

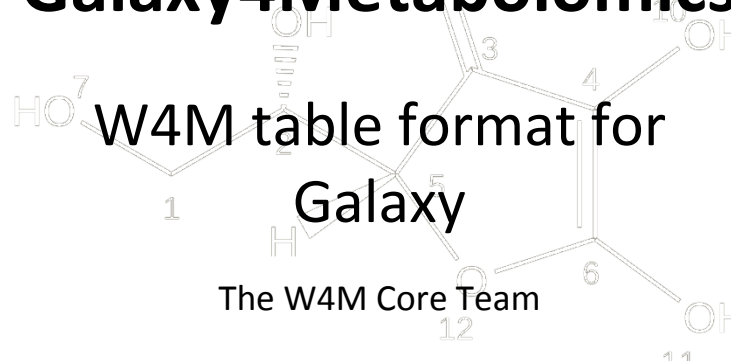


4
Wm

Workflow4metabolomics



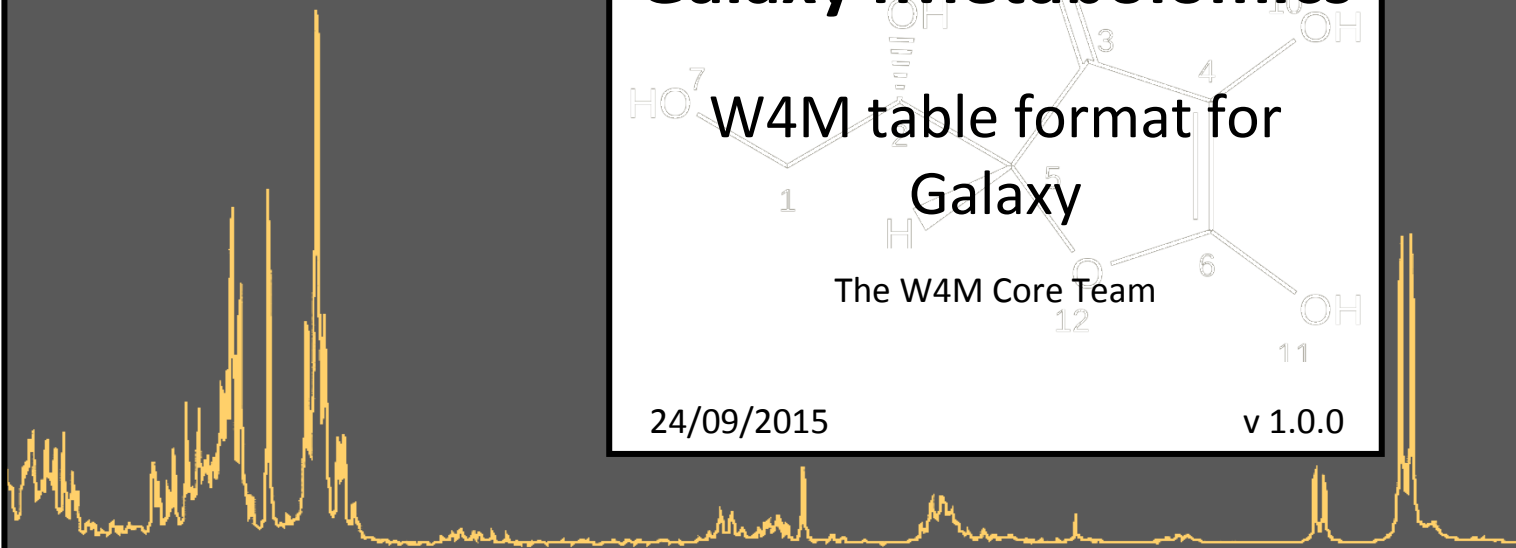
Using Galaxy4Metabolomics



The W4M Core Team

24/09/2015

v 1.0.0

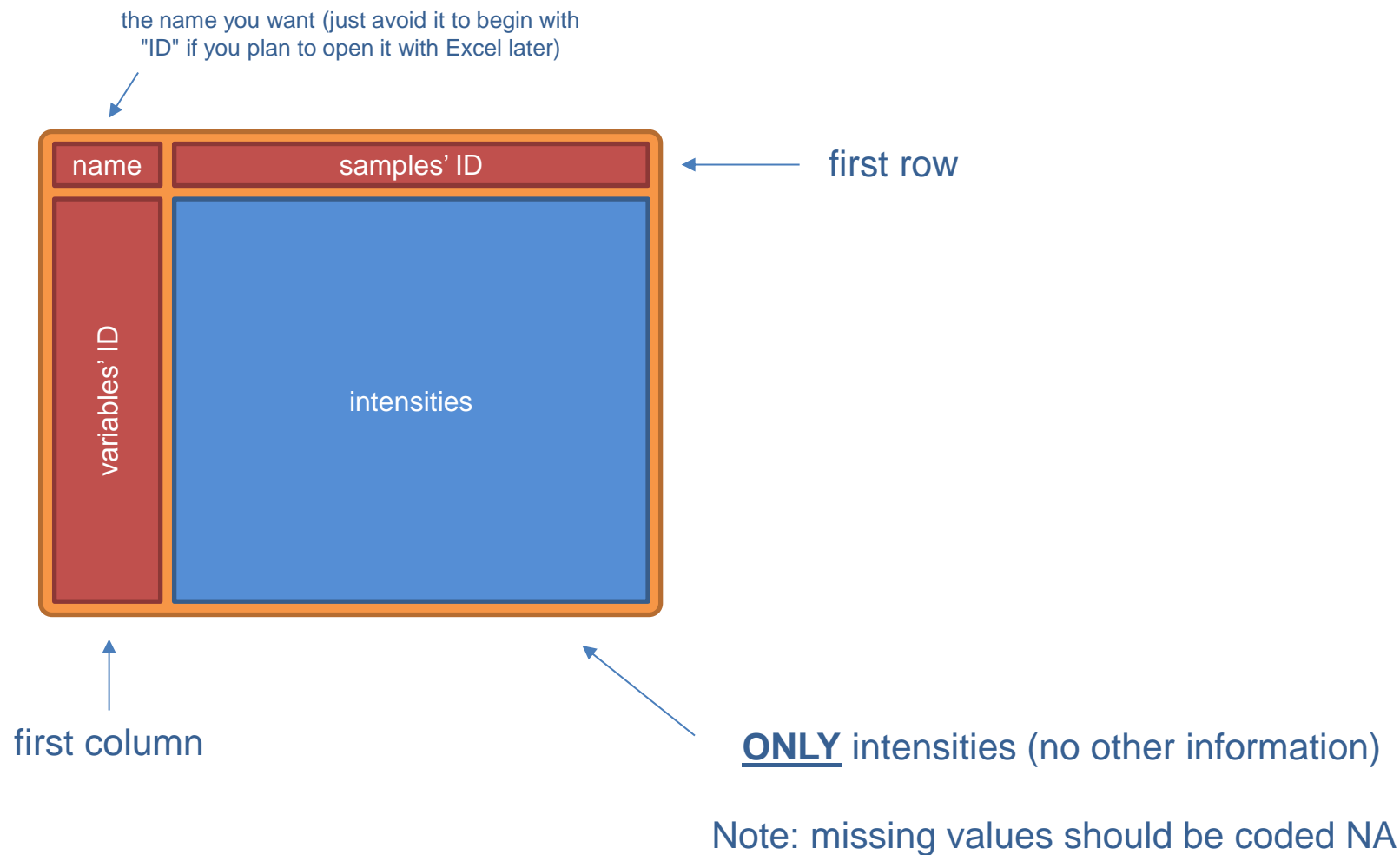


Global structure

