

How to download your data from the 'old' Galaxy

<https://galaxy.workflow4metabolomics.org/>

## **GETTING YOUR DATA BACK**

# Step 1: delete unnecessary datasets

Delete datasets not needed in your workflow (e.g. wrong parameters)

**Galaxy / 4 / Metabolomics** Analyse de données Workflow Visualize Données partagées Aide Utilisateur Using 24.5 GB

**Tools** (search tools)

- Get Data
- LC-MS
- Preprocessing
- Normalisation
- Quality Control
- Statistical Analysis
- Annotation
- GC-MS
- Preprocessing
- Normalisation
- Quality Control
- Statistical Analysis
- Annotation
- NMR
- Preprocessing
- Normalisation
- Quality Control
- Statistical Analysis
- Annotation
- FLUXOMICS
- Isotopic Studies
- MS-MS
- msPurity
- COMMON TOOLS
- Data Handling
- Text Manipulation
- Filter and Sort

## Workflow4metabolomics

**Current version : 3.3**

**Publication:** Franck Giacomoni, Gildas Le Corguillé, Mishal Monsoor, Marion Landi, Pierre Pericard, Mélanie Pétéra, Christophe Dupierier, Marie Tremblay-Franco, Jean-François Martin, Daniel Jacob, Sophie Goullitquer, Etienne A. Thévenot and Christophe Caron (2014). *Workflow4Metabolomics: A collaborative research infrastructure for computational metabolomics*. *Bioinformatics* doi:10.1093/bioinformatics/btu813

**Help and support:** [support@workflow4metabolomics.org](mailto:support@workflow4metabolomics.org)  
**Password manager:** [Forgot your password? or change it!](#)

**Changelog**

- 3.3.4 - 2020-02-14
  - LCMS
    - **UPGRADE** - xcms.\* (3.6.1): upgrade the xcms version from 3.4.4 to 3.6.1
- 3.3.3 - 2020-01-31
- 3.3.2 - 2019-10-22
- 3.3.1 - 2019-09-16
- 3.3.0 - 2019-06-06
- 3.2.1 - 07/03/2019
- 3.2.0 - 19/09/2018
- 3.0.0 - 20/04/2017
- 2.5.1 - 09/03/2016
- 2.5.0 - 24/02/2016
- 2.4.3 - 10/02/2016

**History** (Rechercher des données)

**LCMSextraction**  
27 shown, 5 deleted, 36 hidden  
1.04 GB

- 68: Test5 conclusive\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.quick.Rdata
- 67: Test5 conclusive\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.variableMetadata.tsv
- 61: Test4\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.quick.Rdata
- 60: Test4\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.variableMetadata.tsv
- 59: Test3\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.dataMatrix.tsv
- 58: Test3\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.variableMetadata.tsv
- 57: Test3\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.Rdata
- 56: xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.annotate.dataMatrix.tsv

# Step 2: Extract the workflow from your history

## 1- History options

History

Rechercher des données

History options

LCMSextraction

23 shown, 9 deleted, 36 hidden

1.04 GB

68: Test5\_conclusive\_xs et.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.quick.Rdata

67: Test5\_conclusive\_xs et.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.variable.tsv

57: xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.RData

56: xset.merged.groupChromPeaks.adjustRtime.group.dataMatrix.tsv

55: xset.merged.groupChromPeaks.adjustRtime.group.variableMetadata.tsv

54: xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.plotChromPeakDensity.pdf

53: xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.RData

52: BPIs.pdf

51: TICs.pdf

50: xset.merged.groupChromPeaks.rawVSadjustedRtime.RData

TABLEAUX DES HISTORIQUES

- Historiques sauvegardés
- Historiques partagés avec moi
- CET HISTORIQUE
- Créer un nouveau
- Copier l'Historique
- Partager et publier
- Montrer la structure
- Extraire un Workflow
- Supprimer
- Supprimer définitivement

## 2- 'Extract workflow'

Permissions/Sécurité

- Reprendre les processus en pause
- Réduire les données étendues
- Afficher les données cachées
- Supprimer les données cachées
- Purger les données supprimées

TÉLÉCHARGER

- Exporter les citations des outils
- Exporter l'Historique dans un fichier

AUTRES ACTIONS

- Importer depuis un fichier

53: xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.RData

52: BPIs.pdf

51: TICs.pdf

50: xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.RData

## 3- Customise your workflow name

## 4- 'Create Workflow'

Workflow name

Workflow constructed from history: LCMSextraction

Create Workflow Check all Uncheck all

Tool

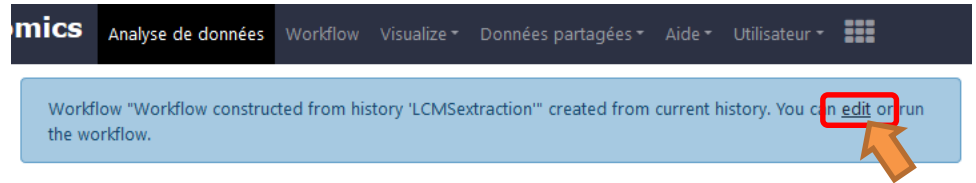
- Dataset Collection Creation  
*Dataset collection created in a way not compatible with workflows*
- MSnbase readMSData  
 Include "MSnbase readMSData" in workflow
- xcms get a sampleMetadata file  
 Include "xcms get a sampleMetadata file" in workflow
- Upload File  
*This tool cannot be used in workflows*
- xcms plot chromatogram  
 Include "xcms plot chromatogram" in workflow
- xcms findChromPeaks (xcmsSet)  
 Include "xcms findChromPeaks (xcmsSet)" in workflow

