0.220571118000746
12-oxo-20-dihydroxy-leukotriene B4	HMDB0012551	366.2048	365.196411	64.12			45	Not Available	0.879195548135019
PE(P-16:0e/0:0)	HMDB0011152	438.3	437.290619	67.6	[30][M]+		49	Not Available	0.0105769947872573
N-Acetylaspartylglutamic acid	HMDB0001067	305.1	304.090668	58.4	[11][M]+		50	Blood; Cerebrospinal Fluid; Urine	0.89573574415104

Showing 1 to 49 of 49 entries

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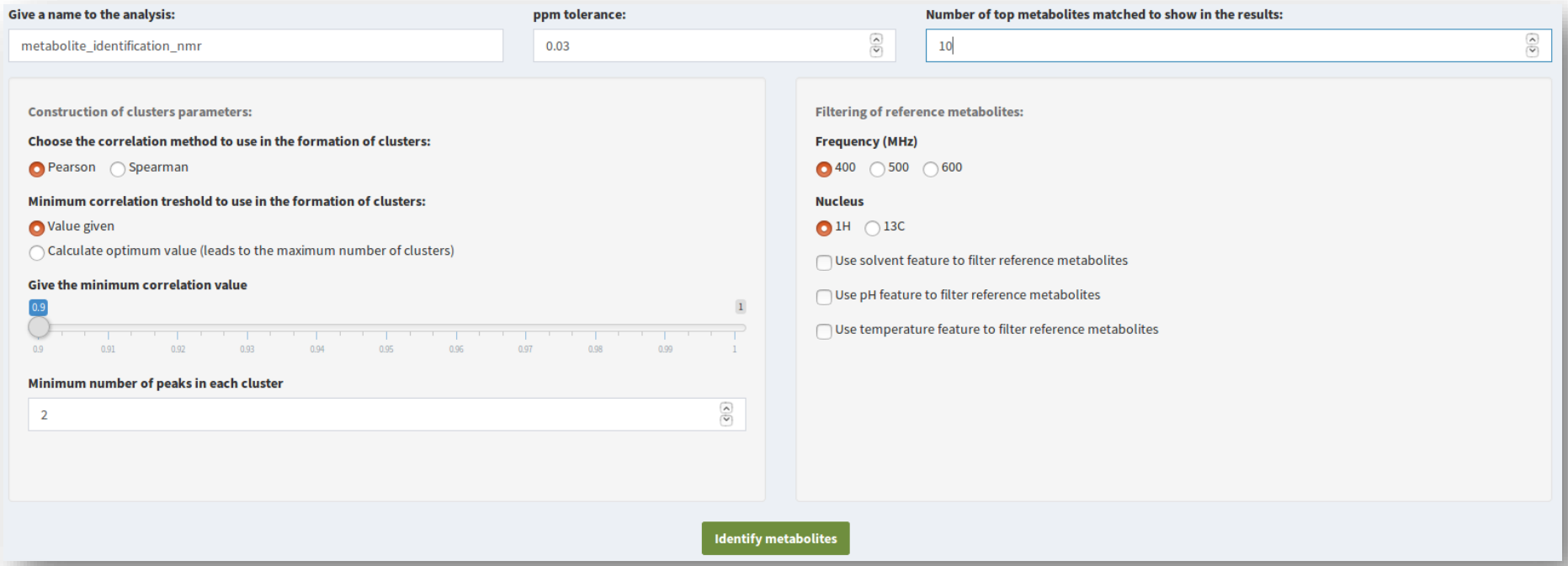
ⓘ Results available for this type of analysis

WebSpecmine: Data Analysis

Metabolite Identification

NMR Data



ⓘ Analysis options

WebSpecmine: Data Analysis

Metabolite Identification

NMR Data

Results Table | Results for each Cluster

Search:

