POMA

Statistical analysis tool for targeted metabolomic data

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Outline

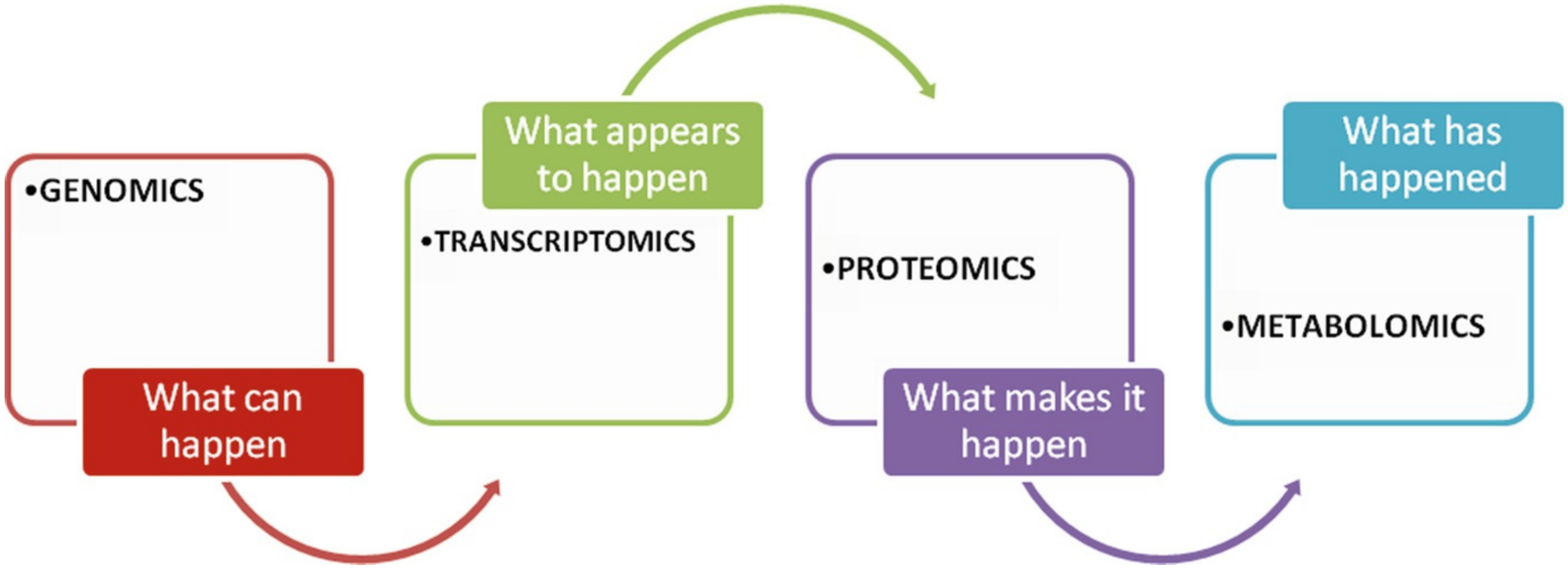
1. Context
2. Motivation & Aims
3. Results
4. Conclusions
5. Future Work

CONTEXT

What’s Metabolomics?

"Metabolomics is the identification and quantification of the small molecule metabolic products (the metabolome) of a biological system. Mass spectrometry and NMR spectroscopy are the techniques most often used for metabolome profiling"[1]

"The Omics Cascade"



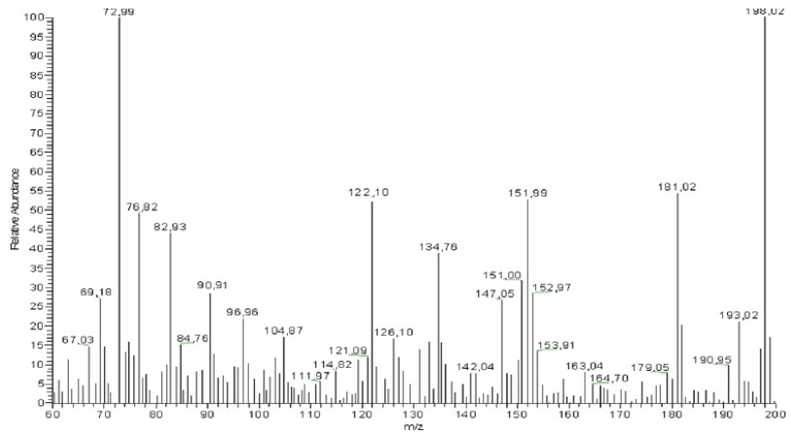
[2]

[1] https://www.nature.com/subjects/metabolomics

[2] Narad P., Kirthanashri S.V. (2018) Introduction to Omics. In: Arivaradarajan P., Misra G. (eds) Omics Approaches, Technologies And Applications. Springer, Singapore

