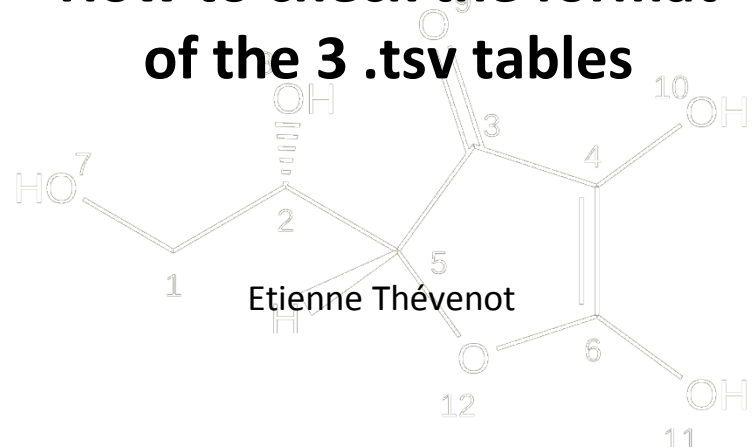




4 Wm

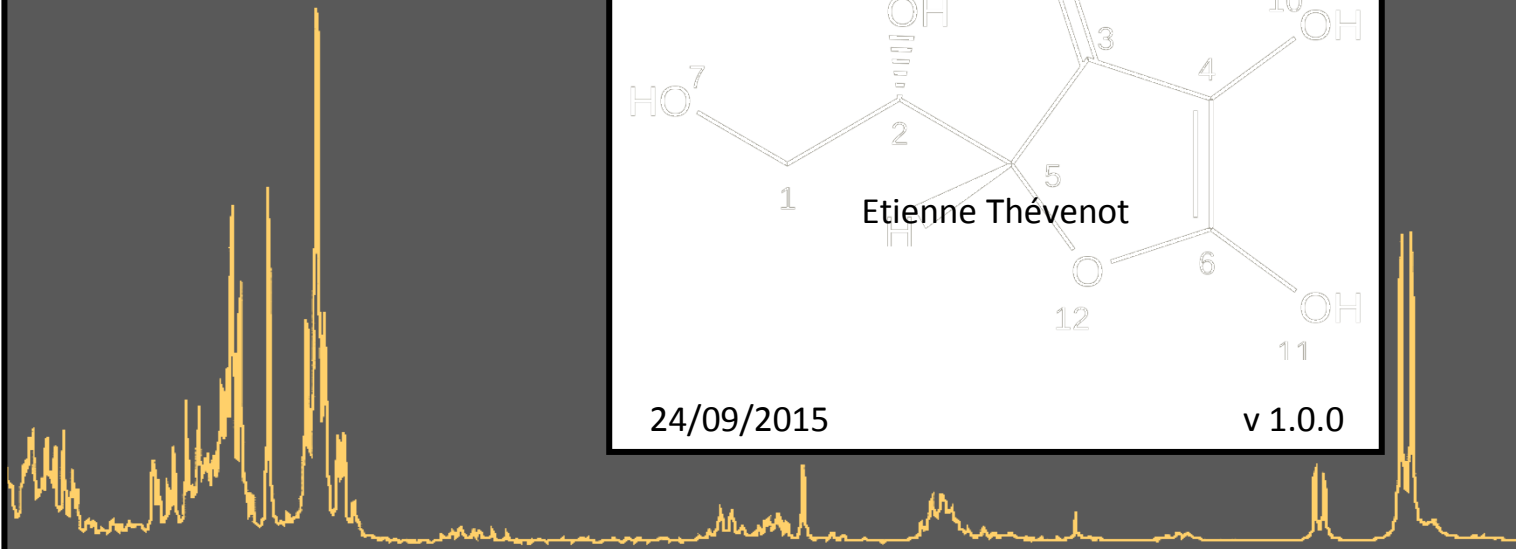
Workflow4metabolomics

How to check the format of the 3 .tsv tables




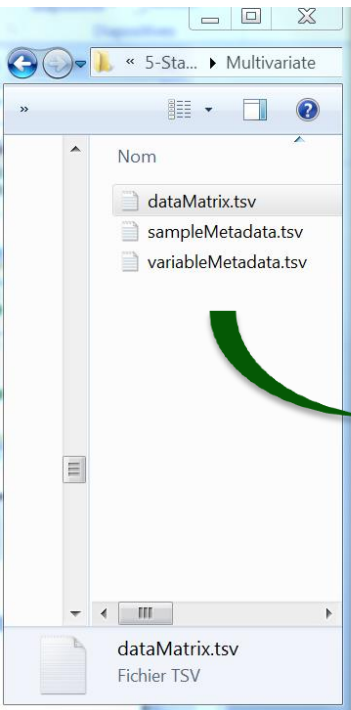
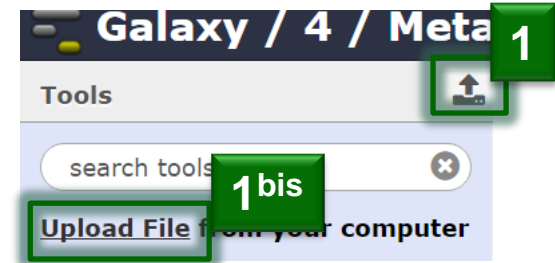
24/09/2015

v 1.0.0






Loading your files into Galaxy

- Upload your three files (dataMatrix.tsv, sampleMetadata.tsv and variableMetadata.tsv)
- either by using  or the "Upload File"
- and drag & dropping the file:



