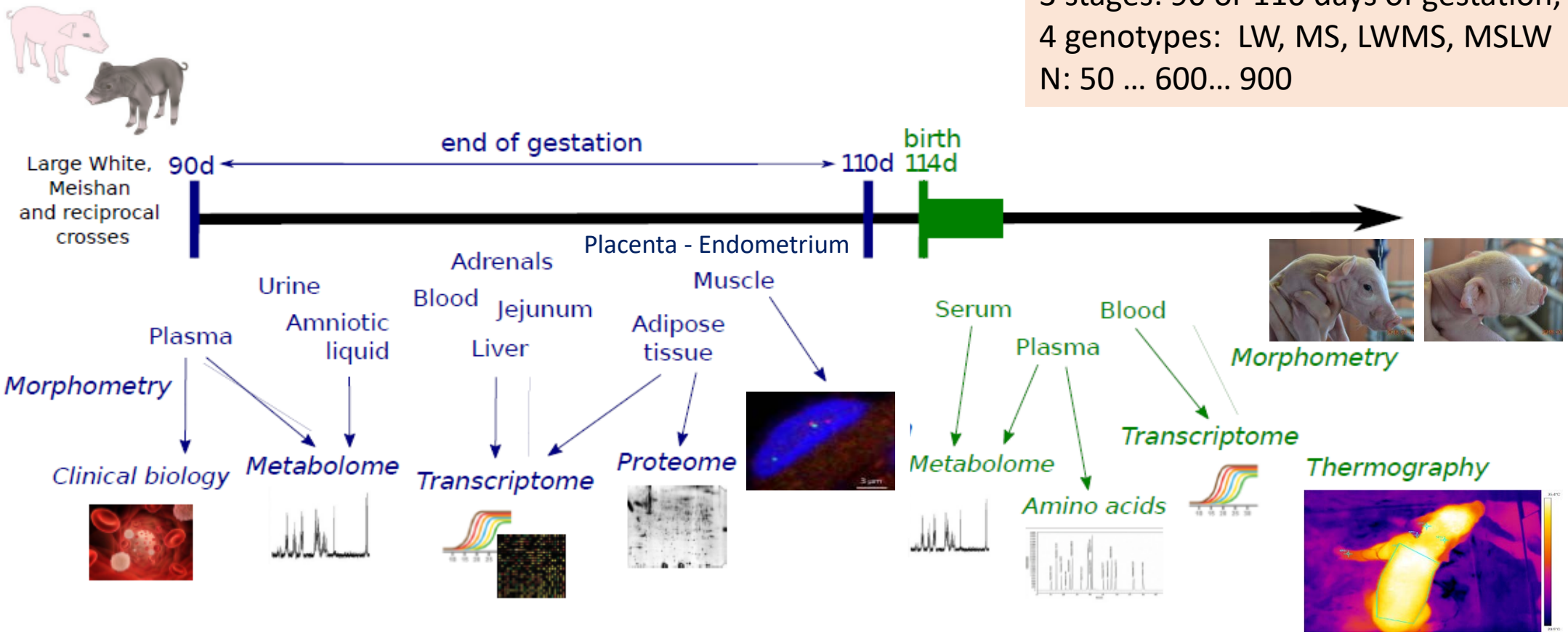
Quelques exemples avec des données multi-omiques et multi-tissus en néonatalité porcine pour illustrer les différentes fonctionnalités d'Asterics.

Élise Maigné, Céline Noirot, Jérôme Mariette, Yaa Adu Kesewaah, Sébastien Déjean, Camille Guilmineau, Julien Henry, Arielle Krebs, **Laurence Liaubet**, Fanny Mathevet, Hyphen-Stat, Christine Gaspin, Nathalie Vialaneix

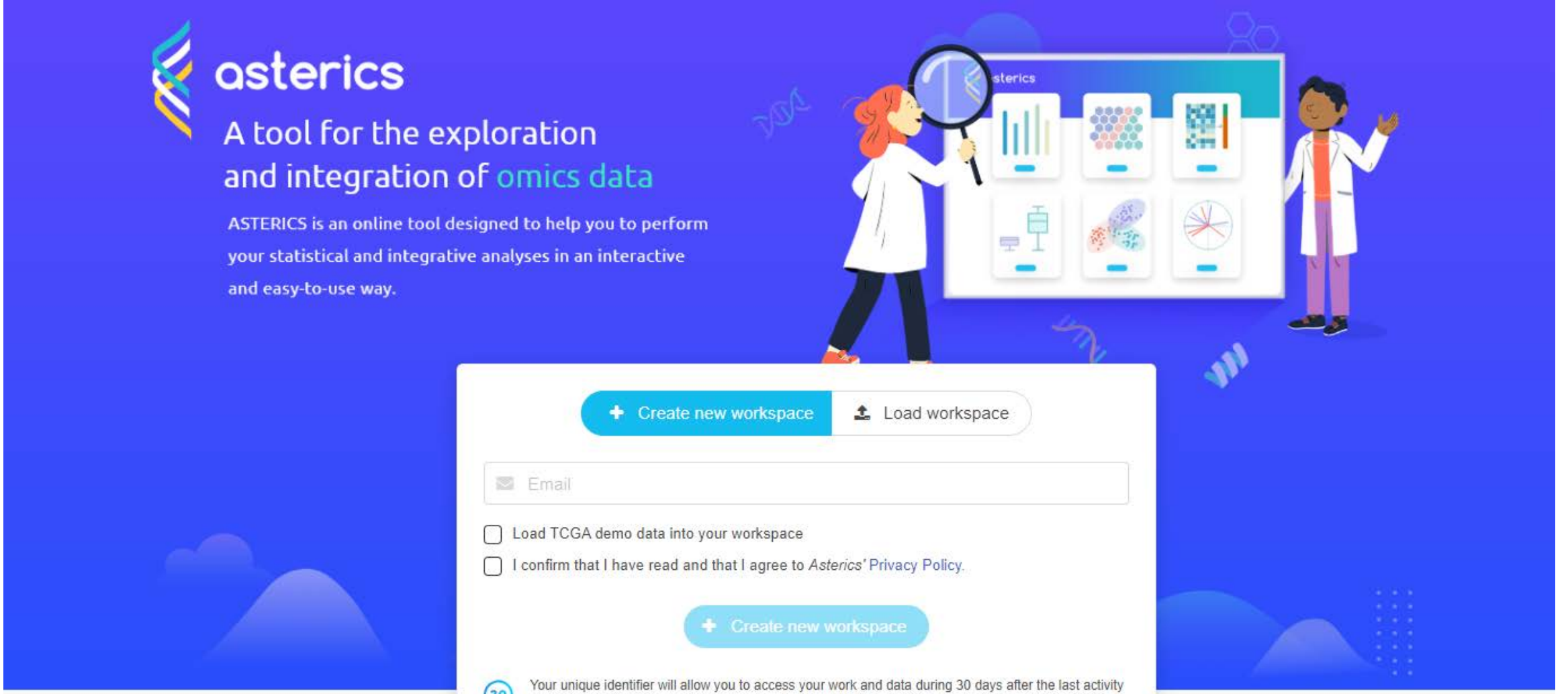
Context: neonatal maturity and birth survival

3 stages: 90 or 110 days of gestation, birth
4 genotypes: LW, MS, LWMS, MSLW
N: 50 … 600… 900



Voillet et al, 2014, 2018; Yao et al.2017 ; Gondret et al, 2018;
Marti-Marimon et al, 2018; Lefort et al, 2020,2021 ; Schmitt et al, 2021

ANR
GISA
Avec la contribution financière du compte d'affectation spéciale développement agricole et rural CASDAR
MINISTÈRE DE L'AGRICULTURE ET DE L'ALIMENTATION
ALLIANCE RD Innovation Durable en Génétique Porcine
INRA SCIENCE & IMPACT Génétique Animale
NeoTec-Vision
ifip institut du porc



https://asterics.miat.inrae.fr/

Project coordinators

Genotoul Bioinfo

Genotoul Biostat

Funder

La Région Occitanie

Partners

MIA Toulouse

INRAE

Dear user,

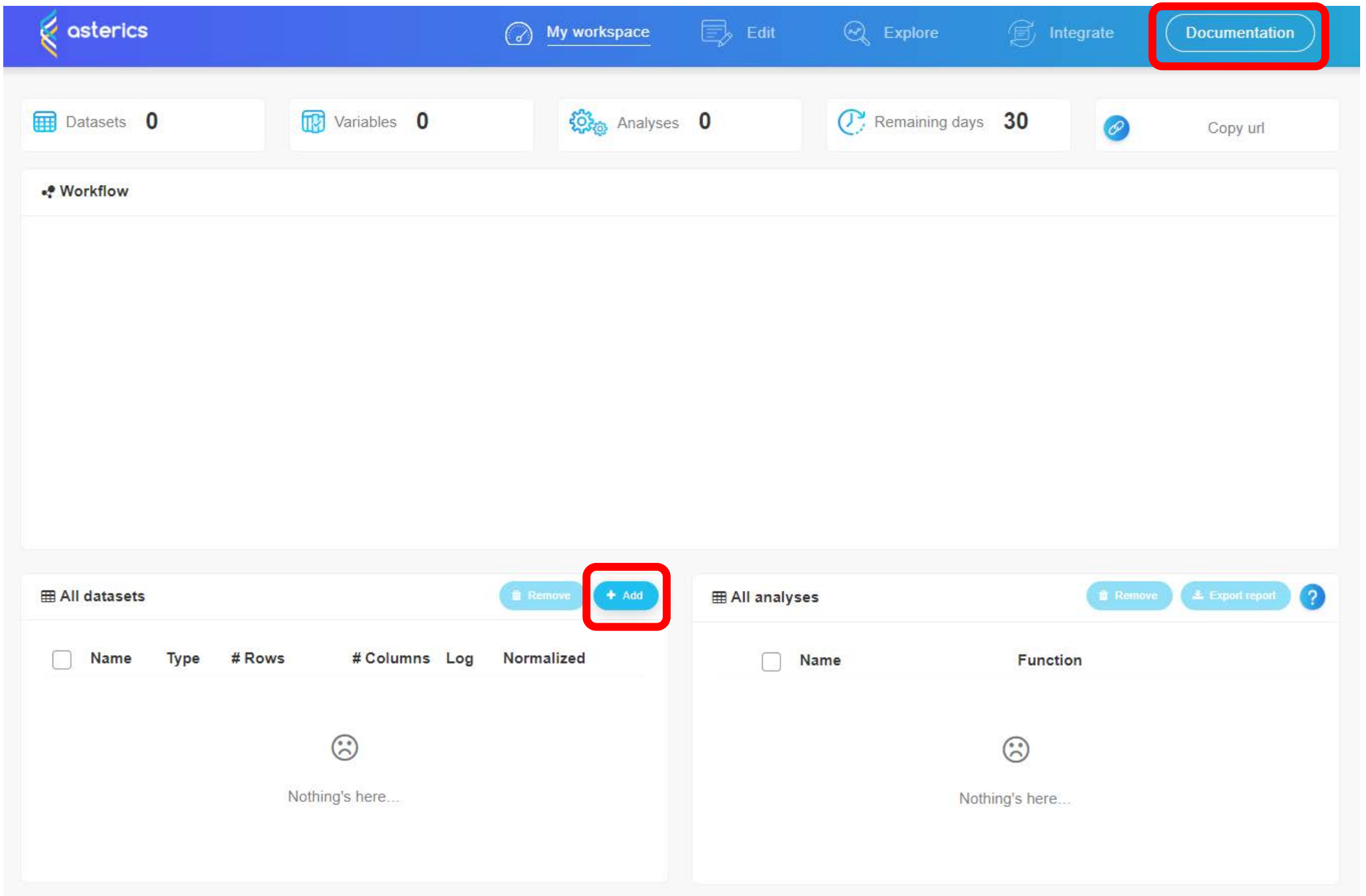
Your workspace has been successfully created at
https://asterics.miat.inrae.fr/workspace/ba20fb6d-4196-45c0-999f-7ff6d522b109.

Thank you for using ASTERICS,
The ASTERICS Team

Dear user,

your workspace https://asterics.miat.inrae.fr/78f3057f-ed70-42c8-ae5c-8d8b7be83484 will be deleted in 3 days.

thanks for using Asterics,
The Asterics Team,


asterics
My workspace
Edit
Explore
Integrate
Documentation
Datasets 0
Variables 0
Analyses 0
Remaining days 30
Copy url
Workflow
All datasets
Remove
+ Add
Name
Type
Rows
Columns
Log
Normalized
Nothing's here...
All analyses
Remove
Export report
Name
Function
Nothing's here...

ASTERICS: User documentation

Maigné Élise, Noirot Céline, Mariette Jérôme, Adu Kesewaah Yaa, Déjean Sébastien,

Guilmineau Camille, Henry Julien, Krebs Arielle, Liaubet Laurence, Mathevet Fanny,

Hyphen-Stat, Gaspin Christine, Vialaneix Nathalie

2022-08-17

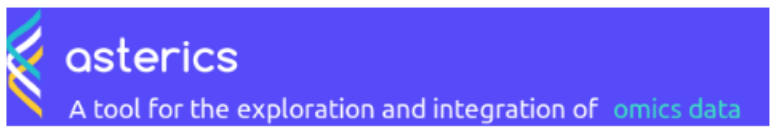
Section 1 Introduction

This document is the user guide for the web tool ASTERICS. *It is still a work-in-progress and mostly incomplete. Come back later for a better version. Thank you for your understanding.*

Link to the application: http://asterics.miat.inrae.fr/

Support for ASTERICS can be obtained at asterics-tlse@inrae.fr.

Bugs can be reported here and suggestions can be made here.



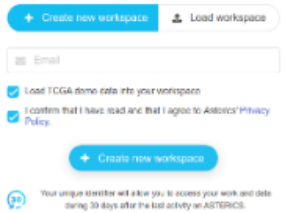
Section 16 Case studies

16.1 Breast cancer

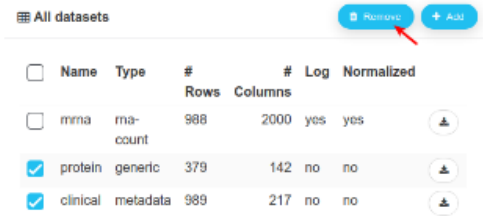
This case study focuses on breast cancer, trying to link omics data to cancer subtypes. There are four breast cancer subtypes that somewhat represent sub-diseases, with different biological mechanisms. Their identification is particularly important when designing / selecting treatments. For this case study, we have mRNA and miRNA data on 988 individuals, as well as the associated subtypes. mRNA data is already normalized and is loaded in ASTERICS by default, whereas miRNA comes in the form of raw counts.
The data is available online (Vialaneix 2021).

16.1.1 Setup

Let us open an empty session and load the TCGA demo data.

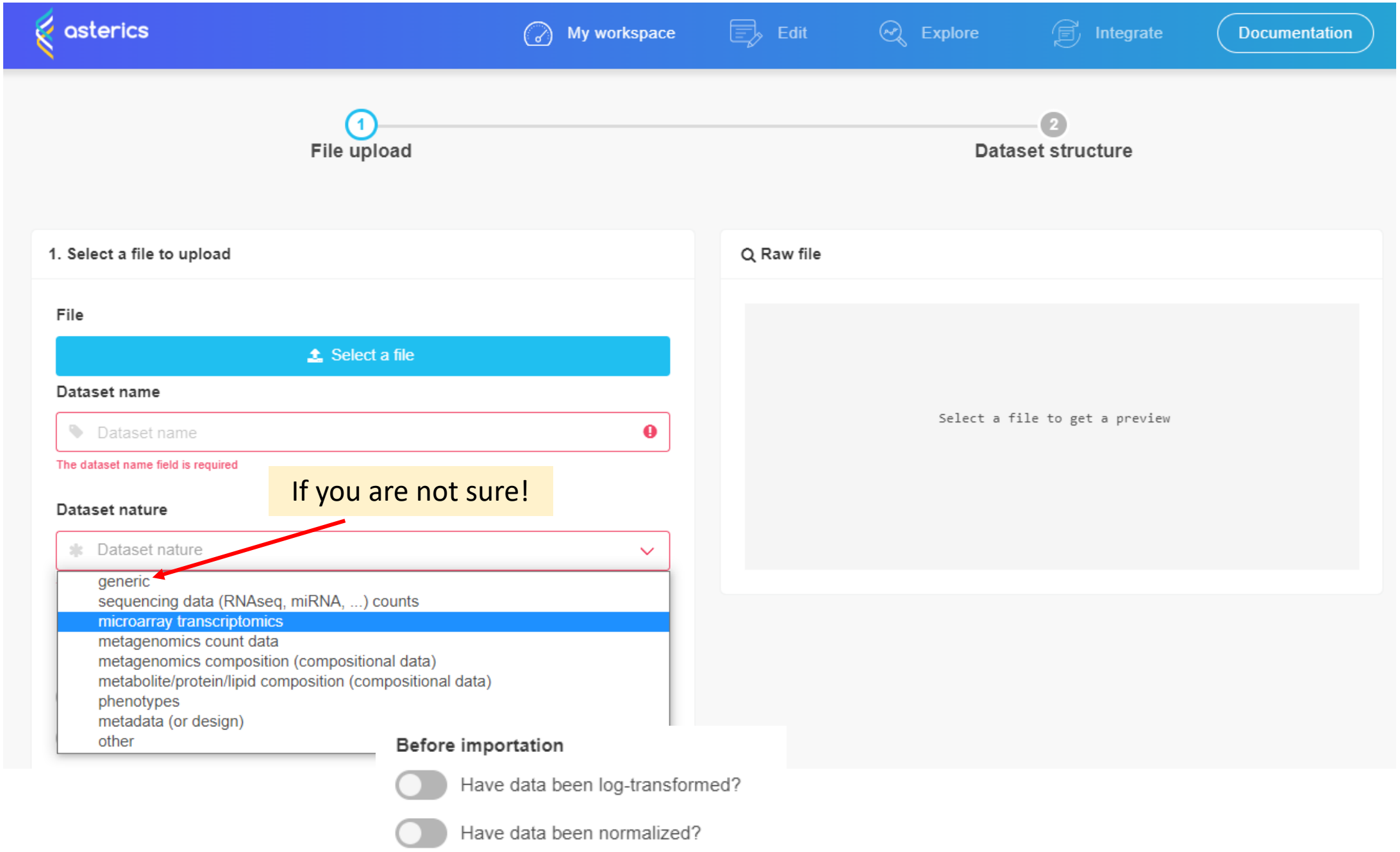


Since we will only use the **mrna** dataset, let us delete the other two.