Metabolite	Metabolite.Name	Reference.Peaks.Matched	Cluster.Peaks.Matched	Cluster	Jaccard.Index
HMDB0001547	Corticosterone	0.931; 0.983; 0.991; 1.01; 1.06; 1.071; 1.092; 1.121; 1.147; 1.402; 1.416; 1.433; 1.462; 1.572; 1.58; 1.606; 1.79; 1.811; 1.994; 2.002; 2.025; 2.05; 2.091; 2.125; 2.178; 2.184; 2.202; 2.235; 2.263; 2.329; 2.36; 2.37; 2.382; 2.41; 2.449; 2.471; 2.502; 3.348; 3.35; 3.358; 4.182; 4.191; 4.206; 4.415; 5.68; 5.683	0.93; 0.96; 0.99; 1.02; 1.06; 1.08; 1.11; 1.15; 1.17; 1.4; 1.43; 1.46; 1.49; 1.55; 1.57; 1.62; 1.82; 1.84; 1.99; 2.01; 2.05; 2.08; 2.11; 2.14; 2.17; 2.2; 2.23; 2.26; 2.29; 2.32; 2.34; 2.38; 2.41; 2.44; 2.47; 2.5; 2.53; 3.32; 3.35; 3.38; 4.17; 4.21; 4.23; 4.4; 5.67; 5.7	1	0.123
HMDB0000016	Deoxycorticosterone	0.695; 0.976; 0.984; 1.003; 1.082; 1.085; 1.092; 1.175; 1.18; 1.192; 1.223; 1.34; 1.348; 1.371; 1.404; 1.431; 1.461; 1.562; 1.57; 1.59; 1.627; 1.66; 1.794; 1.856; 1.937; 1.967; 2.011; 2.023; 2.053; 2.218; 2.223; 2.246; 2.268; 2.298; 2.315; 2.357; 2.384; 2.413; 2.442; 2.479; 2.503; 3.317; 3.319; 4.189; 4.204; 5.736	0.69; 0.96; 0.99; 1.02; 1.06; 1.08; 1.11; 1.15; 1.17; 1.21; 1.24; 1.34; 1.37; 1.4; 1.43; 1.46; 1.49; 1.55; 1.57; 1.62; 1.65; 1.67; 1.82; 1.84; 1.96; 1.99; 2.01; 2.05; 2.08; 2.2; 2.23; 2.26; 2.29; 2.32; 2.34; 2.38; 2.41; 2.44; 2.47; 2.5; 2.53; 3.3; 3.32; 4.17; 4.21; 5.75	1	0.123
HMDB0001830	Progesterone	0.67; 0.982; 0.991; 1.01; 1.163; 1.168; 1.18; 1.211; 1.25; 1.437; 1.449; 1.48; 1.547; 1.556; 1.576; 1.628; 1.632; 1.645; 1.851; 2.025; 2.03; 2.051; 2.083; 2.13; 2.144; 2.175; 2.202; 2.295; 2.301; 2.312; 2.357; 2.38; 2.41; 2.445; 2.522; 2.545; 2.567; 5.735	0.66; 0.96; 0.99; 1.02; 1.15; 1.17; 1.21; 1.24; 1.27; 1.43; 1.46; 1.49; 1.52; 1.55; 1.57; 1.62; 1.65; 1.67; 1.84; 2.01; 2.05; 2.08; 2.11; 2.14; 2.17; 2.2; 2.23; 2.29; 2.32; 2.34; 2.38; 2.41; 2.44; 2.47; 2.5; 2.53; 2.56; 5.75	1	0.103
HMDB0000234	Testosterone	0.794; 0.921; 0.932; 0.962; 0.991; 1.047; 1.058; 1.08; 1.197; 1.285; 1.3; 1.316; 1.414; 1.424; 1.44; 1.461; 1.49; 1.561; 1.57; 1.599; 1.62; 1.654; 1.834; 1.846; 2.007; 2.015; 2.02; 2.053; 2.081; 2.133; 2.286; 2.293; 2.297; 2.351; 2.357; 2.383; 2.418; 3.649; 5.731	0.79; 0.93; 0.96; 0.99; 1.02; 1.06; 1.08; 1.11; 1.17; 1.27; 1.3; 1.34; 1.4; 1.43; 1.46; 1.49; 1.52; 1.55; 1.57; 1.62; 1.65; 1.67; 1.82; 1.84; 1.99; 2.01; 2.05; 2.08; 2.11; 2.14; 2.26; 2.29; 2.32; 2.34; 2.38; 2.41; 2.44; 3.62; 5.75	1	0.103
HMDB0000054	Bilirubin	1.945; 1.961; 1.982; 2.022; 2.073; 2.164; 2.436; 2.455; 2.475; 2.515; 2.52; 2.532; 4.006; 5.285; 5.292; 5.314; 5.597; 5.601; 5.619; 5.645; 6.093; 6.164; 6.208; 6.533; 6.562; 6.577; 6.606; 6.754; 6.784; 6.797; 6.827	1.96; 1.99; 2.01; 2.05; 2.08; 2.14; 2.41; 2.44; 2.47; 2.5; 2.53; 2.56; 4.02; 5.27; 5.31; 5.34; 5.57; 5.61; 5.64; 5.67; 6.11; 6.17; 6.21; 6.51; 6.58; 6.6; 6.62; 6.75; 6.78; 6.81; 6.85	1	0.089
HMDB0000488	4E,15Z-Bilirubin IXa	1.945; 1.961; 1.982; 2.022; 2.073; 2.164; 2.436; 2.455; 2.475; 2.515; 2.52; 2.532; 4.006; 5.285; 5.292; 5.314; 5.597; 5.601; 5.619; 5.645; 6.093; 6.164; 6.208; 6.533; 6.562; 6.577; 6.606; 6.754; 6.784; 6.797; 6.827	1.96; 1.99; 2.01; 2.05; 2.08; 2.14; 2.41; 2.44; 2.47; 2.5; 2.53; 2.56; 4.02; 5.27; 5.31; 5.34; 5.57; 5.61; 5.64; 5.67; 6.11; 6.17; 6.21; 6.51; 6.58; 6.6; 6.62; 6.75; 6.78; 6.81; 6.85	1	0.089

