



4
Wm

Workflow4metabolomics



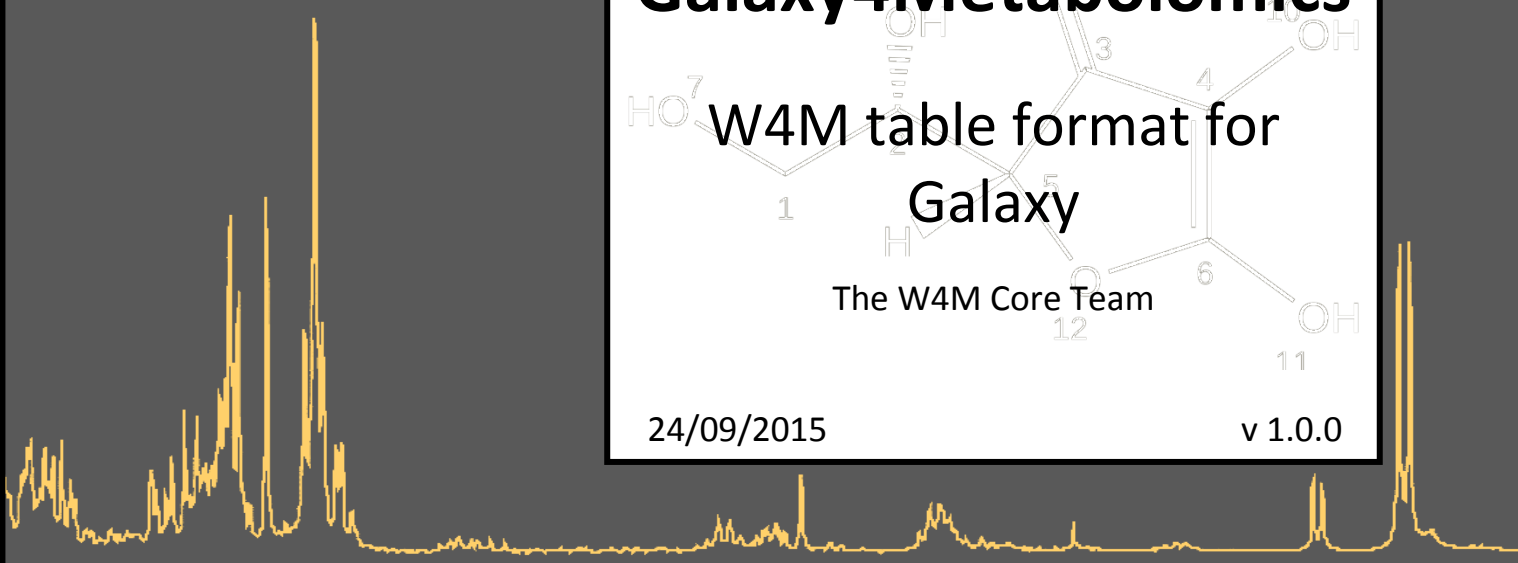
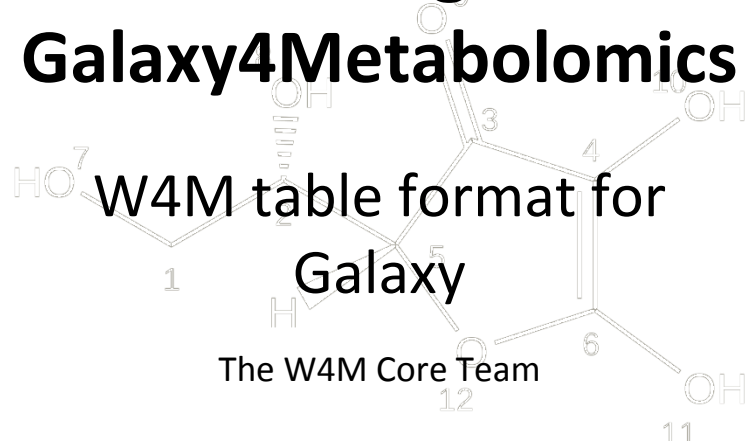
Using Galaxy4Metabolomics