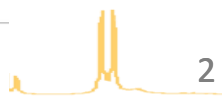
Galaxy / 4 / Metabolomics Workflow Shared Data Visualization Help User Us

Download data directly from web or upload files from your disk

Name	Size	Type	Genome	Settings	Status
 dataMatrix.tsv	2.5 KB	tabular	unspecified (?)		

You added 1 file(s) to the queue. Add more files or click 'Start' to proceed.

Choose local file Paste/Fetch data **Start** **3** Pause Reset Close



Check your data (1/2)

- With the 

Galaxy / 4 / Metabolomics

Analyze Data Workflow Shared Data Visualization Help User Using 2%

	msiLevel	hmdb	chemicalClass
(2-methoxyethoxy)propanoic acid isomer	2		Organi
(gamma)Glu-Leu/Ile	2		AA-pep
1-Methyluric acid	1	HMDB03099	AroHeP:Xenobi
1-Methylxanthine	1	HMDB10738	AroHeP
1,3-Dimethyluric acid	1	HMDB01857	AroHeP
1,7-Dimethyluric acid	1	HMDB11103	AroHeP
2-acetamido-4-methylphenyl acetate	2		AroHoM
2-Amino adipic acid	1	HMDB00510	AA-pep
2-Hydroxybenzyl alcohol	1	HMDB59709	AroHoM
2-Isopropylmalic acid	1	HMDB00402	Organi
2-Methylhippuric acid	1	HMDB11723	AA-pep:AcyGly
2,2-Dimethylglutaric acid	1		Lipids
3-Hydroxybenzyl alcohol	1	HMDB59712	AroHoM
3-Hydroxyphenylacetic acid	1	HMDB00440	AroHoM

Tools

search tools

Upload File from your computer

Export Data

LC-MS

Format Conversion

Preprocessing

Normalisation

Quality Control

Statistical Analysis

Univariate Univariate statistics


Multivariate PCA, PLS and

History

search datasets

Unnamed history

243.4 KB

3: variableMetadata.ts  View data

110 lines

format: tabular, database: ?

uploaded tabular file

1 2



- and with the Check Format module

The screenshot displays the Galaxy 4 Metabolomics interface. The top navigation bar includes 'Galaxy / 4 / Metabolomics', 'Analyze Data', 'Workflow', 'Shared Data', 'Visualization', 'Help', and 'User'. The 'Tools' panel on the left lists various categories: 'Upload File from your computer', 'Export Data', 'LC-MS', 'Format Conversion', 'Preprocessing', 'Normalisation', and 'Quality Control'. The 'Check Format' tool is highlighted in a green box. The main workspace shows the 'Check Format (version 2015.04.25)' tool configuration with three input fields: 'Data matrix file: 1: dataMatrix.tsv', 'Sample metadata file: 2: sampleMetadata.tsv', and 'Variable metadata file: 3: variableMetadata.tsv'. An 'Execute' button is visible below the inputs. The 'History' panel on the right shows a list of datasets: '3: variableMetadata.ts', '2: sampleMetadata.ts', and '1: dataMatrix.tsv'. The 'Check Format' tool description is shown below the configuration, stating it checks the format of the dataMatrix, sampleMetadata, and variableMetadata tables. The 'Workflow position' section shows the tool's placement in a workflow grid.

Tools

search tools

[Upload File from your computer](#)

[Export Data](#)

LC-MS

[Format Conversion](#)

[Preprocessing](#)

[Normalisation](#)

[Quality Control](#)

[ACP ellipsoid by factors](#)

[Metabolites Correlation Analysis](#)

[Generic Filter](#) Removes elements according to numerical or qualitative values

[Determine batch correction](#) to choose between linear, lowess and loess methods

Check Format Checks the formats of the dataMatrix, sampleMetadata, and variableMetadata files

Check Format (version 2015.04.25)

Data matrix file:

1: dataMatrix.tsv

Sample metadata file:

2: sampleMetadata.tsv

Variable metadata file:

3: variableMetadata.tsv

Execute

Author Etienne Thevenot (W4M Core Development Team, MetaboHUB Paris, CEA)

Check Format

Description

Checks the format (row and column names) of the dataMatrix, sampleMetadata and variableMetadata tables

Workflow position

Check Format

History

search datasets

Unnamed history
3 shown, 1 [deleted](#)

278.8 KB

3: variableMetadata.ts

2: sampleMetadata.ts

1: dataMatrix.tsv