The data

Targeted and untargeted metabolomics



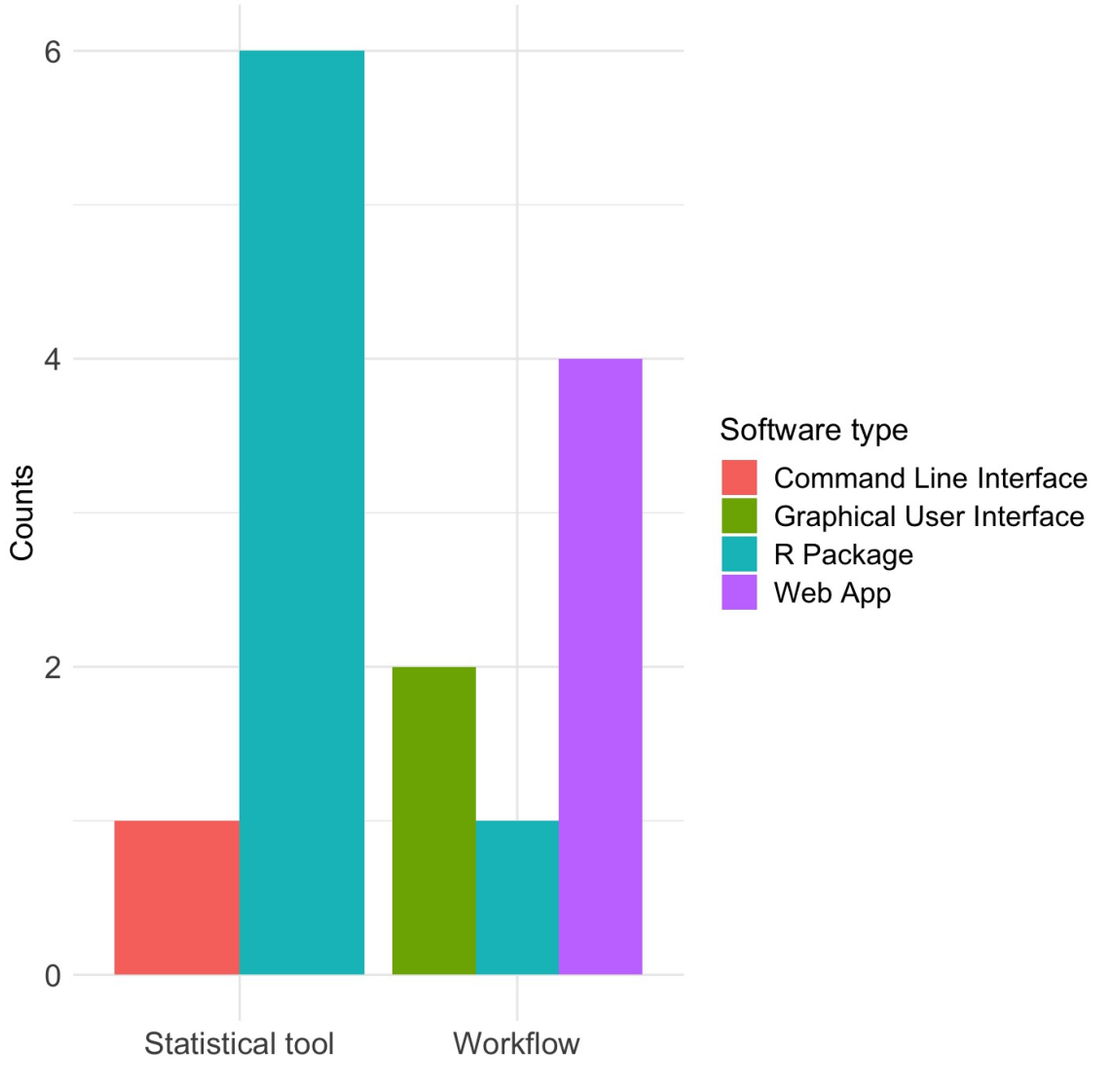
- **Targeted metabolomics:** we know the mass of the metabolites that we want to quantify BEFORE the analysis (hundreds)

- **Untargeted metabolomics:** all metabolites will be acquired, but we will not know exactly which ones are some of them (thousands)

How is the data that we will analize?

- Standard (Omics) matrix: Samples in rows and metabolites (variables) in columns

Freely Available Existing Tools



Web Apps that allows users to perform a statistical analysis[3]

- Workflow4metabolomics
- Galaxy-M
- XCMS Online
- MetaboAnalyst

[3] Spicer, R., Salek, R. M., Moreno, P., Cañueto, D., & Steinbeck, C. (2017). Navigating freely-available software tools for metabolomics analysis. Metabolomics, 13(9), 106.