History items created

- 10 sacurine  
 Treat as input dataset
- 11 sacurine.raw.RData
- 21 sampleMetadata.tsv
- 22 sampleMetadata\_completed.tsv  
 Treat as input dataset
- 23 TICs.pdf
- 24 BPIs.pdf
- 25 sacurine.raw.xset.RData
- 26 sacurine.raw.xset.log.txt

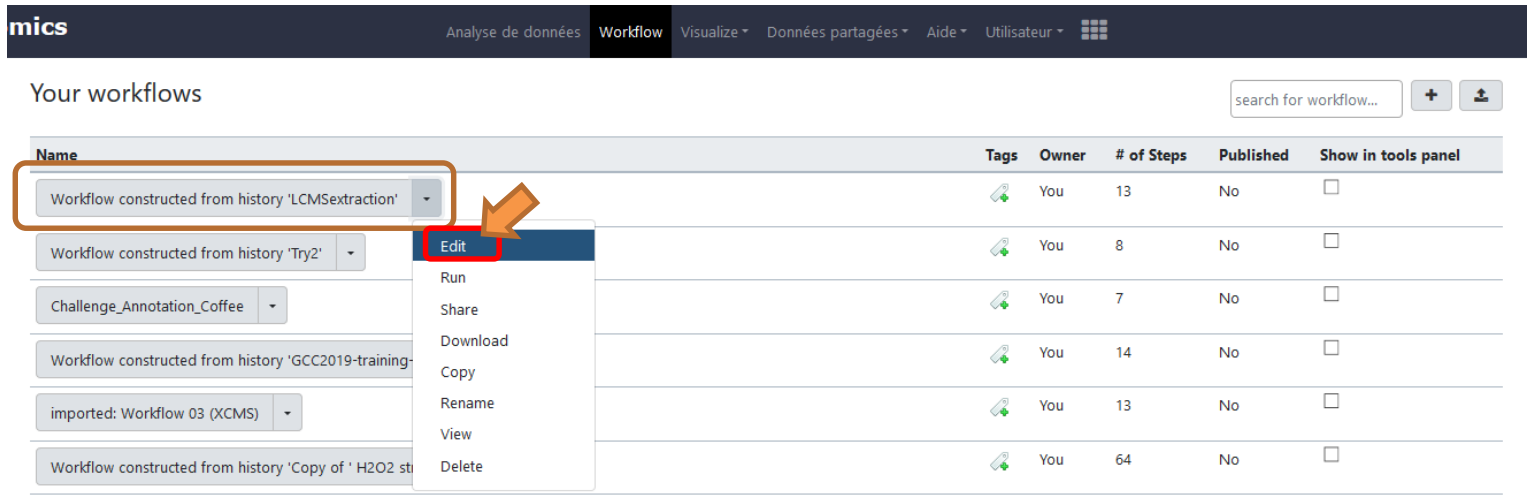
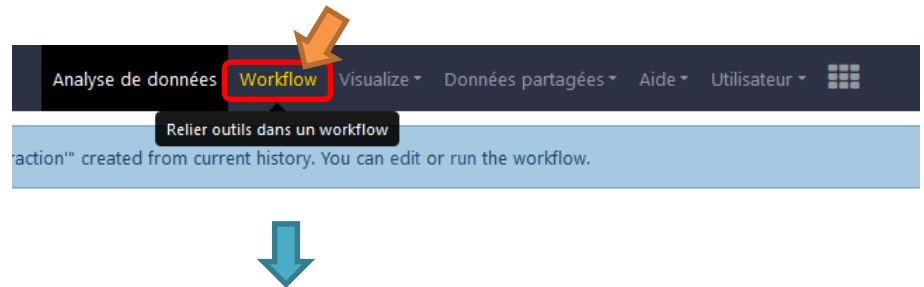
# Step 3: Check your workflow (1)

Access the workflow created by clicking on 'Edit'