Name	Type	# Rows	# Columns	Log	Normalized
mrna	rna-count	988	2000	yes	yes
protein	generic	379	142	no	no
clinical	metadata	989	217	no	no

Here is **mrna** in the workspace:


asterics
My workspace
Edit
Explore
Integrate
Documentation
1
File upload
2
Dataset structure
1. Select a file to upload
File
Select a file
Dataset name
Dataset name
The dataset name field is required
Dataset nature
Dataset nature
generic
sequencing data (RNAseq, miRNA, ...) counts
microarray transcriptomics
metagenomics count data
metagenomics composition (compositional data)
metabolite/protein/lipid composition (compositional data)
phenotypes
metadata (or design)
other
Raw file
Select a file to get a preview
If you are not sure!
Before importation
Have data been log-transformed?
Have data been normalized?

1. Select a file to upload

File

TranscriptomeMuscle50.csv

Dataset name

TranscriptomeMuscle50

Dataset nature

microarray transcriptomics

If you don't know which nature to choose, use "generic".

Before importation

Have data been log-transformed?

Have data been normalized?

Raw file

```
;F405;F409;F411;F449;F455;F458;F469;F476;F481;F485;F498;F500;F524;F525;F53
A1CF_52154;5.6803695954516;5.45610320624039;5.74484272573927;5.92019267767
A2M_40313;5.50693239097091;5.76073759718855;5.5227941006065;5.663677602194
A2M_10645;5.41017364325691;5.79477650004684;6.04237760287688;5.68692117450
A2ML1_14639;5.4491082475774;5.36385961056552;5.17100665288747;5.6208513292
A4GALT_23662;8.36976136324847;7.80328185134206;8.55421636844331;7.22995624
A4GALT_9159;8.82297280814355;8.92285084244449;9.17229076620426;8.834796301
AAAS_61230;5.66491543991508;5.70809268946484;5.85667371223367;6.9757878359
AAAS_2894;5.89283524674721;5.6564212452558;5.66624190687793;6.090788421745
AAAS_18735;7.74349641324072;7.70023645818195;7.43741001836278;8.7585108190
AAAS_24237;6.41516988709249;6.40535808528583;6.82967565563798;7.0901431036
```

2. Set the dataset structure

Column names are included in the first row

File has row labels

Index of the column with row labels

1

File has comment lines

Comment character

#

Switch rows and columns

For ASTERICS, individuals must be in rows.

Separator

, (comma) ; (semicolon) \t (tab) Space Custom :

Quote mark for text

" (double quote)

Decimal mark

. (dot) , (comma)

Encoding

Auto UTF-8 latin1

Missing values are encoded with these strings:

NA Add na.strings

Be patient: large files might take a long time to be uploaded and processed!

Import

Raw file

```
;F476;F481;F560;F578;F688;F455;F485;F498;F738;F899;F900;F469;F557;F559;F67
A1CF_52154;5.82599980707194;5.91662162096354;5.62770189995087;5.974879117
A2M_40313;5.20290966528126;5.71662080795284;5.73529430299502;6.2799406003
A2M_10645;6.05043272137919;5.78608436449946;5.92397285829613;6.3184046337
A2ML1_14639;5.09454305674891;4.89392730422894;5.06610396900029;5.109927232
A4GALT_23662;7.44499238746051;7.88769803161222;7.75157714142366;7.8547880
A4GALT_9159;8.80734586555401;8.74392533000205;8.55935004010872;8.291677946
AAAS_61230;5.82599980707194;5.60366933006277;6.19088825000998;6.690848619
AAAS_2894;5.59207508123505;5.29881778254516;5.87420980899597;5.935500882
AAAS_18735;7.9656631095485;7.65139989082614;7.78415314320795;8.0945502888
AAAS_24237;6.38767805826733;6.53943474153246;6.73107621612731;6.514275437
```

Dataset preview

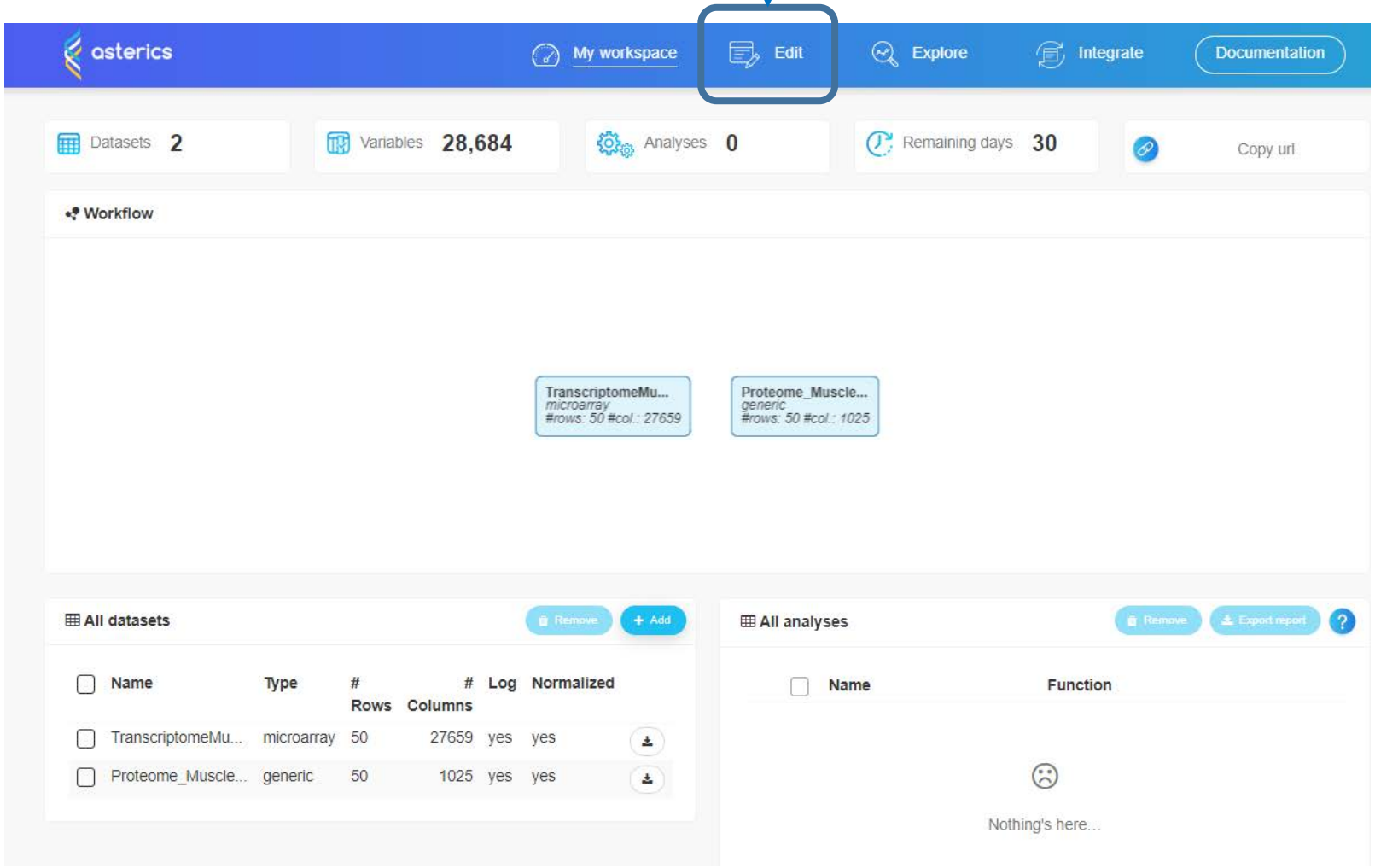
	A1CF_52154 numeric	A2M_40313 numeric	A2M_10645 numeric	A2ML1_14639 numeric	A4GALT_23662 numeric	A4G
F476	5.826	5.2029	6.0504	5.0945	7.445	
F481	5.9166	5.7166	5.7861	4.8939	7.8877	
F560	5.6277	5.7353	5.924	5.0661	7.7516	
F578	5.9749	6.2799	6.3184	5.1099	7.8548	
F688	5.7889	6.434	6.5869	4.7516	8.0703	
F455	5.5397	5.5826	5.8344	5.648	7.4885	
F485	5.8868	6.1856	6.3453	5.661	7.7702	
F498	5.6354	5.81	5.7552	5.8236	7.6827	
F738	5.6221	5.1073	5.5711	5.6786	7.1388	
F899	5.5986	5.5457	5.8591	5.0093	7.3409	
F900	5.781	5.9127	6.1895	5.8663	7.7117	
F469	6.1845	5.7959	5.7232	5.5926	8.0633	

Switch rows and columns !

1 unique identifier per variable, so arrange the name to have the most relevant information !

asterics
A tool for the exploration and integration of omics data

Edit

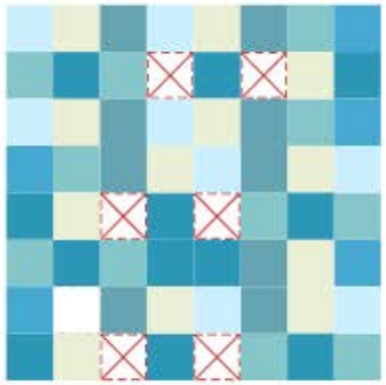


asterics

My workspace | Edit | Explore | Integrate | Documentation

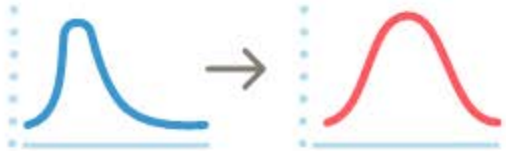
Dataset edition

Provides several ways to modify a dataset.



Missing values

Explore, remove or impute missing values on a dataset.



Normalize dataset

Correct technical biases and prepare your data for further analyses.

Dataset edition

1. Select a dataset and an action

Dataset

Infos_50

Actions

- Transpose
- Change dataset nature
- Change variable (column) types
- Set individual (row) names
- Subset individuals (rows)
- Subset variables (columns)
- Rename categories
- Reorder categories

History

No history to display

Select an action.

Dataset "Infos_50"

# rows	# col.	# missing	% missing	# numeric	# cat.	# logic	# others
50	32	0	0	27	5	0	0

	Sex (categorical, 0.00%)	N_Mother (numeric, 0.00%)	Age (categorical, 0.00%)	TG_Mother (categorical, 0.00%)	TG_Father (categorical, 0.00%)	TG_F (categorical, 0.00%)	Weight (numeric, 0.00%)
F449	M	6	90d	LW	LW	LWLW	733
F458	M	6	90d	LW	LW	LWLW	782
F500	M	8	90d	LW	LW	LWLW	597
F736	M	23	90d	LW	LW	LWLW	597
F744	M	23	90d	LW	LW	LWLW	784
F894	M	33	90d	LW	LW	LWLW	813
F895	M	33	90d	LW	LW	LWLW	389
F455	M	6	90d	LW	MS	MSLW	717
F485	M	8	90d	LW	MS	MSLW	754
F498	M	8	90d	LW	MS	MSLW	704
F738	M	23	90d	LW	MS	MSLW	522
F899	M	33	90d	LW	MS	MSLW	599

‹ 1 2 ... 5 ›

asterics | My workspace | Edit | Explore | Integrate | Documentation

Explore variables in a dataset

1 variable | 2 variables | up to 5 variables | all variables in a dataset

1. Select the dataset to explore

Select a dataset

Infos_50_edited

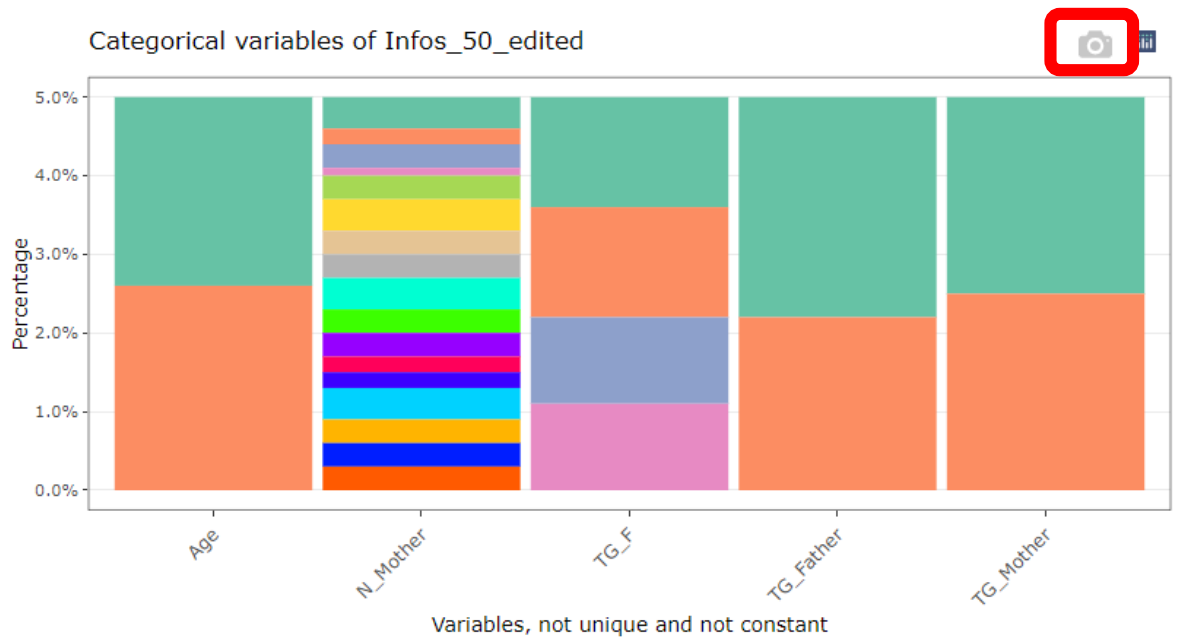
Scale numeric variables in the plot

Explore

2. Plots and numerical summaries

One irrelevant categorical variable (Sex) has been removed from the dataset because it had a unique value or only different values.

Numeric summary | Normality test | Categorical summary | Plots

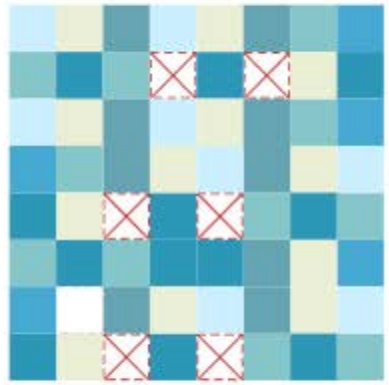


asterics

My workspace | Edit | Explore | Integrate | Documentation

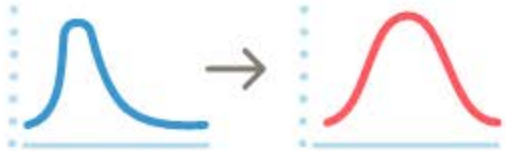
Dataset edition

Provides several ways to modify a dataset.



Missing values

Explore, remove or impute missing values on a dataset.

