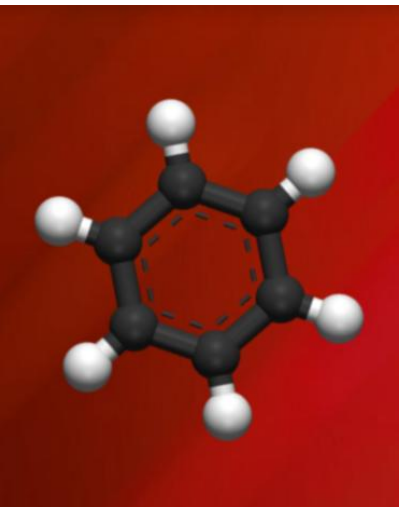


TurbOmics & TurboPutative

A web-server for **multi-omics analysis, data handling** and **metabolite classification** in **untargeted metabolomics**

This website is free to use and open-source to all users and there is no login requirement

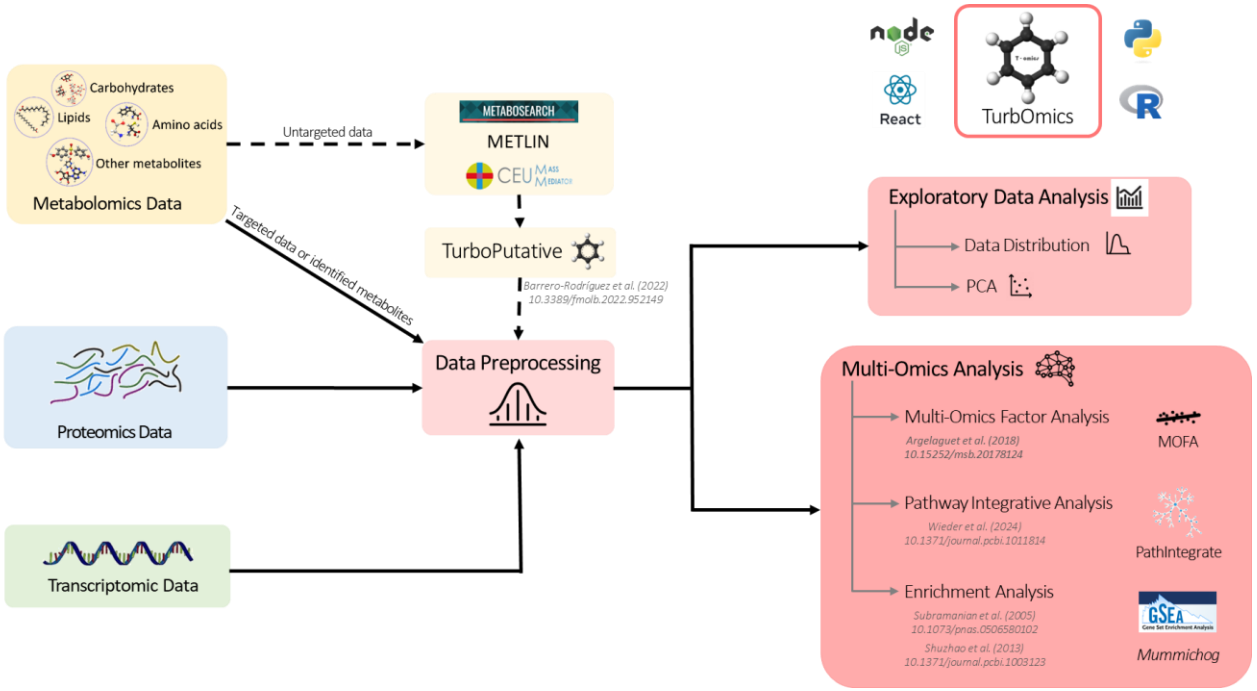
A step-by-step Tutorial

Overview

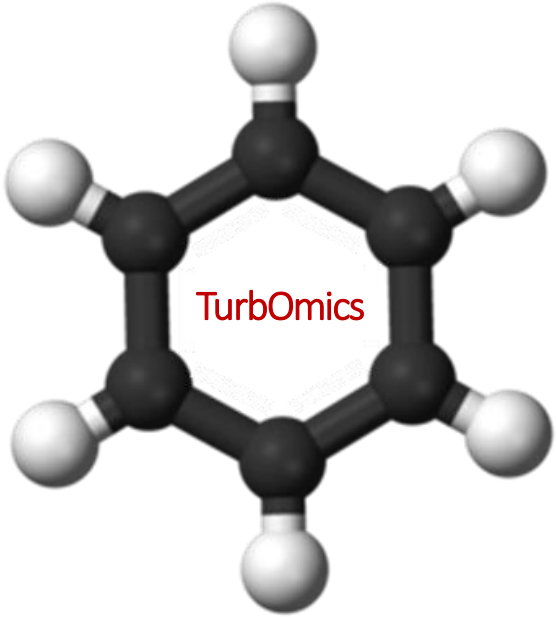
TurbOmics is an intuitive web-based platform designed to facilitate the multi-omics analysis of metabolomics data alongside proteomics and transcriptomics. It supports both **identified metabolites** from targeted-based experiments (LC/CE-MS) as well as those where the metabolite's identification is available (i.e. NMR or GC-MS). Additionally, TurbOmics offers tools to **putatively annotate** features from untargeted metabolomics based on their mass-to-charge (*m/z*) ratio by sequentially and internally running CMM and TurboPutative.

The platform provides a streamlined workflow for **exploratory data analysis** and **multi-omics integration**, through three main modules:

- **Multi-Omics Factor Analysis**
- **Pathway Integrative Analysis**
- **Enrichment Analysis**



Content



- **INTRODUCTION**
- **EXAMPLES**
  - Case study (1): ATHEROSCLEROSIS

    UNTARGETED LIPIDOMICS, PROTEOMICS and TRASCRIPTOMICS from lorenzo *et al*, Nature 2021
    - **DATA PREPARATION**
    - **EXPLORATORY ANALYSIS**
    - **MULTI-OMICS FACTOR ANALYSIS**
    - **ENRICHMENT ANALYSIS**
  - Case study (2): COVID-19

    TARGETED METABOLOMICS and PROTEOMICS from Su *et al.*, Cell 2020
    - **DATA PREPARATION**
    - **PATHWAY INTEGRATIVE ANALYSIS**
- **SUMMARY**

Introduction

Background

Multi-omics integration provides a **comprehensive view of biological systems**, but current bioinformatics tools struggle to incorporate metabolomics data, especially for untargeted annotation and for offering alternatives to predefined knowledge bases. Moreover, advanced integration methods often require programming and statistical expertise, limiting their accessibility to non-specialist users.

The web application

TurbOmics, is a user-friendly web-based platform that enables researchers with diverse backgrounds **to analyze transcriptomics, proteomics, and metabolomics/lipidomics data** using an **integrative workflow** that includes advanced algorithms for **multi-omics integration**, while addressing key challenges associated with untargeted metabolomics data.

Data Formats

TurbOmics uses a structured data frame system composed of three types of tables that should be provided in TSV format :

i. **Experimental metadata** (*e.g.* treatment, sex, time);

ii. **Omics metadata** (*e.g. ChEBI ID, gene names,* annotations, RT, categories)

iii. **Omics quantification** (abundancies or concentrations).

Expected Results

TurbOmics enables users to **map biomolecules** from different omics layer, **facilitating biological interpretation of multiomics results**. Users can explore and export data tables and visualize plots as results of:

i. Exploratory Analysis

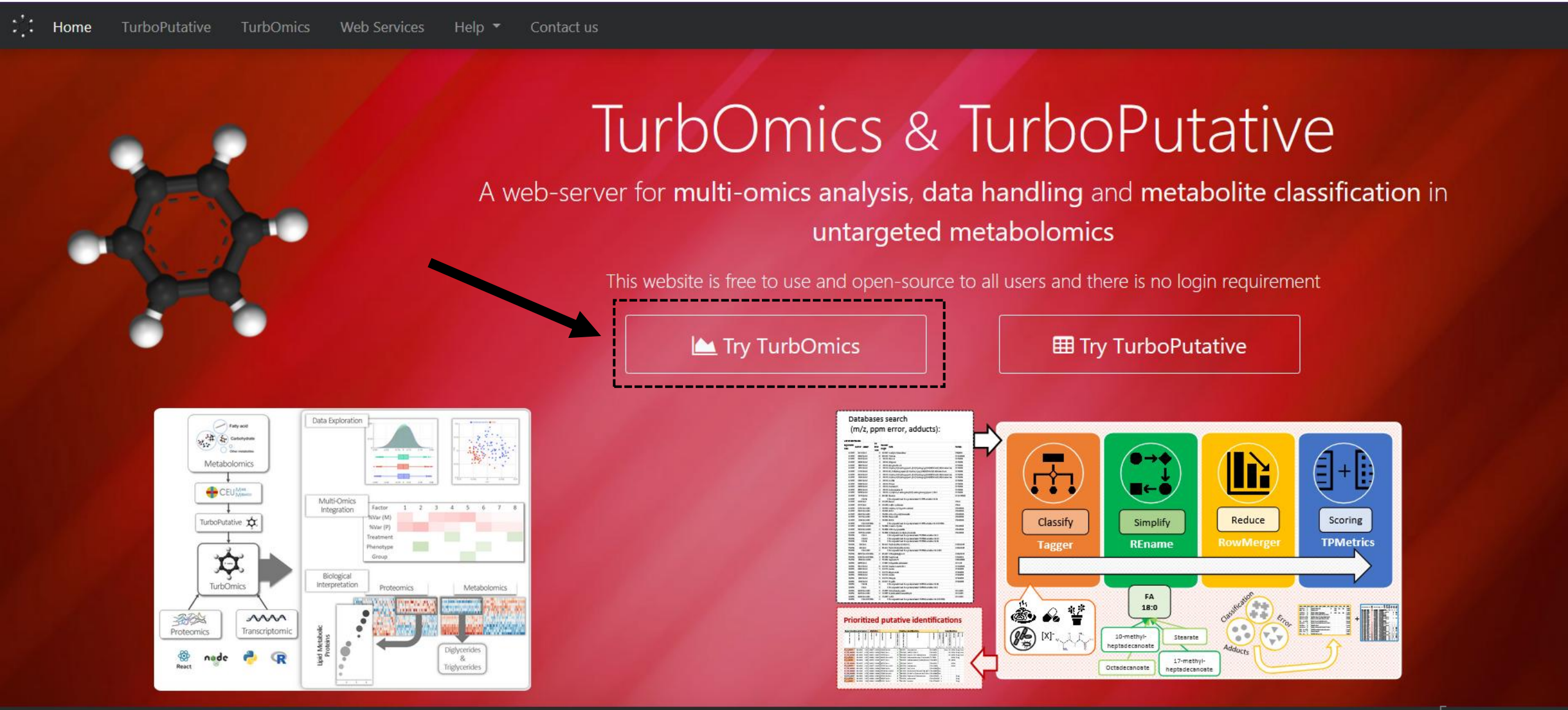
ii. MOFA

iii. Pathway Integrative Analysis

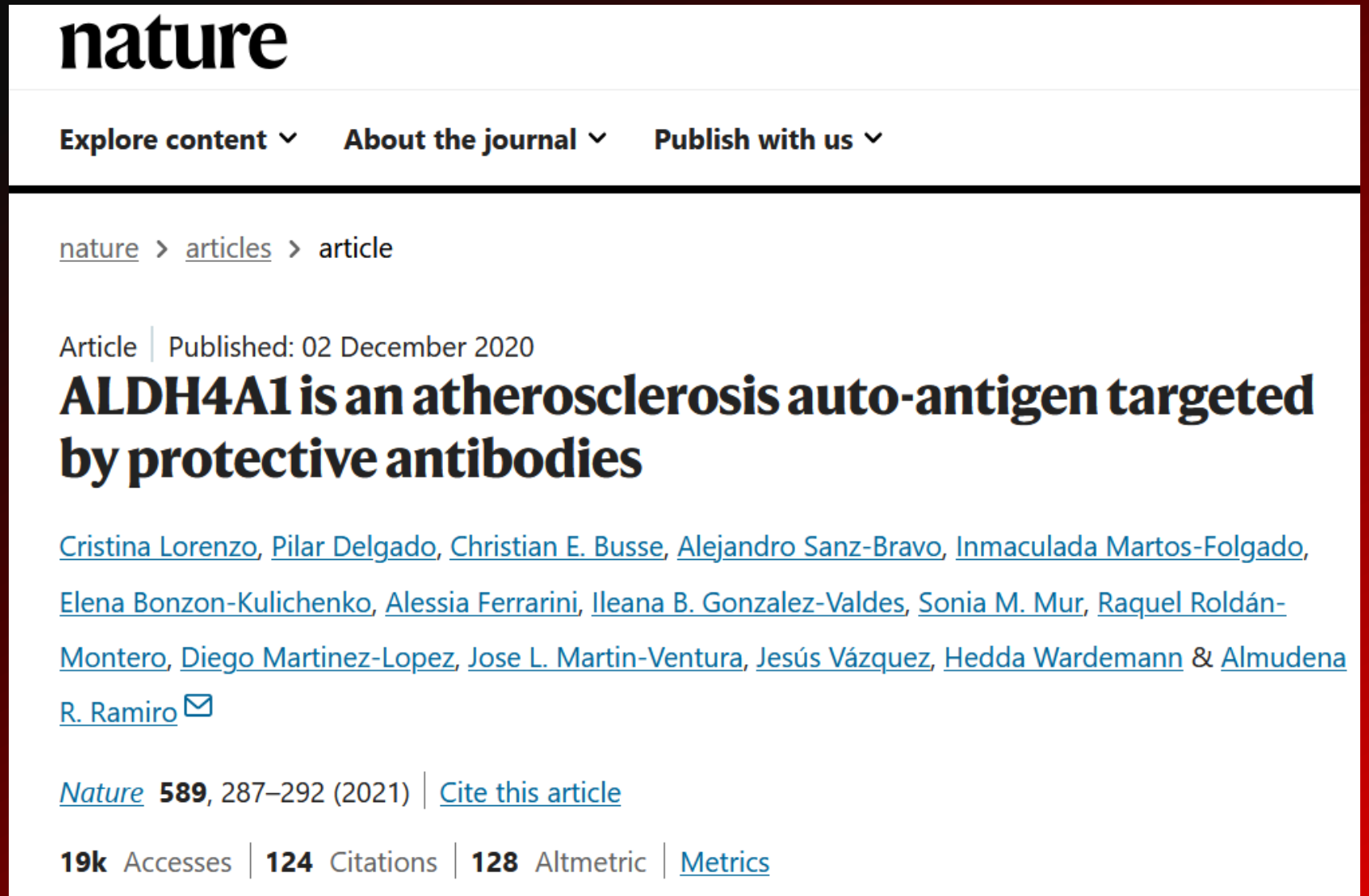
iv. Enrichment Analysis

Try TurbOmics

GO to https://proteomics.cnic.es/TurboPutative/home



Application to multi-omics datasets including untargeted lipidomics data



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Cristina Lorenzo, Pilar Delgado, Christian E. Busse, Alejandro Sanz-Bravo, Inmaculada Martos-Folgado, Elena Bonzon-Kulichenko, Alessia Ferrarini, Ileana B. Gonzalez-Valdes, Sonia M. Mur, Raquel Roldán-Montero, Diego Martinez-Lopez, Jose L. Martin-Ventura, Jesús Vázquez, Hedda Wardemann & Almudena R. Ramiro