MOTIVATION & AIMS

Motivation & Aims

Motivation

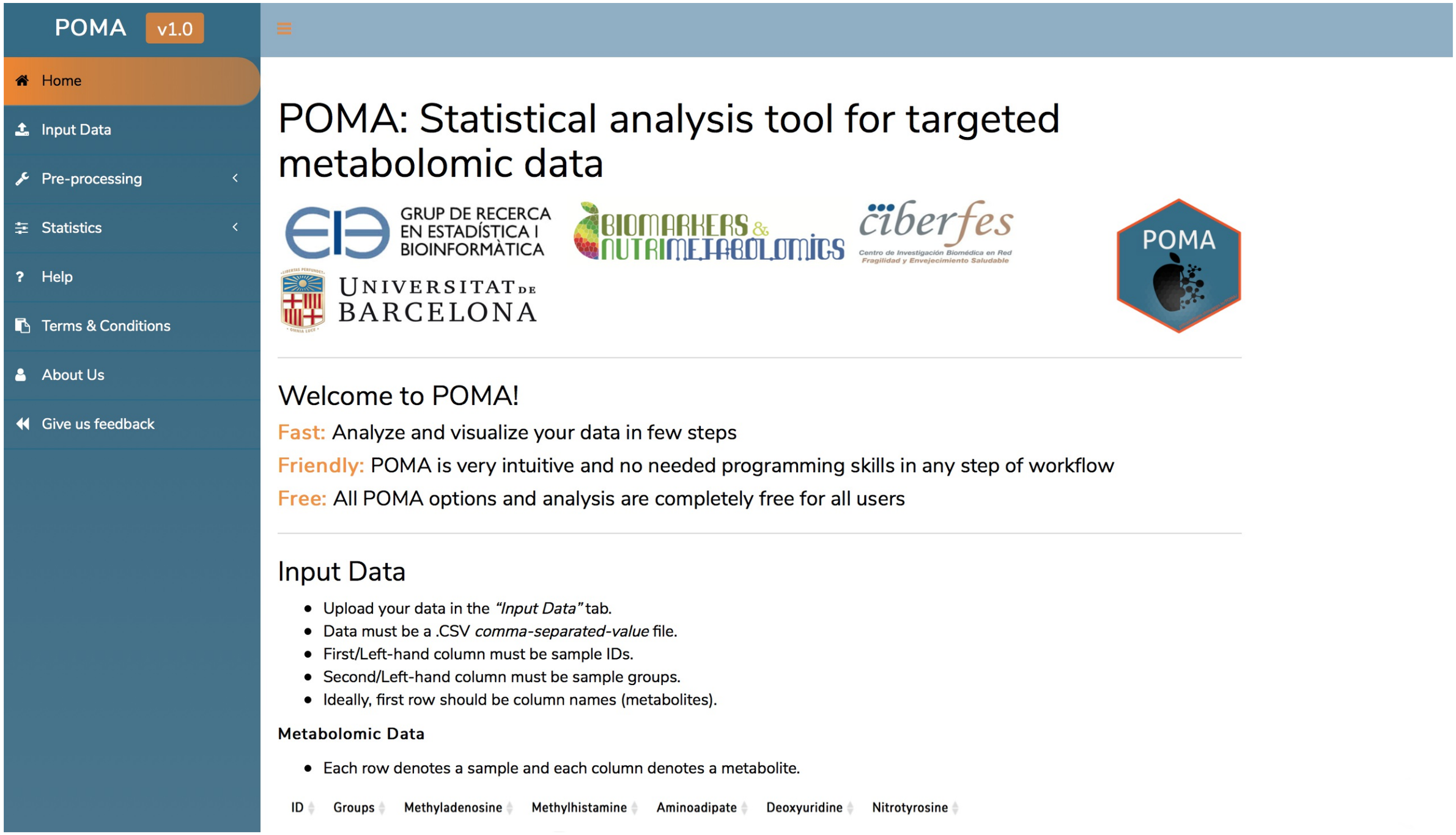
- Biological interpretation of the results is one of the hard points and high knowledge of statistical analysis and computational programming is usually required
- Sometimes, the existing tools don’t accept "complicated" databases

Aims

- Provide users of an **EASY USE** tool that don’t require programming skills
- Allow users to analyze all types of data (simple and complex)
- Lead the user for a good statistical analysis (Documentation & automatic reports)
- Make a completely **REPRODUCIBLE** analysis (Open Source)
- **Our main aim is COMPLETING the existing tools and give other option to users, NOT to COMPETE with the existing tools**