W4M table format for Galaxy

The W4M Core Team

24/09/2015

v 1.0.0

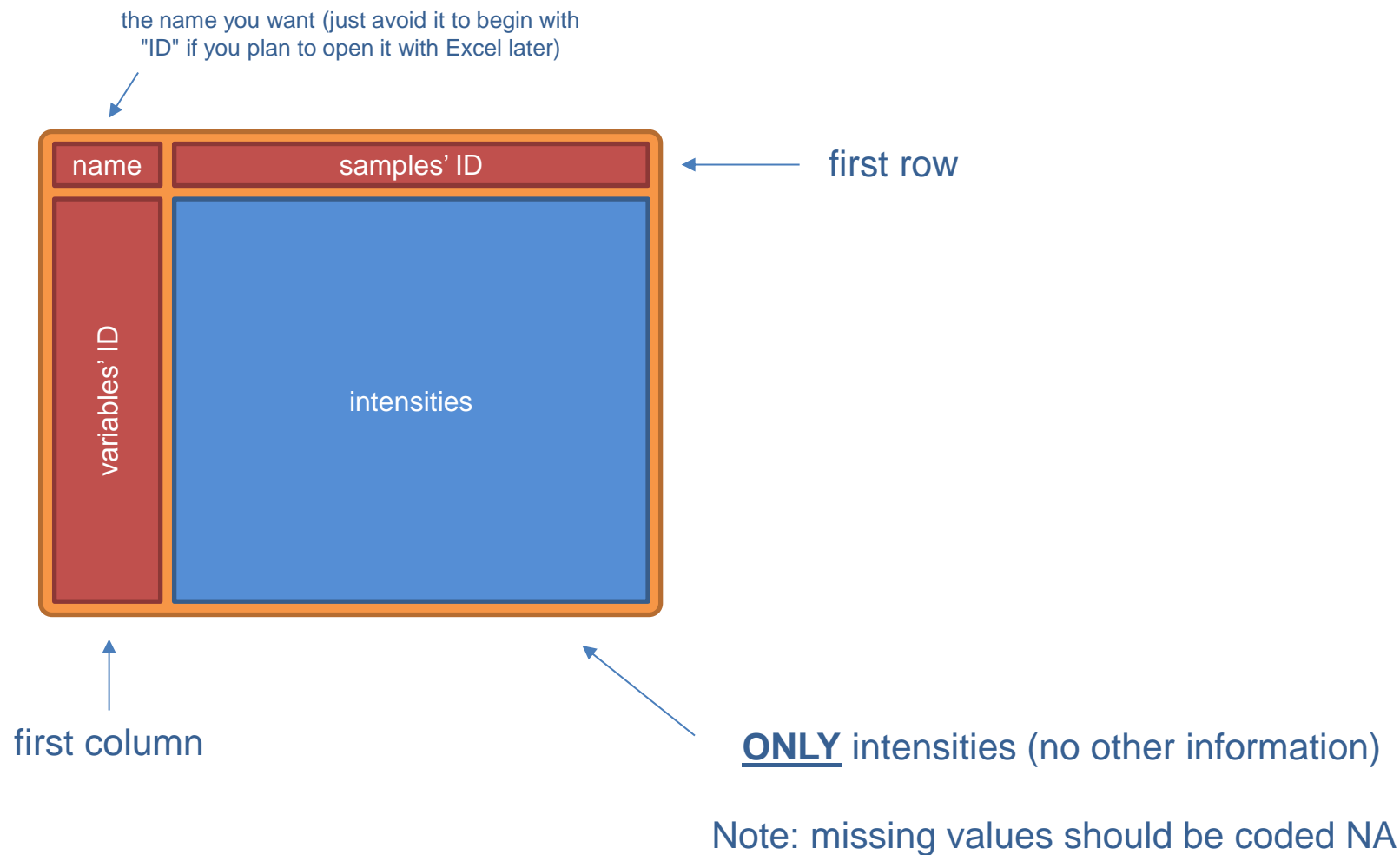


Global structure

- 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)

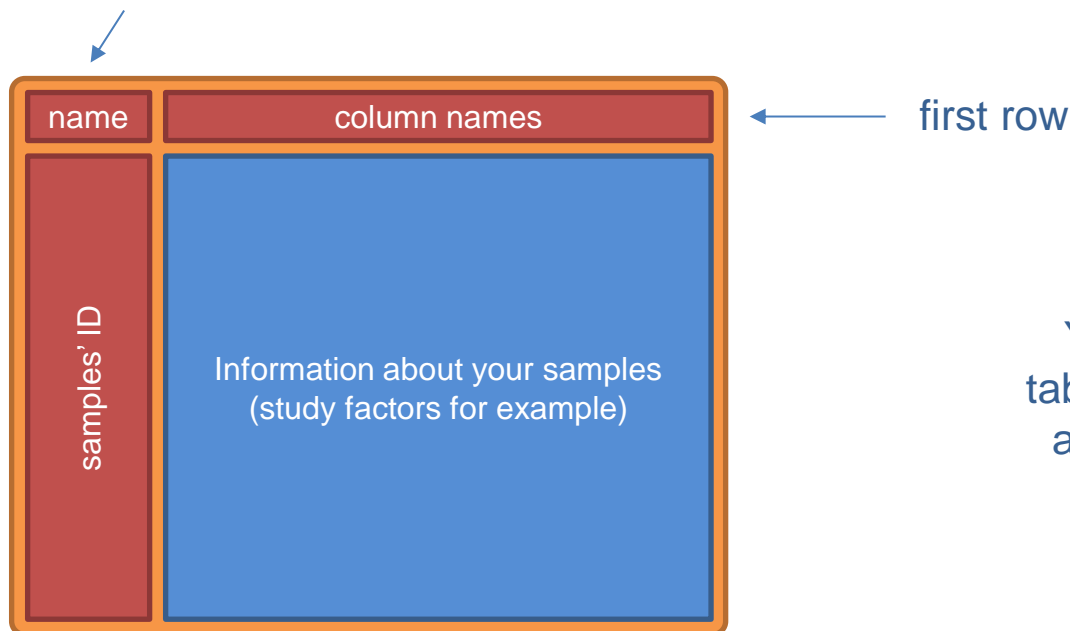


Data matrix



Sample metadata table

the name you want (just avoid it to begin with "ID" if you plan to open it with Excel later)



