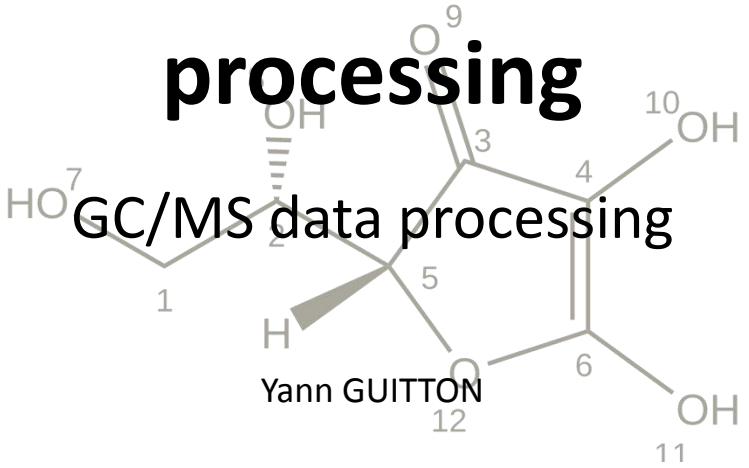
MS data processing

GC/MS data processing

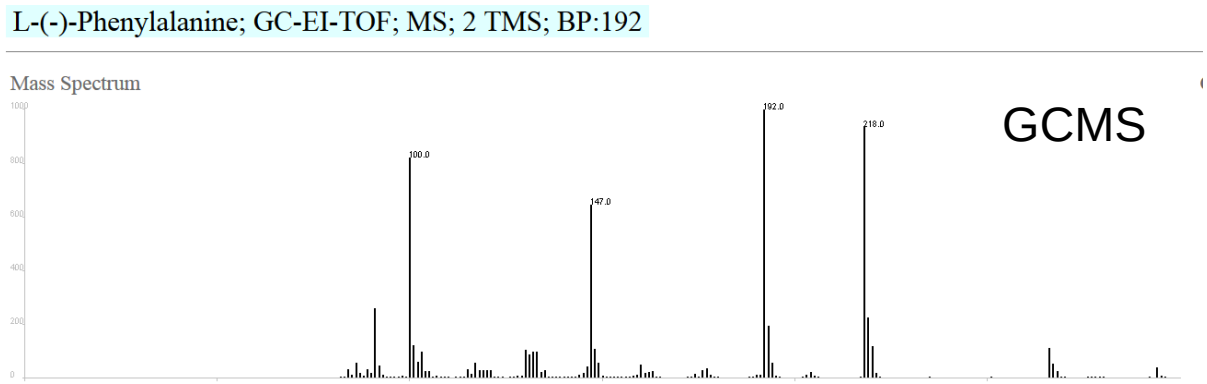


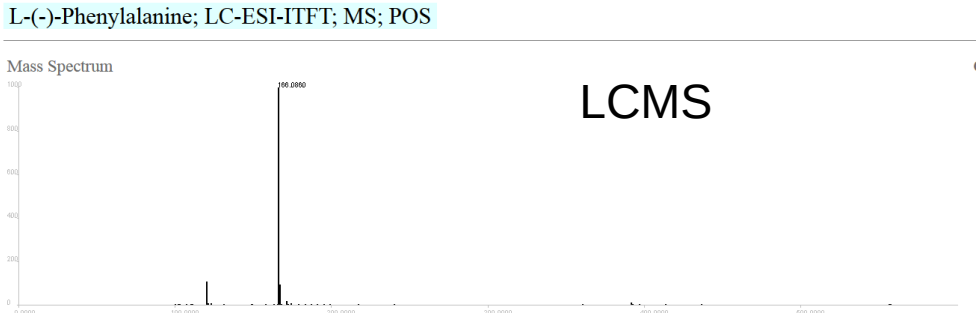
Yann GUITTON

v 1.0.0

Processing GC-MS data in Galaxy

- Why using a specific tool for processing GC-MS data ?
  - GC-MS data have their own specificity
    - First one is higer amount of ions in a mass spectra with EI compared to ESI





Processing GC-MS data in Galaxy

Galaxy / 4 / Metabolomics

Analyze Data | Workflow | Shared Data | Visualization

Tools

search tools

Upload File from your computer

Export Data

LC-MS

Format Conversion

Preprocessing

Normalisation

Quality Control

Statistical Analysis

Annotation

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metaMS.runGC GC-MS data preprocessing using metaMS package

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dbsearch.golm Search GCMS spectra from msp files into Golm Metabolome database