OR

Access the workflow created by accessing the 'Workflow' section



# Step 3: Check your workflow (2)

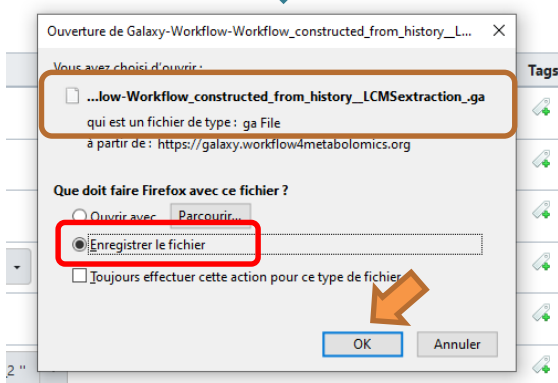
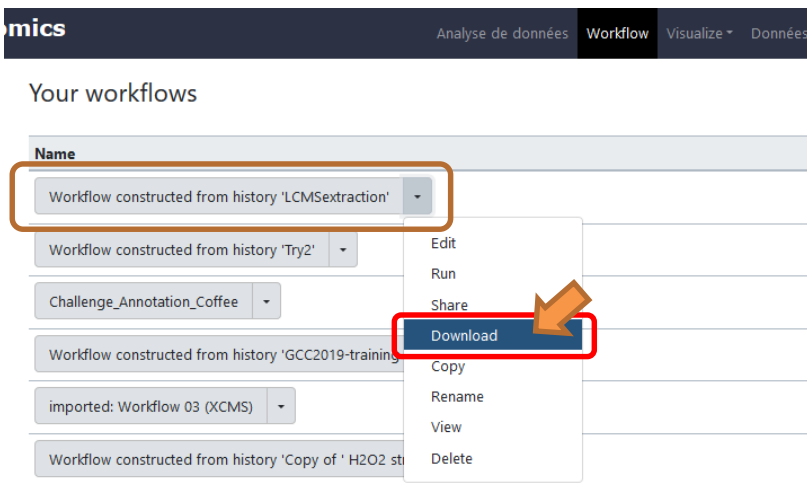
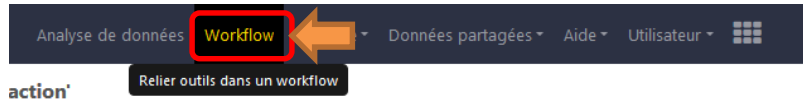
Check that your workflow is complete and no box is alone (at least one link to another box).  
In case of anomaly, check your **history** to identify the issue, solve it and extract again.

The screenshot displays the Workflow4Metabolomics software interface. The main window shows a workflow titled "Workflow constructed from history 'LCMSextraction'". The workflow consists of several interconnected steps:

- Input dataset collection**: Provides an "output" box.
- MSnbase readMSData**: Takes "File(s) from your history containing your chromatograms" and outputs "xsetRData (rdata.msbase.raw)", "sampleMetadata (tabular)", and "sampleMetadata\_complete.tsv".
- xcms get a sampleMetadata file**: Takes "sampleMetadata.tsv (tabular)" and outputs "RData file" and "sampleMetadata.tsv (tabular)".
- xcms findChromPeaks**: Takes "RData file" and "List of regions-of-interest (ROI) representing detected mass traces" and outputs "xsetRData (rdata.xcms.findchrompeaks)", "xsetRData (rdata.xcms.findchrompeaks)", and "log (txt)".
- xcms findChromPeaks Merger**: Takes "RData file" and "Sample metadata file" and outputs "xset.merged.RData (rdata.xcms.findchrompeaks)", "xset.merged.sampleMetadata.tsv (tabular)", and "xset.merged.sampleMetadata.tsv (tabular)".
- xcms plot chromatogram**: Takes "RData file" and "Sample metadata file" and outputs "TICs.pdf (pdf)", "BPIs.pdf (pdf)", and "BPIs.pdf (pdf)".
- xcms adjustTime (retcor)**: Takes "RData file" and "xsetRData (rdata.xcms.retcor)" and outputs "rawVAdjustedPdf (pdf)".
- xcms groupChromPeaks (group)**: Takes "RData file" and "xsetRData (rdata.xcms.group)" and outputs "plotChromPeakDensity (pdf)", "variableMetadata (tabular)", and "dataMatrix (tabular)".
- xcms fillChromPeaks (fillPeaks)**: Takes "RData file" and "xsetRData (rdata.xcms.fillpeaks)" and outputs "variableMetadata (tabular)" and "dataMatrix (tabular)".
- xcms plot chromatogram**: Takes "RData file" and "Sample metadata file" and outputs "TICs.pdf (pdf)", "BPIs.pdf (pdf)", and "BPIs.pdf (pdf)".
- xcms CAMERA.annotate**: Takes "RData file" and "variableMetadata (tabular)" and outputs "rdata\_quick\_true (rdata.camera.quick)".

The right-hand side of the interface shows the "Details" panel for the selected "xcms groupChromPeaks (group)" step. It includes a description: "(group) Perform the correspondence, the grouping of chromatographic peaks within and between samples. (Galaxy Version 3.4.4.0)". It also features a "Label" field, an "Annotation" field, and a "Method to use for grouping" dropdown menu set to "PeakDensity - peak grouping ba...". A "Bandwidth" slider is set to 5.0, with a description: "bandwidth (standard deviation or half width at half maximum) of gaussian smoothing kernel to apply to the peak density chromatogram (bw)".

# Step 4: Download your workflow



1- Go back to the 'Workflow' section

2- 'Download' your workflow

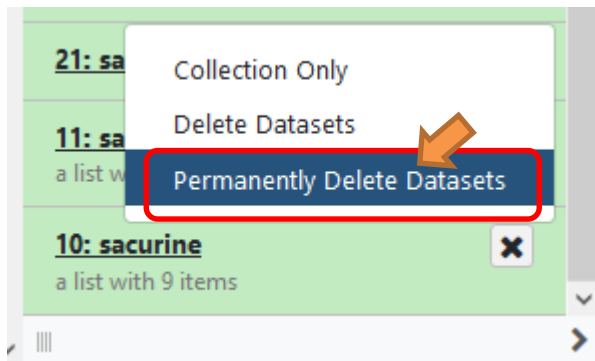
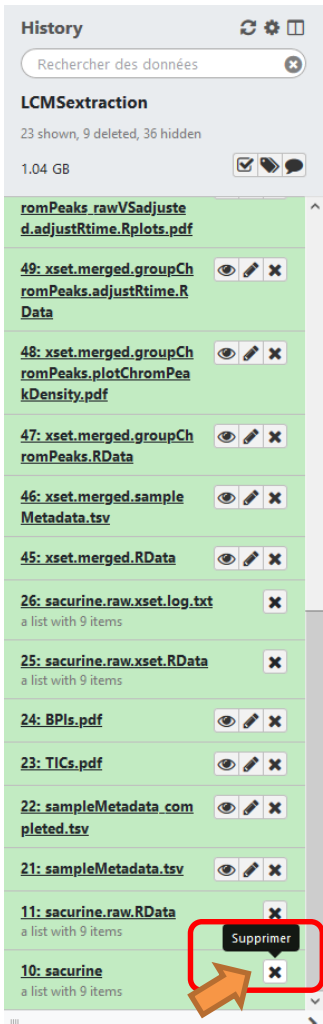
3- Save the file on your computer