Showing 1 to 10 of 10 entries

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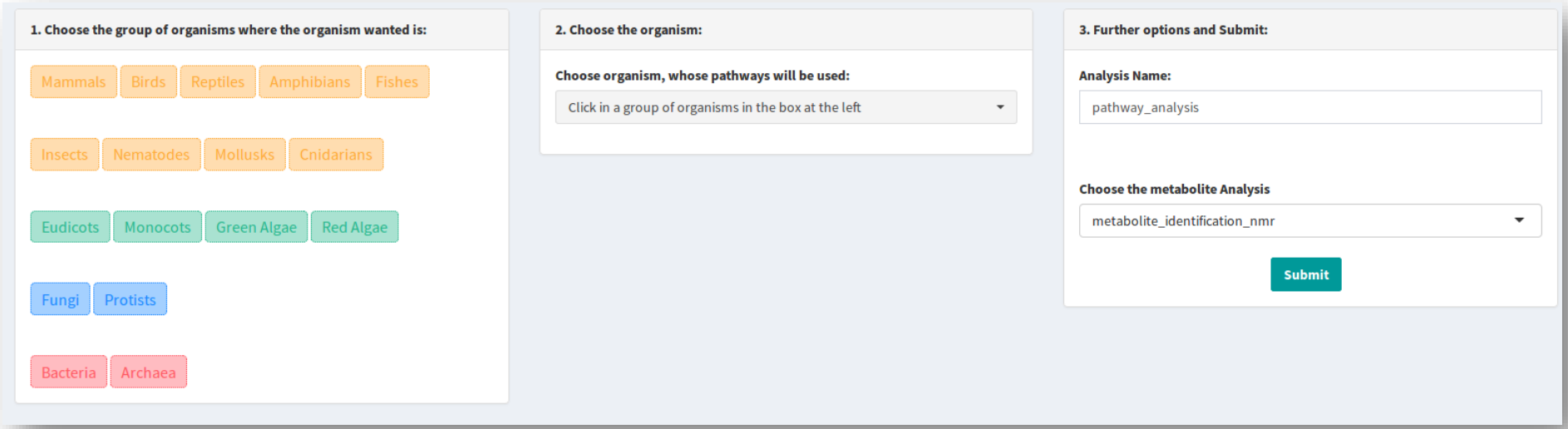
ⓘ Results available for this type of analysis