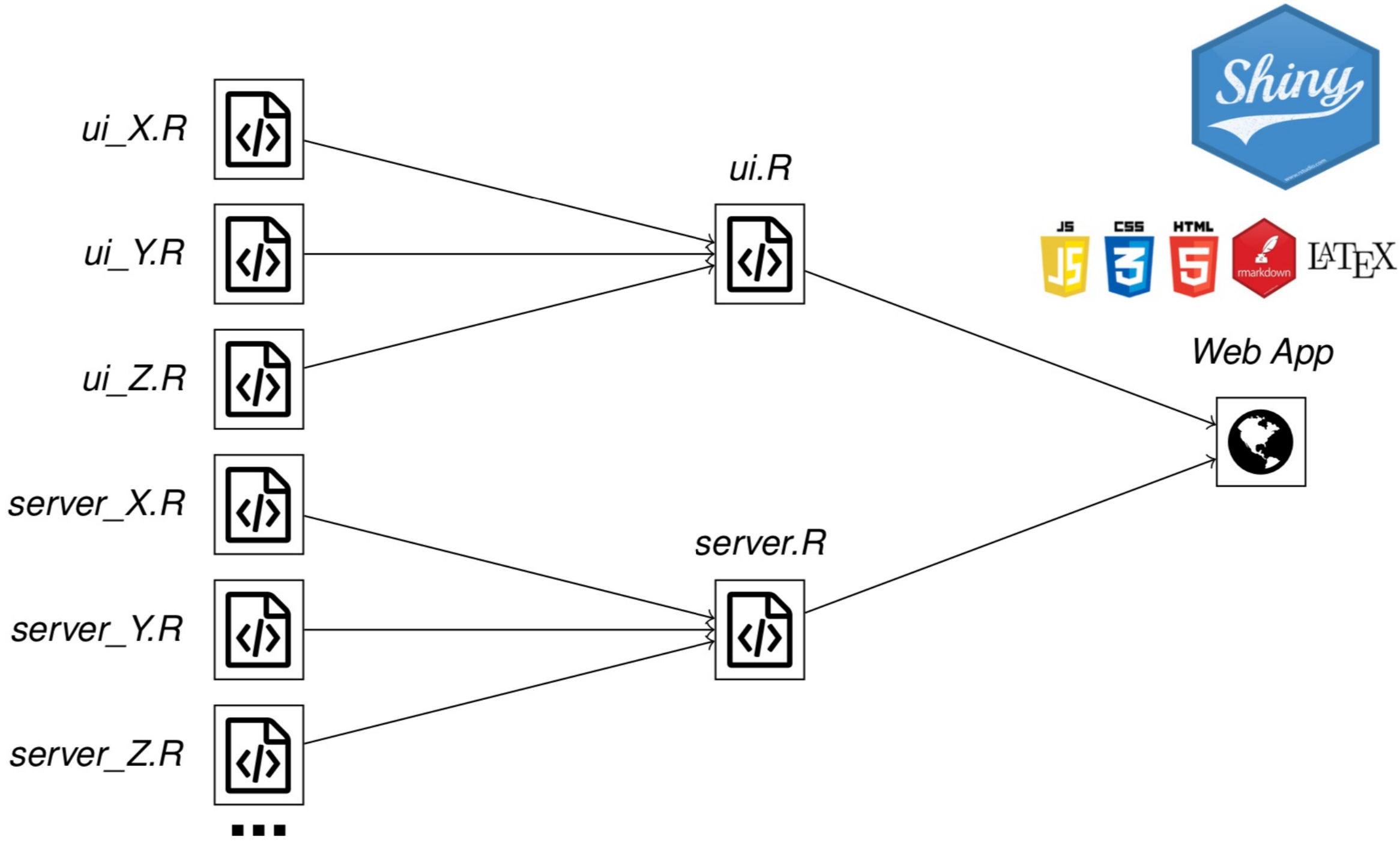
RESULTS

POMA Shiny App



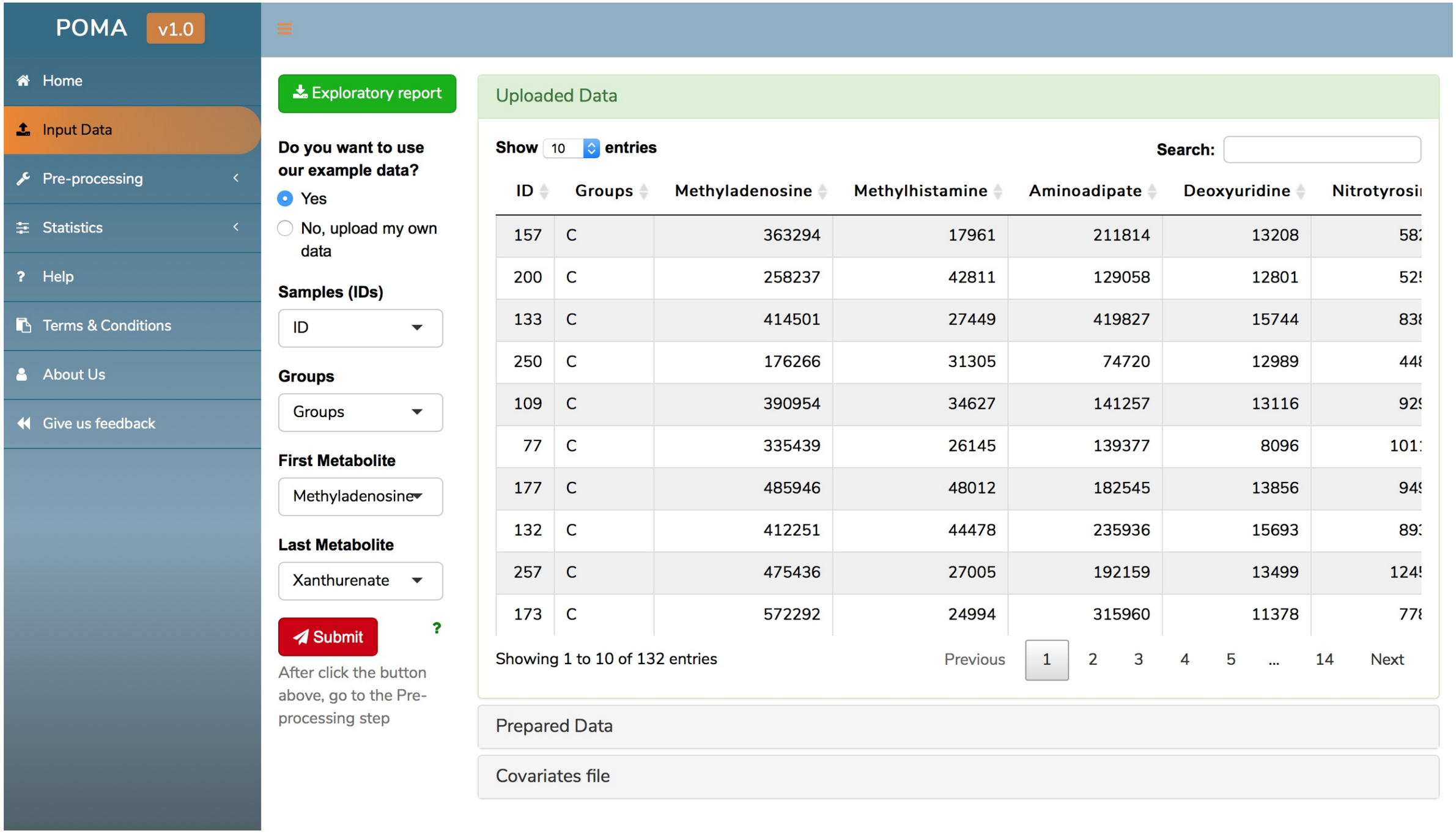
http://polcastellano.shinyapps.io/POMA/

Architecture



Input Data Panel

We have used the `shinydashboard` package for the main structure and the `dashboardthemes` package for customization