This archive file contains the information about the jobs constituting your workflow. Keep it if you need to be able to access the parameters' information in the future.

# Step 5: Clean the raw data (if any)

Raw data (e.g. ‘.mzML’ files in MS) is data you originally uploaded. It has a large size and you already have these files outside from Galaxy. Keeping it in the history you want to download is irrelevant.

If you have any of this kind of data in your history, delete it.



This step deletes **permanently** your dataset collection.

If you are not sure whether your raw data is easily retrievable in your laboratory, **check before proceeding**.

If necessary, remember that you can download the raw files separately **before** doing this cleaning step.



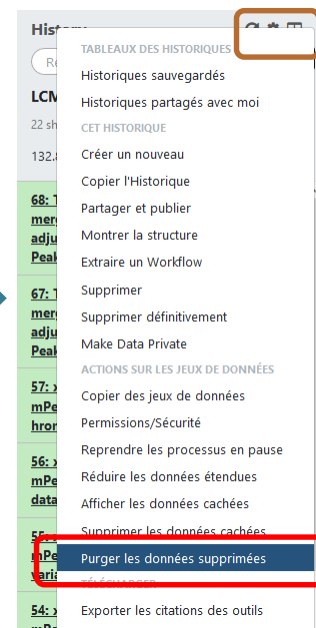
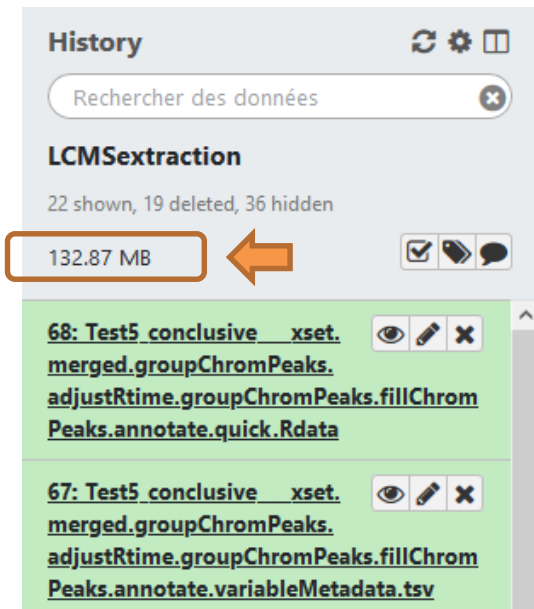
# Step 6: Check the size of your history

You are going to download a potentially large file to get you data files out from Galaxy at once. If your history is huge, the download process may be too long.

Check the size of your history.

- If the size is < 2 Go: you can proceed to the next step
- If the size is > 2 Go:

- You may have large files that have been deleted but not permanently. You can choose to **purge your deleted datasets** and check again your history size. (!/! deleted datasets will be deleted **permanently**)
- If your history still is too large, you need to 'cut' your history in several parts: define groups of datasets (you can use dataset numbers to help) and proceed to the next step **for each of these groups**.



# Step 7: Create a dataset collection

History

Rechercher des données

LCMSextraction

22 shown, 19 deleted, 36 hidden

132.87 MB

Opérer sur plusieurs jeux de données en même temps

68: Test5\_conclusive\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.quick.Rdata

67: Test5\_conclusive\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.variableMetadata.tsv

Activate multiple selection



History

Rechercher des données

LCMSextraction

22 shown, 19 deleted, 36 hidden

132.87 MB

Opérer sur plusieurs jeux de données en même temps

Tout Aucun Pour toute la sélection...

68: Test5\_conclusive\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.quick.Rdata

67: Test5\_conclusive\_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.variableMetadata.tsv

Select all datasets



History

Rechercher des données

LCMSextraction

22 shown, 19 deleted, 36 hidden

132.87 MB

Tout Aucun Pour toute la sélection...

Cacher les jeux de données

Afficher les jeux de données cachés

Supprimer les jeux de données

Restaurer les jeux de données supprimés

Supprimer définitivement les jeux de données

Build Dataset List

Build Dataset Pair

Build List of Dataset Pairs

Build Collection from Rules

56: xset.merged.groupChromPeaks.adjustRtime.group.dataMatrix.tsv

55: xset.merged.groupChromPeaks.adjustRtime.group.variableMetadata.tsv

Create a collection from a list of datasets

Collections of datasets are permanent, ordered lists of datasets that can be passed to tools and workflows in order to have analyses done on each member of the entire group. This interface allows you to create a collection and re-order the final collection...