WebSpecmine: Data Analysis

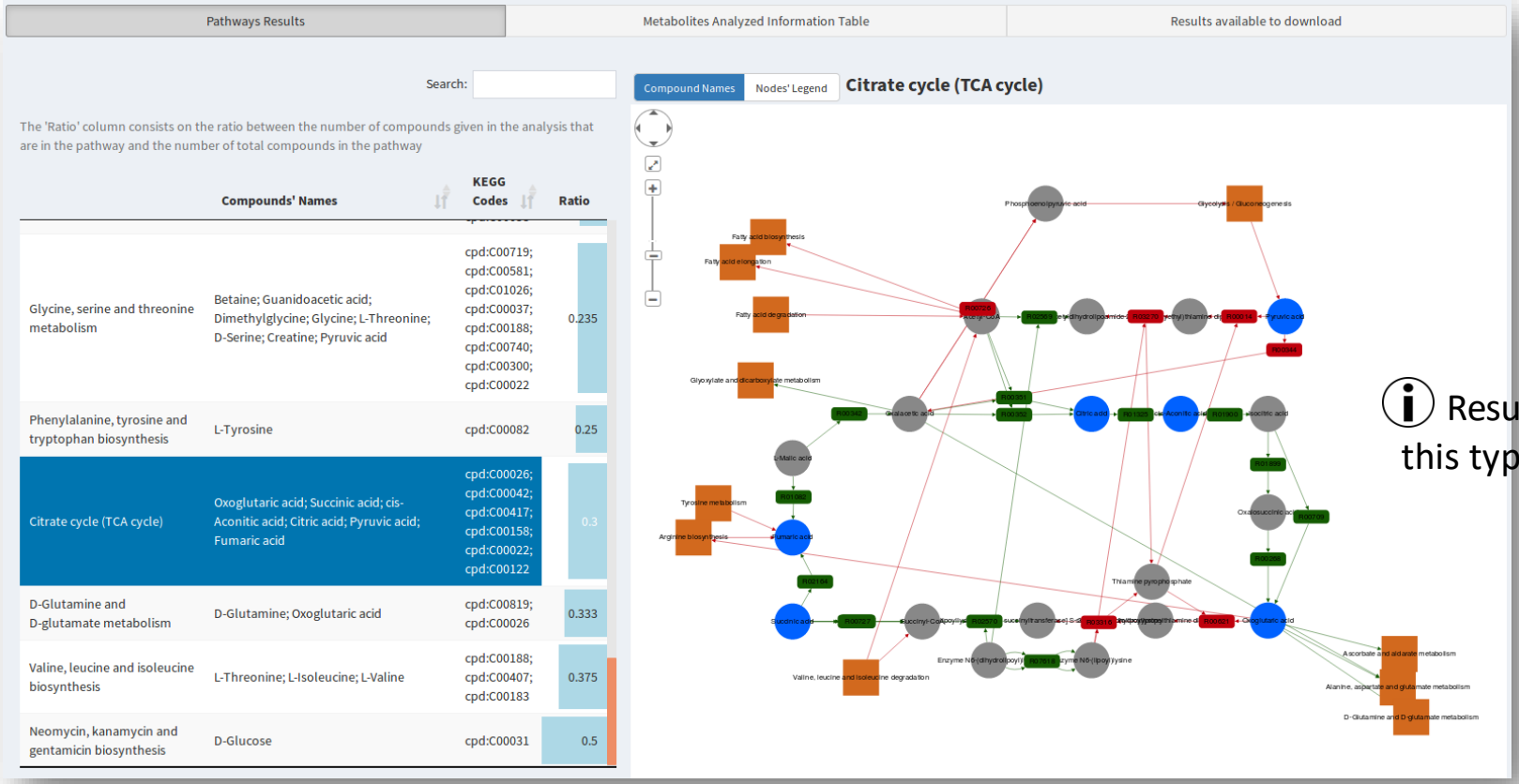
Pathway Analysis



ⓘ Analysis options

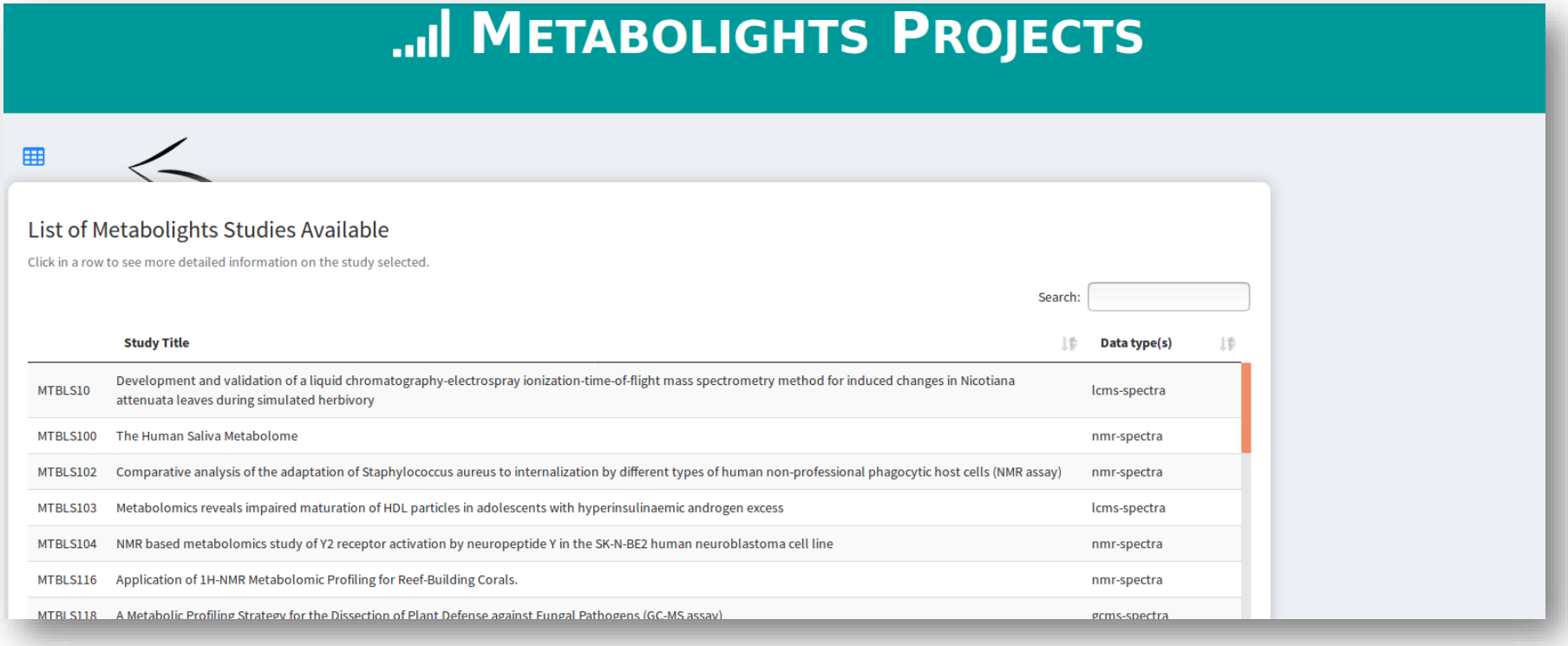