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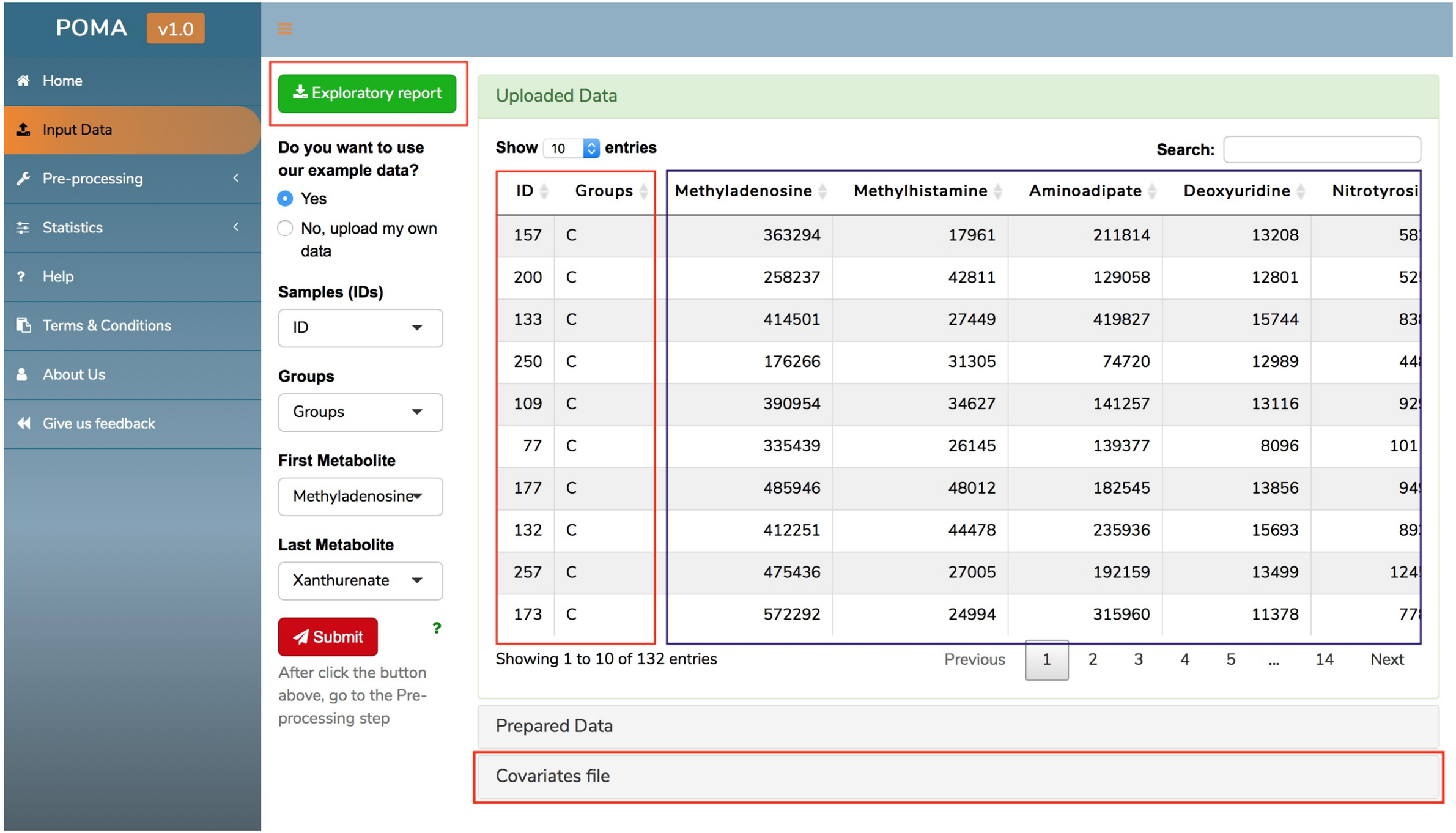
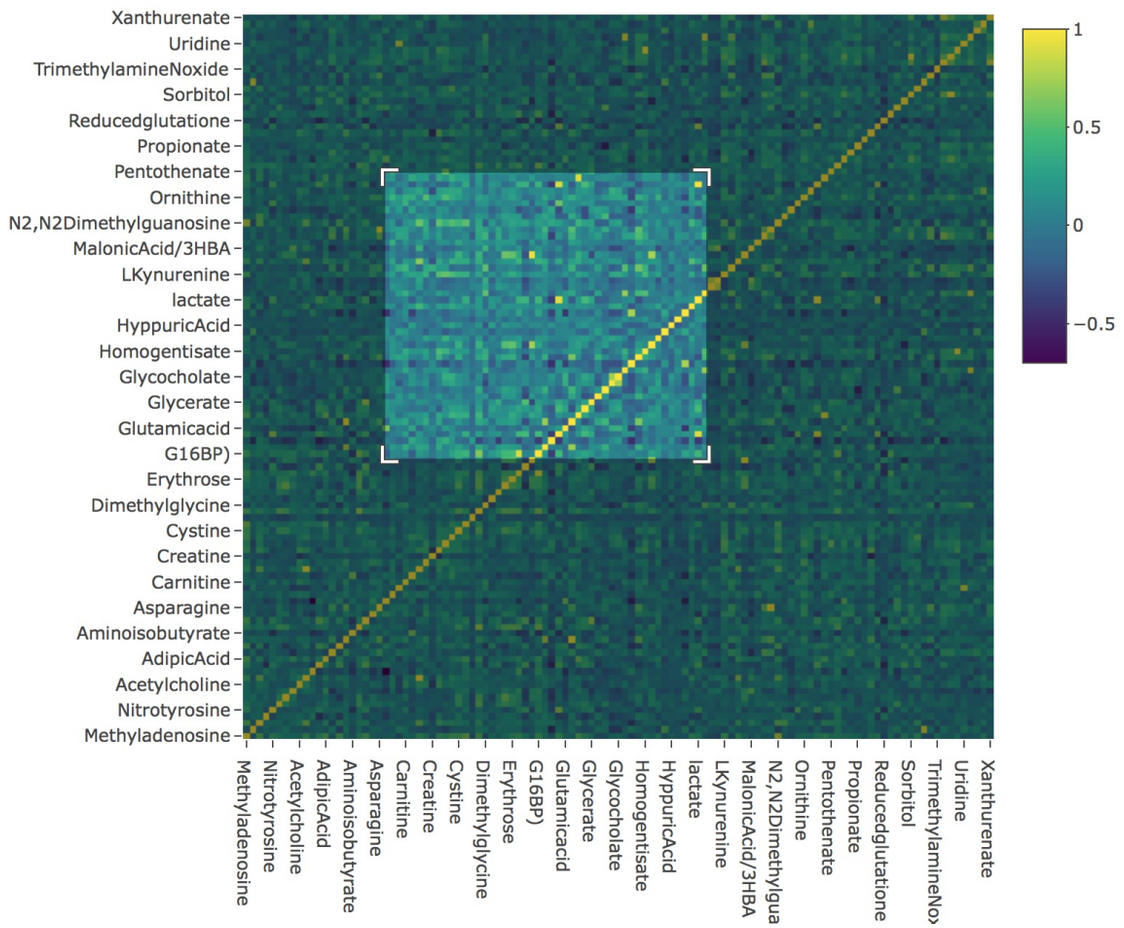
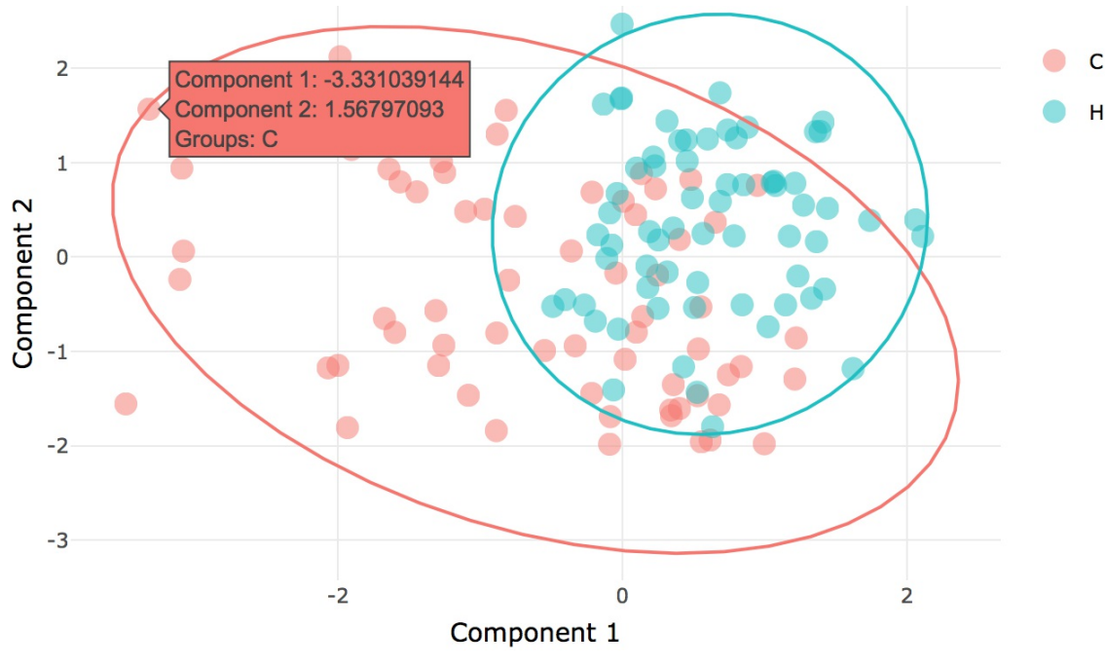