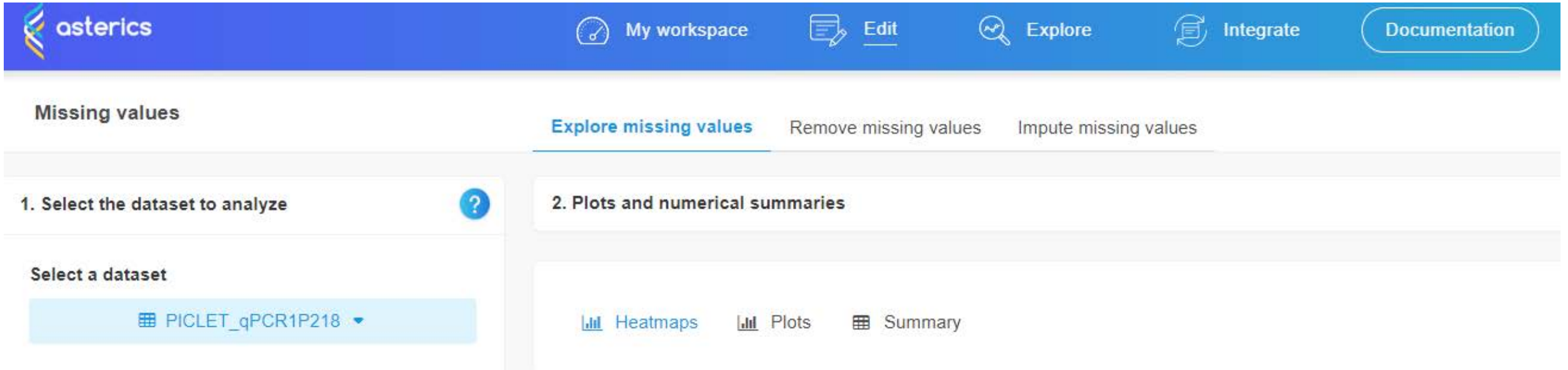


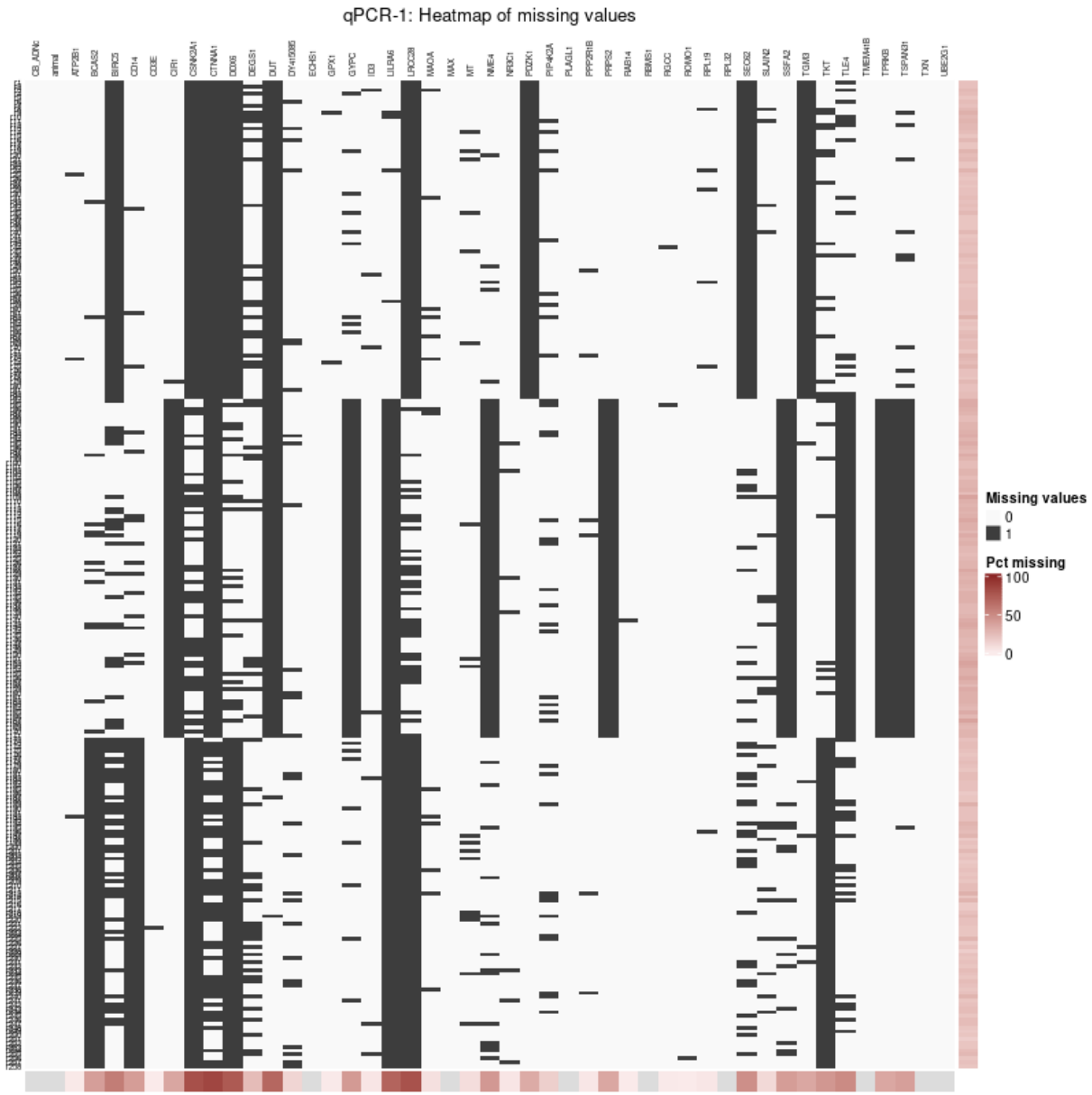
Normalize dataset

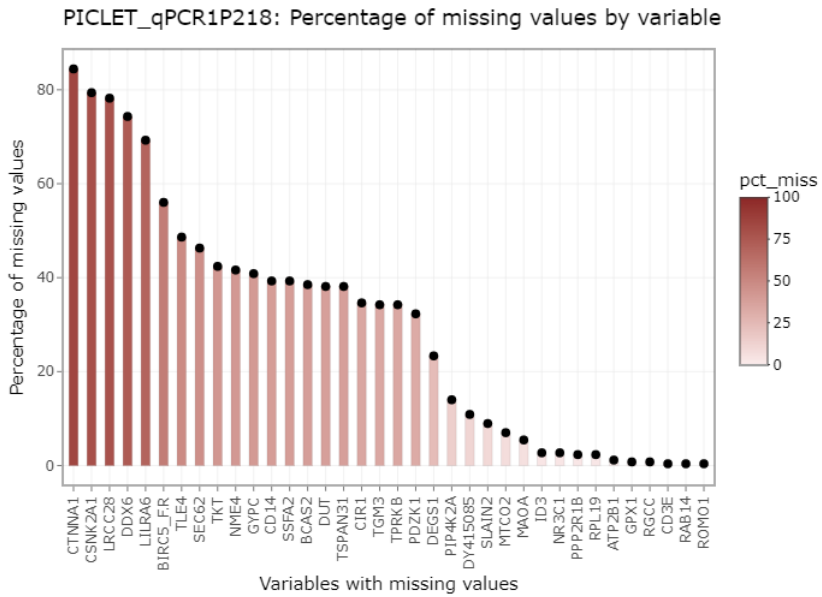
Correct technical biases and prepare your data for further analyses.

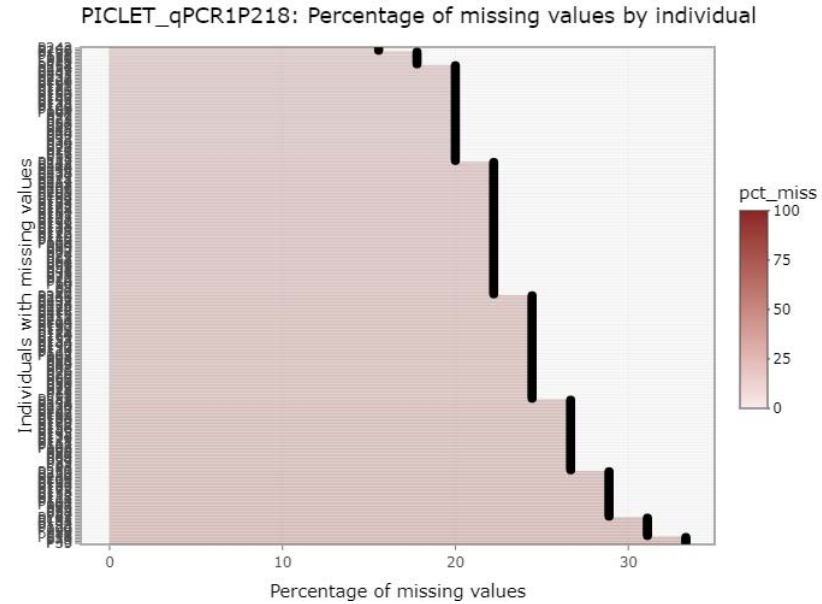
# rows	# col.	# missing	% missing	# numeric	# cat.	# logic	# others
257	45	2760	23.87	45	0	0	0

	ATP2B1 numeric 1.17%	BCAS2 numeric 38.52%	BIRC5_F.R numeric 56.03%	CD14 numeric 39.30%	CD3E numeric 0.39%	CIR1 numeric 34.63%	CSNK2A1 numeric 79.38%	
P1	0.0559	0.0623	NA	0.1167	0.0191	0.0132	NA	NA
P2	0.0521	0.1207	NA	0.042	0.0828	0.0399	NA	NA
P3	0.153	0.0737	NA	0.0761	0.0773	NA	0.0826	NA
P4	0.0644	0.1384	NA	0.2347	0.0495	0.0555	NA	NA
P5	0.2821	0.246	NA	0.3472	0.2379	0.0441	NA	NA
P6	0.1404	0.1411	0.1522	0.0928	0.0943	NA	NA	NA
P7	0.5945	NA	0.1526	NA	0.2019	0.3797	NA	NA
P8	0.1211	0.1025	0.088	0.1648	0.141	NA	NA	NA


asterics
My workspace
Edit
Explore
Integrate
Documentation
Missing values
Explore missing values
Remove missing values
Impute missing values
1. Select the dataset to analyze
Select a dataset
PICLET_qPCR1P218
2. Plots and numerical summaries
Heatmaps
Plots
Summary


qPCR-1: Heatmap of missing values
Missing values
0
1
Pct missing
100
50
0


PICLET_qPCR1P218: Percentage of missing values by variable
Percentage of missing values
0
20
40
60
80
CTNNA1
CSNK2A1
LRCC28
DDX6
LILRA6
BIRC5_FR
TLE4
SEC62
TKT
NME4
GYPC
CD14
SSFA2
BCAS2
DUT
TSPAN31
CIR1
TGM3
TPRKB
PDZK1
DEGS1
PIP4K2A
DY41508S
SLAIN2
MTCO2
MAOA
ID3
NR3C1
PPP2R1B
RPL19
ATP2B1
GPX1
RGCC
CD3E
RAB14
ROMO1
Variables with missing values
pct_miss
100
75
50
25
0


PICLET_qPCR1P218: Percentage of missing values by individual
Individuals with missing values
0
10
20
30
Percentage of missing values
pct_miss
100
75
50
25
0

Missing values

Explore missing values | **Remove missing values** | Impute missing values

1. Select the dataset to analyze

Select a dataset

PICLET_qPCR1P218

Direction

Individuals (rows)

Maximum % of acceptable missingness in individuals/variables

0 — 30 — 100

Run

2. Plots and numerical summaries

Purpose of Missing values:

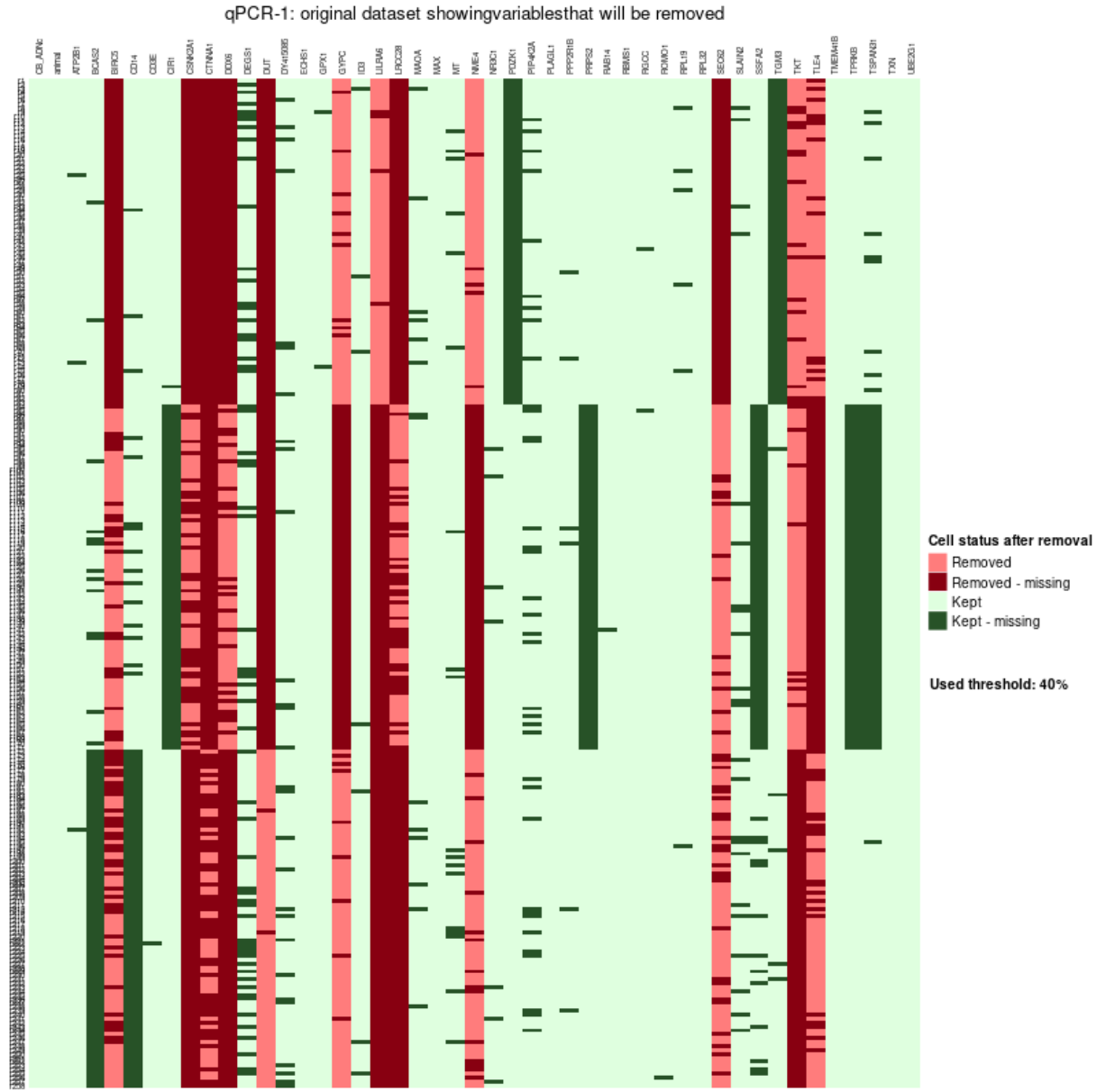
Handle missing values in your datasets

- Explore the distribution of missing values in your dataset
- **Impute** missing values with PCA, k-means or by zero.
- OR **remove** individuals / variables with the largest proportions of missing values.

How to set options?

- "Direction" is used to choose to remove either entire individuals (rows) or entire variables (columns).
- The chosen percentage corresponds to the maximum acceptable missingness. For instance, if 30% is chosen, it means that all individuals or variables with more than 30% of missing values will be removed.

Check help for further advice.


qPCR-1: original dataset showingvariablesthat will be removed
Cell status after removal
Removed
Removed - missing
Kept
Kept - missing
Used threshold: 40%

Missing values

Explore missing values | Remove missing values | **Impute missing values**

1. Select the dataset to analyze

Select a dataset

PICLET_qPCR1P218

Imputation method

PCA

Type of variables to impute

Auto

Run

2. Plots and numerical summaries

Purpose of Missing values:

Handle missing values in your datasets

- Explore the distribution of missing values in your dataset
- **Impute** missing values with PCA, k-means or by zero.
- OR **remove** individuals / variables with the largest proportions of missing values.

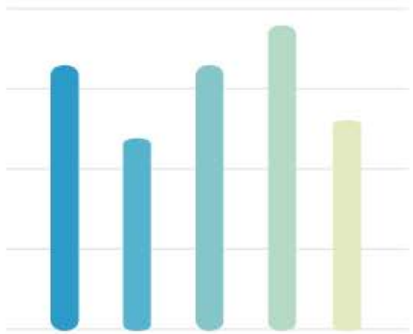
How to set options?

Imputation method can be chosen according to what you know on the missing values and subsequent analyses:

- **imputation by zeros** is dedicated to cases where missing values are due to a measurements below the detection threshold. It is a very basic approach to address this problem but certainly not the best;
- **imputation by PCA** is well designed when you want to use PCA, MFA, or PLS (for instance) afterwards because it best preserves the projection of your individuals on PC axes;
- **imputation by k-nearest neighbors** is based on the idea that two individuals that are similar on observed values also have similar values for unobserved variables. It best preserves the distances between individuals and is well adapted prior clustering.

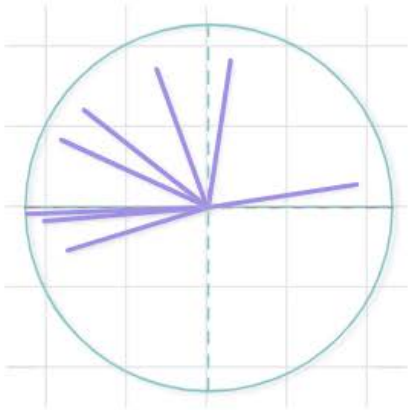
The last two methods are only valid when data are missing at random.

In addition, for PCA and KNN you can choose to impute **only certain types of variables** (only numerical or only categorical variables). Setting this option to “Auto” imputes only variables of the most present type while “Mixed” imputes both numerical and categorical variables.



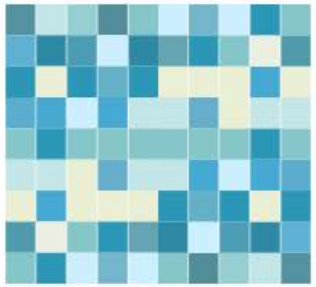
Explore variables in a dataset

Obtain numerical summaries and plots for a few variables.



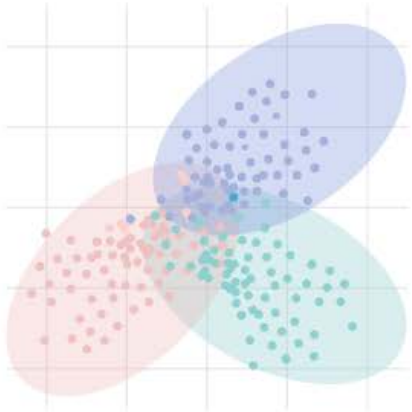
Explore a dataset with PCA

Perform Principal Component Analysis on a dataset.



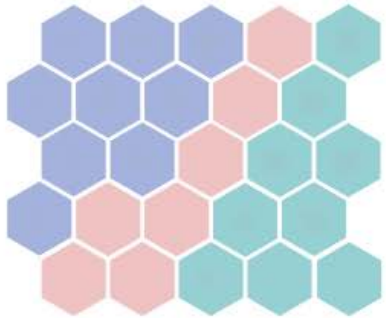
Explore a dataset with a heatmap

Obtain the heatmap of a dataset.



Clustering

Cluster the individuals of a dataset.