WebSpecmine: Data Analysis

Pathway Analysis



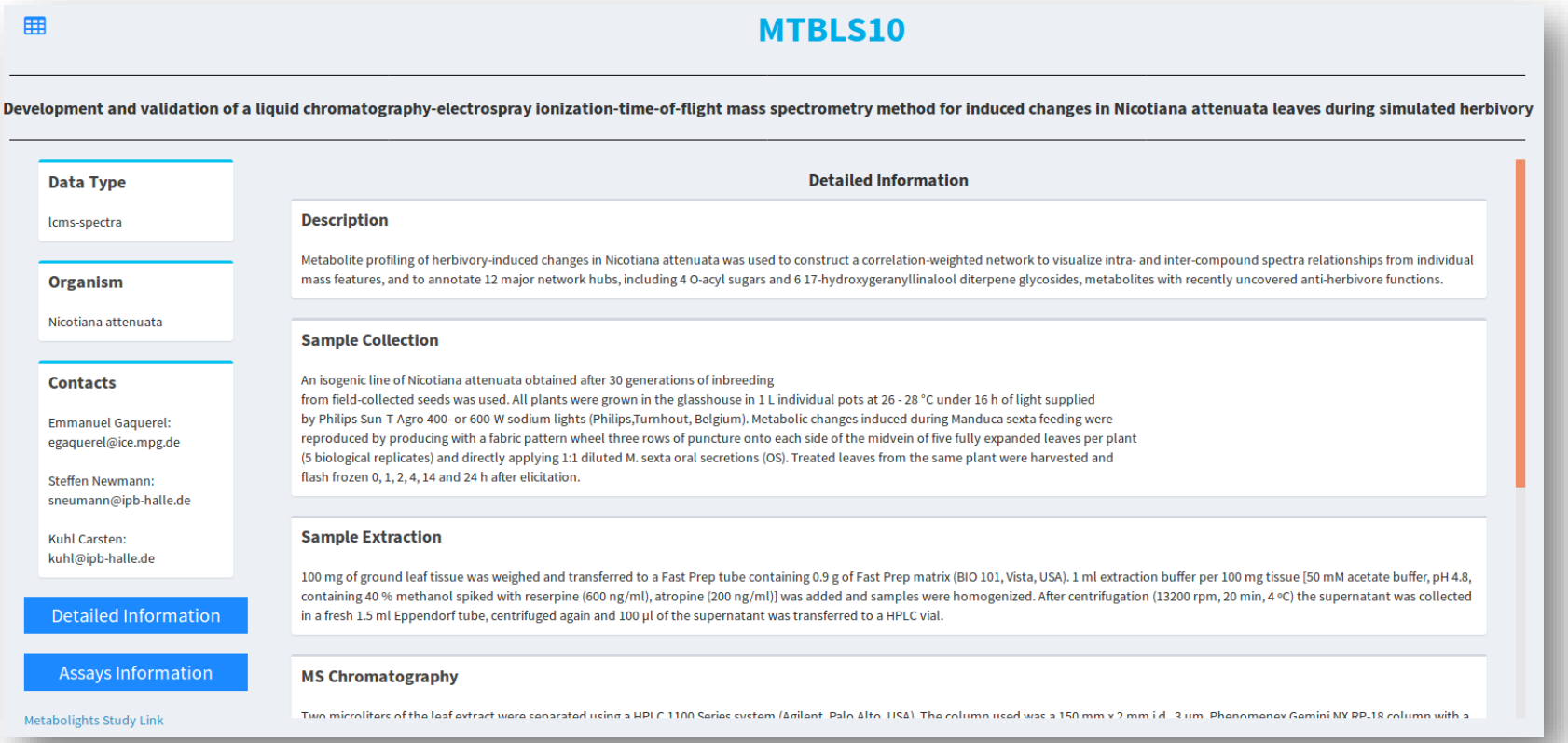
Results available for this type of analysis