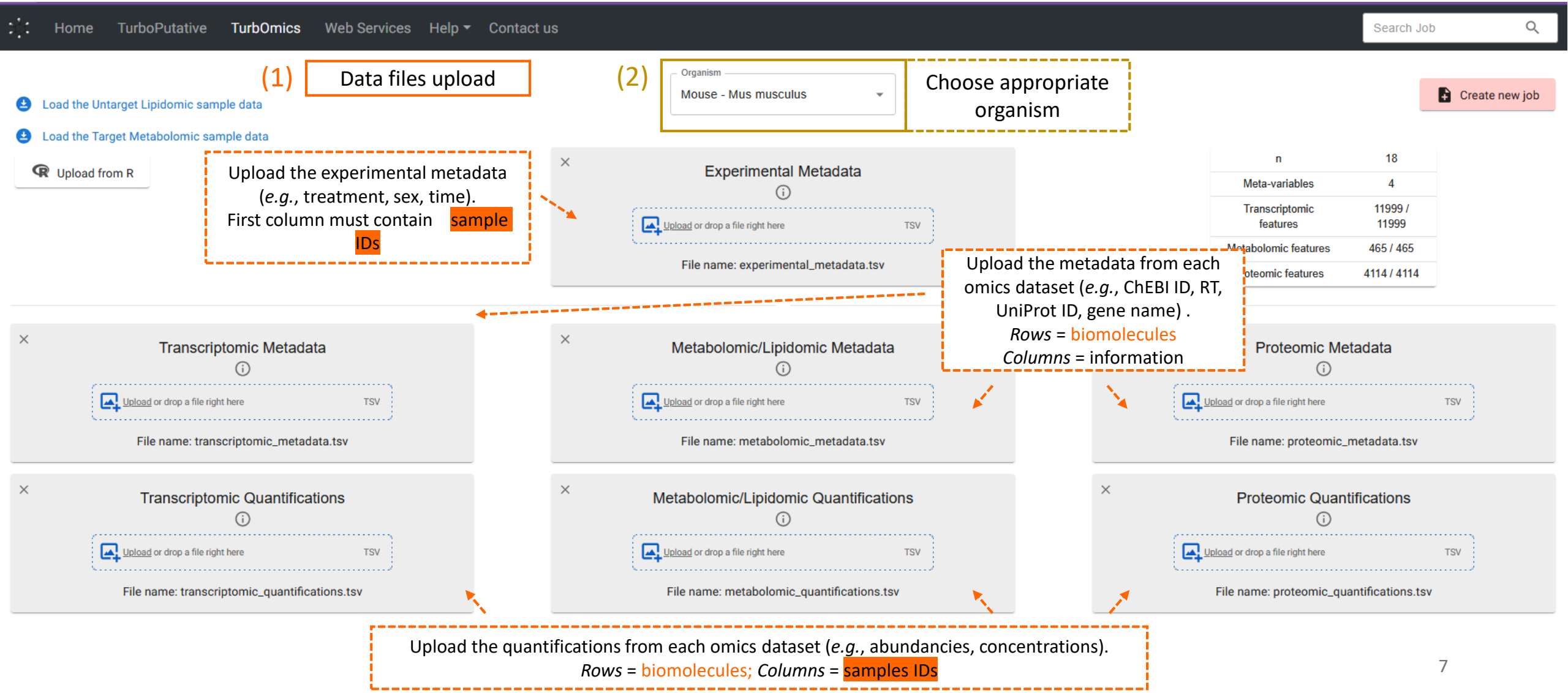
Nature **589**, 287–292 (2021) | Cite this article

19k Accesses | **124** Citations | **128** Altmetric | Metrics

- UNTARGTED LIPIDOMICS
- PROTEOMICS
- TRANSCRIPTOMICS

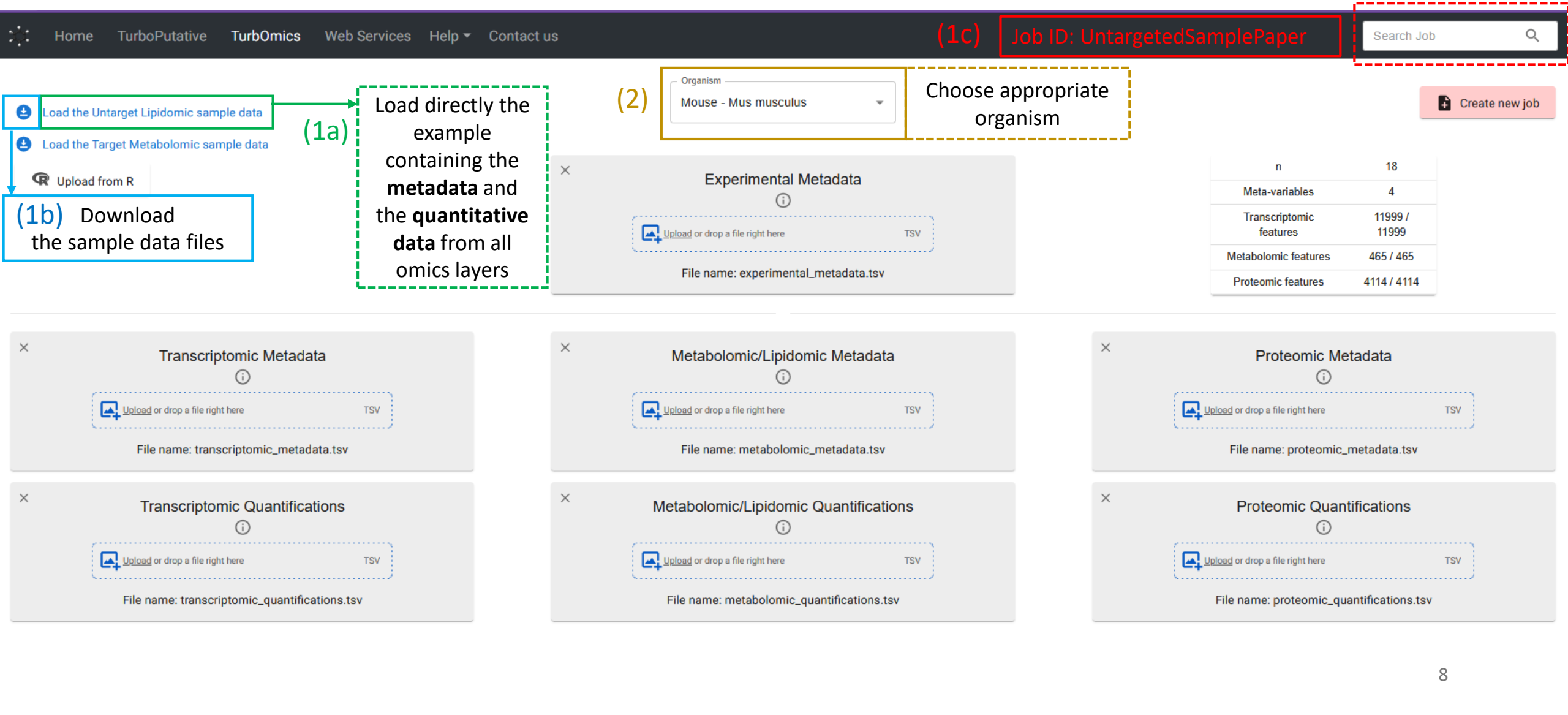
i. New data upload

To get started, users can upload their experimental data directly from the **Main Page**. Previous analyses can be accessed using the **Find Job** field by entering the corresponding job ID. Once a dataset is loaded, the **Results** section provides access to a suite of tools for in-depth analysis and interpretation.

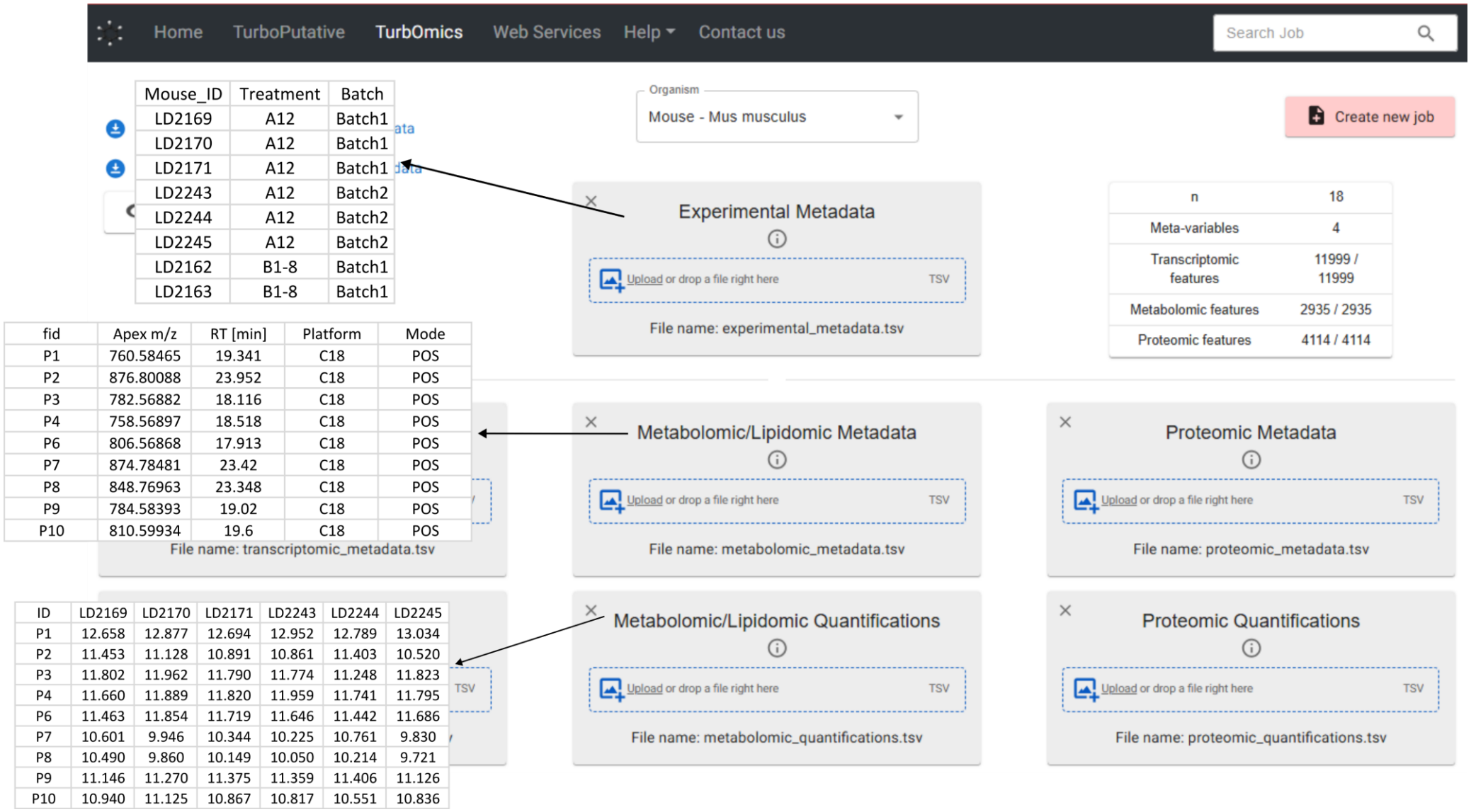


ii. Load example dataset

To get started, users can upload their experimental data directly from the **Main Page**. Previous analyses can be accessed using the **Find Job** field by entering the corresponding job ID. Once a dataset is loaded, the **Results** section provides access to a suite of tools for in-depth analysis and interpretation.



Example of uploaded untargeted lipidomics dataset by TSV format



Mouse_ID	Treatment	Batch
LD2169	A12	Batch1
LD2170	A12	Batch1
LD2171	A12	Batch1
LD2243	A12	Batch2
LD2244	A12	Batch2
LD2245	A12	Batch2
LD2162	B1-8	Batch1
LD2163	B1-8	Batch1

n	18
Meta-variables	4
Transcriptomic features	11999 / 11999
Metabolomic features	2935 / 2935
Proteomic features	4114 / 4114

fid	Apex m/z	RT [min]	Platform	Mode
P1	760.58465	19.341	C18	POS
P2	876.80088	23.952	C18	POS
P3	782.56882	18.116	C18	POS
P4	758.56897	18.518	C18	POS
P6	806.56868	17.913	C18	POS
P7	874.78481	23.42	C18	POS
P8	848.76963	23.348	C18	POS
P9	784.58393	19.02	C18	POS
P10	810.59934	19.6	C18	POS

ID	LD2169	LD2170	LD2171	LD2243	LD2244	LD2245
P1	12.658	12.877	12.694	12.952	12.789	13.034
P2	11.453	11.128	10.891	10.861	11.403	10.520
P3	11.802	11.962	11.790	11.774	11.248	11.823
P4	11.660	11.889	11.820	11.959	11.741	11.795
P6	11.463	11.854	11.719	11.646	11.442	11.686
P7	10.601	9.946	10.344	10.225	10.761	9.830
P8	10.490	9.860	10.149	10.050	10.214	9.721
P9	11.146	11.270	11.375	11.359	11.406	11.126
P10	10.940	11.125	10.867	10.817	10.551	10.836

Data format for the three uploaded tables

The consistency and linkage between these tables rely on matching identifiers. Therefore, it is essential that:

- The sample identifiers in the first column of the experimental metadata table match the column headers (i.e., the first row) of the omic quantification tables.
- The biomolecule identifiers in the first column of both the omics metadata and omics quantification tables match exactly.

Experimental Metadata

Sample_ID	Condition	Treatment	Batch
S001	Control	None	Batch1
S002	Control	None	Batch1
S003	Control	None	Batch2
S004	Control	None	Batch2
S005	Control	Drug_A	Batch1
S006	Control	Drug_A	Batch1
S007	Control	Drug_A	Batch2
S008	Control	Drug_A	Batch2
S009	Control	Drug_B	Batch1
S010	Control	Drug_B	Batch1
S011	Control	Drug_B	Batch2
S012	Control	Drug_B	Batch2
S013	Disease	None	Batch1
S014	Disease	None	Batch1
S015	Disease	None	Batch2
S016	Disease	None	Batch2
S017	Disease	Drug_A	Batch1
S018	Disease	Drug_A	Batch1
S019	Disease	Drug_A	Batch2
S020	Disease	Drug_A	Batch2
S021	Disease	Drug_B	Batch1
S022	Disease	Drug_B	Batch1
S023	Disease	Drug_B	Batch2
S024	Disease	Drug_B	Batch2

Metabolomics Metadata

Metabolite_ID	Name	Biol_Function	Chemical_Class	ChEBI_ID	Pathway
HMDB0000122	Glucose	Energy metabolism	Carbohydrate	17234	Glycolysis
HMDB0000190	Lactate	Anaerobic metabolism	Organic acid	24996	Cori cycle
HMDB0000538	ATP	Cellular energy	Nucleotide	15422	Oxidative Phospho.
⋮	⋮	⋮	⋮	⋮	⋮
HMDB0000259	Serotonin				
HMDB0000562	Creatinine				
HMDB0000243	Pyruvate				

Metabolomics Quantification

Metabolite_ID	S001	S002	S003	...	S010	S011	S012
HMDB0000122	5.3	6.1	5.8	...	5.9	5.4	4.8
HMDB0000190	10.5	11.2	9.9	...	10.9	10.3	9.5
HMDB0000538	7.9	8.4	7.5	...	7.8	7.1	6.8
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
HMDB0000259	25.7	26.3	24.9	...	25.4	24.1	23.3
HMDB0000562	6.8	7.2	6.5	...	6.7	6.3	5.8
HMDB0000243	3.2	3.8	3.1	...	3.5	3.2	2.8

Transcriptomics Metadata

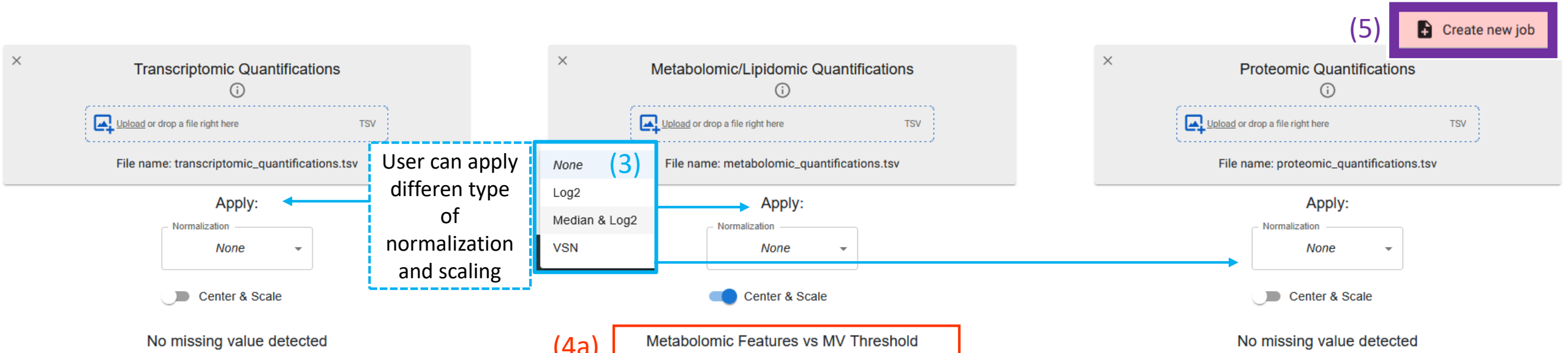
Transcript_ID	Gene_Name	Biol_Function	Chromosome	Pathway_Association
ENST00000269305	TP53	Tumor suppression	17	p53 signaling
ENST00000352993	BRCA1	DNA repair	17	Homologous recomb.
ENST00000229239	GAPDH	Glycolysis	12	Metabolism
⋮	⋮			⋮
ENST00000324450	VEGF			
ENST00000377970	MYC			
ENST00000361624	MT-C			

Transcriptomics Quantification

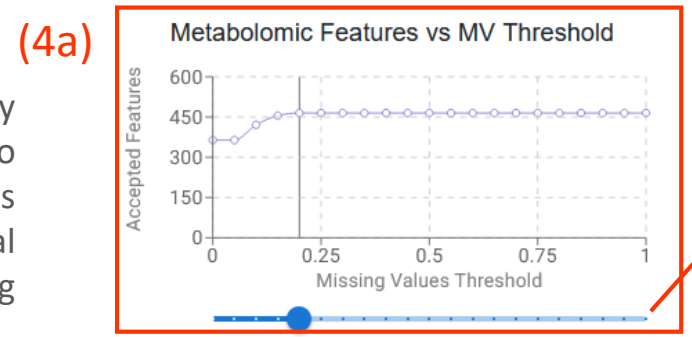
Transcript_ID	S001	S002	S003	...	S010	S011	S012
ENST00000269305	12.3	14.2	11.8	...	12.8	11.9	10.7
ENST00000352993	8.7	9.1	8.5	...	8.4	7.9	7.2
ENST00000229239	20.4	21.2	19.8	...	19.5	18.6	17.3
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
ENST00000324450	10.5	11.2	9.9	...	10.3	9.5	8.7
ENST00000377970	7.9	8.4	7.5	...	7.1	6.8	6
ENST00000361624	25.7	26.3	24.9	...	24.1	23.3	22

iii. Normalization, scaling and Missing values Imputation

- **Normalization techniques** are used to correct for systemic and technical variations that can obscure biological signals and lead to misleading conclusions.
- Different omics datasets often exhibit varying value ranges due to differences in technological platforms and the normalization methods applied during data generation. These disparities can be addressed **standardizing** omics data by setting the mean of each biomolecule to 0 and the standard deviation to 1.
- Once these parameters are set, the user can launch the analysis > create new job



- TurbOmics handles **missing values** independently for each omic type. This design allows users to apply different filtering and imputation methods tailored to the technical and methodological characteristics of each omics dataset, increasing the flexibility and robustness of the workflow.