Self-Organizing Map

Use SOM as a clustering and visualization method.

asterics

Explore a dataset with PCA

1. Display individuals on components

Component to display on X (horizontal)

1

Component to display on Y (vertical)

2

Color

PICLET_qPCR... | Select a variable

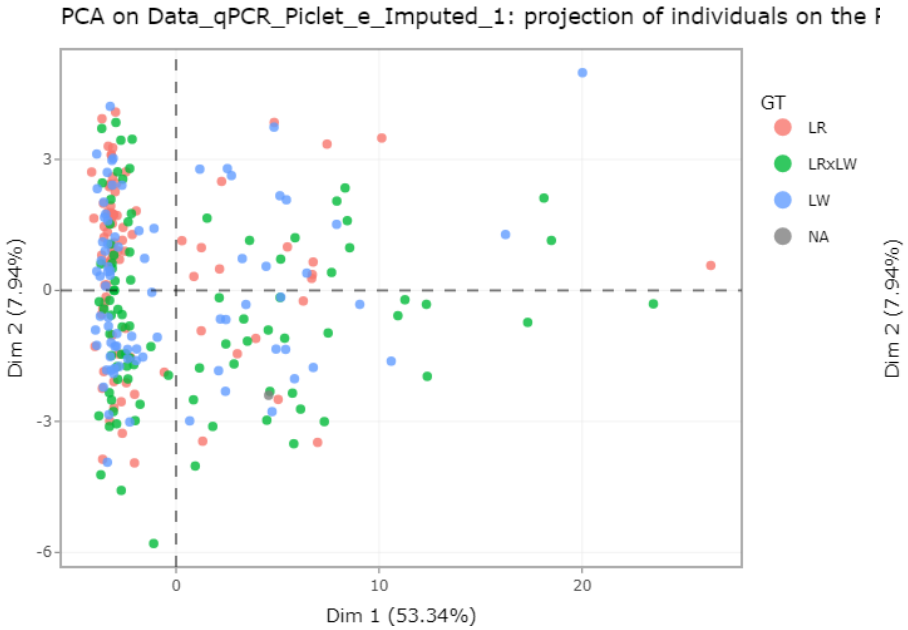
Shape

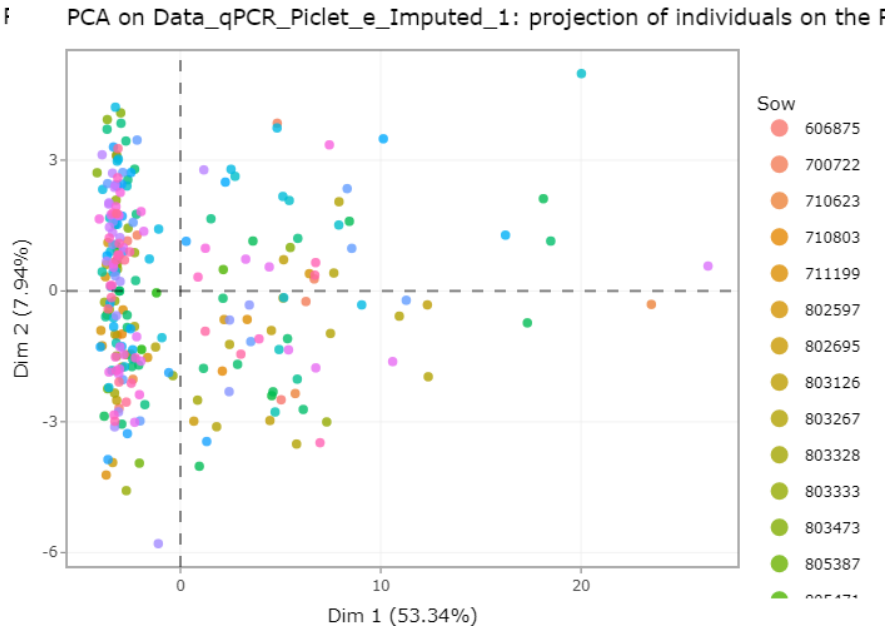
Dataset | Select a variable

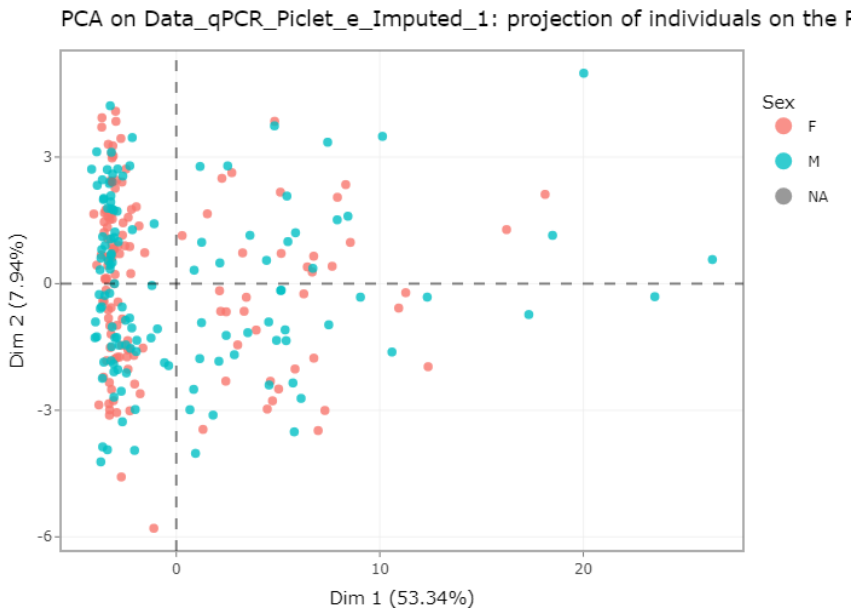
Size

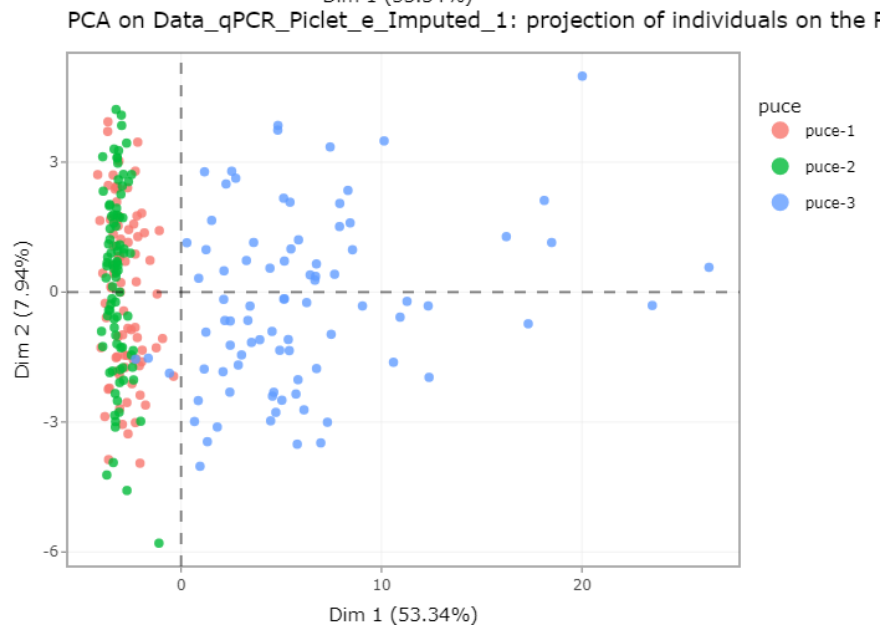
Dataset | Select a variable

Plot individuals







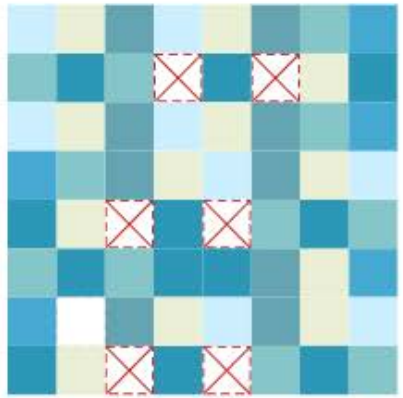


asterics

My workspace | Edit | Explore | Integrate | Documentation

Dataset edition

Provides several ways to modify a dataset.



Missing values

Explore, remove or impute missing values on a dataset.

Normalize dataset

Correct technical biases and prepare your data for further analyses.

Normalize dataset

1. Select a dataset, choose a normalization type and set options

Select a dataset

PICLET_qPCR1P218_Imputed_2

Choose normalization type

Correct batch effect

- Log-transformation
- Centering and scaling to unit variance
- Correct batch effect
- Quantile normalization

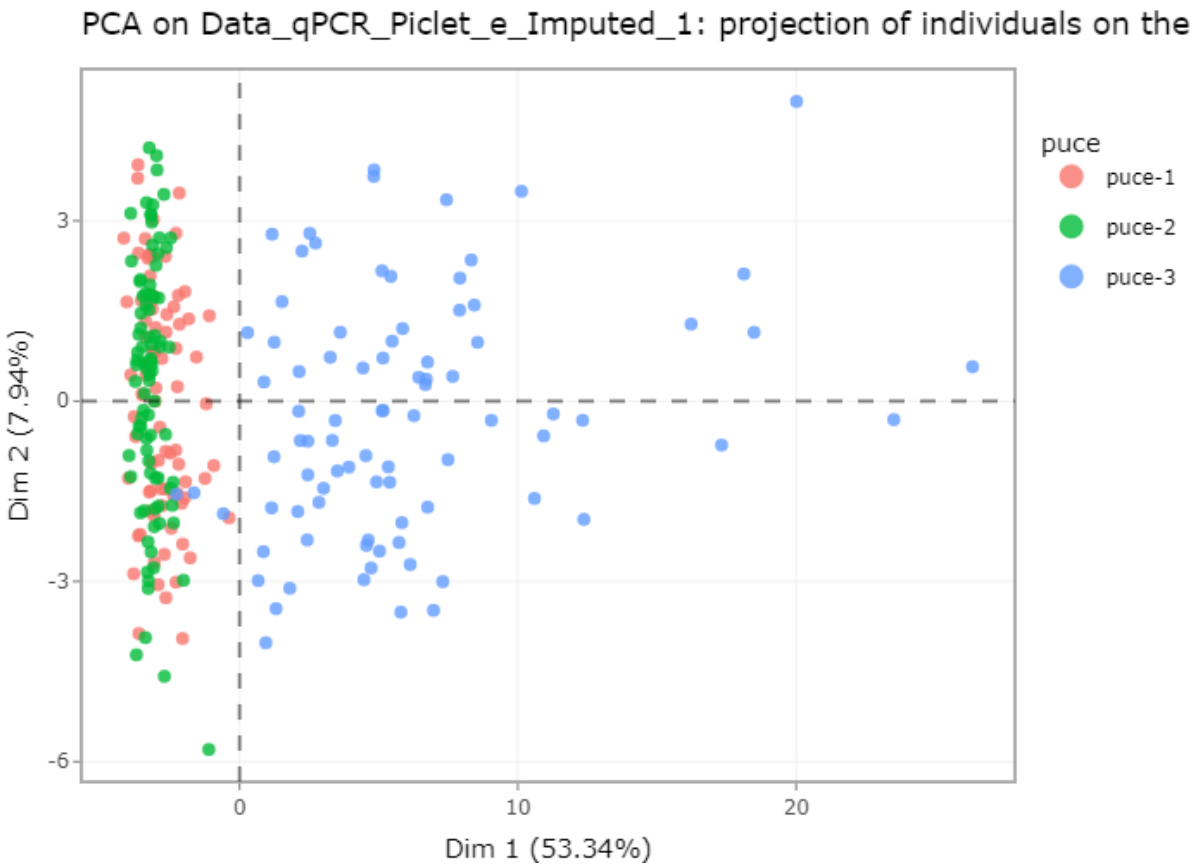
Run

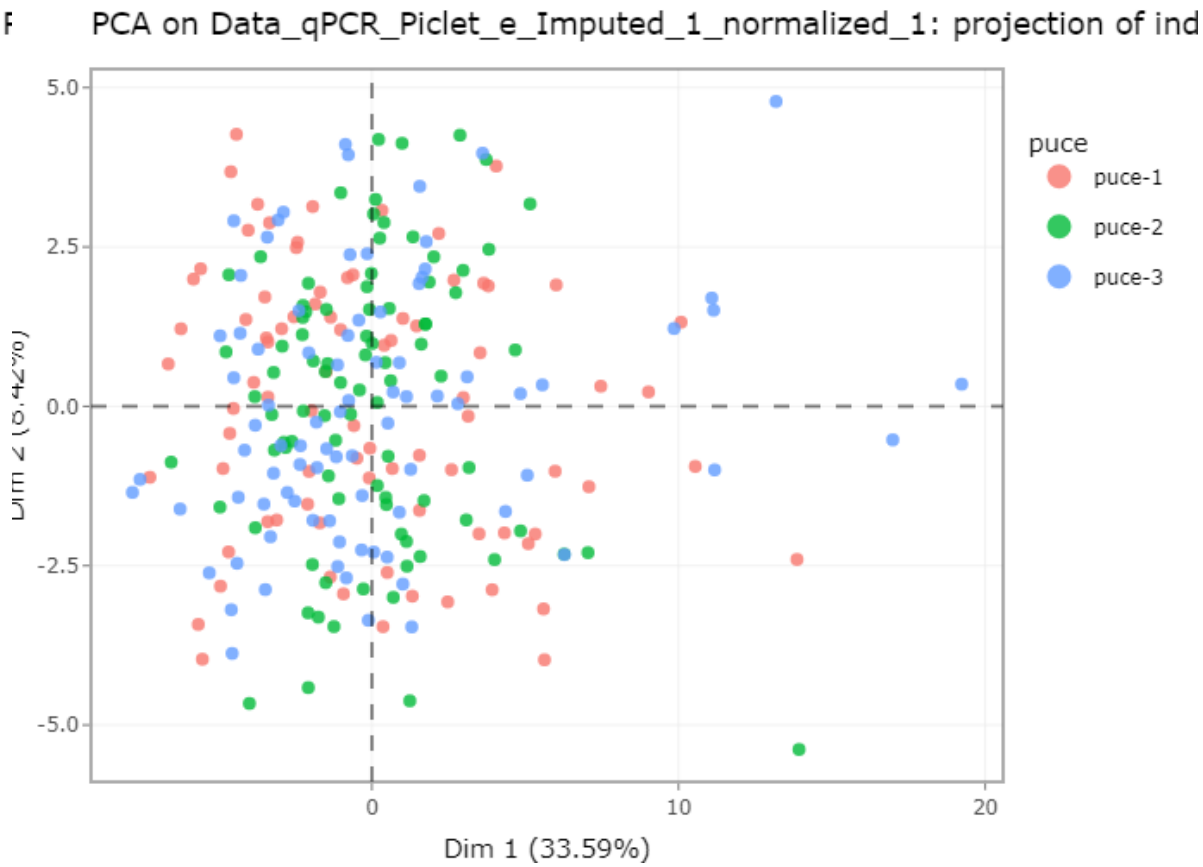
2. Dataset

Purpose of Normalize dataset:

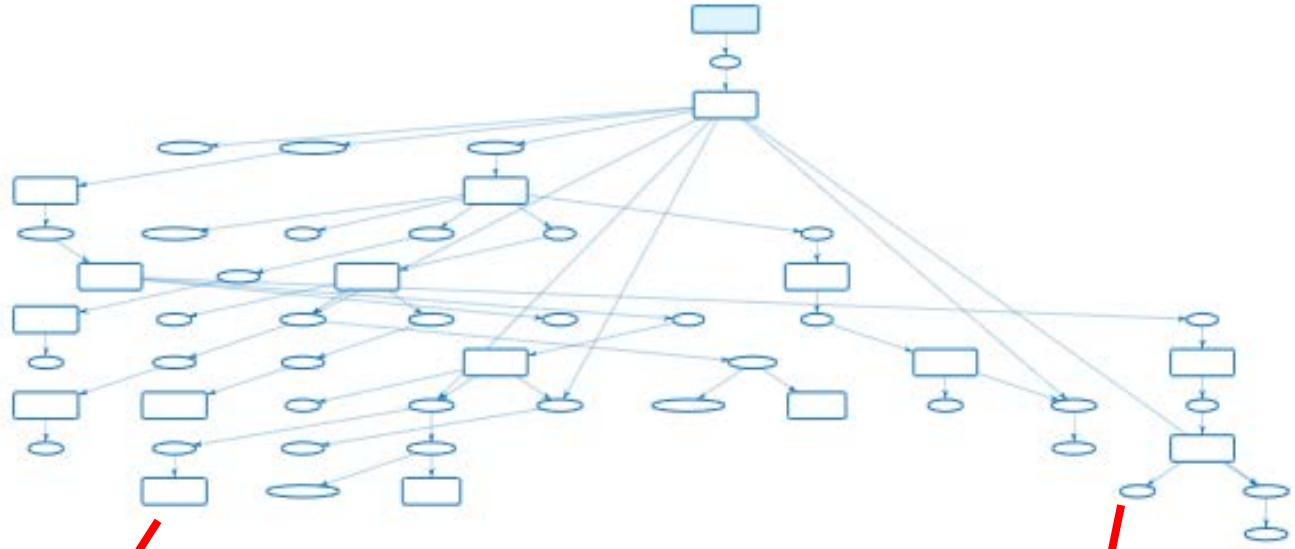
Correct technical biases and prepare your datasets for further analyses

- **Basic transformations** (log, ...).
- **Normalizations specific of certain data types** (RNA-seq, ...).
- Normalization for the **correction of an explicit batch effect**.
- All normalization methods come with **diagnostic plots**.