Start over

Test5_conclusive_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.quick.Rdata	Discard
Test5_conclusive_xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.annotate.variableMetadata.tsv	Discard
xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.fillChromPeaks.RData	Discard
xset.merged.groupChromPeaks.adjustRtime.group.dataMatrix.tsv	Discard
xset.merged.groupChromPeaks.adjustRtime.group.variableMetadata.tsv	Discard
xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.plotChromPeakDensity.pdf	Discard
xset.merged.groupChromPeaks.adjustRtime.groupChromPeaks.RData	Discard
BPIs.pdf	Discard
TICs.pdf	Discard
xset.merged.groupChromPeaks_rawVSadjusted.adjustRtime.Rplots.pdf	Discard
xset.merged.groupChromPeaks.adjustRtime.RData	Discard
xset.merged.groupChromPeaks.plotChromPeakDensity.pdf	Discard

Hide original elements?



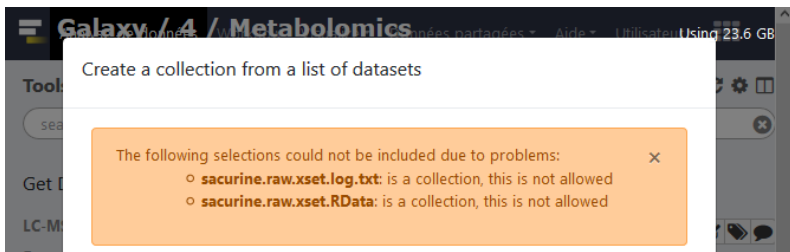
Cancel

Name: MyHistoryCollection

Create list

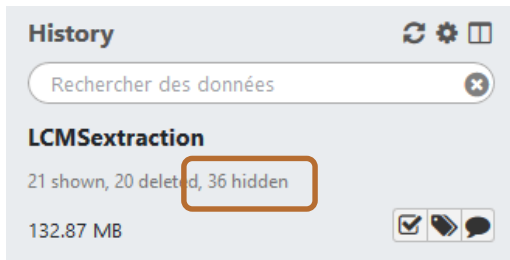
# Note: case of already existing dataset collections

Already existing dataset collections can not be included in another dataset collection.



If you already have other dataset collections, you can either:

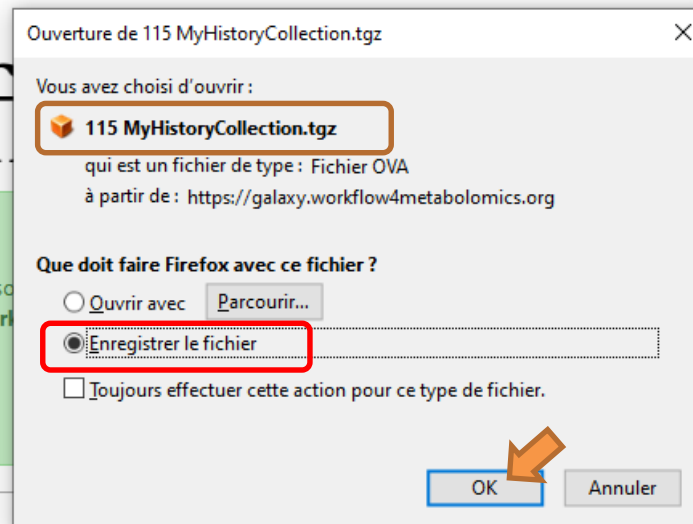
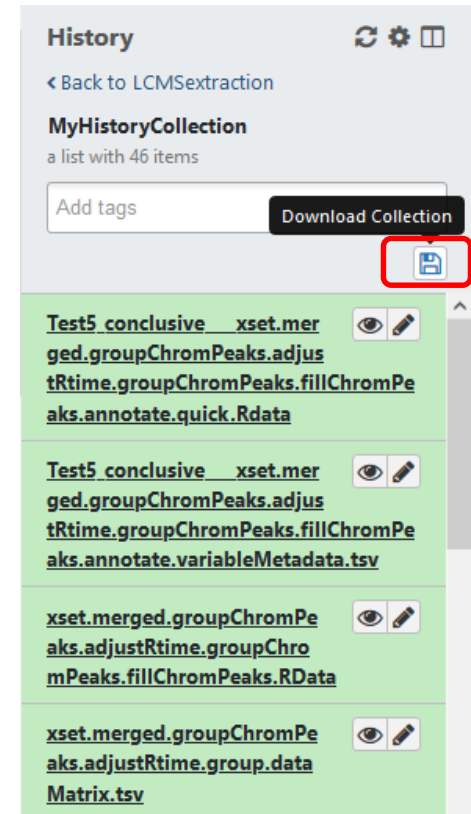
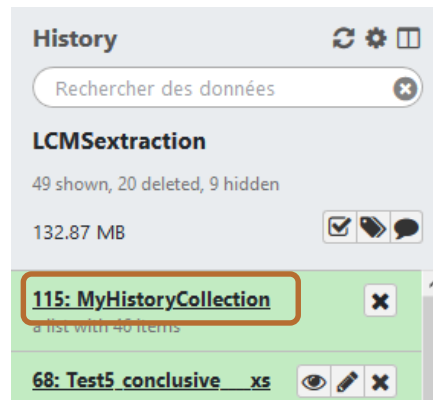
- download them independently (see next step)
- include corresponding datasets in the previous one by 'unhiding' corresponding datasets if hidden



⚠ If you choose the 'unhiding' strategy, proceed to it **before** doing step 7

# Step 8: Download the dataset collection

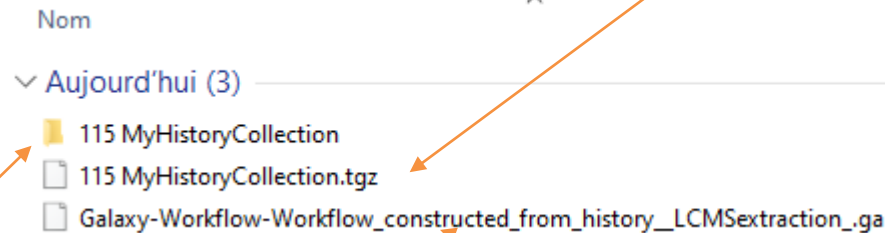
Click on the name of your dataset collection



This archive file contains all the files of the dataset collection. You can unzip the archive to get the individual files.