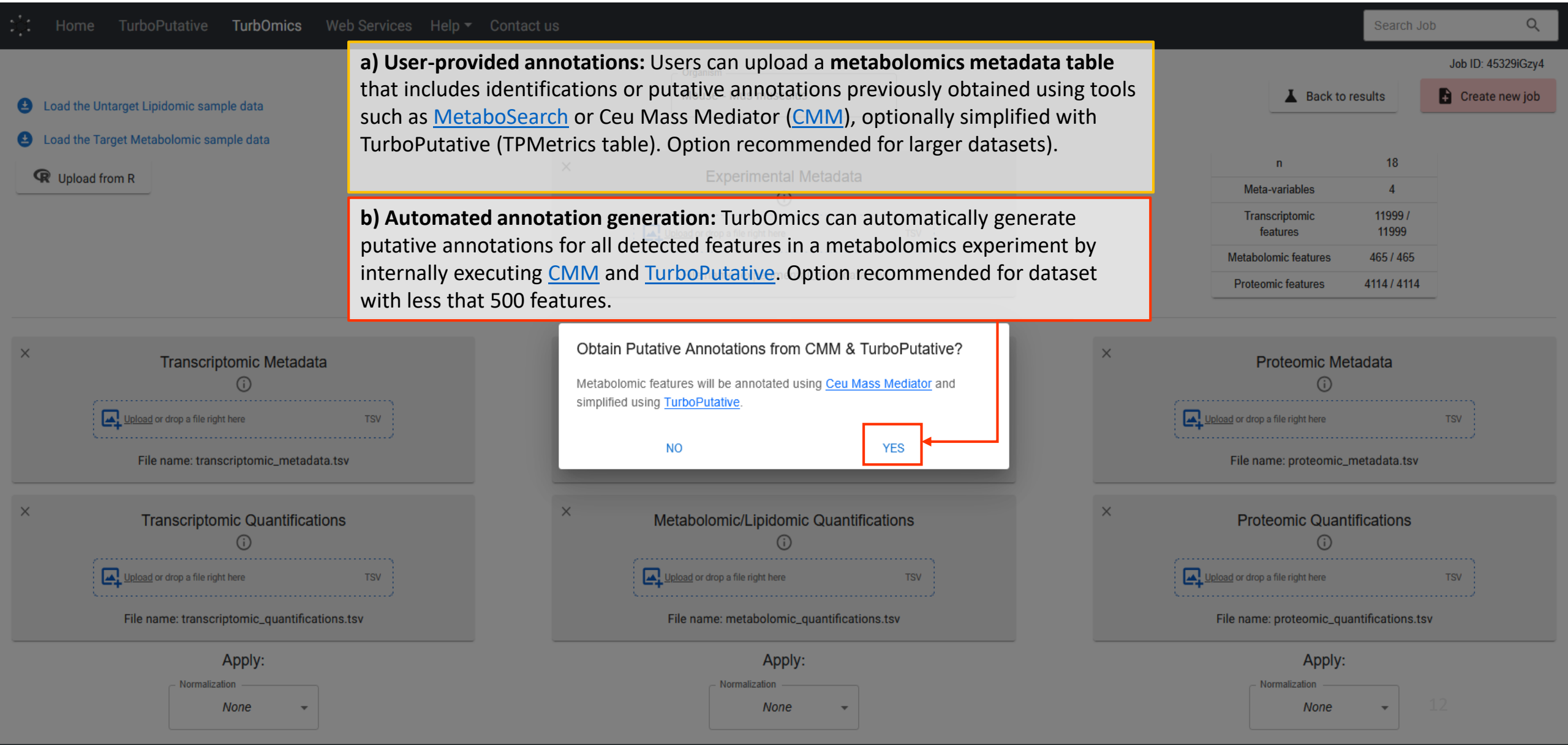
Users can interactively adjust this threshold and observe in real time how many biomolecules are retained.

KNN
Minimum
Mean
Median

Choose from several imputation techniques to handle missing values in the remaining biomolecules

Putative Annotation

TurbOmics provides two alternative approaches for handling putative annotations of metabolite:



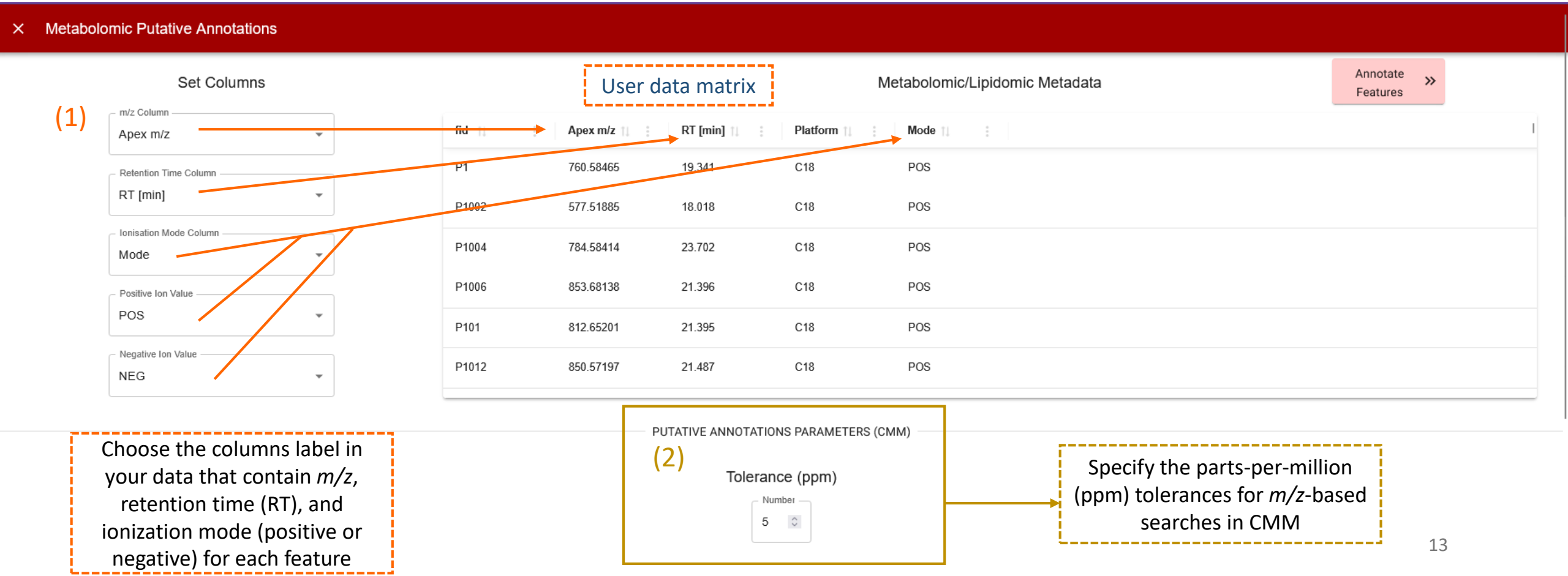
a) User-provided annotations: Users can upload a **metabolomics metadata table** that includes identifications or putative annotations previously obtained using tools such as MetaboSearch or Ceu Mass Mediator (CMM), optionally simplified with TurboPutative (TPMetrics table). Option recommended for larger datasets).

b) Automated annotation generation: TurbOmics can automatically generate putative annotations for all detected features in a metabolomics experiment by internally executing CMM and TurboPutative. Option recommended for dataset with less that 500 features.

Putative Annotation

To enable automated annotation, users must upload a metadata table containing the ***m/z*, retention time (RT), and ionization mode** (positive or negative) for each feature.
CMM compares the *m/z* values of detected features against in-house libraries and external databases such as HMDB, LipidMaps, METLIN, and KEGG.
The resulting candidate annotations are then processed by the four modules of TurboPutative: **Tagger**, **REname**, **RowMerger**, and **TPMetrics**. The final output, **TPFilter**, provides the most likely annotation for each feature and is integrated with the user-supplied metabolomics/lipidomics metadata table.

i. Upload the metabolomics/lipidomics metadata table

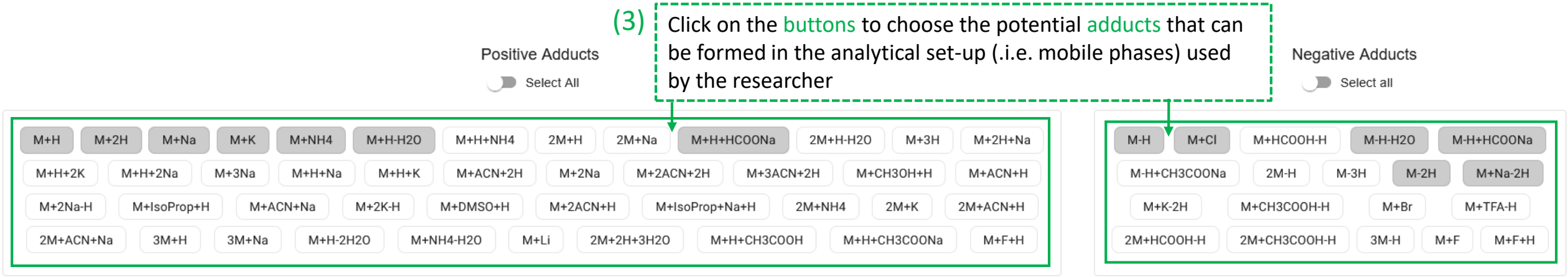


Choose the columns label in your data that contain *m/z*, retention time (RT), and ionization mode (positive or negative) for each feature

Specify the parts-per-million (ppm) tolerances for *m/z*-based searches in CMM

Putative Annotation

ii. Select potential adducts for both positive and negative ionization modes



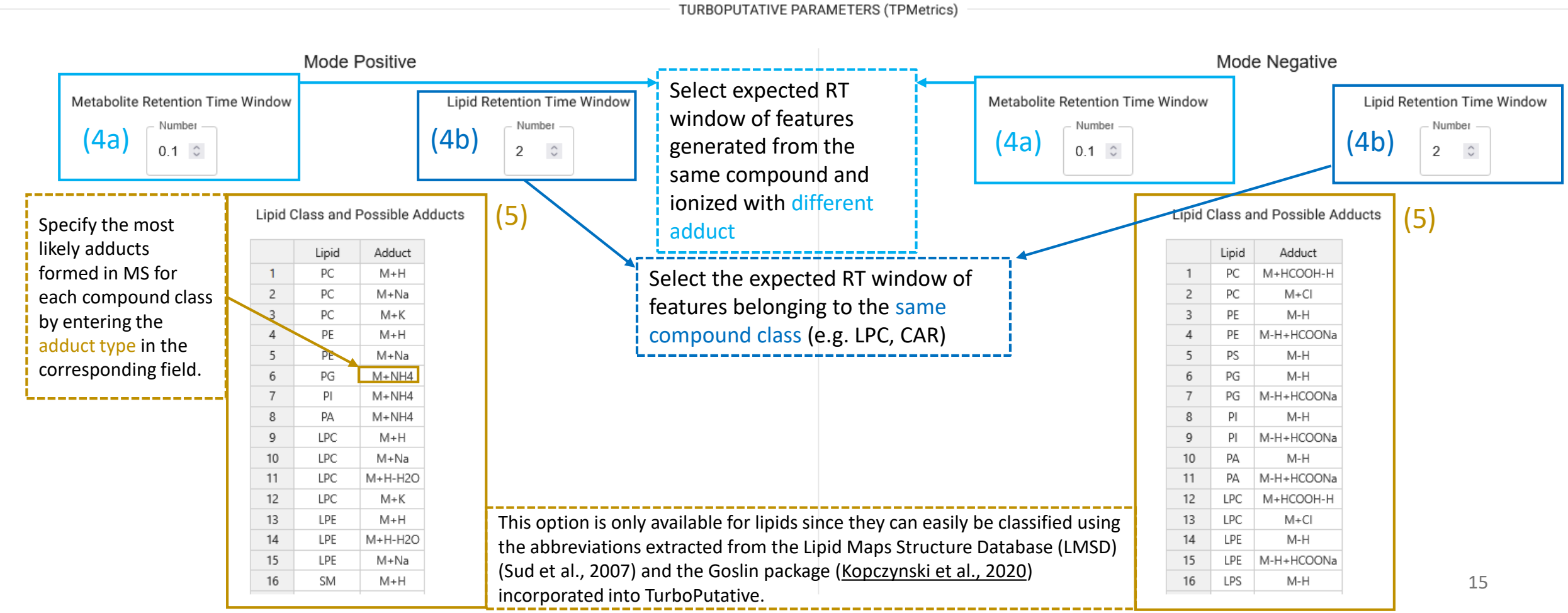
Putative Annotations

iii. Select TPMetric parameters (Turboputative)

(6) Annotate Features »

RT is used by the TPMetrics module to prioritize annotations based on correlation analyses between features.
These criteria are based on the concept that signals coming from the same molecular entity and those sharing the same biochemical class show a common elution behavior in the LC-MS and a similar correlation pattern across the samples.

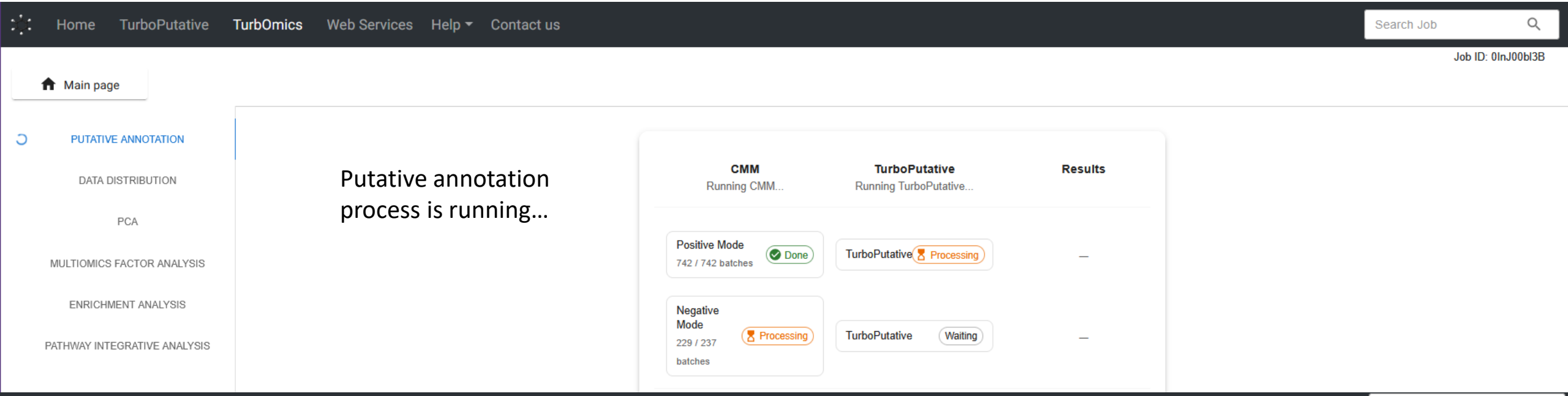
- Once these parameters are set, the user can launch the analysis > annotate features