PCA on Data_qPCR_Piclet_e_Imputed_1: projection of individuals on the F
puce
puce-1
puce-2
puce-3
Dim 2 (7.94%)
Dim 1 (53.34%)
3
0
-3
-6
0
10
20


PCA on Data_qPCR_Piclet_e_Imputed_1_normalized_1: projection of ind
puce
puce-1
puce-2
puce-3
Dim 1 (33.59%)
5.0
2.5
0.0
-2.5
-5.0
0
10
20

Workflow



All datasets

Remove | Add

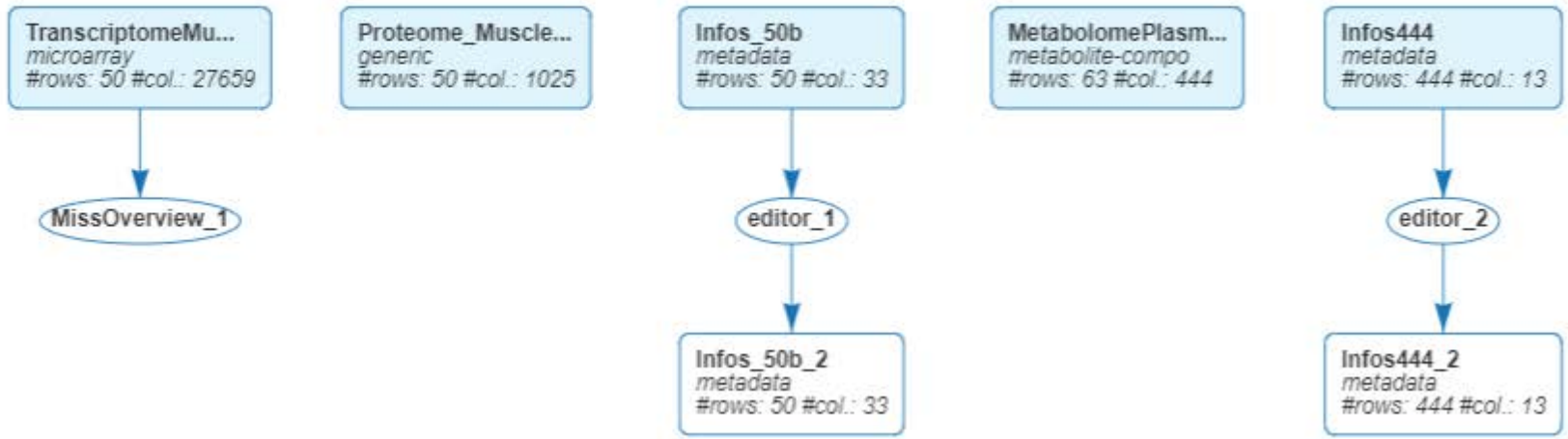
Name	Type	# Rows	# Columns	Log	Normalized
PICLET_qPCR1P21...	generic	257	45	no	no
PICLET_qPCR1P21...	generic	257	25	nc	nc
PICLET_qPCR1P21...	generic	257	45	nc	nc
PICLET_qPCR1P21...	generic	257	25	nc	nc

All analyses

Remove | Export report

Name	Function
editor_1	r_edit_dataset
UnivariateDatas...	r_univariate_dataset
MissOverview_1	r_missing_overview
MissShowRemove_...	r_missing_showremove
MissShowRemove_...	r_missing_showremove
PCAobj_1	r_famd
imputeMissing_1	r_missing_impute
imputeMissing_2	r_missing_impute

Workflow


TranscriptomeMu...
microarray
#rows: 50 #col.: 27659
Proteome_Muscle...
generic
#rows: 50 #col.: 1025
Infos_50b
metadata
#rows: 50 #col.: 33
MetabolomePlasm...
metabolite-compo
#rows: 63 #col.: 444
Infos444
metadata
#rows: 444 #col.: 13
MissOverview_1
editor_1
editor_2
Infos_50b_2
metadata
#rows: 50 #col.: 33
Infos444_2
metadata
#rows: 444 #col.: 13

asterics

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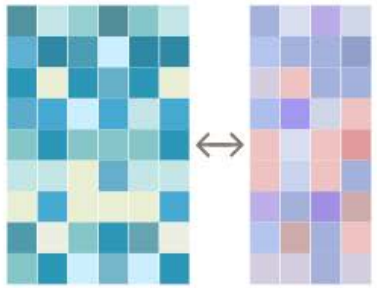
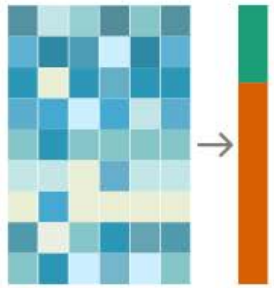


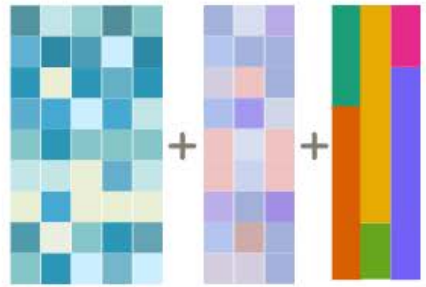
Integrate two datasets with PLS

Performs Partial Least Squares analysis on two datasets.



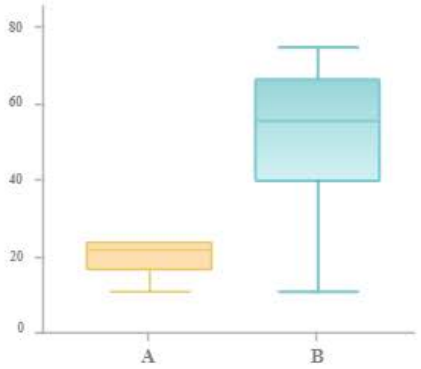
Integrate two datasets with PLS-DA

Performs Partial Least Squares analysis on two datasets.



Integrate datasets with MFA

Perform Multiple Factor Analysis on several datasets.



Differential analysis

Perform differential analysis for all numeric variables of a dataset.

Integrate two datasets with PLS

1. Select the datasets to integrate

Datasets

Proteome_Muscle_50 Infos_50_edited

Integrate

2. Plots and summaries

General information | Venn diagram | Upset plot

Description of datasets before filtering common individuals (rows)

Name	# rows	# col.	# missing	% missing	# numeric	# cat.	# logic	# others
Infos_50_edited	50	32	0	0	26	6	0	0
Proteome_Muscle...	50	1025	0	0	1025	0	0	0

Description of datasets after filtering common individuals (rows)

Name	# rows	# col.	# missing	% missing	# numeric	# cat.	# logic	# others
Infos_50_edited	50	32	0	0	26	6	0	0
Proteome_Muscle...	50	1025	0	0	1025	0	0	0

Integrate two datasets with PLS

1. Display individuals on components

Component to display on X (horizontal)

1

Component to display on Y (vertical)

2

Color

Info_50b_... TG_F

Shape

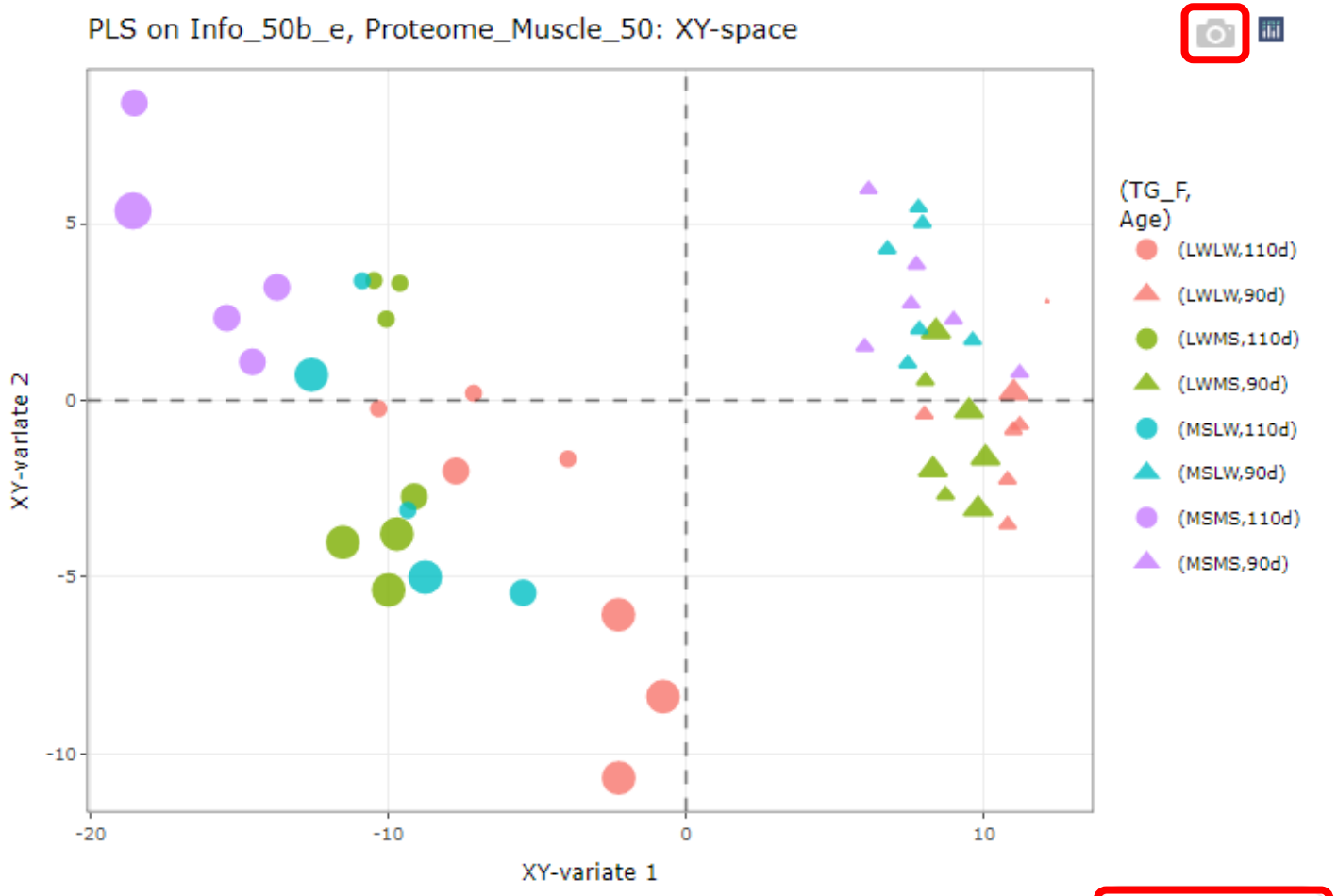
Info_50b_... Age

Size

Info_50b_... Weight

Plot individuals

2. Plot individuals on components



Add to report

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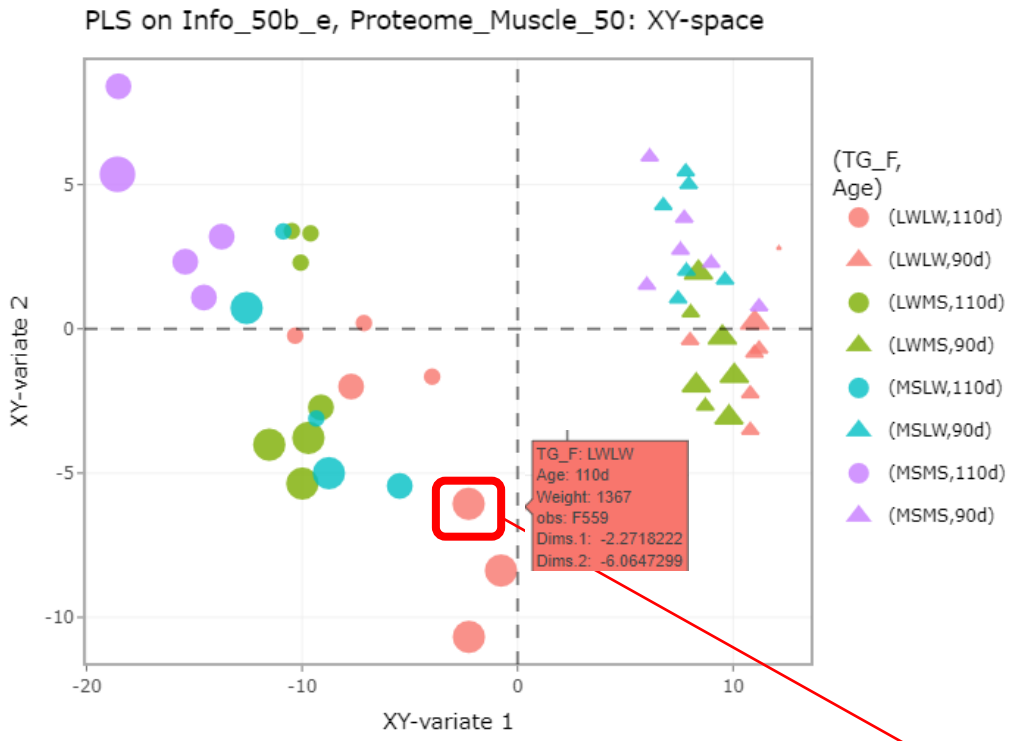
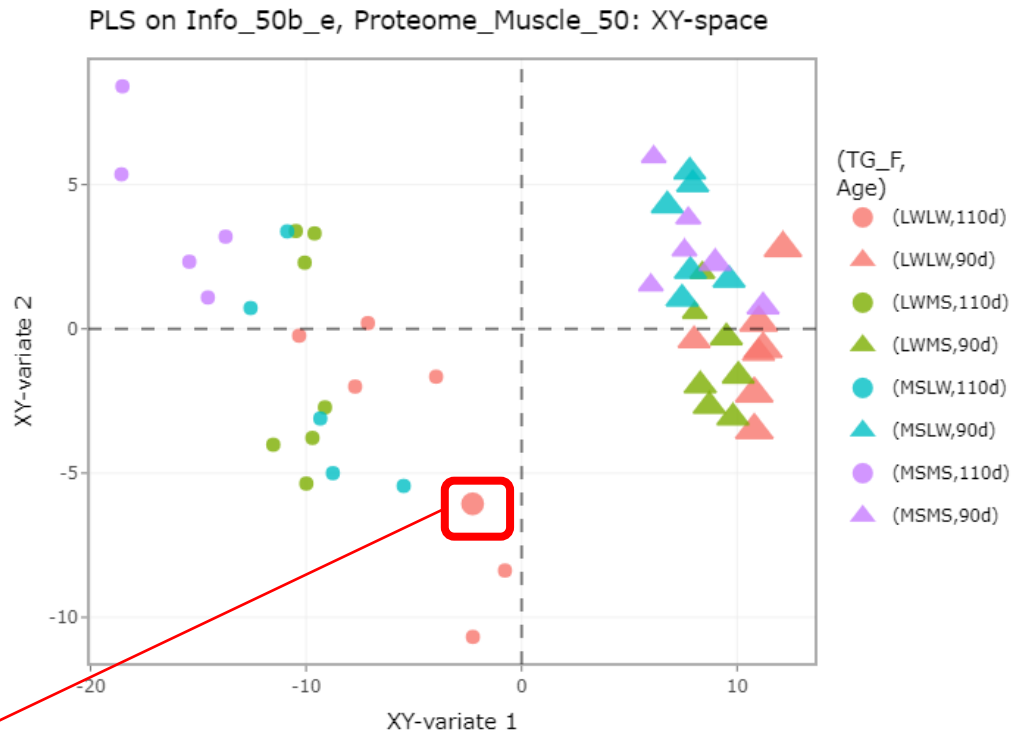
Integrate two datasets with PLS

Preprocessing | Run PLS | **Explore individuals** | Explore variables | Extract new data