# Your downloaded data

Archive containing your history files



Unzip folder of you  
history files

Archive containing the workflow  
(information about jobs)

## Notes about unzipping your history folder

- ❖ To unzip the archive obtained by downloading your history dataset collection, you need a dedicated software on your computer.  
If you do not have one, you can download the free software « **7-zip** »
- ❖ Please note that the Windows-built-in unzipping solution may not handle correctly this kind of archive.

# Notes concerning XCMS histories (1)

Want to gather all your XCMS parameters in a row?

→ Do not forget to run the '*xcms\_process\_history*' tool on the last step of your XCMS workflow! (before constructing your dataset collection to include it in the archive)

**Note:** If you are interested in keeping a trace of your XCMS parameters only, the HTML file generated by this tool can replace the workflow extraction regarding traceability.

**Galaxy / 4 / Metabolomics** Analyse de données Workflow Visualize Données partagées Aide Utilisateur Using 23.6 GB

**Tools**  
search tools

Get Data  
LC-MS  
Preprocessing  
**xcms\_process\_history** Create a summary of XCMS analysis

**XCMS analysis summary using Workflow4Metabolomics**  
By: melanie.petera@clermont.inra.fr - Date: 200612-16:38:27

**Samples used:**

sample	filename	md5sum*
QC1_014	QC1_014.mzML	cb133446f5137d0cf50ad9709f9c55f7
QC1_008	QC1_008.mzML	881d4e94b0de1f6aa7ae931e897348c8
QC1_002	QC1_002.mzML	77cf3c9ed4a9c00d05ec83308f69d6e
HU_neg_192	HU_neg_192.mzML	e1e50308e9c440d885e8530302a1e2a2
HU_neg_173	HU_neg_173.mzML	5a23e8996d4cb5d020c3399f9fad044e
HU_neg_157	HU_neg_157.mzML	5f60b7526c5dbf93972cfe1941739c2c
HU_neg_123	HU_neg_123.mzML	79b4ca15faab323ebd6608c5427b5448
HU_neg_090	HU_neg_090.mzML	b609cb66b0cd926a833d63cf5c529622
HU_neg_048	HU_neg_048.mzML	9e093906811d11c0b14de7a9c2171a75

\*The program md5sum is designed to verify data integrity. So you can check if the data were uploaded correctly or if the data were changed during the process.

**Function launched:**

timestamp***	function	argument	value
Wed Jun 26 17:52:30 2019	Peak detection	Object of class: CentWaveParam Parameters: ppm: 3 peakwidth: 5, 20 snthresh: 10 prefilter: 3, 5000 mzCenterFun: wMean integrate: 1 mzdiff: -0.001 fitgauss: FALSE noise: 1000 verboseColumns: FALSE roiList length: 0 firstBaselineCheck TRUE roiScales length: 0	

**History**  
Rechercher des données

**LCMSExtraction**  
50 shown, 22 deleted, 55 hidden  
132.87 MB

118: xcms summary.html  
115: MyHistoryCollection  
68: Test5 conclusive\_xs  
67: Test5 conclusive\_xs  
57: xset.merged.groupChromPeaks.adjustTime.groupChromPeaks.fillChromPeaks.Rdata  
56: xset.merged.groupChromPeaks.adjustTime.group.dataMatrix.tsv  
55: xset.merged.groupChromPeaks.adjustTime.group.variableMetadata.tsv  
54: xset.merged.groupChromPeaks.adjustTime.groupChromPeaks.plotChromPeakDensity.pdf  
53: xset.merged.groupChromPeaks.adjustTime.gr

# Notes concerning XCMS histories (2)

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Most XCMS histories contain **dataset collections** for the first steps of the extraction process ('Msnbase\_readMSData', 'xcms\_findChromPeaks\_(xcmsSet)').

As explained previously you can either *download these collections individually* or include them in the overall dataset collection by *unhiding the concerned data files beforehand*.

Please note that these dataset collections contain **one file per sample in each collection**. This can easily leads to a **huge number of files in the archive** if you choose the 'unhiding datasets' option.

- If your main objective is to download the file in a storage goal, you may consider using the 'unhiding' option.
- Otherwise, individual downloads of these collections may be the best option.

# Notes concerning XCMS histories (3)

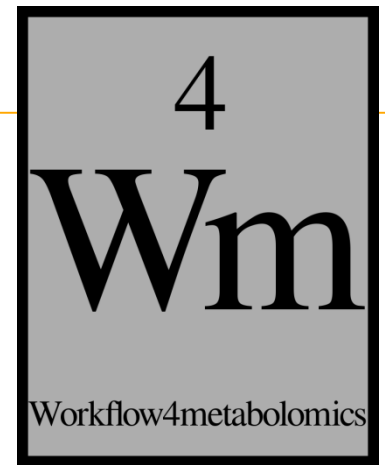
As previously mentioned, **raw data** (.mzML, .mzXML, .cdf...) is **not meant to be downloaded from Galaxy** as it was not generated by Galaxy. Since you uploaded it in the first place, you should be able to find the data elsewhere.