WebSpecmine: Analysis of MetaboLights Studies



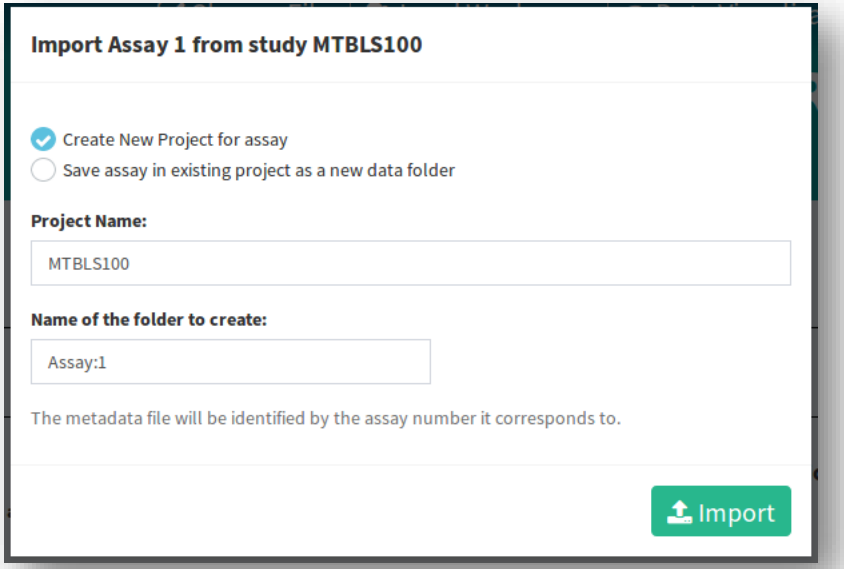
ⓘ You can see information on some of the MetaboLights studies

WebSpecmine: Analysis of MetaboLights Studies



ⓘ You can see detailed information on the protocol and metadata information on each assay

WebSpecmine: Analysis of MetaboLights Studies



ⓘ You can download the data and metadata of an assay into your private account and analyse it

Conclusions

✓ We were able to create an easy-to-use and freely available website with many advantages:

- Wide variety of techniques and data formats supported
- Wide variety of pre-processing methods
- Wide variety of analysis methods
- Flexible Pipeline
- User Account

✓ However, more analyses could be added, to add more biological meaning to data, such as:

- Enrichment Analysis
- Biomarker Analysis

For More Detailed Information ...

Website Link: https://webspecmine.bio.di.uminho.pt/ 

We have Tutorials and a complete User Guide at the *?Help* page.

We have a troubleshooting window, from where the users can report any problems and see the problems already encountered, but still being solved.

Acknowledgments

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