Visualization

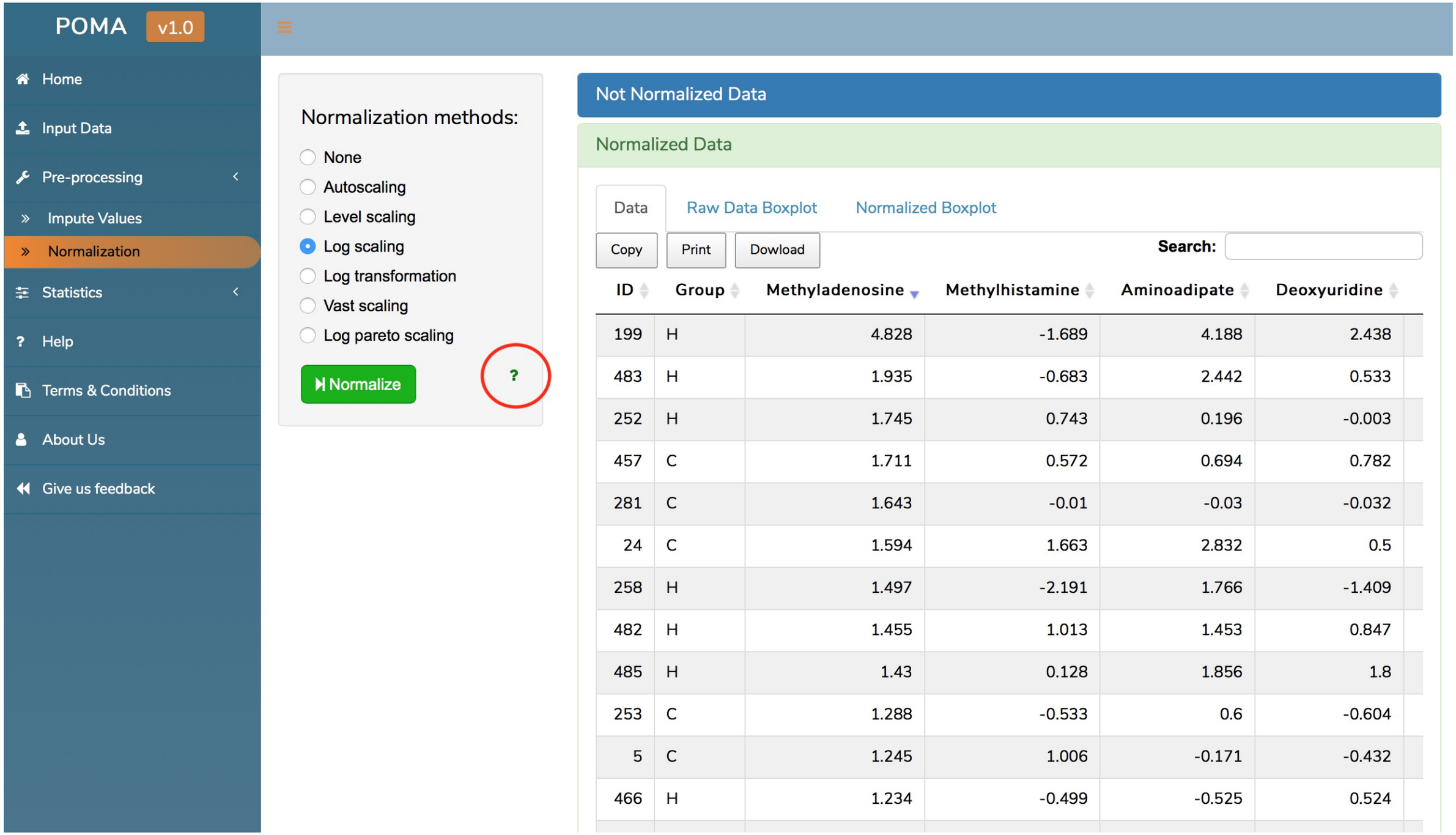
All plots in the app are designed using `plotly` package. It make all plots interactive allowing users to zoom in or zoom out in a plots, select points to see the individual information, hide all points of one group and download plots in a easy way!