Size = weight



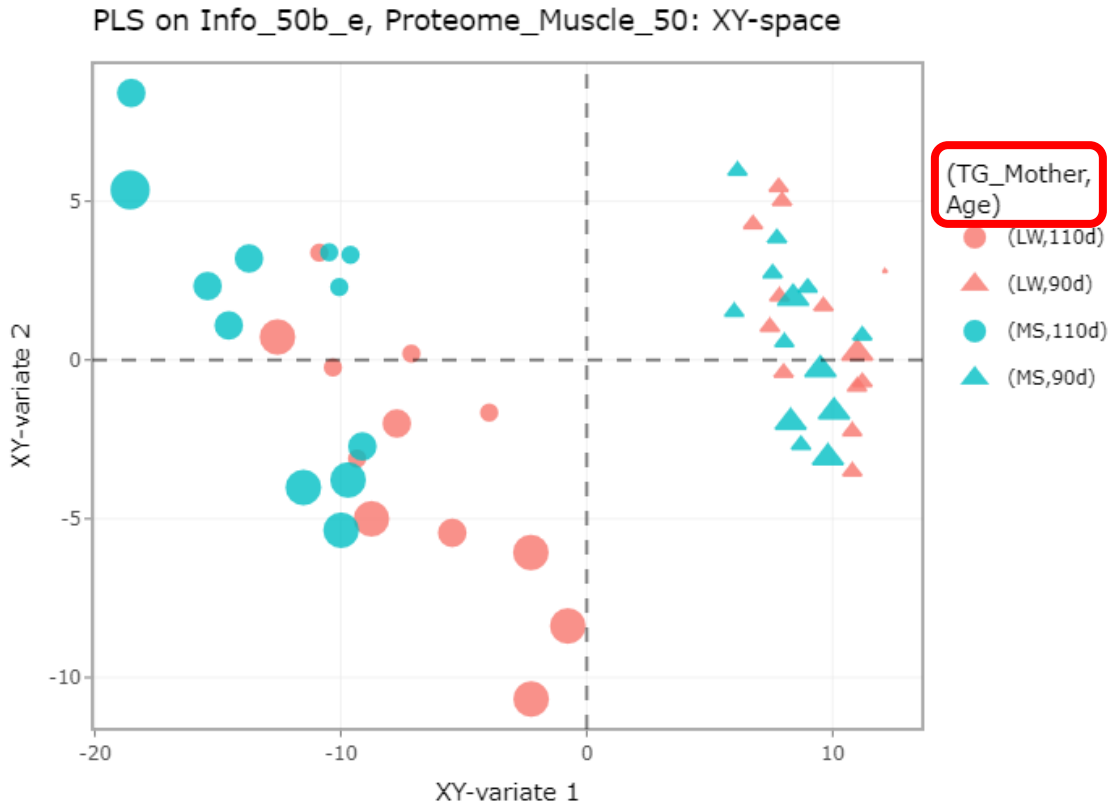
Size = MHC_E

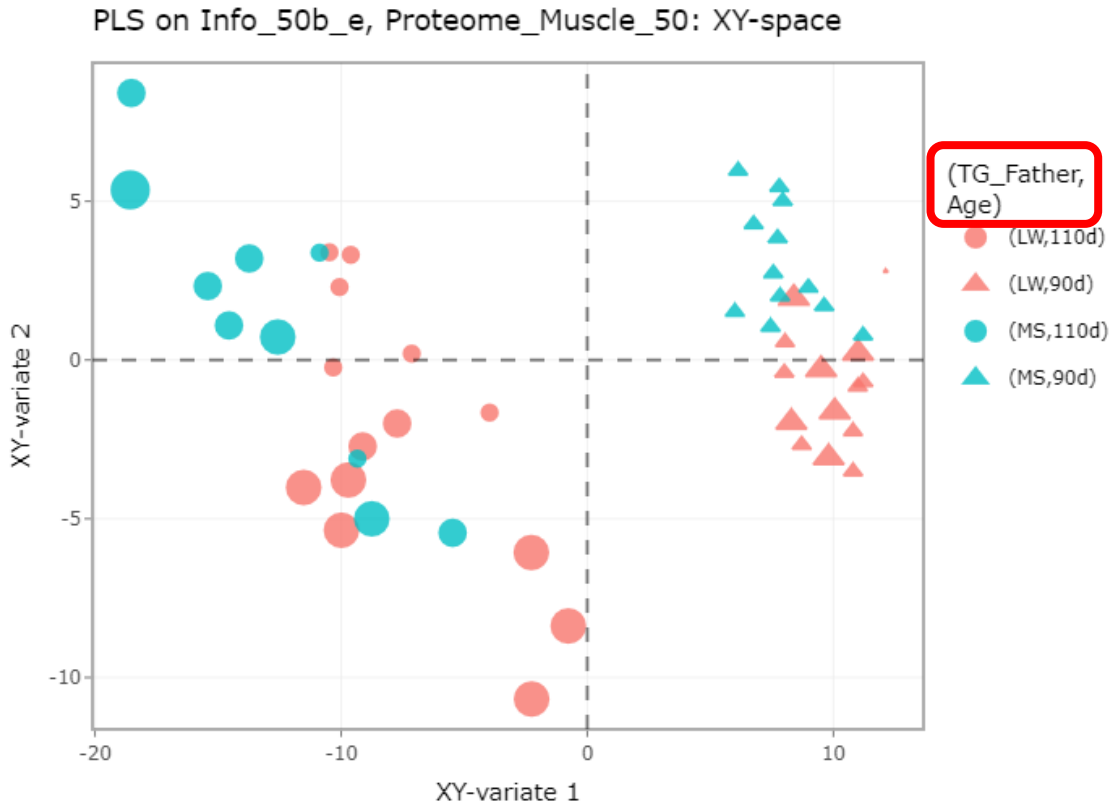


Heavy but developmental delay

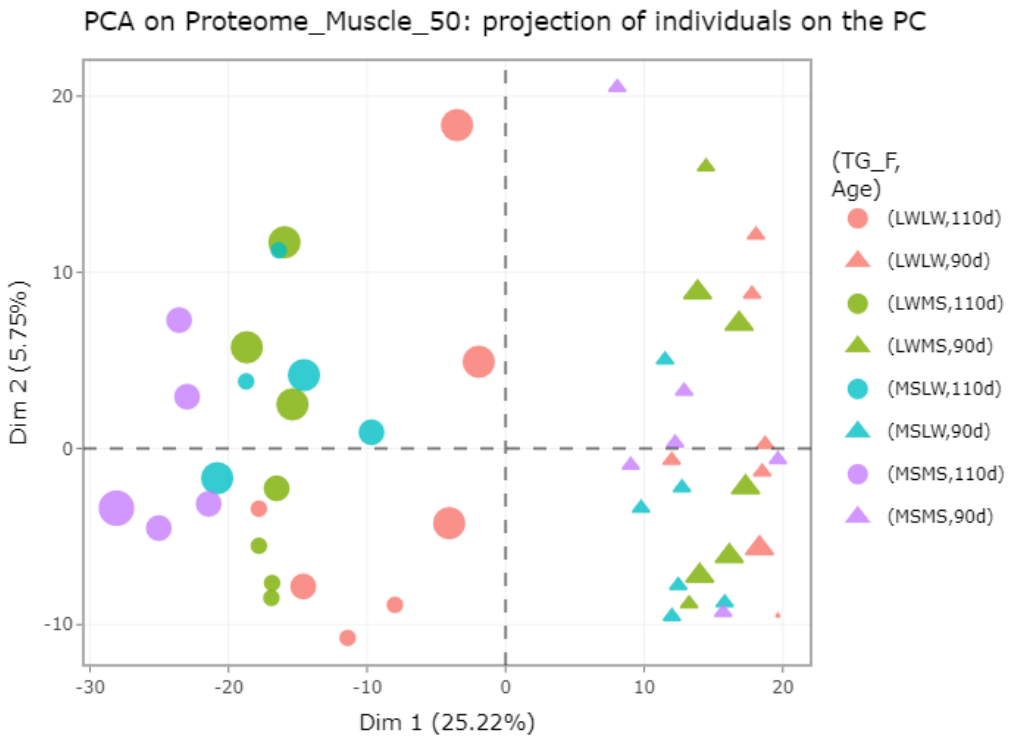
Integrate two datasets with PLS

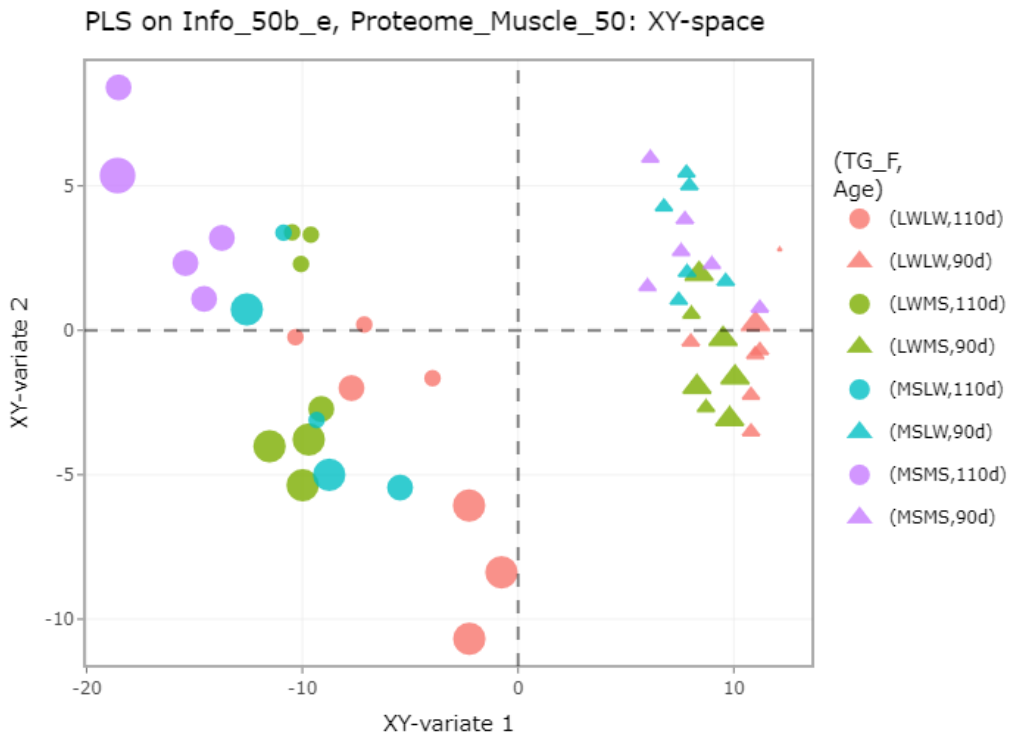
Size = weight





PCA vs PLS

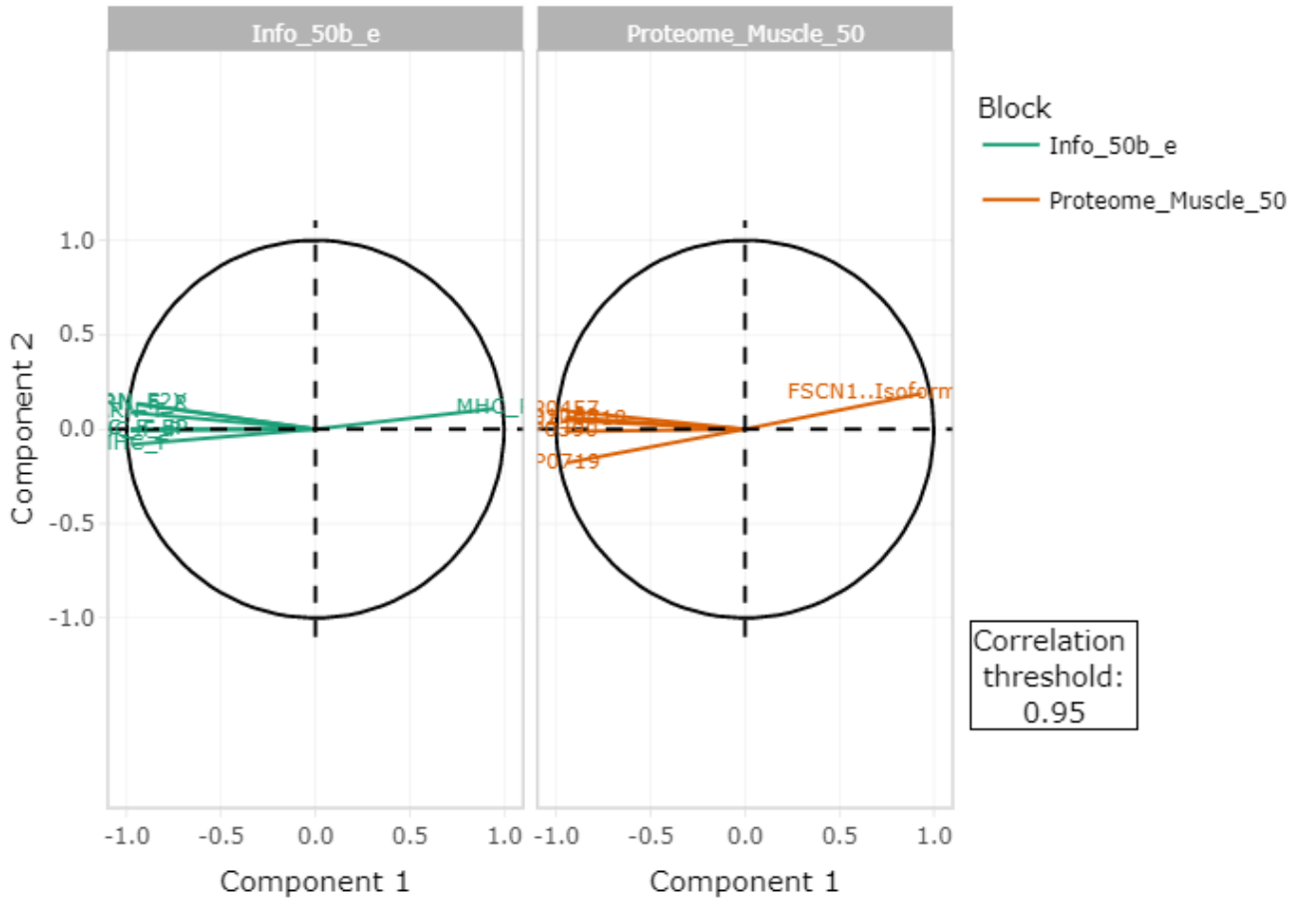


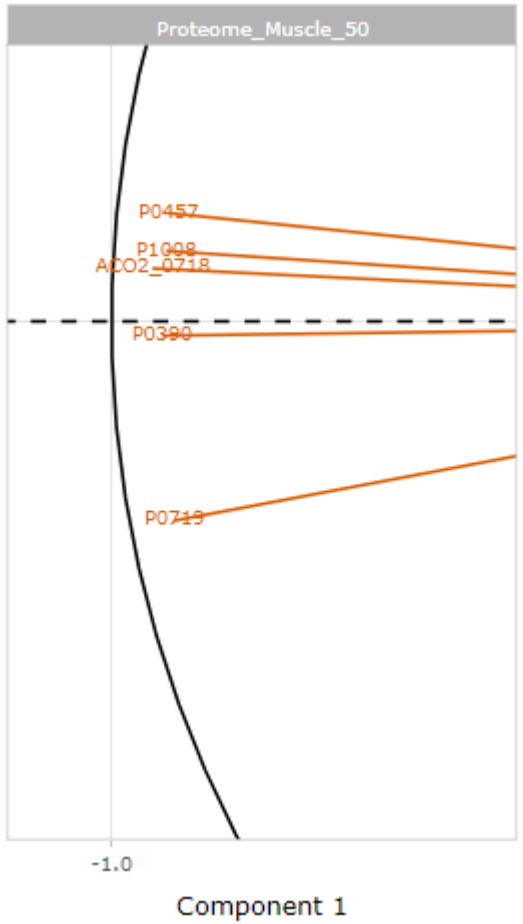


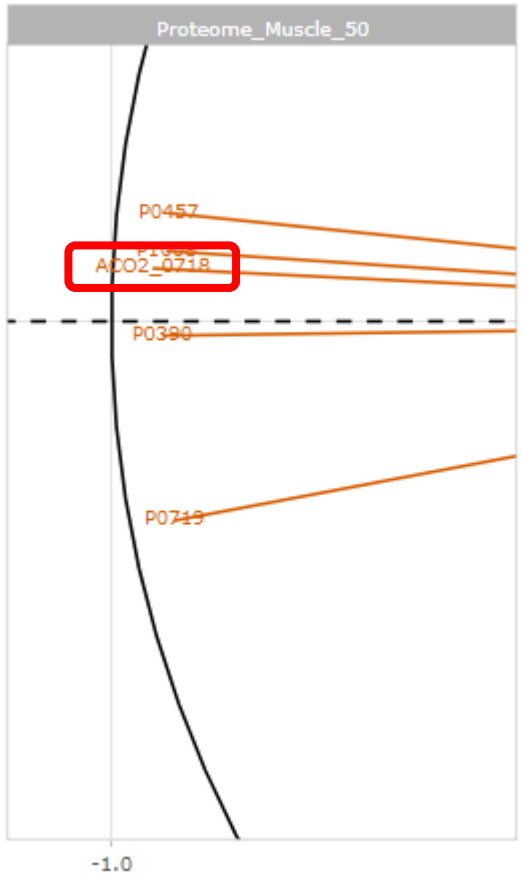
Size = weight

Integrate two datasets with PLS

PLS on Info_50b_e, Proteome_Muscle_50: correlations of variables with



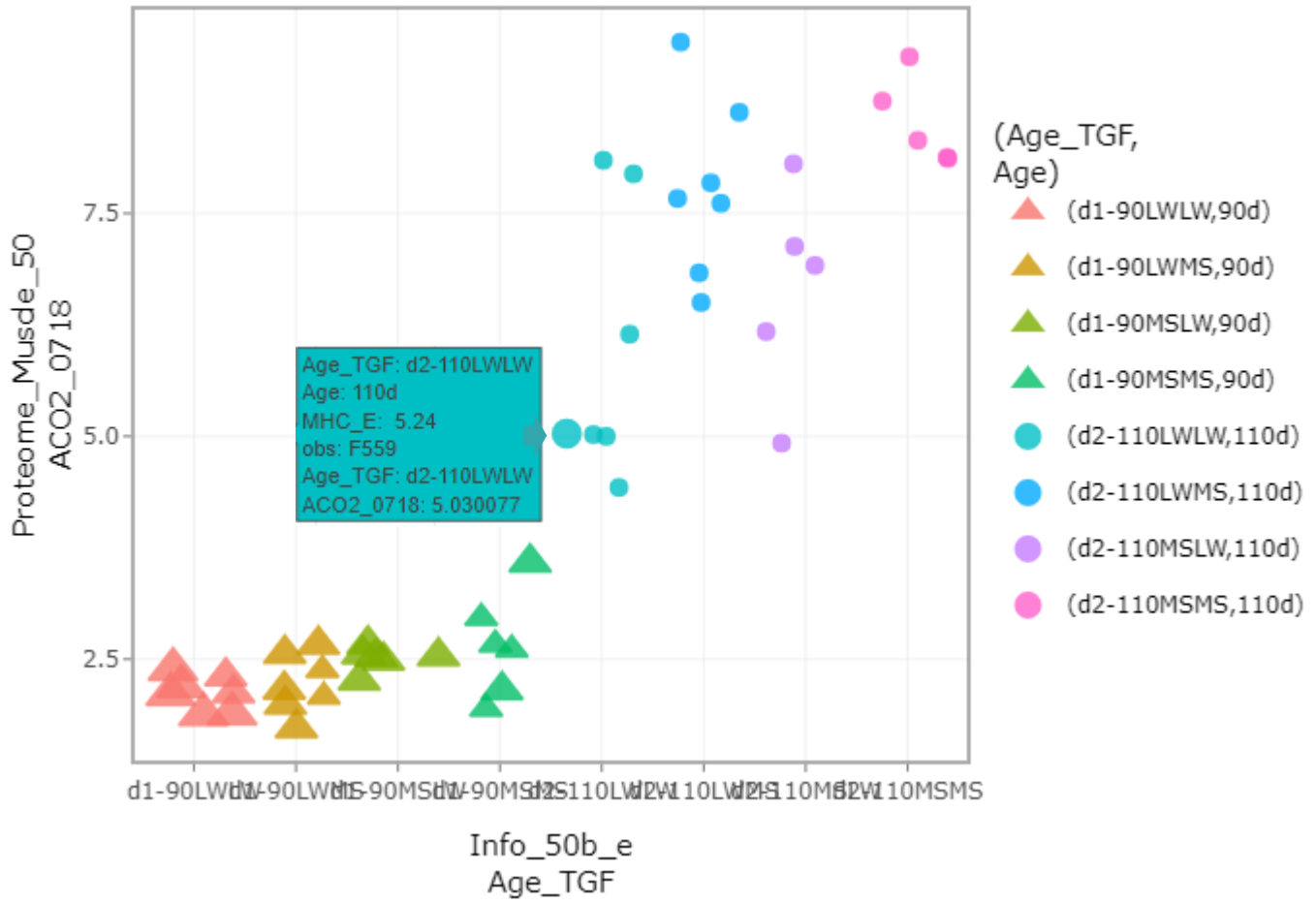




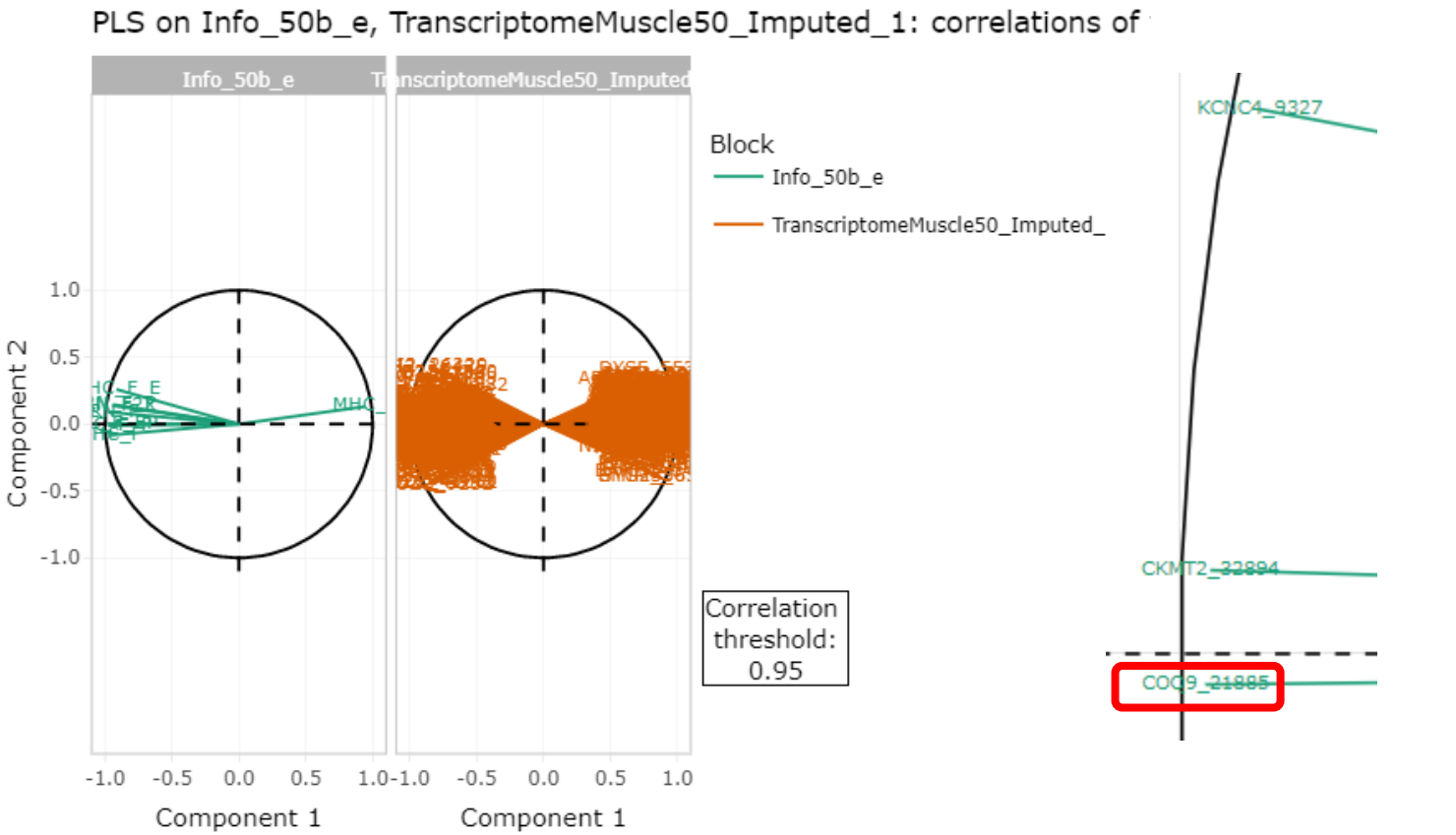
asterics

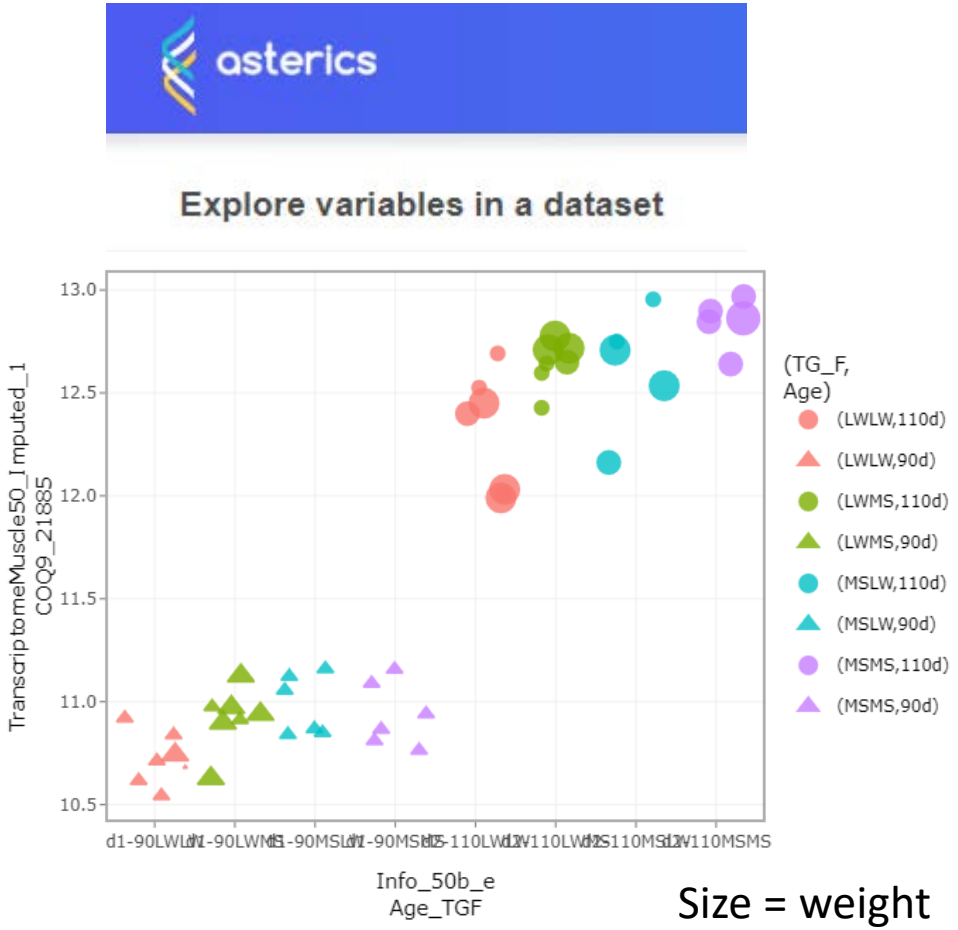
Explore variables in a dataset

Size = MHC_E



Integrate two datasets with PLS

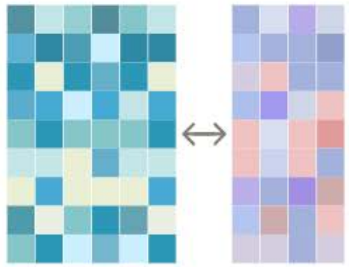




Size = weight

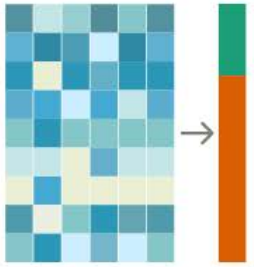
