

➤ TP Conversion de fichiers

Binta Diémé, IR biologiste en analyse de données, PFEM



1

Download from web or upload from disk

Regular

Composite

Collection

2 Rule-based

You added 2 file(s) to the queue. Add more files or click 'Start' to proceed.

	Name	Size	Status	
	053_Plasma_FS_70k_01.raw	328 MB	0%	
	056_Plasma_FS_70k_ddMS2.raw	165.5 MB	0%	

Collection Type: List

File Type: thermo.raw

Genome (set all): ----- Additional ...

Choose local files

Paste/Fetch data

Pause

Reset

4 Start

Build

Close

Tools

search tools

Get Data

Send Data

Collection Operations

Expression Tools

GENERAL TEXT TOOLS

Text Manipulation

Filter and Sort

Join, Subtract and Group

GENOMIC FILE MANIPULATION

Convert Formats

FASTA/FASTQ

FASTQ Quality Control

Quality Control

SAM/BAM

BED

VCF/BCF

Variant

msconvert Convert and/or f

Input unrefined MS data



No mzML

Do you agree to the vendor li

Yes No

This tool uses proprietary vendo

Output Type

mzML

Data Processing Filters

Apply peak picking?

Yes No

Peak Peaking - Apply to M

All Levels (1-)

Peak Picking - Algorithm

Prefer vendor algorithm, fallback to local-maximum

The vendor method only works on Agilent, Bruker, Sciex, Thermo data, and only on Windows (although some vendors work on Wine)

Apply m/z refinement with identification data?

Download from web or upload from disk

Regular

Composite

Collection

Rule-based

	Name	Size	Status
	053_Plasma_FS_70k_01.raw	328 MB	100% ✓
	056_Plasma_FS_70k_ddMS2.raw	165.5 MB	100% ✓

Collection Type:

List

File Type:

Auto-detect

Genome (set all):

----- Additional S...

Choose local files

Paste/Fetch data

Pause

Reset

Start

Build

Close



INRAE

Design d'une étude métabolomique

04-06-2020 / Production at analyse de données métabolomiques / Binta Diémé

Cliquez sur **Build** et nommer votre dossier

← → ↻ usegalaxy.eu

Galaxy / Europe

Tools

msconvert 1

Convert Formats

msms_extractor Extract MS/MS scans from the mzML file(s) based on PSM report

idconvert Convert mass spectrometry identification files

msconvert Convert and/or filter mass spectrometry files

msconvert Subset Peak List against list of scan numbers or indices.

Proteomics

DIA_Umpire_SE DIA signal extraction

Metabolomics

Process Scans (and SIM-Stitch) - Read, filter and average MS scans

Workflows

All workflows



msconvert Convert and/or filter mass spectrometry files (Galaxy Version 3.0.19052.0) Versions Options

Input unrefined MS data

8: 3 ia_FS_70k_ddMS2.mzML

Do you agree to the vendor licenses?

☒ Yes ☐ No

This tool uses proprietary vendor libraries; to run it you must agree to the vendor licenses. Read them at <http://www.proteowizard.org/licenses.html>

Output Type

mzML

Data Processing Filters

Apply peak picking?

☒ Yes ☐ No 4

Peak Peaking - Apply to MS Levels

All Levels (1-)

Peak Picking - Algorithm

Prefer vendor algorithm, fallback to local-maximum

The vendor method only works on Agilent, Bruker, Sciex, Thermo data, and only on Windows (although some vendors work on Wine)

Apply m/z refinement with identification data?

☐ Yes ☒ No

(Re-)calculate charge states?

no

Filter by Threshold

+ Insert Filter by Threshold

Filter m/z Window

☐ Yes ☒ No

Filter out ETD precursor peaks?



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Design d'une étude métabolique

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