Documentation

The implementation of `shinyhelper` package allows each panel to have an individual help



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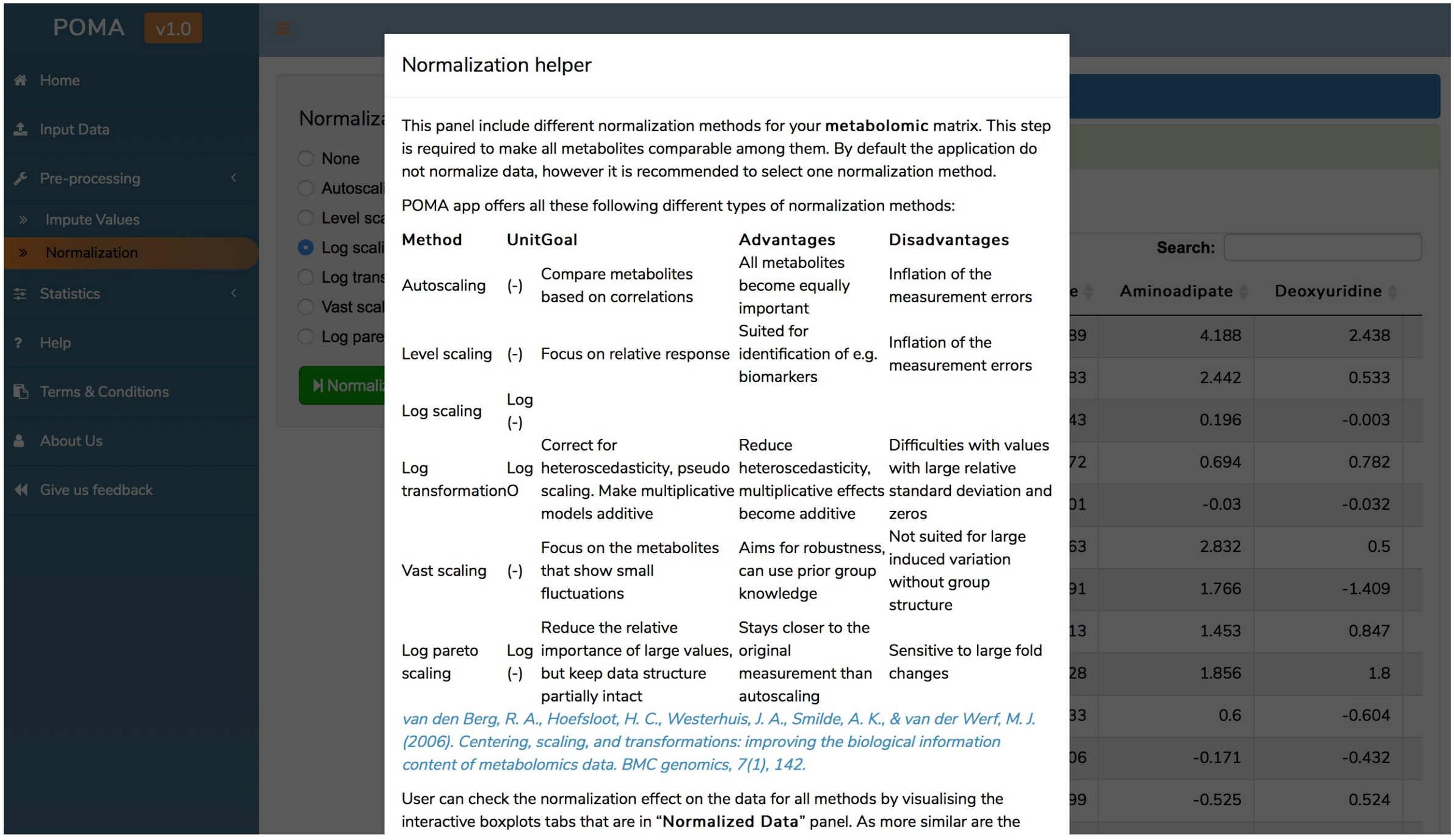
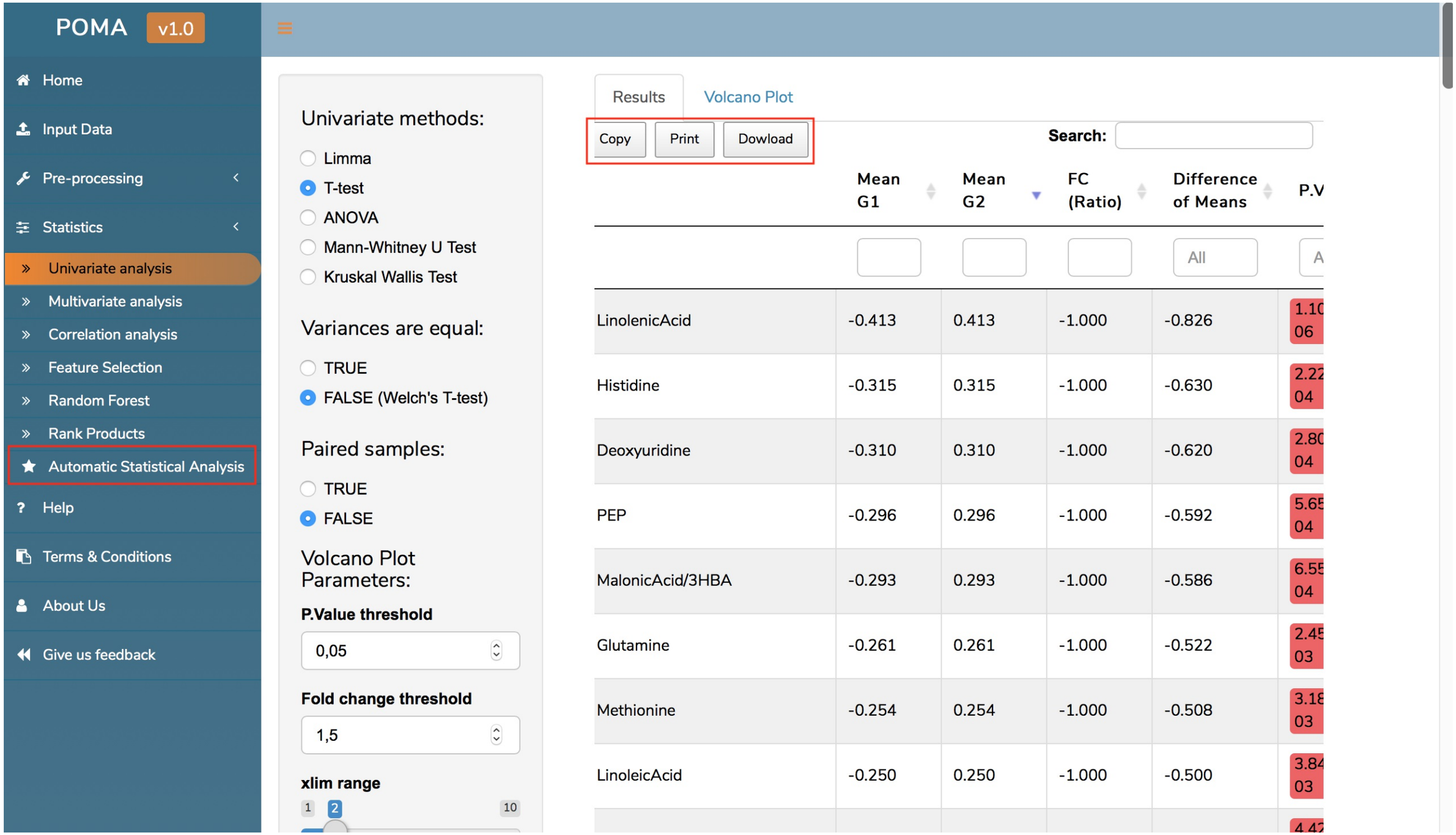