asterics | My workspace | Edit | Explore | Integrate | Documentation

Let's integrate data!



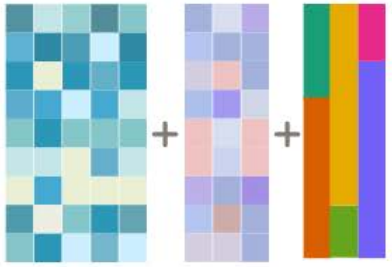
Integrate two datasets with PLS

Performs Partial Least Squares analysis on two datasets.



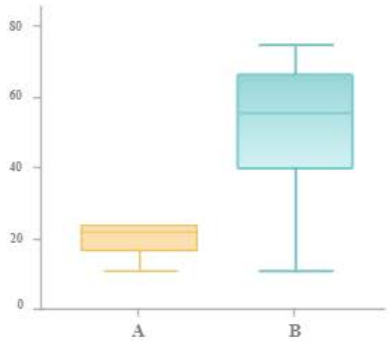
Integrate two datasets with PLS-DA

Performs Partial Least Squares analysis on two datasets.



Integrate datasets with MFA

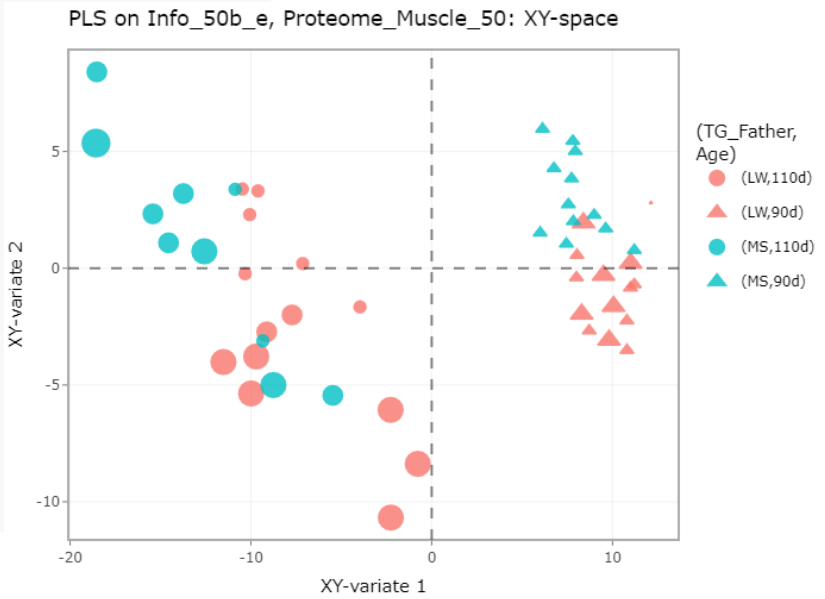
Perform Multiple Factor Analysis on several datasets.



Differential analysis

Perform differential analysis for all numeric variables of a dataset.

It is easy to discriminate the age but what about the genotype?



asterics | My workspace | Edit | Explore | Integrate | Documentation

Integrate two datasets with PLS-DA

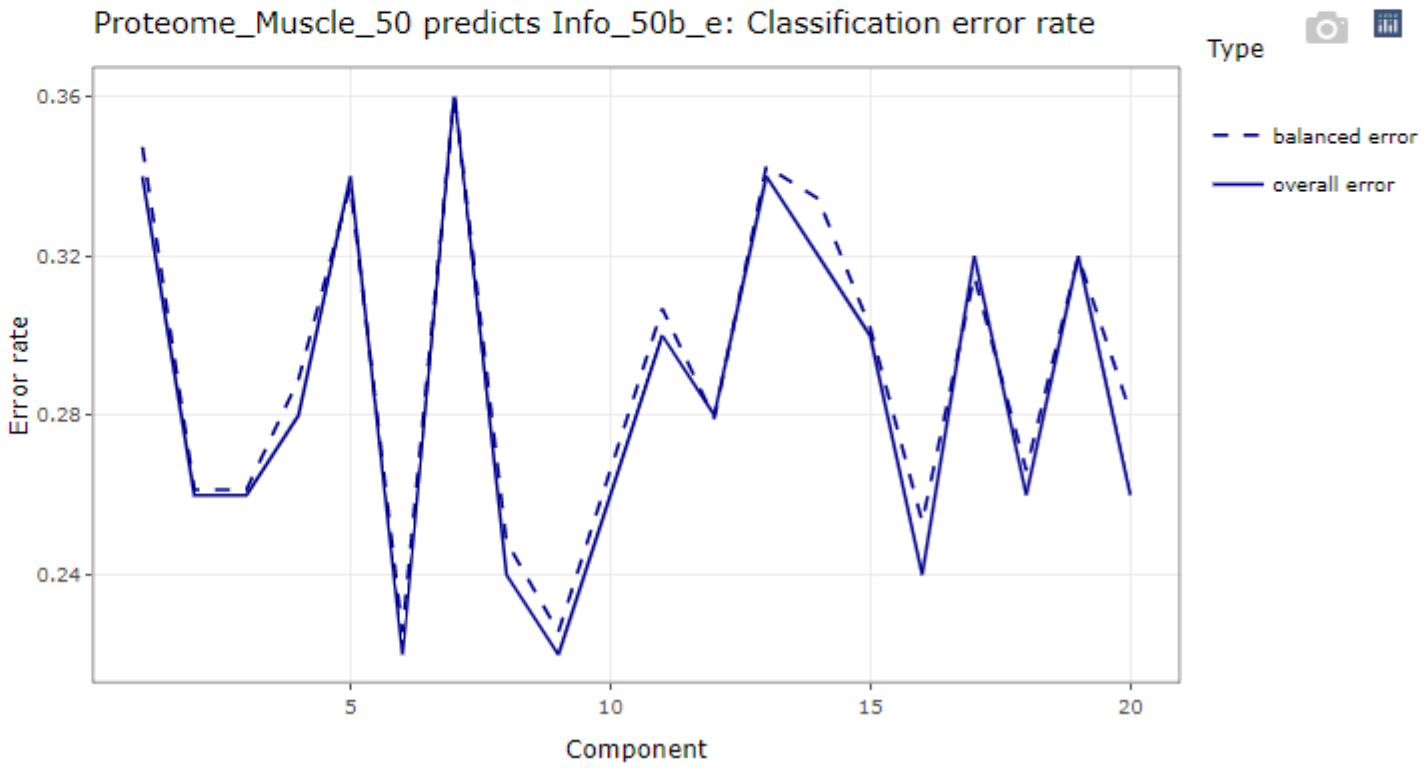
Preprocessing | Run PLS-DA | Explore individuals | Explore variables | Extract new data