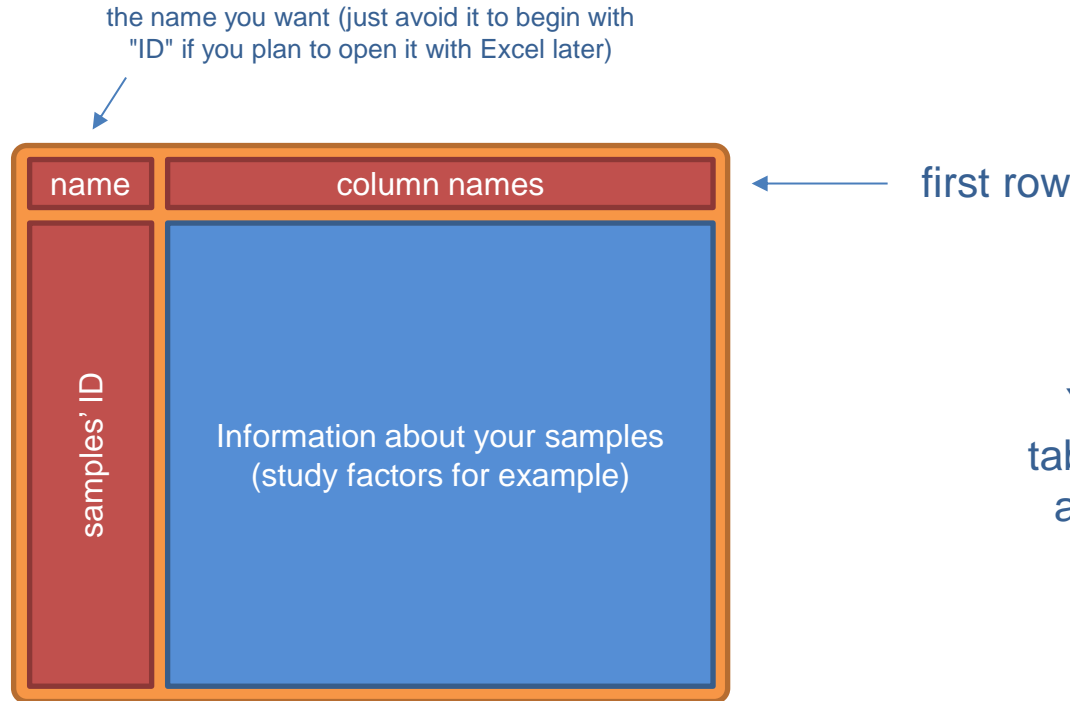
- 3 tables gathering all the information
 - the **data matrix**: intensities of ions or buckets
 - the **sample metadata** file: information concerning your samples
 - the **variable metadata** file: information concerning your ions or buckets
- Note that this 3 tables structure is already generated from the XCMS or bucketing modules
 - **/!** you must complete the sample metadata file with your samples' information (technical information about your samples, or factors of interest for example)