*If for any reason you still need to download the data from Galaxy, please note that the files' extension you will get will be 'doubled' compared to the original files. For example, a file originally named 'Myrawdata1.mzML' will get que name 'Myrawdata1.mzML.mzml'. Thus, if you want your files to match your sampleMetadata table, you will need to get rid of the added '.mzml' extension first.*

## Can't find out where your raw data is? Adopt the **Metabolights** attitude!

- ❖ Such data repositories combine the advantage of (i) storing your data with easy access and DOI and (ii) promoting open-science by going one step further to FAIR.
- ❖ Metabolights is the reference data repository in the metabolomics community. Find out more about it here: <https://www.ebi.ac.uk/metabolights/>
- ❖ W4M highly promotes FAIR practices. **Tip: in Galaxy we provide a downloader enabling data retrieval directly from Metabolights!**

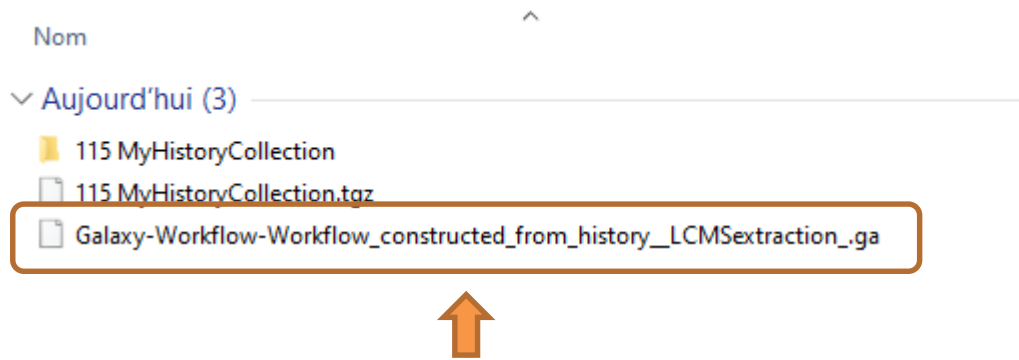




This step is highly recommended, **at least to check that your workflow can be imported smoothly** in the new *workflow4metabolomics.usegalaxy.fr* instance

## **PUTTING YOUR DATA BACK INTO GALAXY**

# Step 1: the workflow archive



Make sure you have your workflow archive on your computer

# Step 2: Go to the 'Workflow' section

## 1 - Log in workflow4metabolomics.usegalaxy.fr

If you have not got an account yet, you can create one (auto-registration)

## 2 – Go to the 'Workflow' section

The screenshot shows the Galaxy Workflow4Metabolomics interface. At the top, the navigation bar includes 'Galaxy / Workflow4Metabolomics' and several menu items: 'Analyse de données', 'Workflow' (highlighted with a red box and an orange arrow), 'Visualize', 'Données partagées', 'Aide', and 'Utilisateur'. Below the navigation bar, there is a search bar for tools and a list of tool categories on the left side, including 'Get Data', 'Collection Operations', 'Text Manipulation', and various 'Preprocessing' and 'Quality processing' tools. The main content area features the 'Workflow4metabolomics' logo and title, a 'Term Of Use' notice, a tweet from @galaxyproject, and a 'Current version: 3.3' section with publication details.

# Step 3: Import your workflow

Workflow4metabolomics

Analyse de données Workflow Visualize Données partagées Aide Utilisateur

Search Workflows

+ Create Import

Name	Tags	Created	Bookmark
Challenge_Annotation_Coffee (imported from uploaded file)		11 days ago	
'Challenge_Annotation'		2 months ago	
wf test ceci est un test		3 months ago	
Workflow imported: SGA20 etat des lieux_part		3 months ago	
imported: Mass spectrometry: LC-MS analysis		3 months ago	

### Import Workflow

Please provide a Galaxy workflow export URL or a workflow file.

Archived Workflow URL

If the workflow is accessible via a URL, enter the URL above and click Import.

Archived Workflow File

No file chosen Browse

If the workflow is in a file on your computer, choose it and then click Import.

Import workflow

Import a Workflow from myExperiment

Visit myExperiment

Click the link above to visit myExperiment and search for Galaxy workflows.

### Import Workflow

Please provide a Galaxy workflow export URL or a workflow file.

Archived Workflow URL

If the workflow is accessible via a URL, enter the URL above and click Import.

Archived Workflow File

Galaxy-Workflow-Workflow\_constructed\_from\_history\_LCMSextraction\_ga Browse

If the workflow is in a file on your computer, choose it and then click Import.

Import workflow

Import a Workflow from myExperiment

Visit myExperiment

Click the link above to visit myExperiment and search for Galaxy workflows.