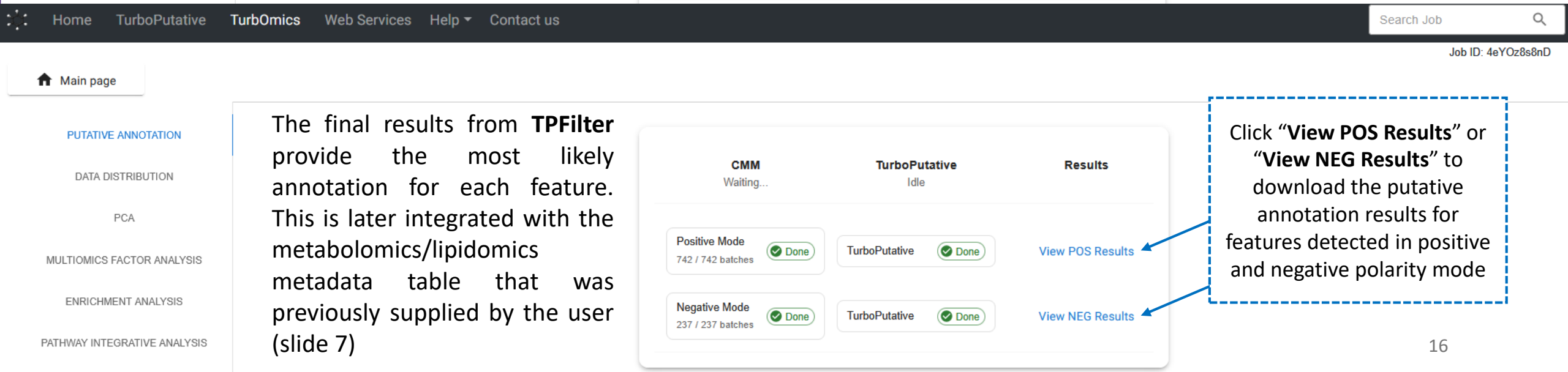
	Lipid	Adduct
1	PC	M+H
2	PC	M+Na
3	PC	M+K
4	PE	M+H
5	PE	M+Na
6	PG	M+NH4
7	PI	M+NH4
8	PA	M+NH4
9	LPC	M+H
10	LPC	M+Na
11	LPC	M+H-H2O
12	LPC	M+K
13	LPE	M+H
14	LPE	M+H-H2O
15	LPE	M+Na
16	SM	M+H

	Lipid	Adduct
1	PC	M+HCOOH-H
2	PC	M+Cl
3	PE	M-H
4	PE	M-H+HCOONa
5	PS	M-H
6	PG	M-H
7	PG	M-H+HCOONa
8	PI	M-H
9	PI	M-H+HCOONa
10	PA	M-H
11	PA	M-H+HCOONa
12	LPC	M+HCOOH-H
13	LPC	M+Cl
14	LPE	M-H
15	LPE	M-H+HCOONa
16	LPS	M-H

Putative Annotation



Putative annotation process is running…

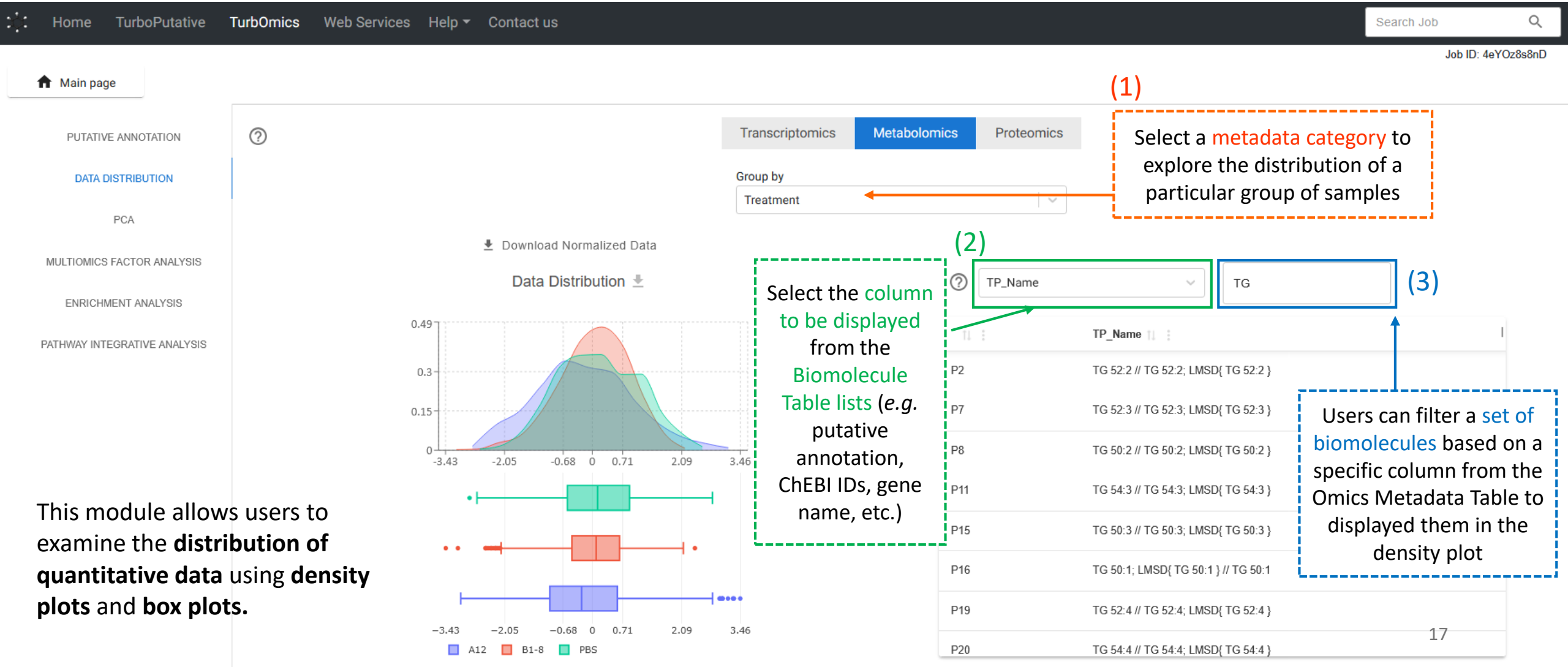


The final results from **TPFilter** provide the most likely annotation for each feature. This is later integrated with the metabolomics/lipidomics metadata table that was previously supplied by the user (slide 7)

Click "**View POS Results**" or "**View NEG Results**" to download the putative annotation results for features detected in positive and negative polarity mode

Exploratory data analysis: Data Distribution

The Exploratory Data Analysis module provides researchers with an **initial overview and visualization of the data uploaded to the platform**.
In TurbOmics, exploratory analysis is conducted independently for each omics dataset.
To support this process, the platform includes two dedicated modules: Data Distribution and Principal Component Analysis (PCA).



This module allows users to examine the **distribution of quantitative data** using **density plots** and **box plots.**

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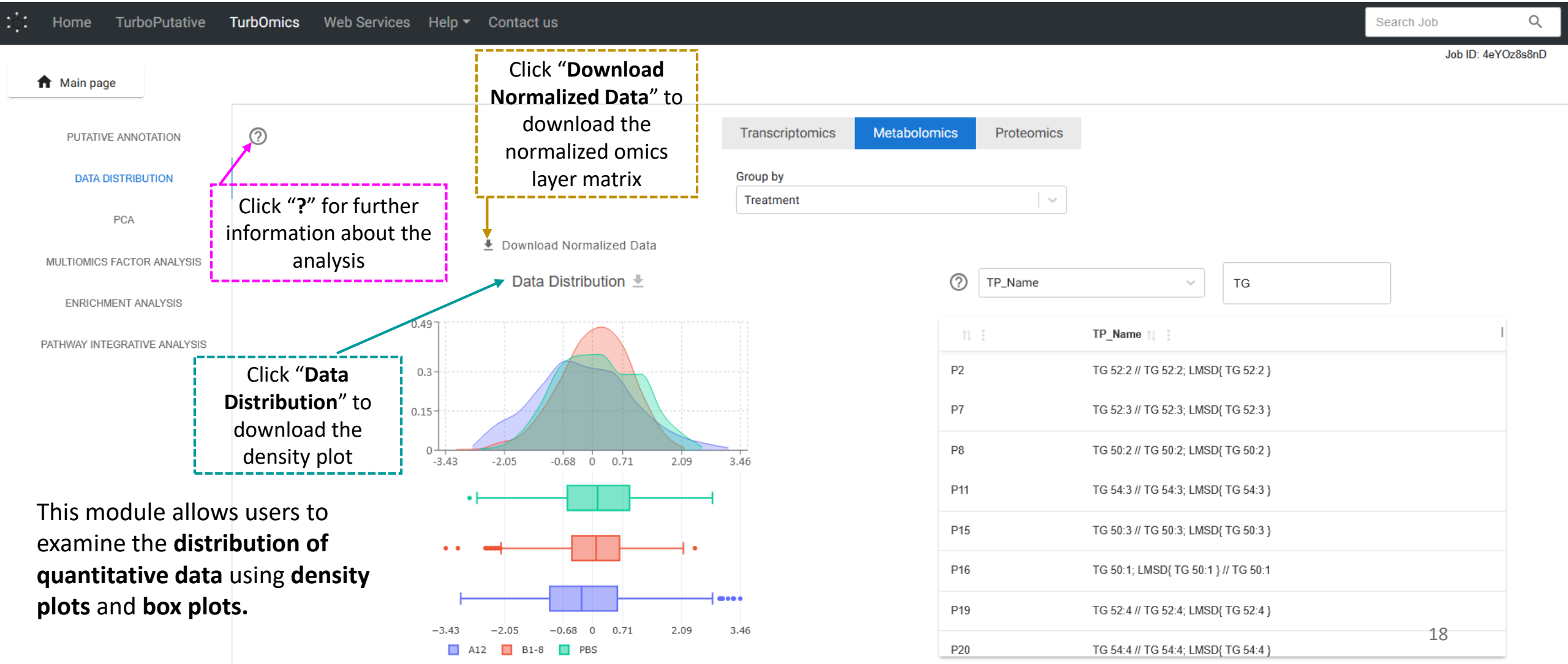


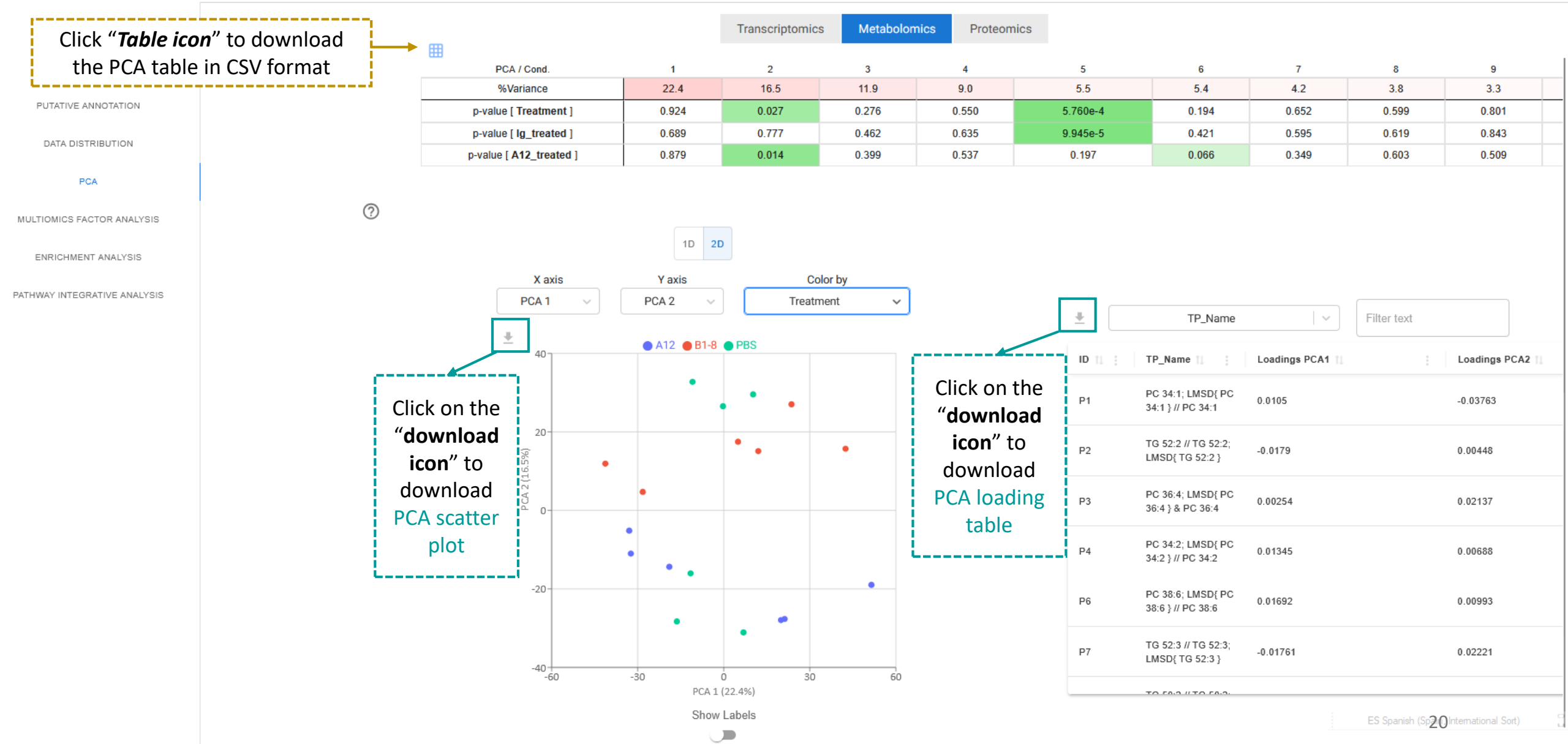
This module allows users to examine the **distribution of quantitative data** using **density plots** and **box plots.**

Exploratory data analysis: Principal Component Analysis (PCA)

TurbOmics computes the first ten principal components (PCs) and calculates correlations between the component scores and metadata variables. The percentage of variance explained by each component, along with the p-values from the correlations, is shown in a color-coded table, allowing users to quickly identify associations between quantitative data and metadata.

Exploratory data analysis: Principal Component Analysis (PCA)

Click "***Table icon***" to download the PCA table in CSV format



PCA / Cond.	1	2	3	4	5	6	7	8	9
%Variance	22.4	16.5	11.9	9.0	5.5	5.4	4.2	3.8	3.3
p-value [**Treatment**]	0.924	0.027	0.276	0.550	5.760e-4	0.194	0.652	0.599	0.801
p-value [**lg_treated**]	0.689	0.777	0.462	0.635	9.945e-5	0.421	0.595	0.619	0.843
p-value [**A12_treated**]	0.879	0.014	0.399	0.537	0.197	0.066	0.349	0.603	0.509

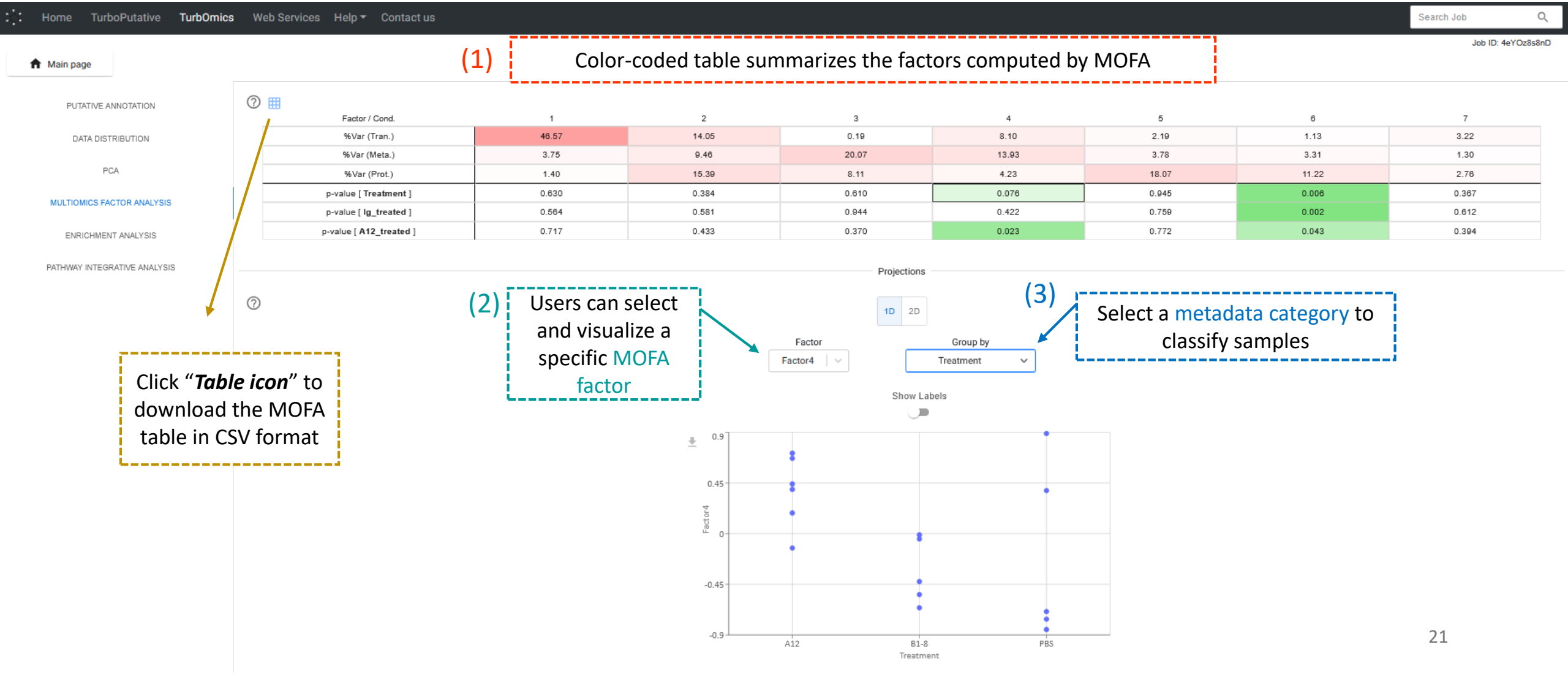
Click on the "**download icon**" to download PCA scatter plot