Data matrix



Sample metadata table

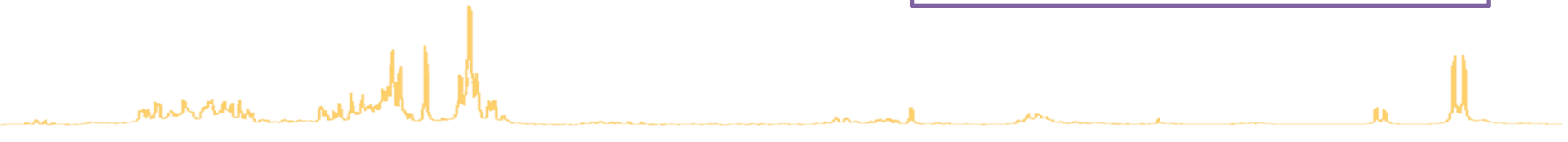


You can add to this table as many columns as you want or need

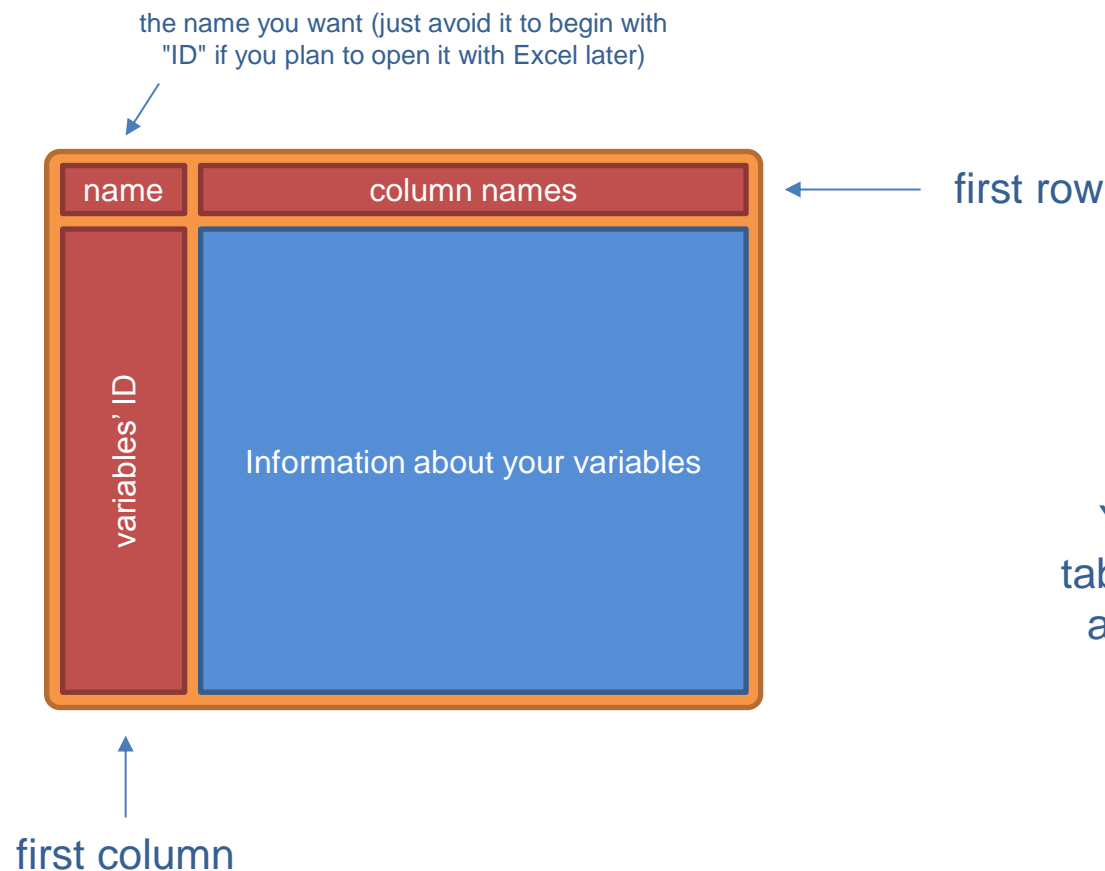
Note: some modules may need some specific columns with particular names (e.g. 'sampleType', 'injectionOrder' or 'batch' for the Batch Correction module) Refer to the module's help section for more information

first column

Samples' ID **must absolutely match** those in the data matrix file



Variable metadata table



You can add to this table as many columns as you want or need

Variables' ID **must absolutely match** those in the data matrix file



Technical aspect

- The files must be tabulated
 - TSV files
 - TXT files with tabulation as separator
- Convention for identifiers and column names
 - It **should not** contain any duplicate
 - Rather use only alphanumeric characters, and points (.) and underscores (_)



Example with Generic Filter module

The screenshot shows the Galaxy 4 Metabolomics interface with the Generic_Filter module (version 2014.12.11) configured. The module has three input files: dataMatrix.txt, sampleMetadata.txt, and variableMetadata.txt. It is set to filter based on numerical values, specifically removing values lower than 10.5 for the 'var1' column. The history panel on the right shows the resulting output files: Generic_Filter_variableMetadata.txt, Generic_Filter_sampleMetadata.txt, and Generic_Filter_dataMatrix.txt.

Input files: dataMatrix.txt, sampleMetadata.txt, variableMetadata.txt

Output files: Generic_Filter_variableMetadata.txt, Generic_Filter_sampleMetadata.txt, Generic_Filter_dataMatrix.txt

The 3 tables as input files

The 3 tables filtered according to specified parameters as output files