### Envoi du fichier

Ce PC > Téléchargements

Organiser Nouveau dossier

Choose your workflow archive

- Aujourd'hui (3)
  - 115 MyHistoryCollection... 09/06/2020 19:24
  - Galaxy-Workflow-Workflow\_constructed\_from\_history\_LCMSextraction\_ga 09/06/2020 17:48
  - 115 MyHistoryCollection 09/06/2020 19:31
- Le mois dernier (7)
- Plus tôt cette année (75)
- Il y a longtemps (7)

Nom du fichier: Galaxy-Workflow-Workflow\_constructed\_from\_history\_ Tous les fichiers

Ouvrir Annuler

# Your workflow is ready to be used!

Metabolomics

Analyse de données Workflow Visualize Données partagées Aide Utilisateur

Search Workflows + Create Import

Name	Tags	Created	Bookmark
Workflow constructed from history 'LCMSextraction' (imported from uploaded file)		a few seconds ago	<input type="checkbox"/> <span>▶</span>
Challenge_Annotation_Coffee (imported from uploaded file)		11 days ago	<input type="checkbox"/> <span>▶</span>
'Challenge_Annotation'		2 months ago	<input type="checkbox"/> <span>▶</span>
wf test ceci est un test		3 months ago	<input type="checkbox"/> <span>▶</span>
Workflow imported: SGA20 etat des lieux_part		3 months ago	<input type="checkbox"/> <span>▶</span>
imported: Mass spectrometry: LC-MS analysis		3 months ago	<input type="checkbox"/> <span>▶</span>

You can either:

- ❖ View it to get access to the jobs and parameters you used
- ❖ Use it to relaunch your analysis – in a new history, simply upload from your computer the input data needed, then run the workflow on these data

# Workflow troubleshooting (1)

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*'I have never used workflows before. How do I recreate my history in the new instance?'*

As mentioned previously, all you need to do is to **upload the input data needed** for your workflow (e.g. in case of XCMS your raw data and the completed sampleMetadata file) in a new history, and then to **launch the workflow** using it.

If you are not familiar with how to launch a workflow, you can find out how following the **'Galaxy 101' GTN tutorial**:  
<https://galaxyproject.github.io/training-material/topics/introduction/tutorials/galaxy-intro-101-everyone/tutorial.html>

You can focus on the **'Galaxy management'** chapter.

# Workflow troubleshooting (2)

*'It seems I can not import all my workflow in the new galaxy instance... What should I do?'*

There are two configurations that you might run into while facing workflow import issues:

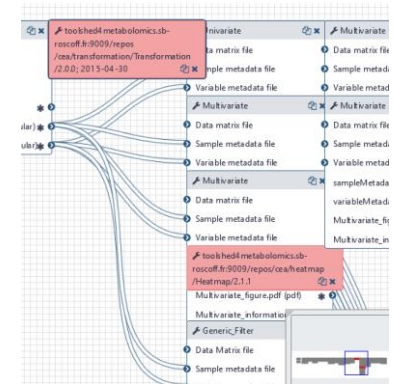
- The tool is missing – you get 'red boxes' in your workflow

While trying running it:

Following tools missing: toolshed4metabolomics.sb-roscoff.fr:9009/repos/cea/transformation/Transformation/2.0.0; 2015-04-30, toolshed4metabolomics.sb-roscoff.fr:9009/repos/cea/heatmap/Heatmap/2.1.1

While trying editing it:

- Step 13: toolshed4metabolomics.sb-roscoff.fr:9009/repos/cea/transformation/Transformation/2.0.0; 2015-04-30
  - Tool is not installed



- The tool exists however the version that have been used is not available – the tool box is displayed in your workflow but with default parameter values

While trying running it:

Some tools in this workflow may have changed since it was last saved or some errors were found. The workflow may still run, but any new options will have default values. Please review the messages below to make a decision about whether the changes will affect your analysis.

While trying editing it:

- Step 7: xcms fillChromPeaks (fillPeaks)
  - No value found for 'Convert retention time (seconds) into minutes'. Using default: 'False'.
  - No value found for 'Reported intensity values'. Using default: 'into'.

If you run into one of these issues, please visit the “Troubleshooting – Workflows” post on the IFB forum for more information <https://community.france-bioinformatique.fr/t/troubleshooting-workflows/615>

# Workflow troubleshooting (3)

*'I relaunched my workflow but I do not see resulting jobs in my history. What should I do?'*

It sometimes happens that while using imported workflows, job outputs appear as 'hidden datasets' in your history. To put it back to standard display, you simply need to select concerned datasets and to unhide them.

The sequence of screenshots illustrates the process of un hiding hidden datasets:

- Initial State:** The 'History' panel shows 'My\_relaunched\_history\_from\_workflow' with '3 shown, 55 hidden' datasets. A red box highlights this status, and an arrow points to the settings gear icon.
- Opening Menu:** The settings gear icon is clicked, opening a 'History Actions' menu. A red box highlights the gear icon, and an arrow points to the 'Afficher les données cachées' option.
- Selecting Action:** The 'Afficher les données cachées' option is selected in the menu. A red box highlights this option, and an arrow points to it. A text box 'Unhide hidden datasets' is placed below the menu.
- Confirmation:** A dialog box asks 'Really unhide all hidden datasets?' with 'OK' and 'Annuler' buttons. A red box highlights the 'OK' button, and an arrow points to it.
- Final State:** The 'History' panel now shows '82 shown, 3 hidden' datasets, indicating that the hidden datasets have been successfully un hidden.



# See you on W4M!

Website:

<https://workflow4metabolomics.org/>

Galaxy instance:

<https://workflow4metabolomics.usegalaxy.fr/>

Need some help?

<https://community.france-bioinformatique.fr/c/workflow4metabolomics/10>