Click on the "**download icon**" to download PCA loading table

ID	TP_Name	Loadings PCA1	Loadings PCA2
P1	PC 34:1; LMSD{ PC 34:1 } // PC 34:1	0.0105	-0.03763
P2	TG 52:2 // TG 52:2; LMSD{ TG 52:2 }	-0.0179	0.00448
P3	PC 36:4; LMSD{ PC 36:4 } & PC 36:4	0.00254	0.02137
P4	PC 34:2; LMSD{ PC 34:2 } // PC 34:2	0.01345	0.00688
P6	PC 38:6; LMSD{ PC 38:6 } // PC 38:6	0.01692	0.00993
P7	TG 52:3 // TG 52:3; LMSD{ TG 52:3 }	-0.01761	0.02221

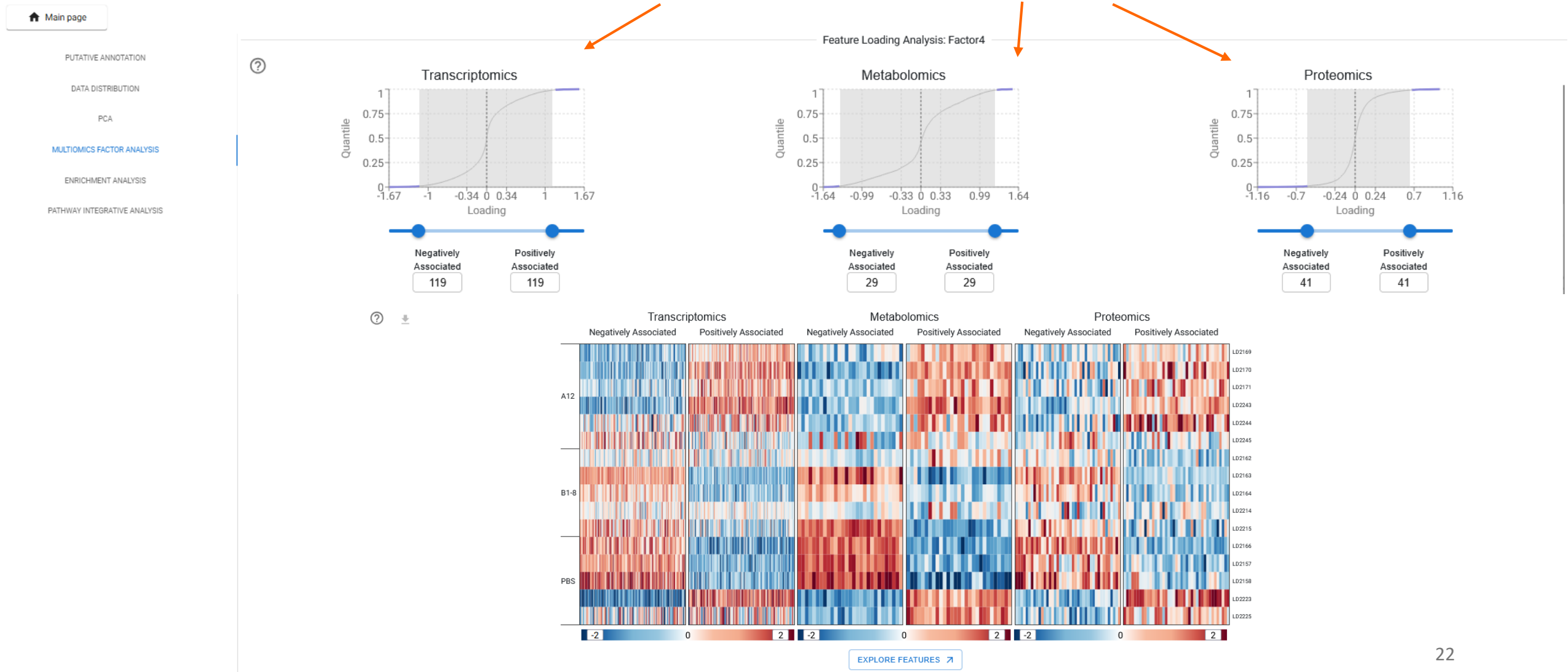
Multi-Omics Factor Analysis

The **Multi-Omics Factor Analysis** module enables the unbiased and integrative decomposition of multi-omics quantitative data into latent factors. This module is based on the MOFA framework, which identifies latent factors that capture the main sources of variation across the analyzed datasets. TurbOmics supports the visualization of sample subgroups and shared patterns across different omics layers.

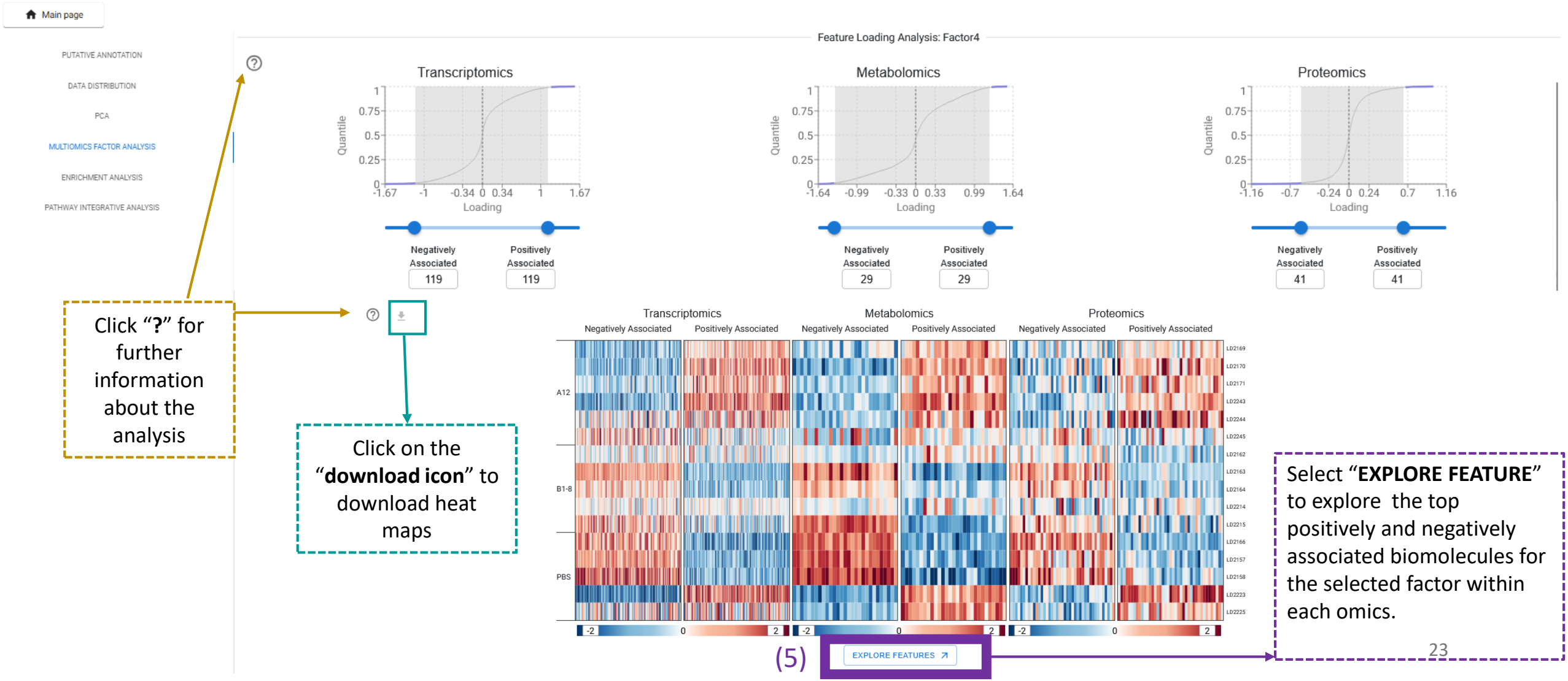


Multi-Omics Factor Analysis: Feature Loading Analysis

(4) Users can examine the distribution of factor loadings for each omics dataset and select the top-n biomolecules with the highest positive or negative loadings for visualization in a heatmap.

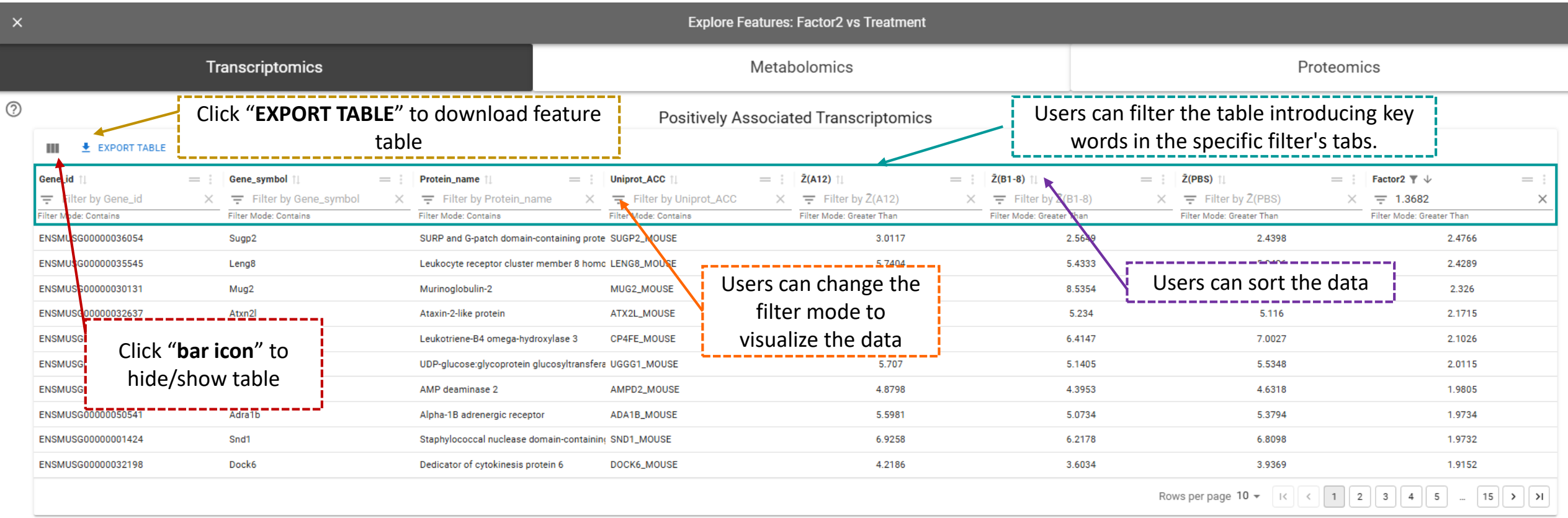


Multi-Omics Factor Analysis: Feature Loading Analysis



Multi-Omics Factor Analysis

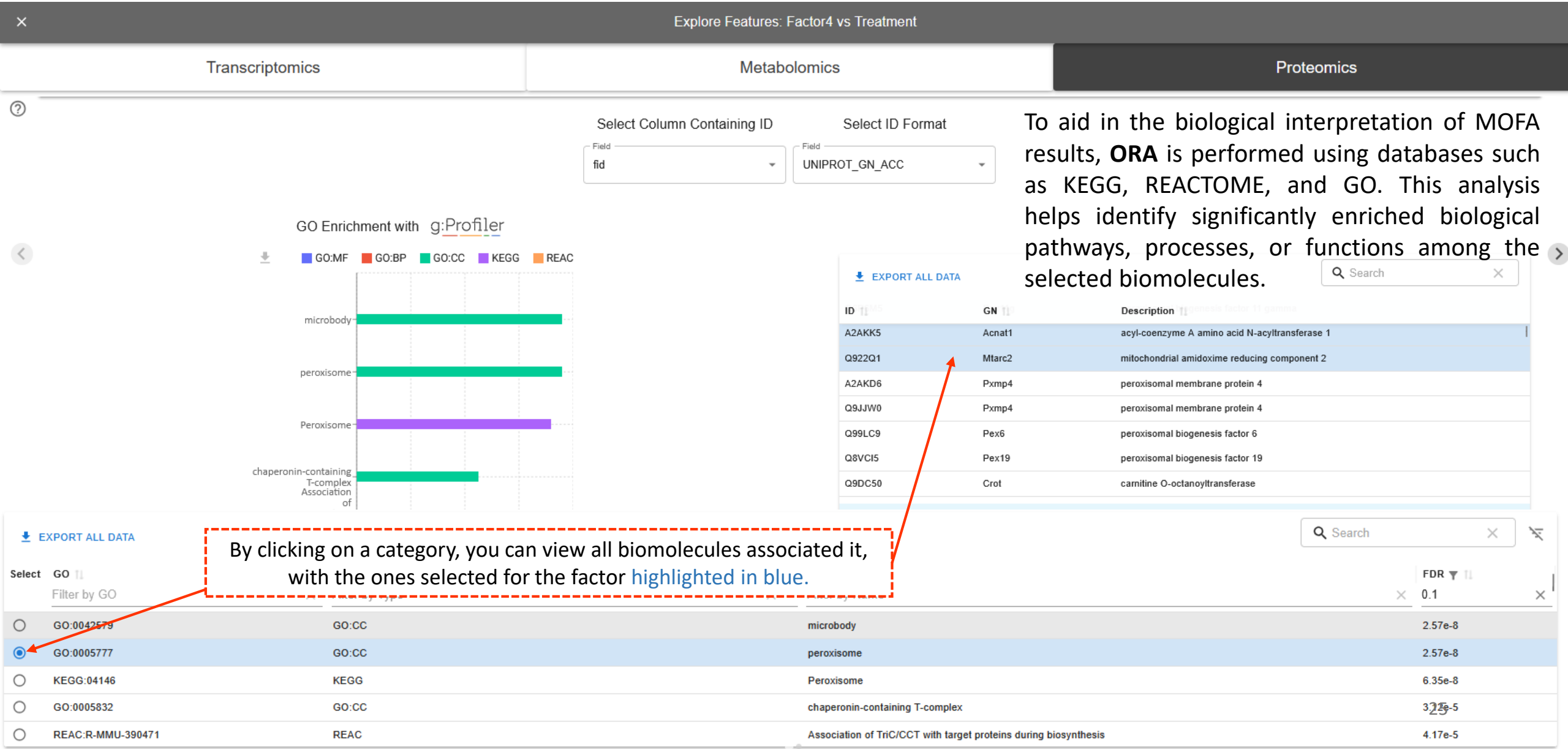
- Example of ORA (over-representation analysis) of the transcriptomics data within Factor 2 in MOFA



This table lists the selected biomolecules and provides additional context by displaying the average quantitative value of each biomolecule across different sample groups.

Multi-Omics Factor Analysis

➢ Example of ORA (over-representation analysis) of the proteomics data within Factor 4 in MOFA

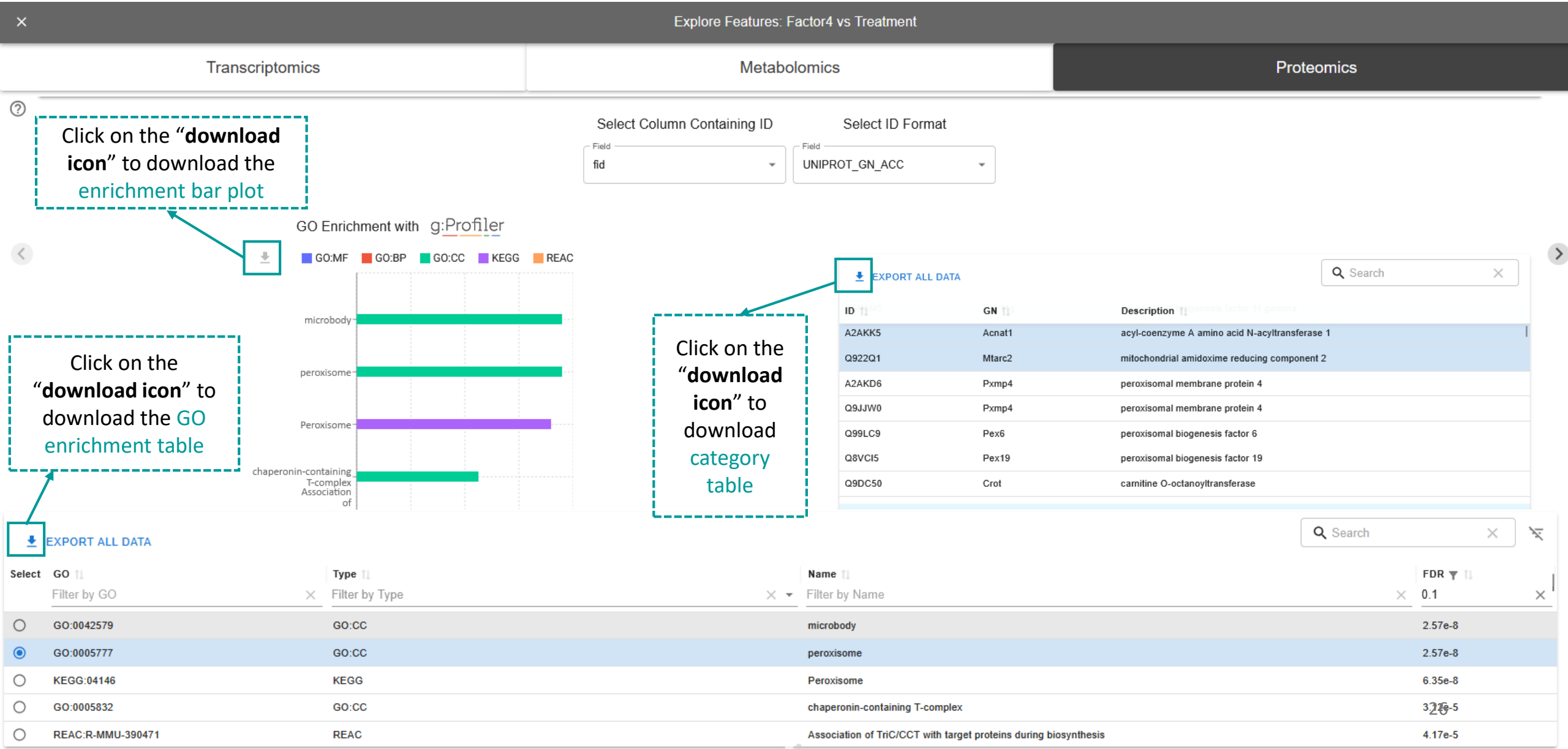


To aid in the biological interpretation of MOFA results, **ORA** is performed using databases such as KEGG, REACTOME, and GO. This analysis helps identify significantly enriched biological pathways, processes, or functions among the selected biomolecules.