Statistical Analysis

The aim is to offer to tune as many parameters as possible to avoid the "black box" effect



Automatic Statistical Report

POMA: Statistical analysis tool for targeted metabolomic data

Intelligent Statistical Analysis: Metabolomic analysis for 2 groups using default 'Pre-processing' by POMA

July, 2019

- 1 Parametric tests
  - 1.1 T-test
    - 1.1.1 Metabolites with NORMAL distribution & variance HOMOSCEDASTICITY
    - 1.1.2 Metabolites with NORMAL distribution & variance HETEROSCEDASTICITY
  - 1.2 ANOVA
    - 1.2.1 Metabolites with NORMAL distribution ANOVA model
- 2 Non Parametric tests
  - 2.1 Mann-Whitney U Test (Wilcoxon Signed Rank Test if the data is paired)
    - 2.1.1 Metabolites with NON NORMAL distribution

1 Parametric tests

1.1 T-test

1.1.1 Metabolites with NORMAL distribution & HOMOSCEDASTICITY

Metabolite	Mean G1	Mean G2	FC (Ratio)	Difference of Means	P.Value	adj.P.Val
Deoxyuridine	4.050	4.097	1.012	-0.047	0.00028	0.01593
Glycochenodeoxycholate	5.526	5.183	0.938	0.343	0.00074	0.02104
MaleicAcid)	6.297	6.240	0.991	0.057	0.00114	0.02173
Methionine	5.782	5.832	1.009	-0.050	0.00315	0.04493
Allantoin	5.034	4.921	0.978	0.113	0.00650	0.07409

CONCLUSIONS

Conclusions

- **We have developed a FAST, FRIENDLY and FREE software that is called POMA**
- **POMA is full-based in R language and uses a Shiny system to run**
- **POMA provides an accurate DOCUMENTATION ("HELP") at each step of analysis that coluld improve the results and facilitate the interpretation of it**
- **POMA can generate two types of AUTOMATIC REPORTS: Exploratory report and Statistical report**
- **POMA is in a constant development. According to this, we are totally open to user bug reports to keep improving our app**

Future Work

(In order of importance...)

- Finishing the **documentation** as accurately as possible
- Make the code more **efficient**
- Develop a **package** with all POMA functions

Thank you all!

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To the useR! 2019 organizers, for allowing me to show this work

Slides created via the R package xaringan

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