1. Run PLS-DA

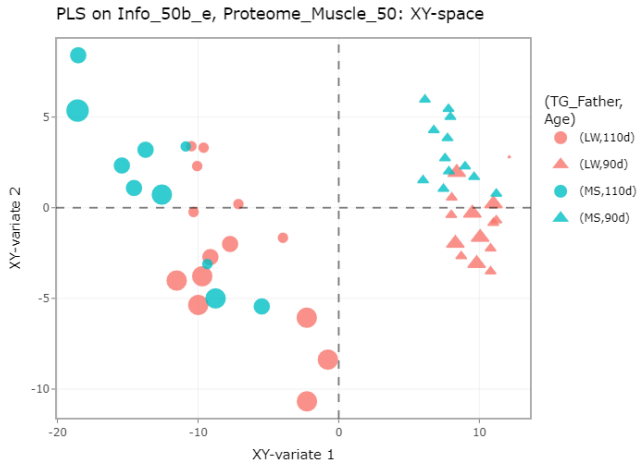
Run

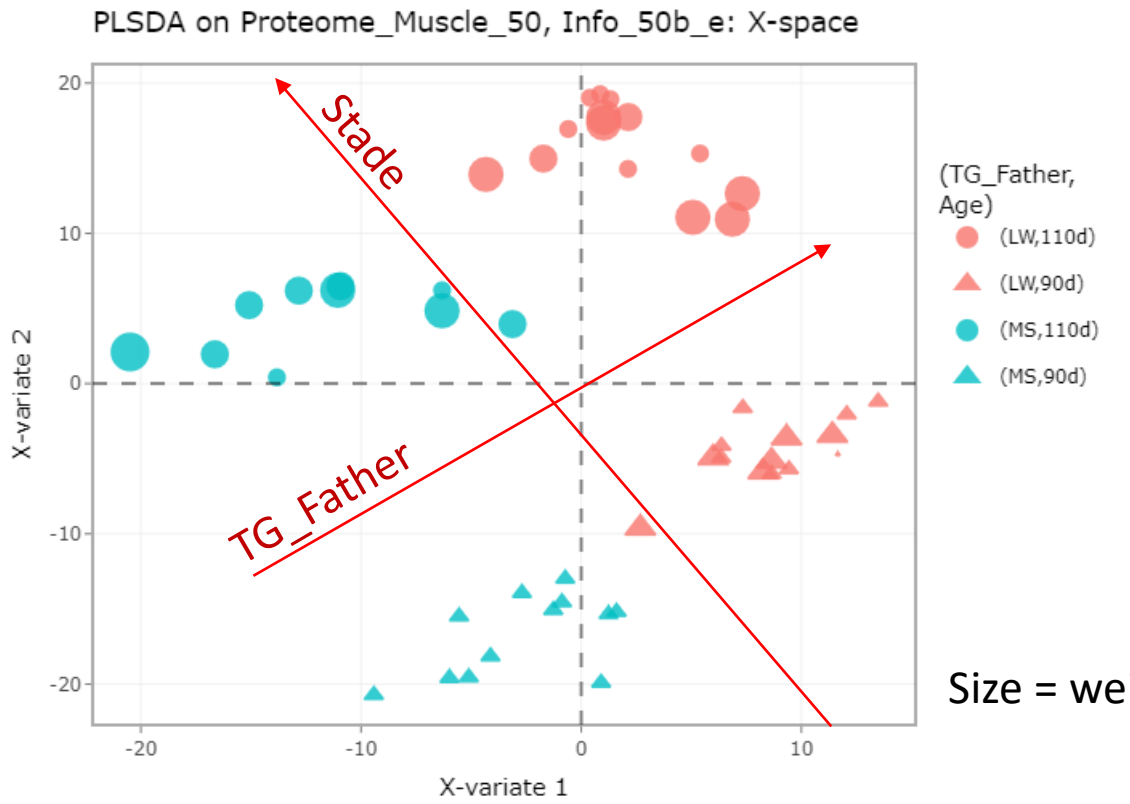
TG_Father

2. Plots



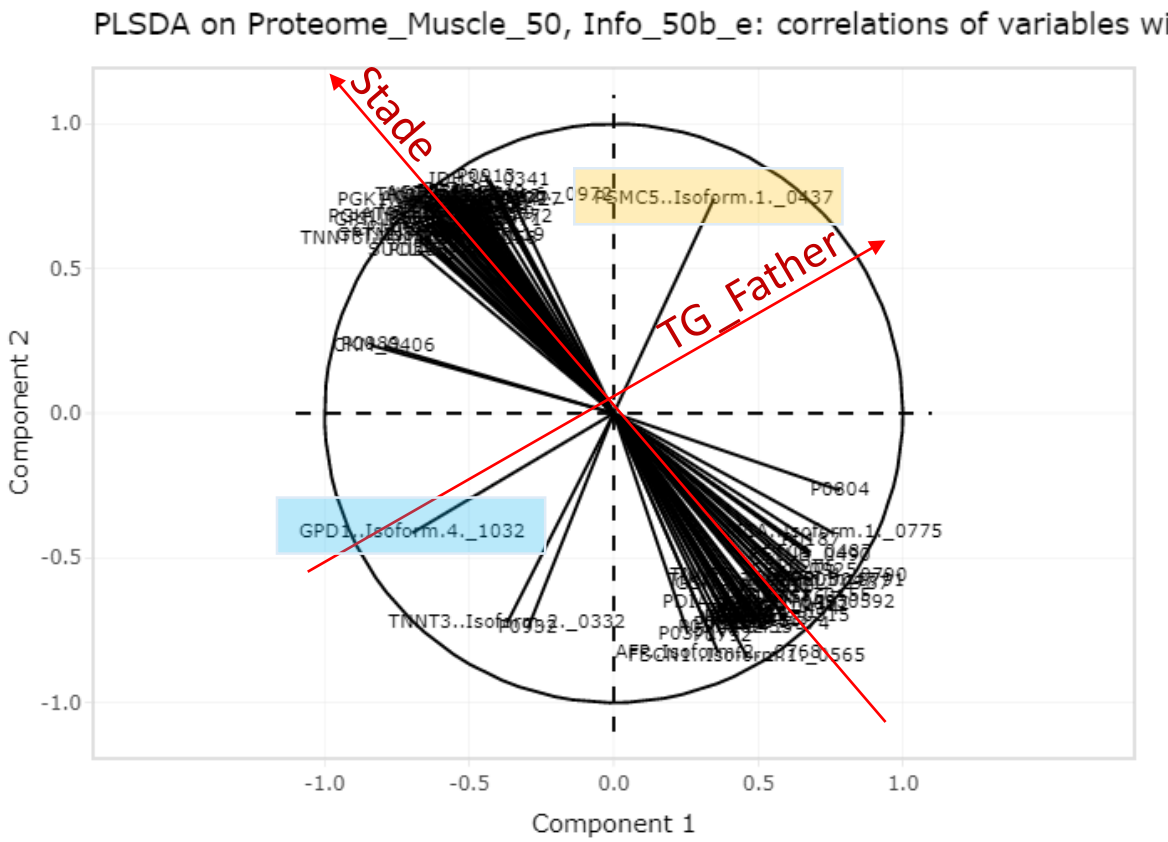
Integrate two datasets with PLS-DA

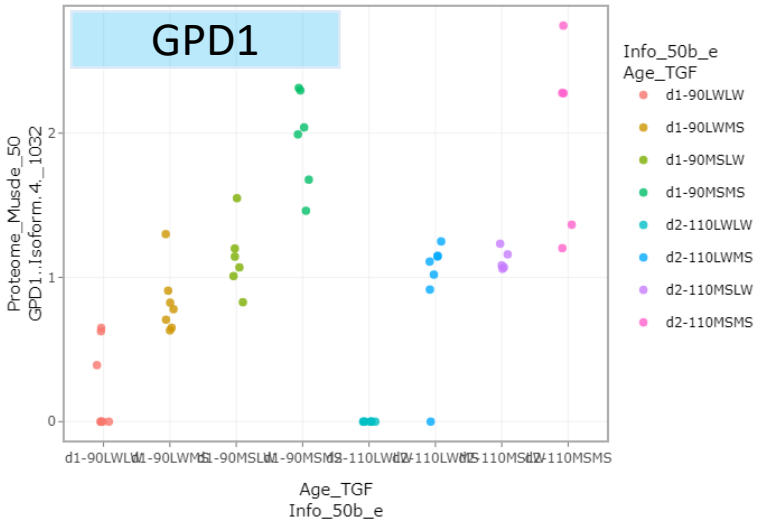


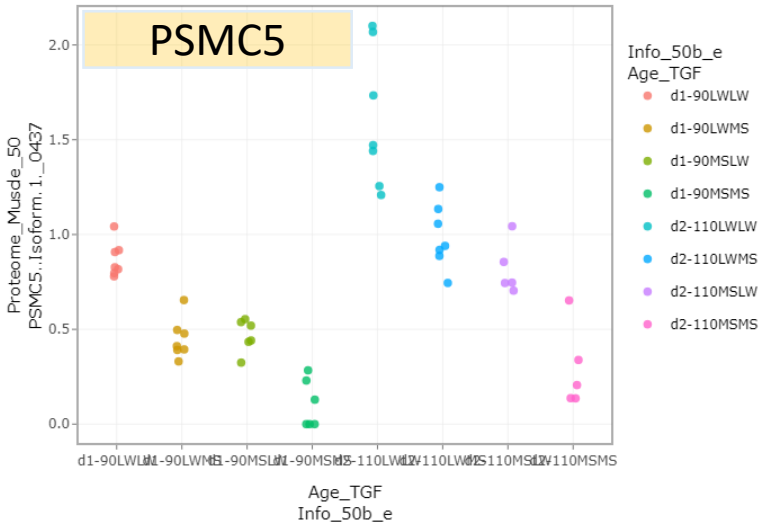


Size = weight

Integrate two datasets with PLS-DA

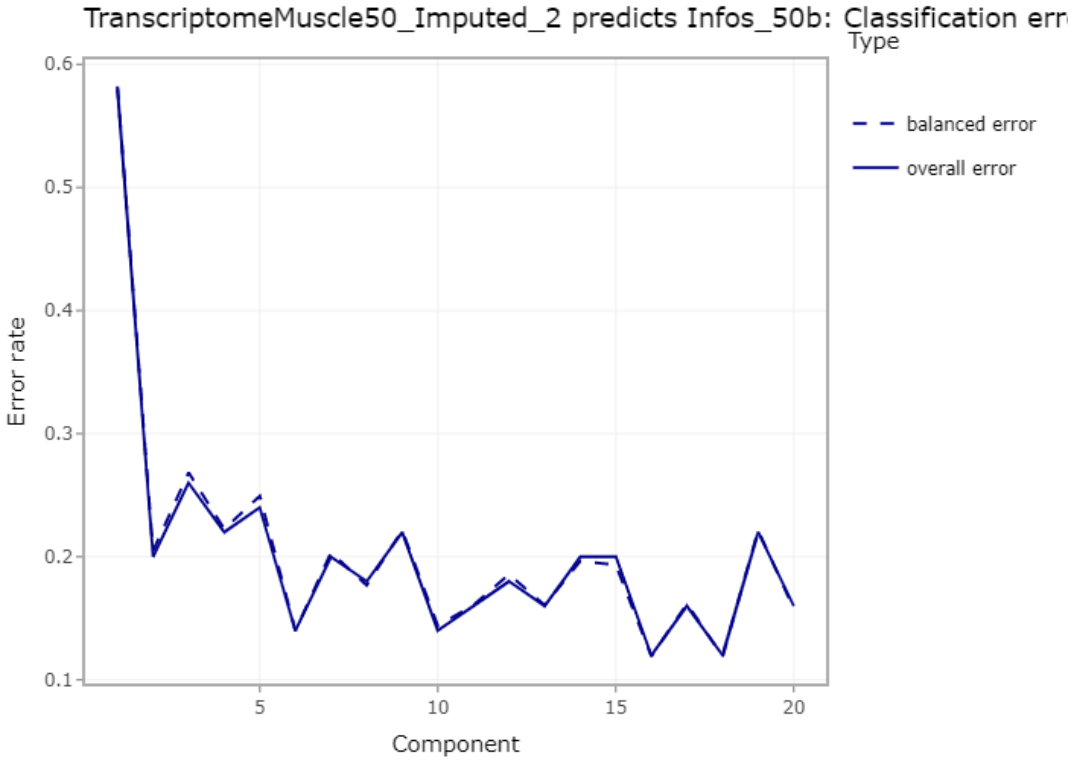


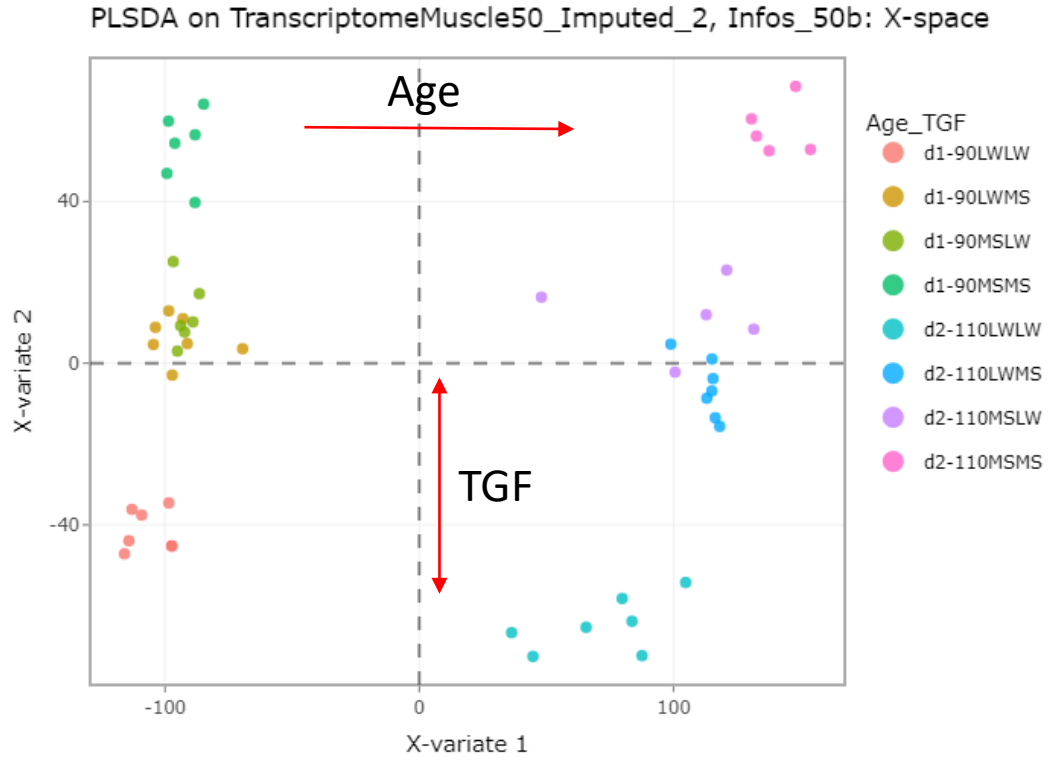


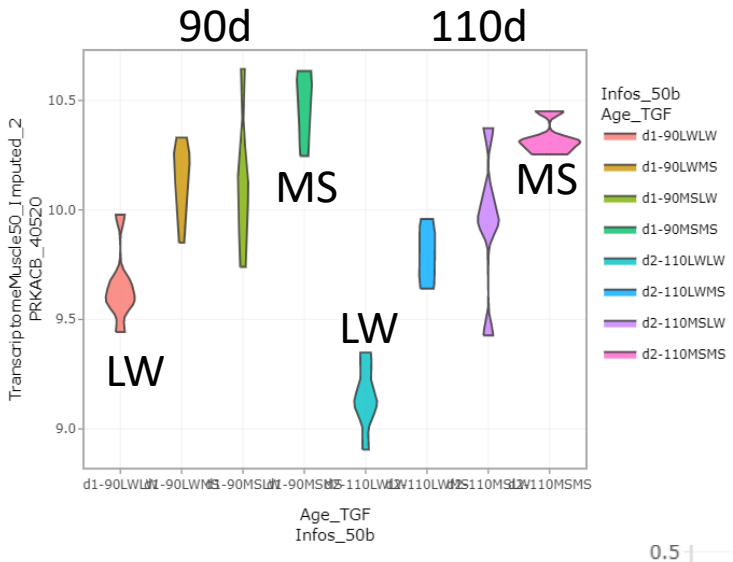


Integrate two datasets with PLS-DA

Age_TGF



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MS
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LW
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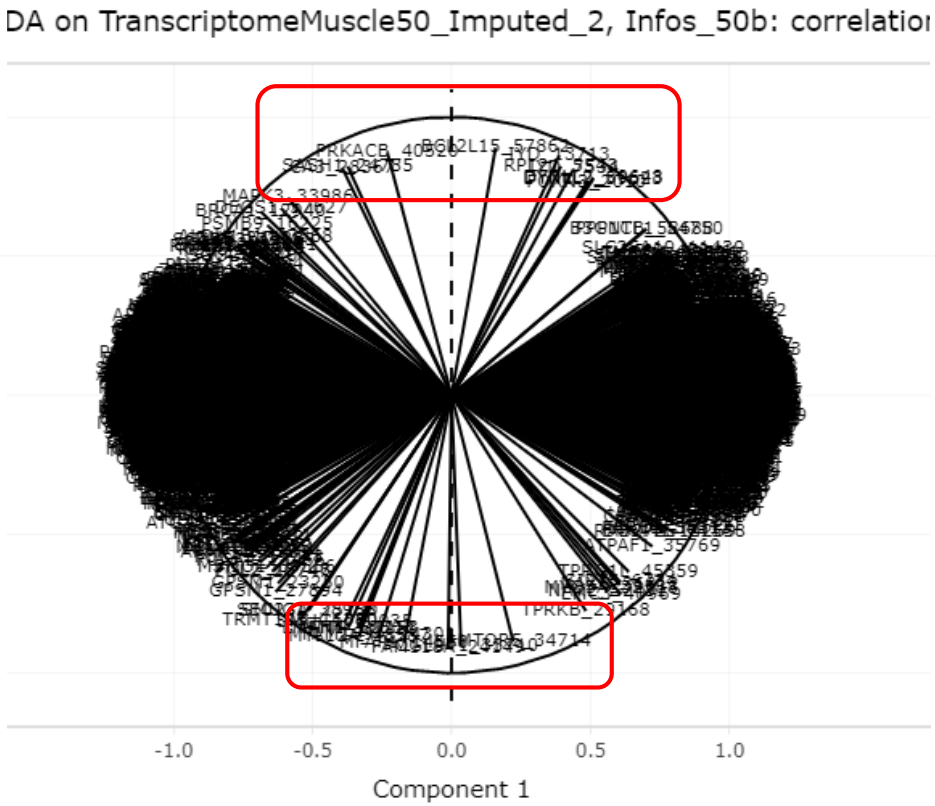
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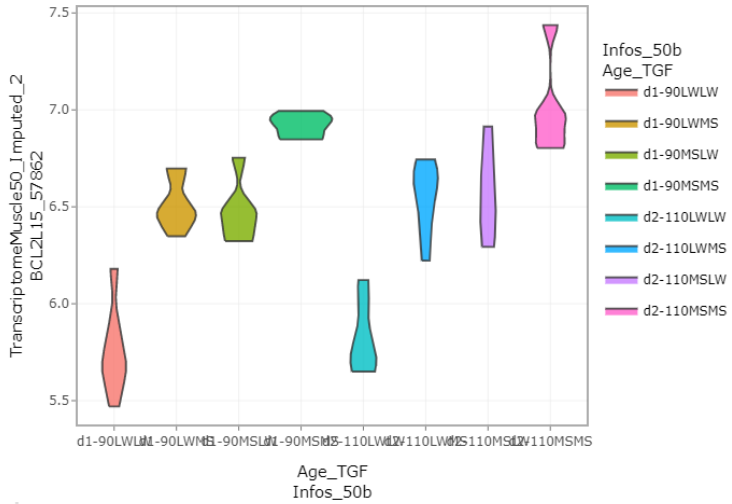
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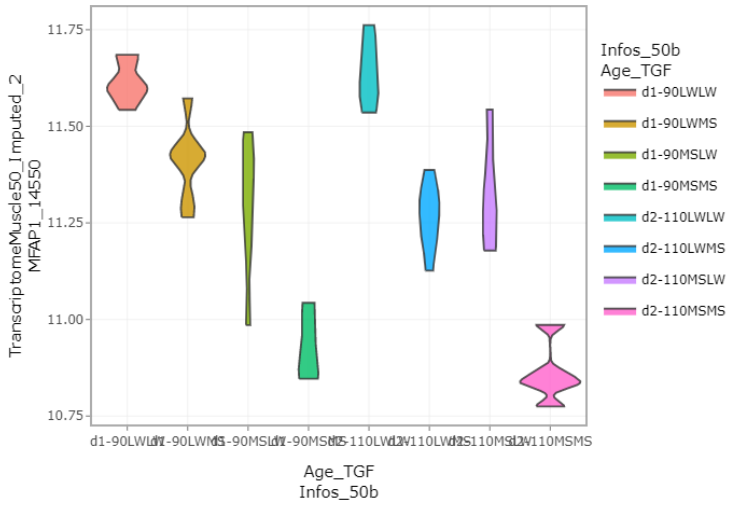
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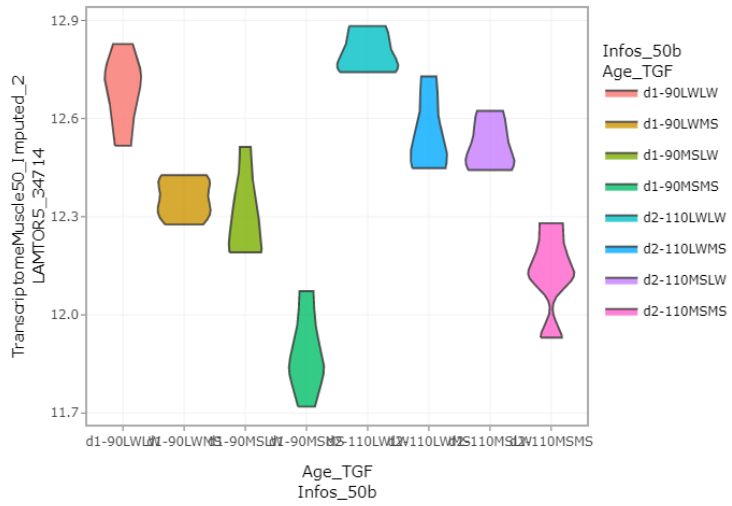
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Merci pour votre attention !