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

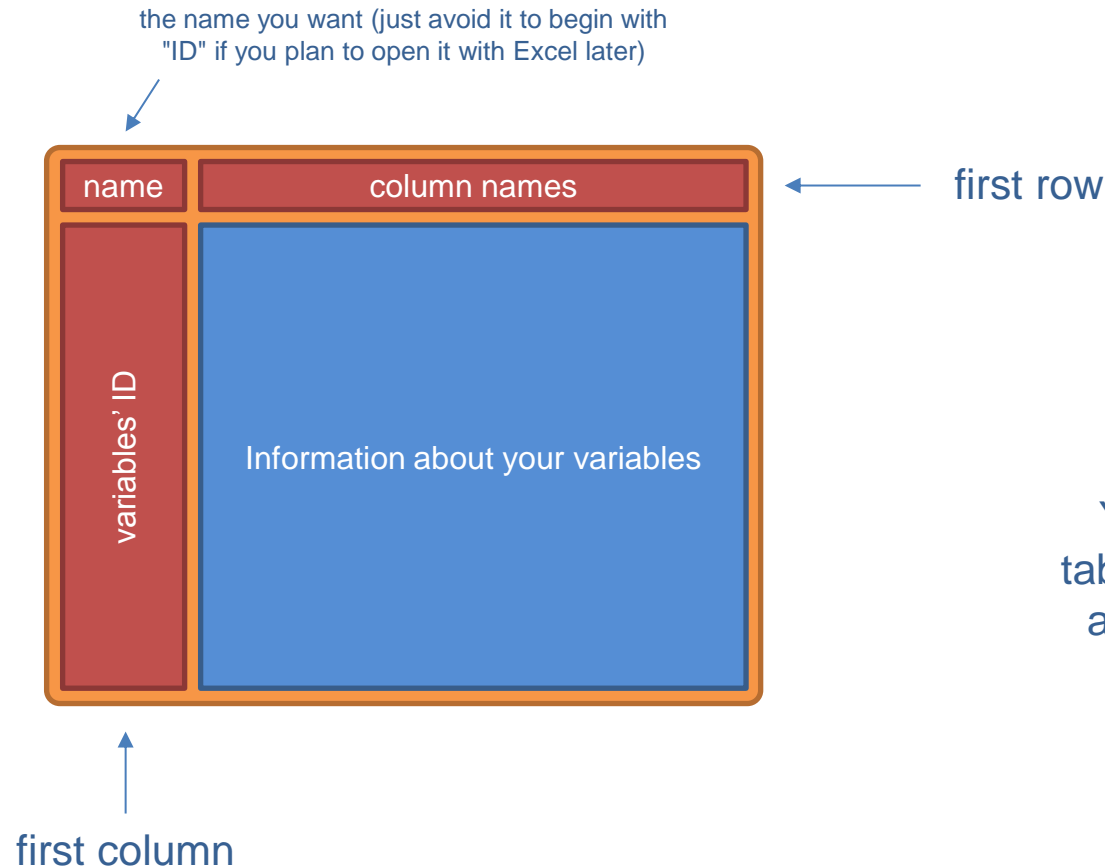
first column

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

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



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 displays the Galaxy 4 Metabolomics interface. The central panel shows the configuration for the **Generic_Filter** module (version 2014.12.11). The configuration includes three input file fields: **Data Matrix file:** 1: dataMatrix.txt, **Sample metadata file:** 2: sampleMetadata.txt, and **Variable metadata file:** 3: variableMetadata.txt. Below these are sections for filtering based on numerical and qualitative values, with an **Execute** button at the bottom.

On the right, the **History** panel shows a list of datasets. Three datasets are highlighted with a purple box and labeled as **Input files**: **3: variableMetadata.txt**, **2: sampleMetadata.txt**, and **1: dataMatrix.txt**. Three other datasets are highlighted with an orange box and labeled as **Output files**: **6: Generic_Filter_variableMetadata.txt**, **5: Generic_Filter_sampleMetadata.txt**, and **4: Generic_Filter_dataMatrix.txt**. Purple arrows point from the input files in the history to their respective fields in the module configuration.

A text box at the bottom right contains the following text:

The 3 tables as input files

The 3 tables filtered according to specified parameters as output files