By clicking on a category, you can view all biomolecules associated it, with the ones selected for the factor highlighted in blue.

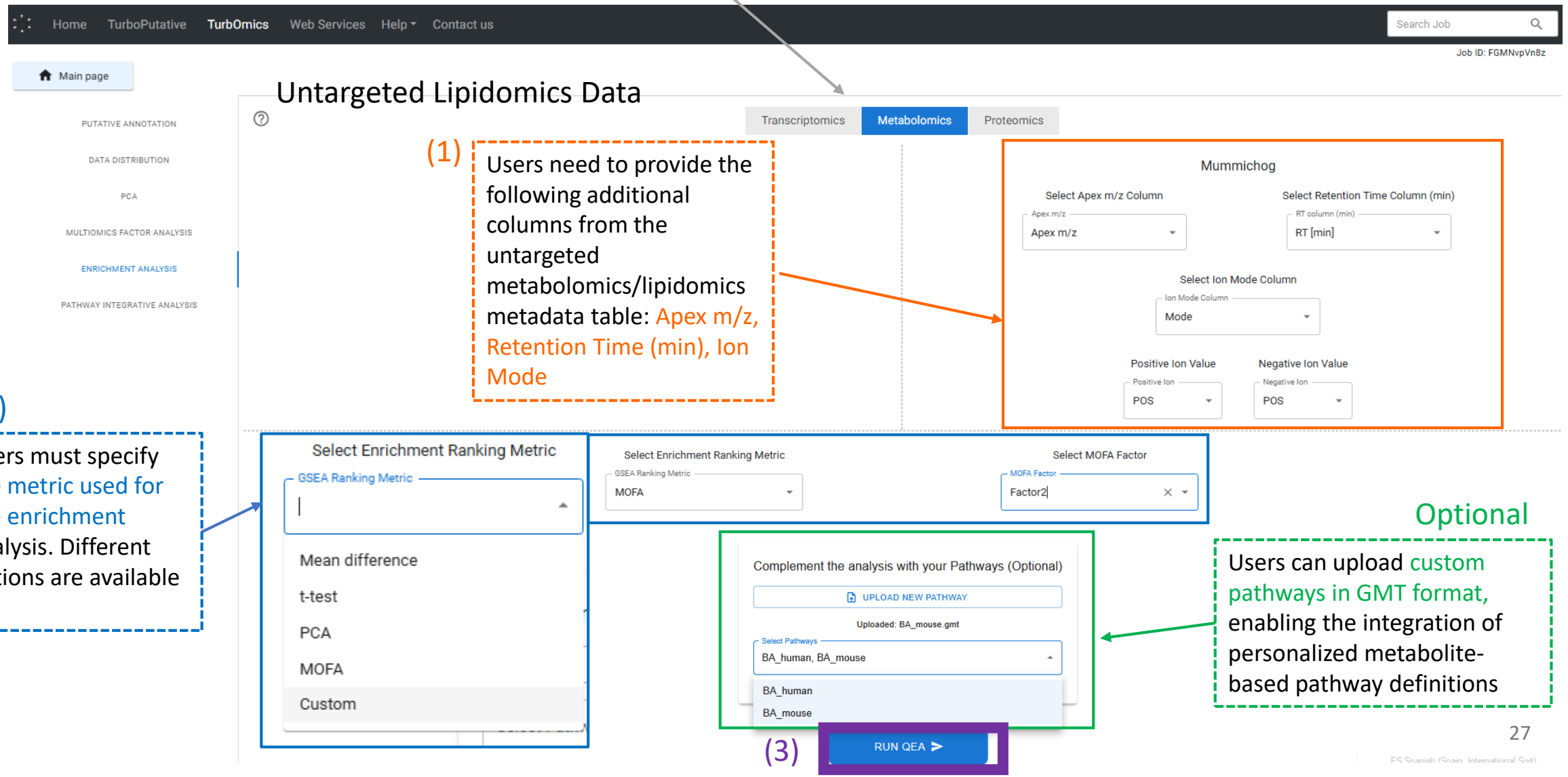
Multi-Omics Factor Analysis

➢ Example of ORA (over-representation analysis) of the proteomics data within Factor 4 in MOFA



Enrichment Analysis

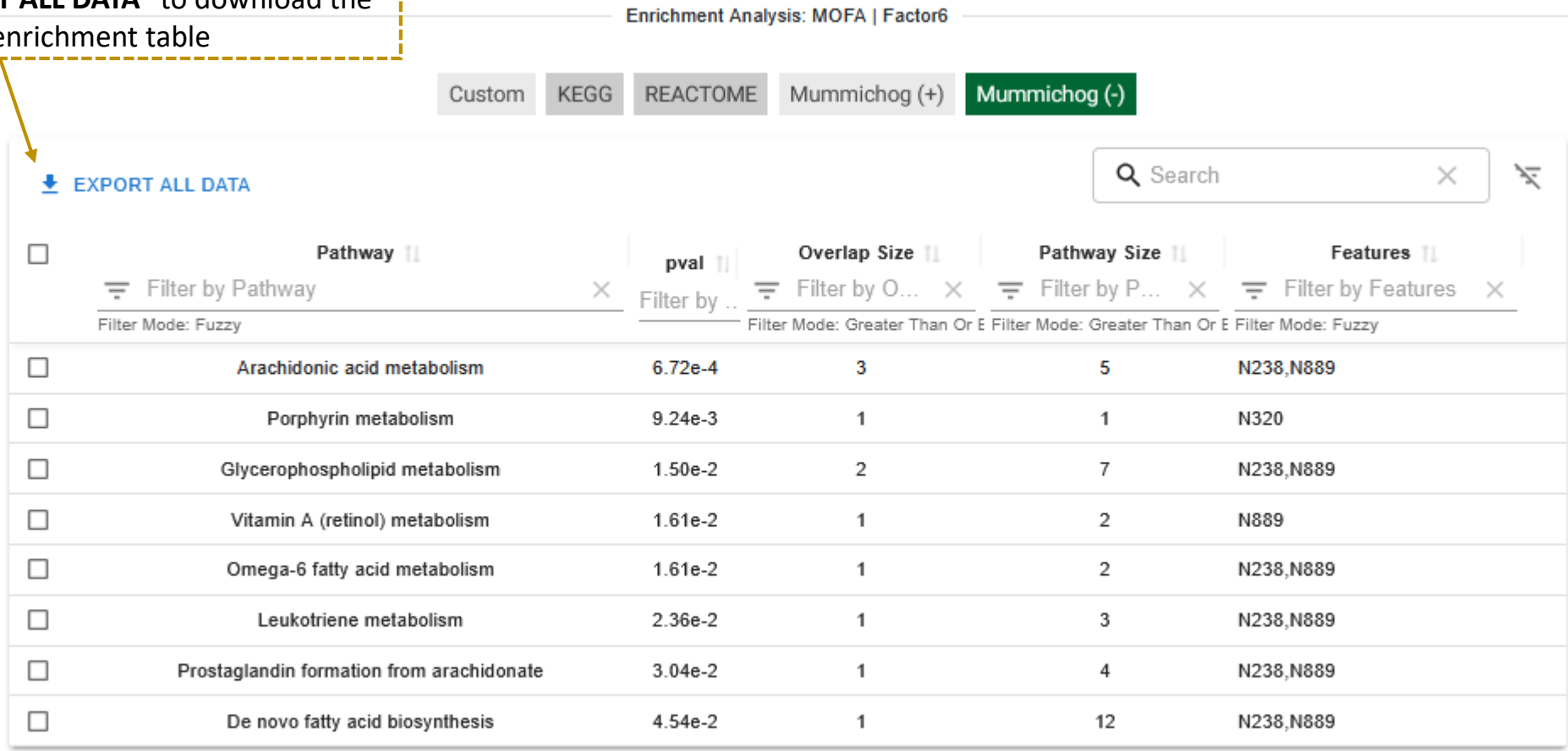
This module allows the user to perform Enrichment Analysis using the **Gene Set Enrichment Analysis (GSEA)** algorithm on each omics dataset independently. Users can switch between omics using the navigator bar at the top of the page to explore results for different data types.
If you are working with **untargeted metabolomics/lipidomics data**, you can choose to perform enrichment analysis using the **Mummichog algorithm**.



Enrichment Analysis: example using untargeted lipidomics data

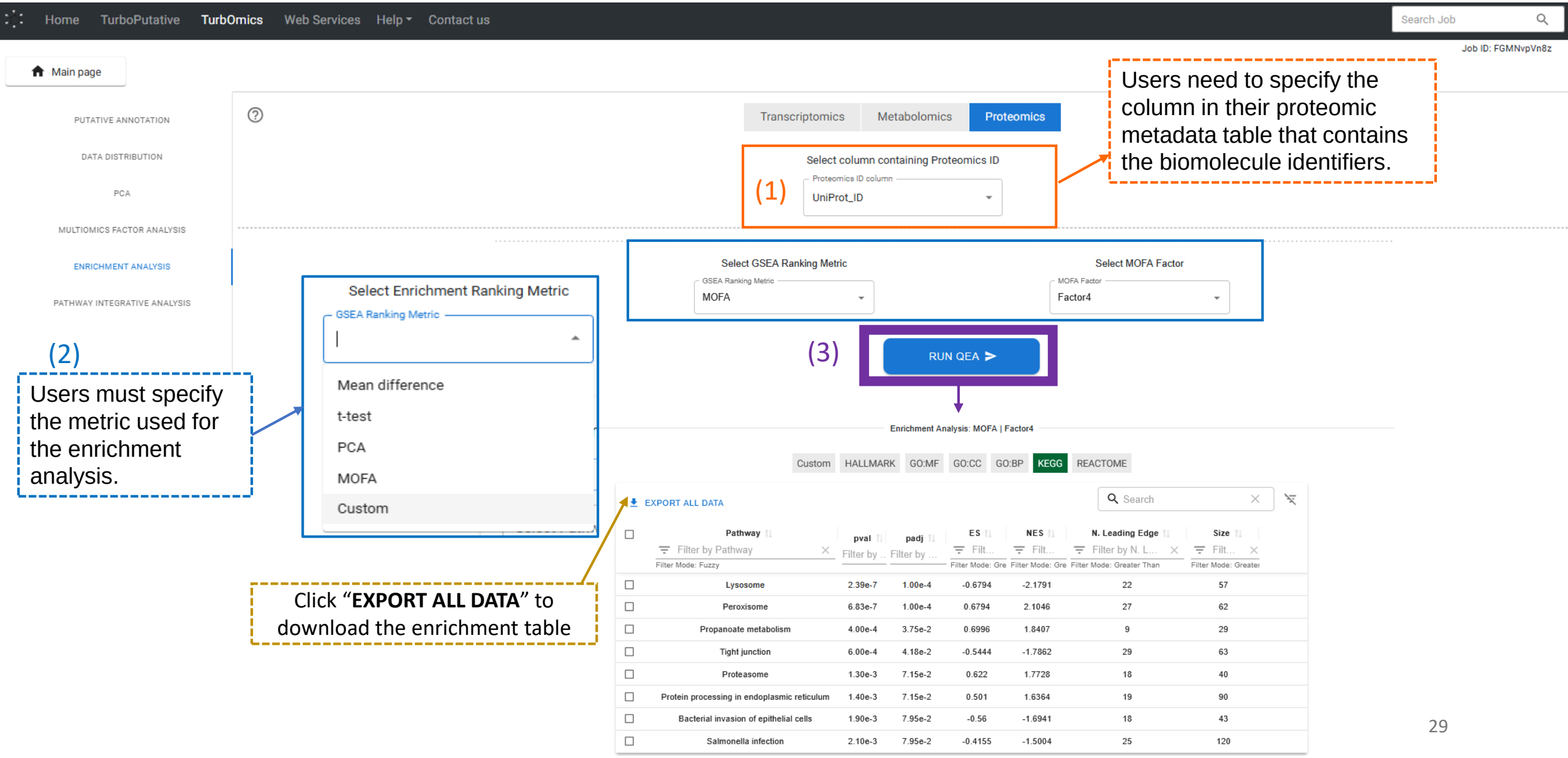
Results of the Enrichment Analysis can be explored, providing insights into the biological pathways, processes, or functions that are significantly associated with the conditions or experimental groups in the study.

Click "**EXPORT ALL DATA**" to download the enrichment table



Pathway	pval	Overlap Size	Pathway Size	Features
Arachidonic acid metabolism	6.72e-4	3	5	N238,N889
Porphyrin metabolism	9.24e-3	1	1	N320
Glycerophospholipid metabolism	1.50e-2	2	7	N238,N889
Vitamin A (retinol) metabolism	1.61e-2	1	2	N889
Omega-6 fatty acid metabolism	1.61e-2	1	2	N238,N889
Leukotriene metabolism	2.36e-2	1	3	N238,N889
Prostaglandin formation from arachidonate	3.04e-2	1	4	N238,N889
De novo fatty acid biosynthesis	4.54e-2	1	12	N238,N889

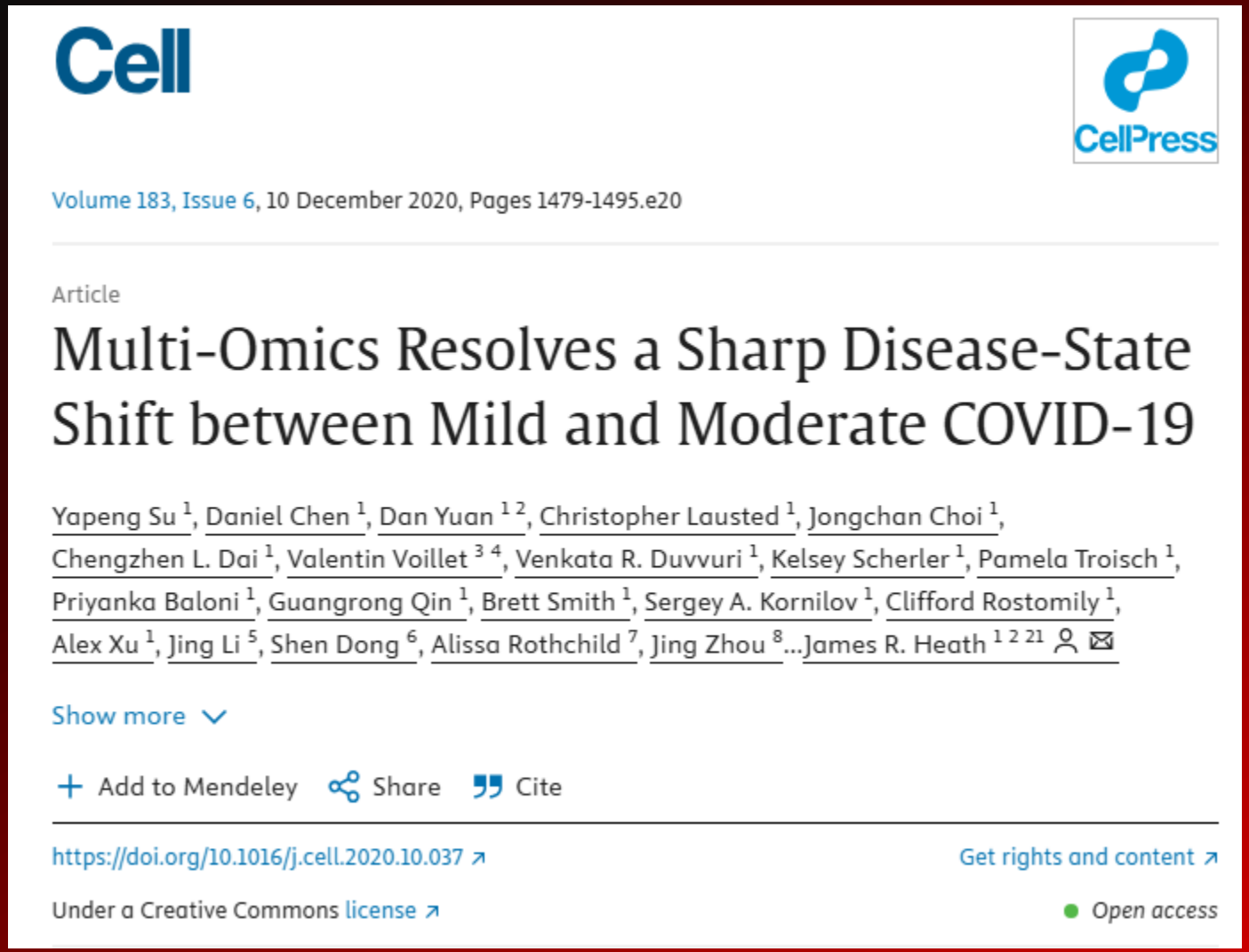
Enrichment Analysis: example using proteomics data



Pathway	pval	padj	ES	NES	N. Leading Edge	Size
Lysosome	2.39e-7	1.00e-4	-0.6794	-2.1791	22	57
Peroxisome	6.83e-7	1.00e-4	0.6794	2.1046	27	62
Propanoate metabolism	4.00e-4	3.75e-2	0.6996	1.8407	9	29
Tight junction	6.00e-4	4.18e-2	-0.5444	-1.7862	29	63
Proteasome	1.30e-3	7.15e-2	0.622	1.7728	18	40
Protein processing in endoplasmic reticulum	1.40e-3	7.15e-2	0.501	1.6364	19	90
Bacterial invasion of epithelial cells	1.90e-3	7.95e-2	-0.56	-1.6941	18	43
Salmonella infection	2.10e-3	7.95e-2	-0.4155	-1.5004	25	120

✓ For Pathway Integrative Analysis see slides 36-40 of the present tutorial

Application to multi-omics datasets in a COVID-19 study, including targeted metabolomics data



Cell

CellPress

Volume 183, Issue 6, 10 December 2020, Pages 1479-1495.e20

Article

Multi-Omics Resolves a Sharp Disease-State Shift between Mild and Moderate COVID-19

Yapeng Su [1], Daniel Chen [1], Dan Yuan [1 2], Christopher Lausted [1], Jongchan Choi [1], Chengzhen L. Dai [1], Valentin Voillet [3 4], Venkata R. Duvvuri [1], Kelsey Scherler [1], Pamela Troisch [1], Priyanka Baloni [1], Guangrong Qin [1], Brett Smith [1], Sergey A. Kornilov [1], Clifford Rostomily [1], Alex Xu [1], Jing Li [5], Shen Dong [6], Alissa Rothchild [7], Jing Zhou [8]...James R. Heath [1 2 21]

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https://doi.org/10.1016/j.cell.2020.10.037

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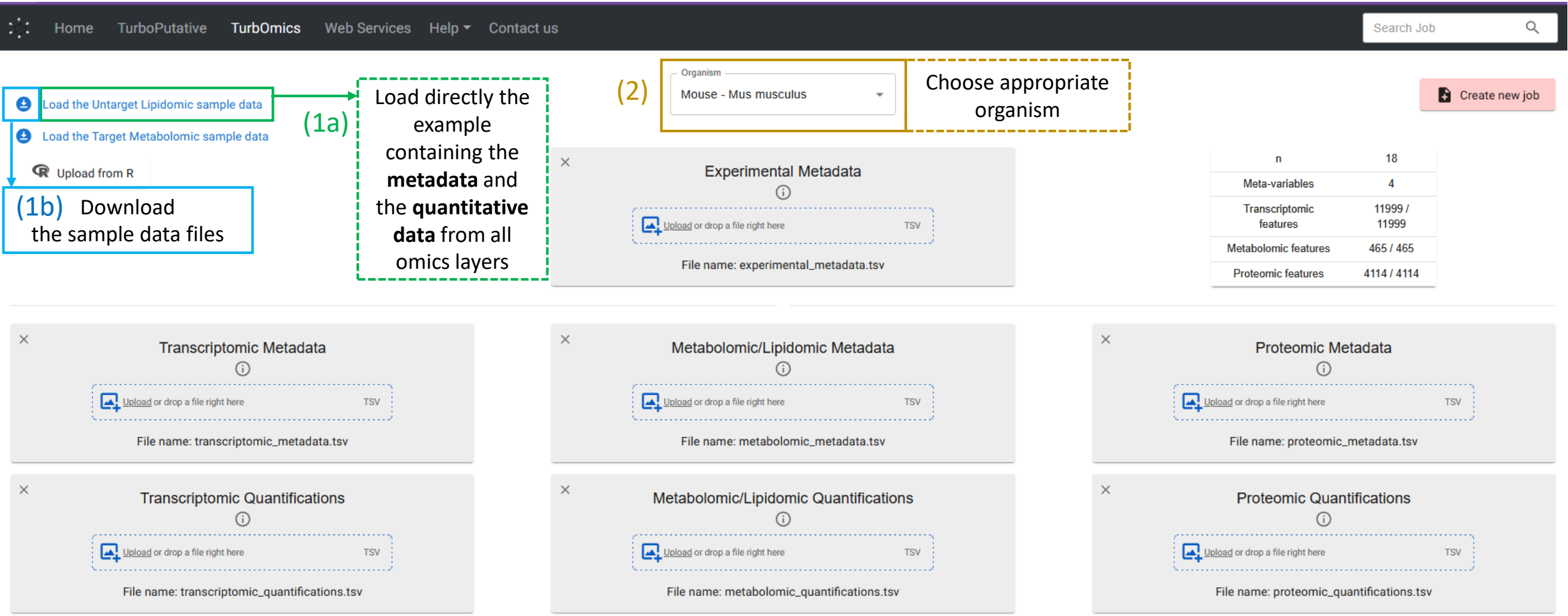
- TARGTED METABOLOMICS
- PROTEOMICS
- TRANSCRIPTOMICS

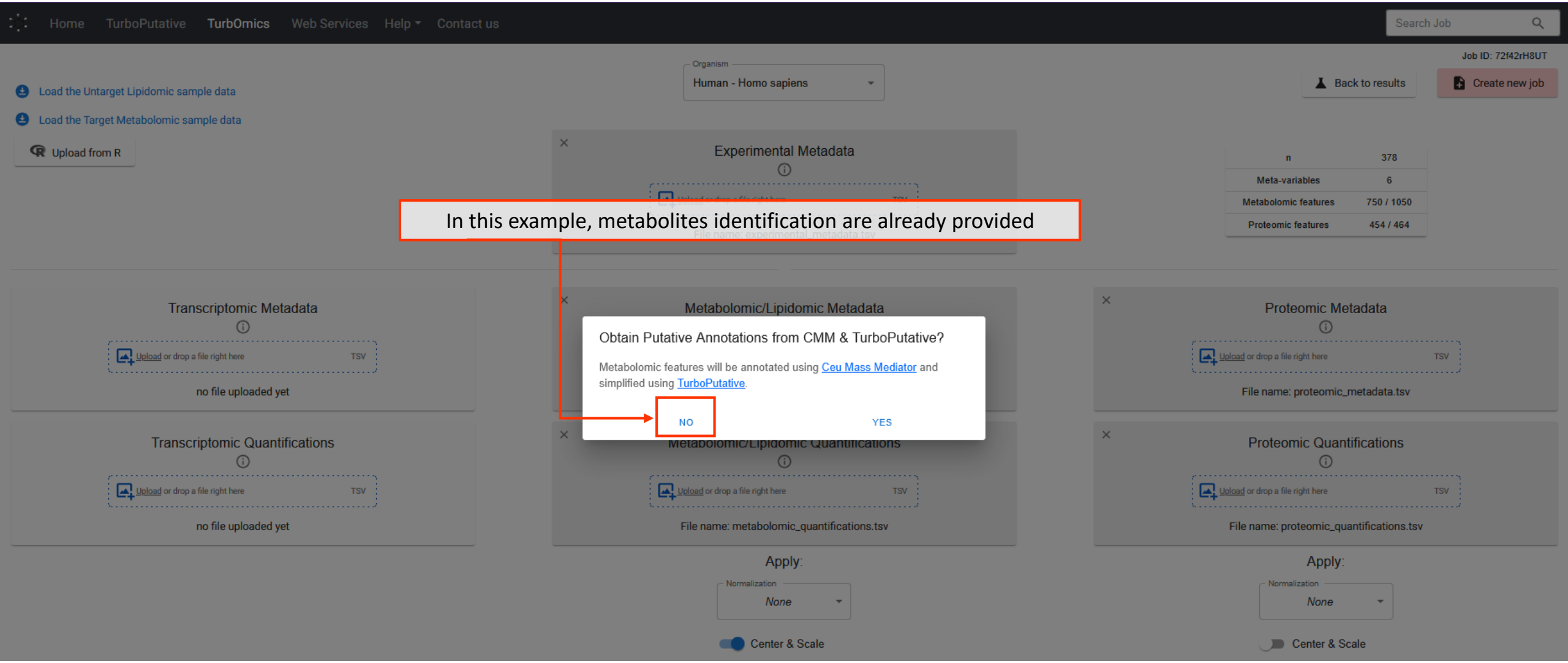
Load example dataset

To get started, users can upload their experimental data directly from the **Main Page**. Previous analyses can be accessed using the **Find Job** field by entering the corresponding job ID. Once a dataset is loaded, the **Results** section provides access to a suite of tools for in-depth analysis and interpretation.



- ✓ For Normalization, Scaling and Missing Values Imputation see slide 11 of the present tutorial

Putative Annotation

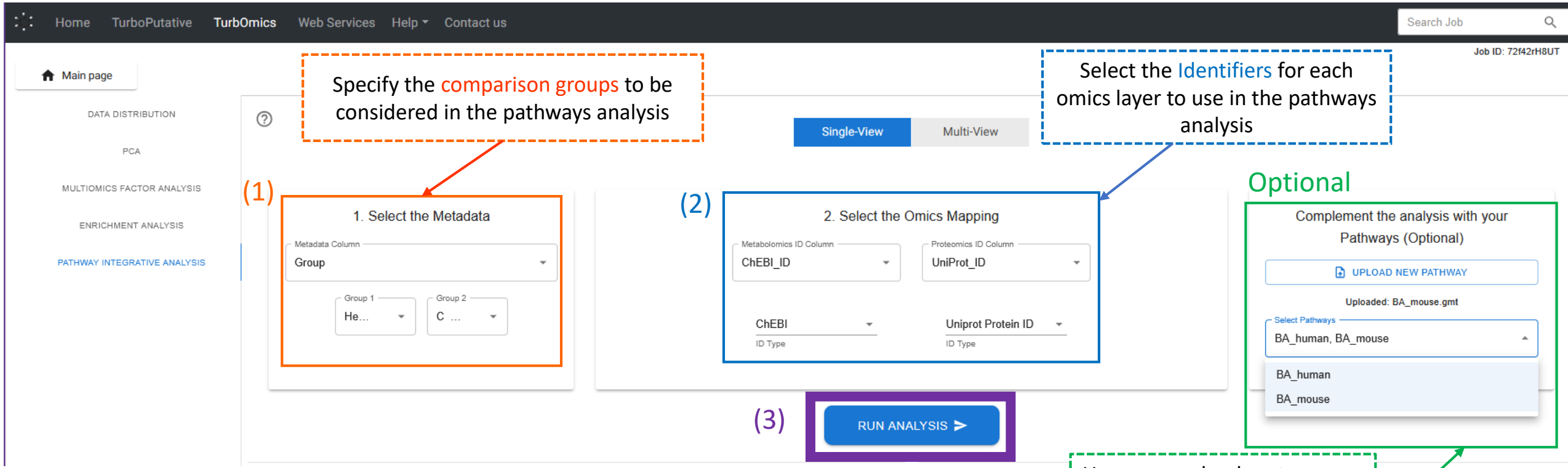


- ✓ For Exploratory analysis see pp.17-20 of the present tutorial
- ✓ For Multiomics Factor Analysis (MOFA) see pp. 21-26 of the present tutorial
- ✓ For Enrichment Analysis see pp. 27-29 of the present tutorial

Pathway Integrative Analysis

This section leverages the **PathIntegrate** library to identify pathways that are most strongly associated with a condition of interest. By using single-sample pathway analysis (ssPA) approaches, PathIntegrate transforms molecular-level abundance data into pathway-level matrices, enabling a more comprehensive understanding of how different pathways contribute to the observed biological outcomes. In this implementation, Principal Component Analysis (PCA) is used for summarizing the data at the pathway level.

➢ Single-View Framework



Single-View approach computes more comprehensive pathway scores, using Partial Least Squares Discriminant Analysis (PLS-DA) on a single pathway-level matrix that combines information from all omics

Users can upload custom pathways in GMT format, enabling the integration of personalized metabolite-based pathway definitions

Pathway Integrative Analysis

R-squared (R^2) value representing the proportion of variance in the response variable explained by the model. An **empirical p-value** is, calculated by performing ten permutations on the response vector (y) and comparing the simulated R^2 values with the actual one. The minimum p-value that can be obtained is 0.1, reflecting the reliability of the model.

➢ Single-View Framework results

DATA DISTRIBUTION

PCA

MULTIOMICS FACTOR ANALYSIS

ENRICHMENT ANALYSIS

PATHWAY INTEGRATIVE ANALYSIS

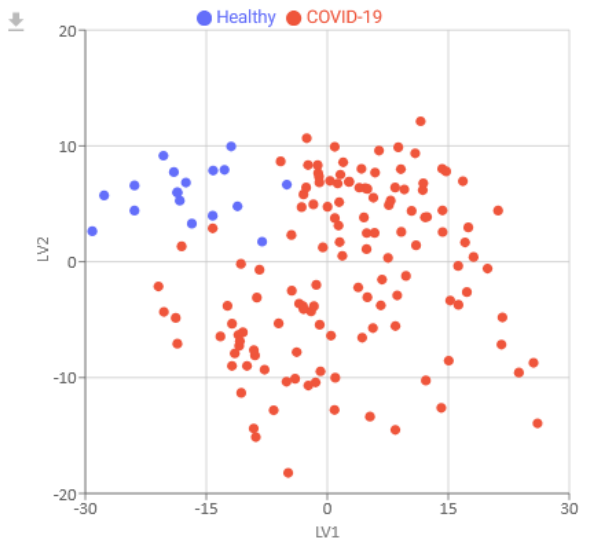
EXPORT TABLE

Summary statistics

Model R2 = 0.8287

p-value ≤ 0.1

Latent Variable	R2	p-value
1	0.2998	4.97e-13
2	0.0973	0.00011
3	0.1609	3.97e-7
4	0.1911	2.48e-8
5	0.0796	0.00049



Show Labels

X Axis
LV1

Y Axis
LV2

EXPORT TABLE

Select	Path_ID	Name	N.	VIP
	Filter by Path_ID	Filter by Name	Filter by N.	Filter by ...
○	R-HSA-216083	Integrin cell surface interactions	4	3.1342
◉	R-HSA-156580	Phase II - Conjugation of compounds	9	2.4516
○	R-HSA-448424	Interleukin-17 signaling	5	2.3862
○	R-HSA-5687128	MAPK6/MAPK4 signaling	4	2.2312
○	R-HSA-83936	Transport of nucleosides and free purine and pyrimidine bases across the plasma membrane	4	2.1508
○	R-HSA-74217	Purine salvage	4	2.0680

EXPORT TABLE

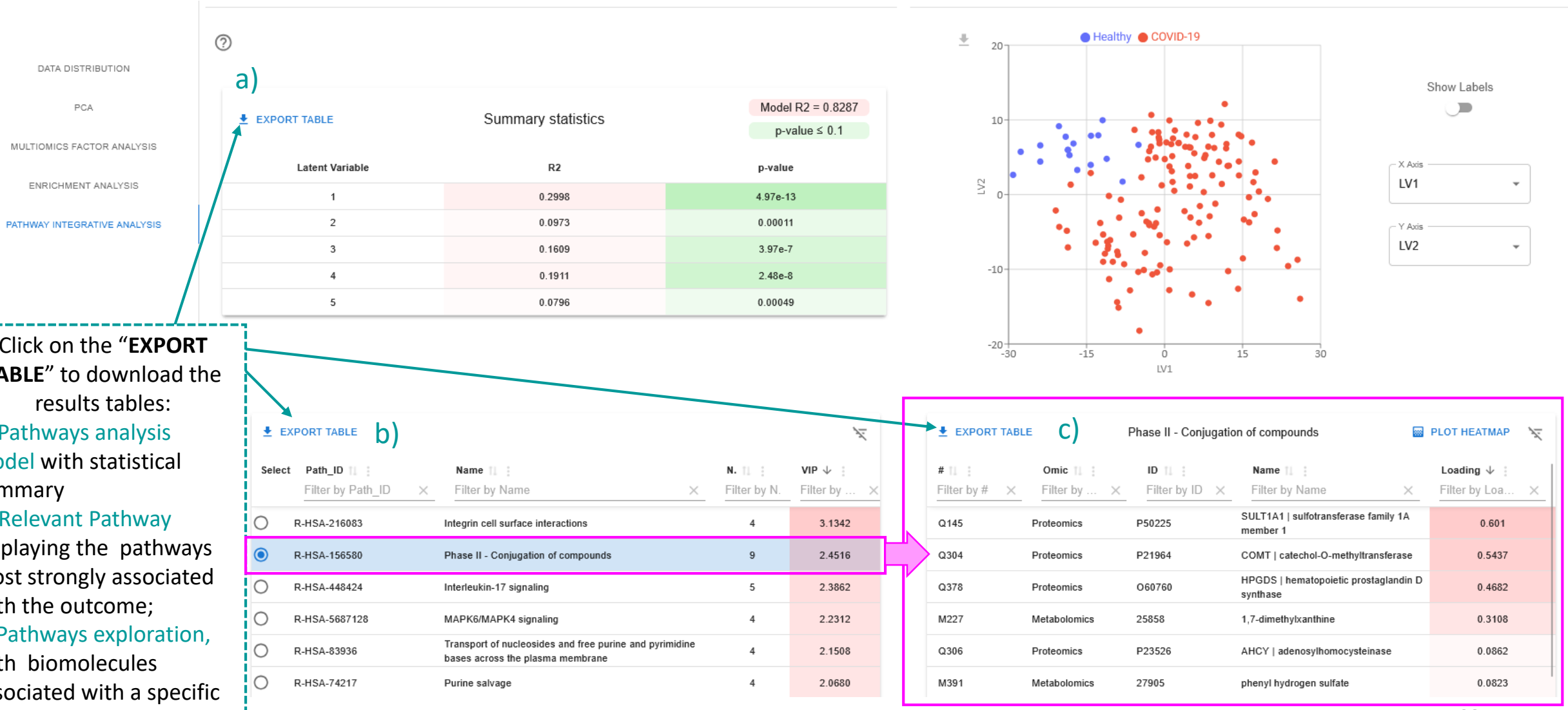
Phase II - Conjugation of compounds

PLOT HEATMAP

#	Omic	ID	Name	Loading
Filter by #	Filter by ...	Filter by ID	Filter by Name	Filter by Loa...
Q145	Proteomics	P50225	SULT1A1 | sulfotransferase family 1A member 1	0.601
Q304	Proteomics	P21964	COMT | catechol-O-methyltransferase	0.5437
Q378	Proteomics	O60760	HPGDS | hematopoietic prostaglandin D synthase	0.4682
M227	Metabolomics	25858	1,7-dimethylxanthine	0.3108
Q306	Proteomics	P23526	AHCY | adenosylhomocysteinase	0.0862
M391	Metabolomics	27905	phenyl hydrogen sulfate	0.0823

Pathway Integrative Analysis

➢ Single-View Framework results



Click on the "**EXPORT TABLE**" to download the results tables:

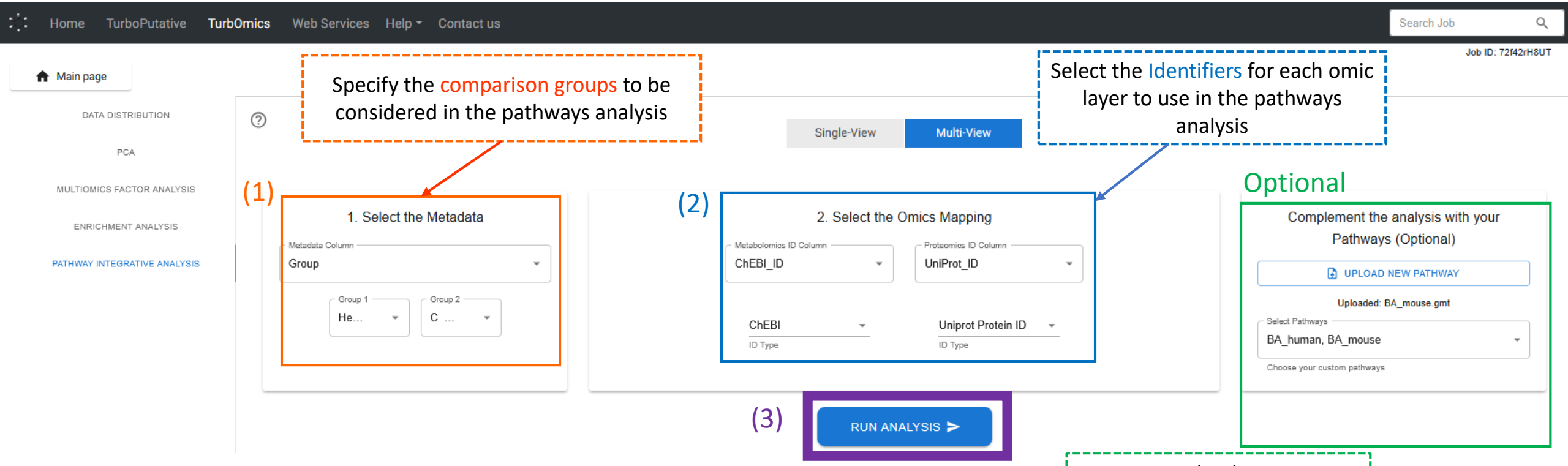
a) Pathways analysis model with statistical summary

b) Relevant Pathway displaying the pathways most strongly associated with the outcome;

c) Pathways exploration, with biomolecules associated with a specific pathway

Pathway Integrative Analysis

- Multi-View Framework



Multi-View approach employs a multi-block partial least squares (MB-PLS) latent variable model. It preserves the block structure of each omics view, enabling you to see the contribution of each omics dataset to the prediction of the outcome variable.

Users can upload custom pathways in GMT format, enabling the integration of personalized metabolite-based pathway definitions

Pathway Integrative Analysis

- Multi-View Framework results

DATA DISTRIBUTION

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MULTIOMICS FACTOR ANALYSIS

ENRICHMENT ANALYSIS

PATHWAY INTEGRATIVE ANALYSIS

Click on the "**EXPORT TABLE**" to download results :
a) Pathways analysis model with statistical summary;
b) Relevant Pathway displaying the pathways most strongly associated with the outcome;
c) Pathways exploration with biomolecules associated with a specific pathway

a)

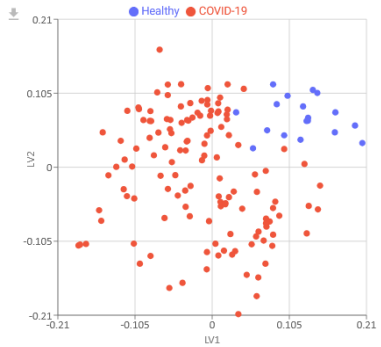
EXPORT TABLE

Summary statistics

Model R2 = 0.7864

p-value ≤ 0.1

Latent Variable	Metabolomics (%)	Proteomics (%)	R2	p-value
1	16.44	83.56	0.3007	4.54e-13
2	55.46	44.54	0.1025	6.88e-5
3	53.56	46.44	0.142	2.17e-6
4	85.37	14.63	0.1777	8.60e-8
5	88.31	11.69	0.0635	0.00194



b1) Metabolomics

EXPORT TABLE

Select	Path_ID	Name	N.	VIP
	Filter by Path_ID	Filter by Name	Filter by N.	Filter by ...
○	R-HSA-373076	Class A/1 (Rhodopsin-like receptors)	6	2.5551
◉	R-HSA-156580	Phase II - Conjugation of compounds	5	2.5417
○	R-HSA-556833	Metabolism of lipids	11	2.5026
○	R-HSA-416476	G alpha (q) signalling events	4	2.4952
○	R-HSA-1483206	Glycerophospholipid biosynthesis	4	2.4916
○	R-HSA-425393	Transport of inorganic cations/anions and amino acids/ oligopeptides	5	2.4465
○	R-HSA-5619102	SLC transporter disorders	11	2.4452

b2) Proteomics

EXPORT TABLE

Select	Path_ID	Name	N.	VIP
	Filter by Path_ID	Filter by Name	Filter by N.	Filter by ...
○	R-HSA-5669034	TNFs bind their physiological receptors	7	1.5163
◉	R-HSA-156580	Phase II - Conjugation of compounds	4	1.5101
○	R-HSA-8957322	Metabolism of steroids	4	1.5058
○	R-HSA-8979227	Triglyceride metabolism	4	1.4659
○	R-HSA-163560	Triglyceride catabolism	4	1.4659
○	R-HSA-168255	Influenza Infection	4	1.4357
○	R-HSA-5218859	Regulated Necrosis	8	1.4325

c1) Phase II - Conjugation of compounds

EXPORT TABLE PLOT HEATMAP

#	ID	Name	Loading
Filter by #	Filter by ID	Filter by Name	Filter by Loading
M227	25858	1,7-dimethylxanthine	0.7268
M391	27905	phenyl hydrogen sulfate	0.3355
M710	37946	dopamine 3-O-sulfate	-0.065
M82	9008	salicyluric acid	-0.0822
M435	17864	taurolithocholic acid sulfate	-0.5902

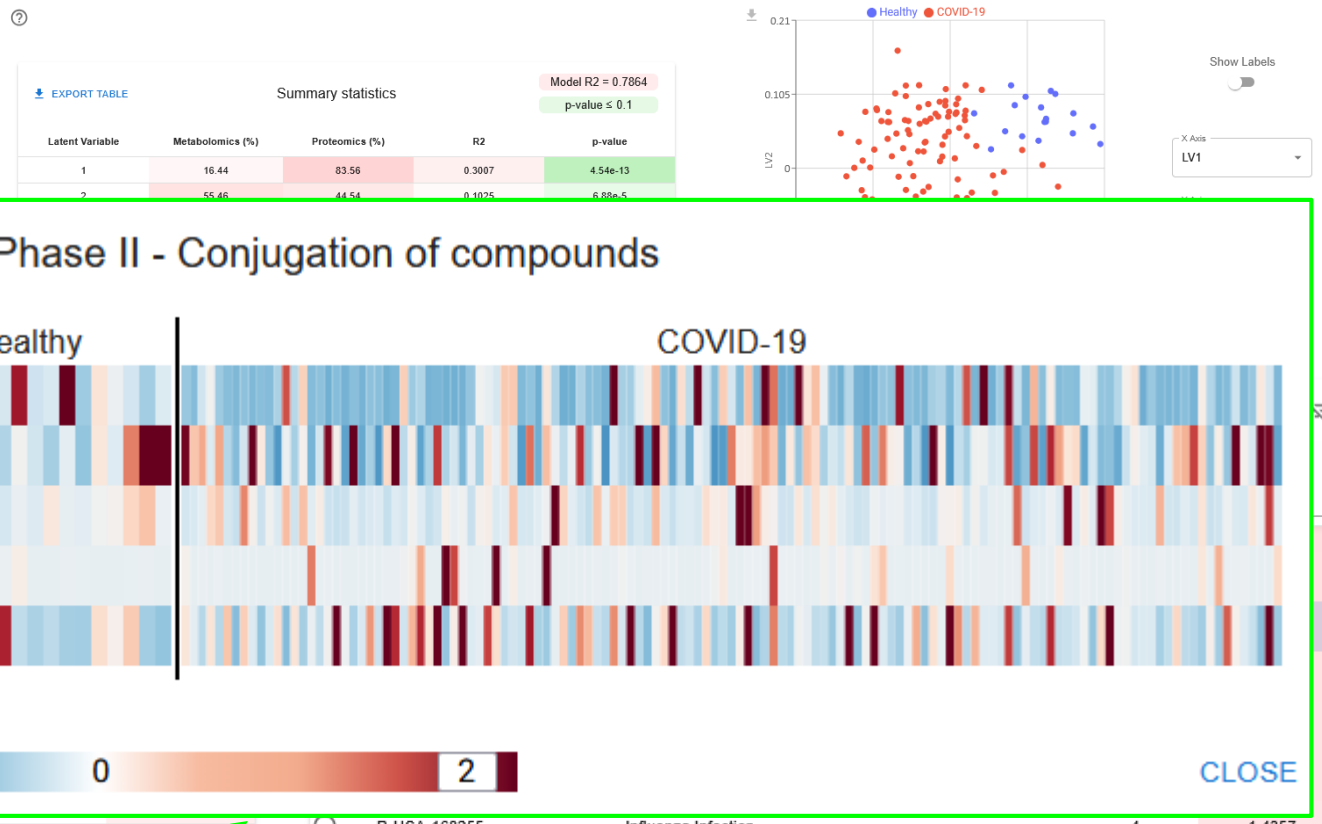
c2) Phase II - Conjugation of compounds

EXPORT TABLE PLOT HEATMAP

#	ID	Name	Loading
Filter by #	Filter by ID	Filter by Name	Filter by Loading
Q145	P50225	SULT1A1 | sulfotransferase family 1A member 1	0.6379
Q304	P21964	COMT | catechol-O-methyltransferase	0.6269
Q378	O60760	HPGDS | hematopoietic prostaglandin D synthase	0.3758
Q306	P23526	AHCY | adenosylhomocysteinase	0.2426

Pathway Integrative Analysis

- Multi-View Framework results



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PCA

MULTIOMICS FACTOR ANALYSIS

ENRICHMENT ANALYSIS

PATHWAY INTEGRATIVE ANALYSIS

EXPORT TABLE

Select	Path_ID	Name		
	R-HSA-373076	Class A/1 (Rho		
◉	R-HSA-156580	Phase II - Conj		
	R-HSA-556833	Metabolism of l		
	R-HSA-416476	G alpha (q) sig		
	R-HSA-1483206	Glycerophosph		
	R-HSA-425393	Transport of inc oligopeptides		
	R-HSA-5619102	SLC transporter disorders	11	2.4452
	R-HSA-168255	Influenza Infection	4	1.4357
	R-HSA-5218859	Regulated Necrosis	8	1.4325

Click on "**PLOT HEATMAPS**" to show heatmap visualization of biomolecule abundance or quantification values associated with the selected pathway

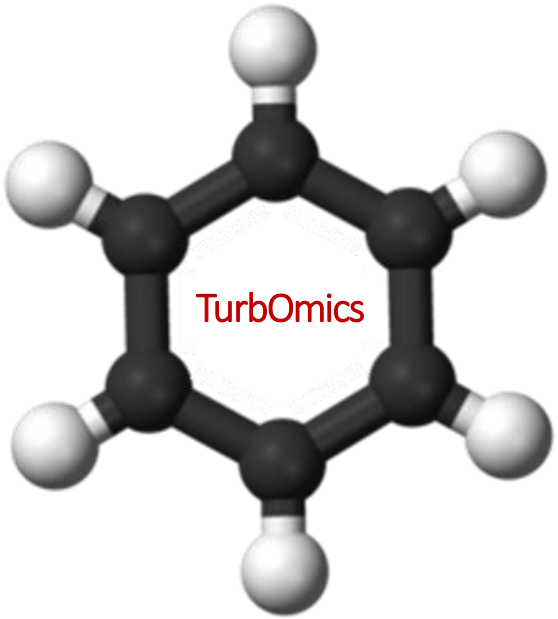
Phase II - Conjugation of compounds — PLOT HEATMAP

ID	Name	Loading
5858	1,7-dimethylxanthine	0.7268
7905	phenyl hydrogen sulfate	0.3355
M710	37946 dopamine 3-O-sulfate	-0.065
M82	9008 salicyluric acid	-0.0822
M435	17864 taurolithocholic acid sulfate	-0.5902

c2) EXPORT TABLE — Phase II - Conjugation of compounds — PLOT HEATMAP

#	ID	Name	Loading
Q145	P50225	SULT1A1 | sulfotransferase family 1A member 1	0.6379
Q304	P21964	COMT | catechol-O-methyltransferase	0.6269
Q378	O60760	HPGDS | hematopoietic prostaglandin D synthase	0.3758
Q306	P23526	AHCY | adenosylhomocysteinase	0.2426

Summary



For additional details and explanation, please visit:
https://proteomics.cnic.es/TurboPutative/turbomicshelp

If you have any questions, please contact us:
metabolomics.cnic@gmail.com

- TurbOmics is an intuitive web-based platform designed to facilitate the **multi-omics analysis of metabolomic/ lipidomics data alongside proteomics and transcriptomics**.
- It supports both **targeted** experiments and those where metabolite **identification** is available (e.g., LC/CE-MS/MS, NMR or GC-MS data).
- Additionally, TurbOmics offers tools to **putatively annotate features** from untargeted metabolomics based on their mass-to-charge (m/z) ratio.
- The platform provides a streamlined workflow for **exploratory data analysis** and **multi-omics integration** through **i) Multi-Omics Factor Analysis, ii) Pathway Integrative Analysis** and **iii) Enrichment Analysis.**
- Users can upload their experimental data directly from the **Main Page**. Previous analyses can be accessed using the **Find Job** field by entering the corresponding job ID.
- Once a dataset is loaded, the **Results** section provides access to a suite of tools for in-depth analysis and interpretation where users can explore and export data tables and visualize plots of the results.