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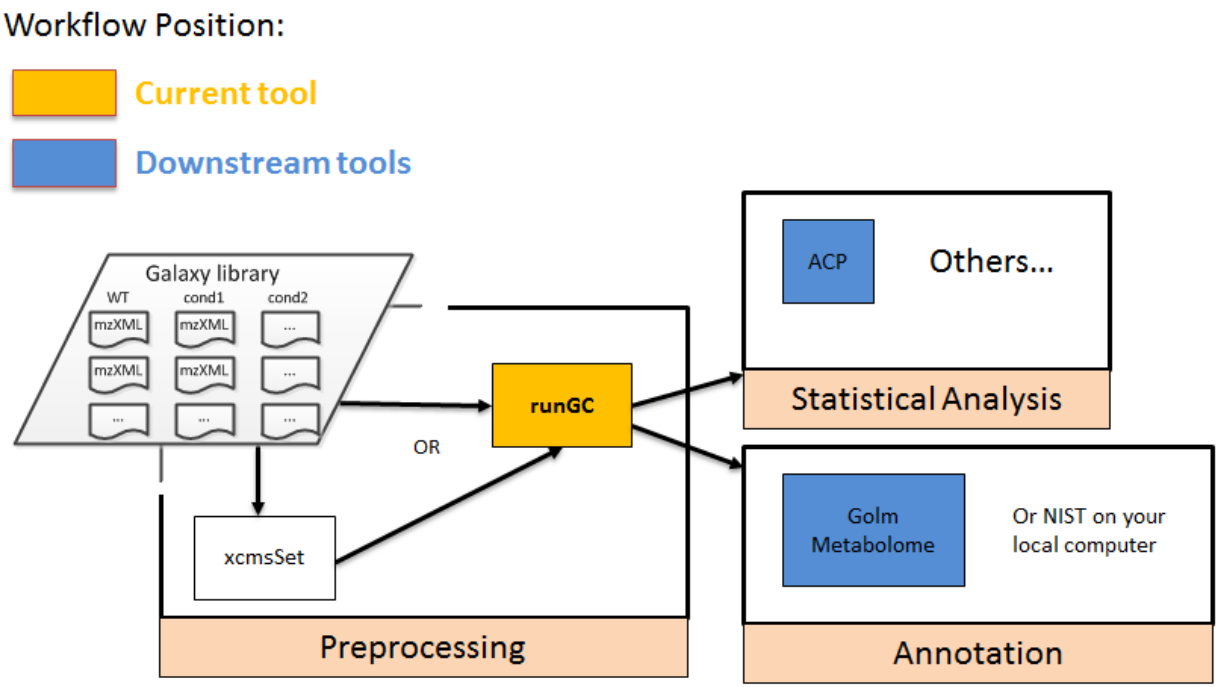
Downstream tools

Name	Output file	Format
Determine Vdk or Lowess	dataMatrix.tsv	Tabular
Normalization Vdk/Lowess	dataMatrix.tsv	Tabular
Anova	dataMatrix.tsv	Tabular
PCA	dataMatrix.tsv	Tabular
Hierarchical Clustering	dataMatrix.tsv	Tabular
Golm Metabolome Search	peakspectra.msp	Text

General schema of the metabolomic workflow for GCMS



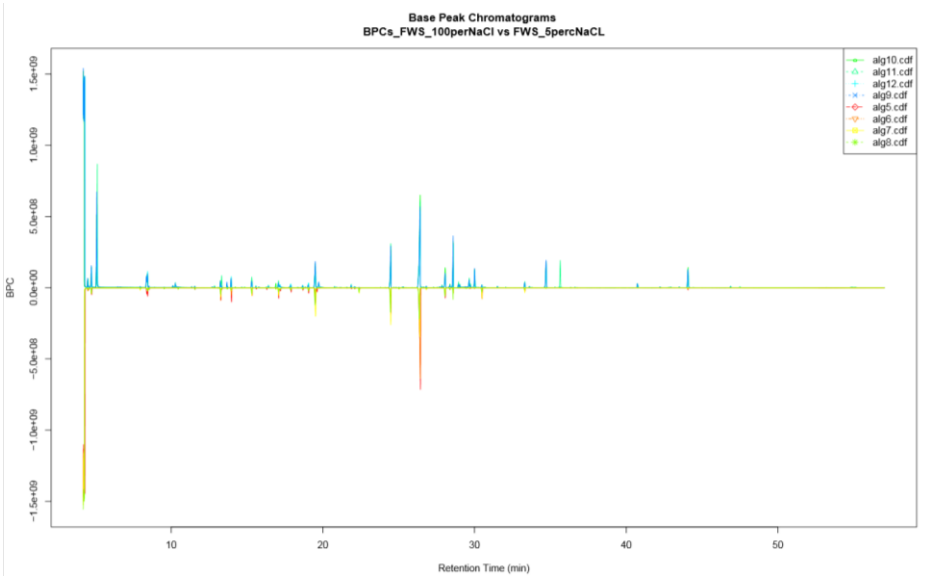
Processing GC-MS data in Galaxy

- *In fine* that tool use xcms/CAMERA under metaMS R package from R. Wehrens

metaMS : Wehrens, R.; Weingart, G.; Mattivi, F. Journal of Chromatography B.

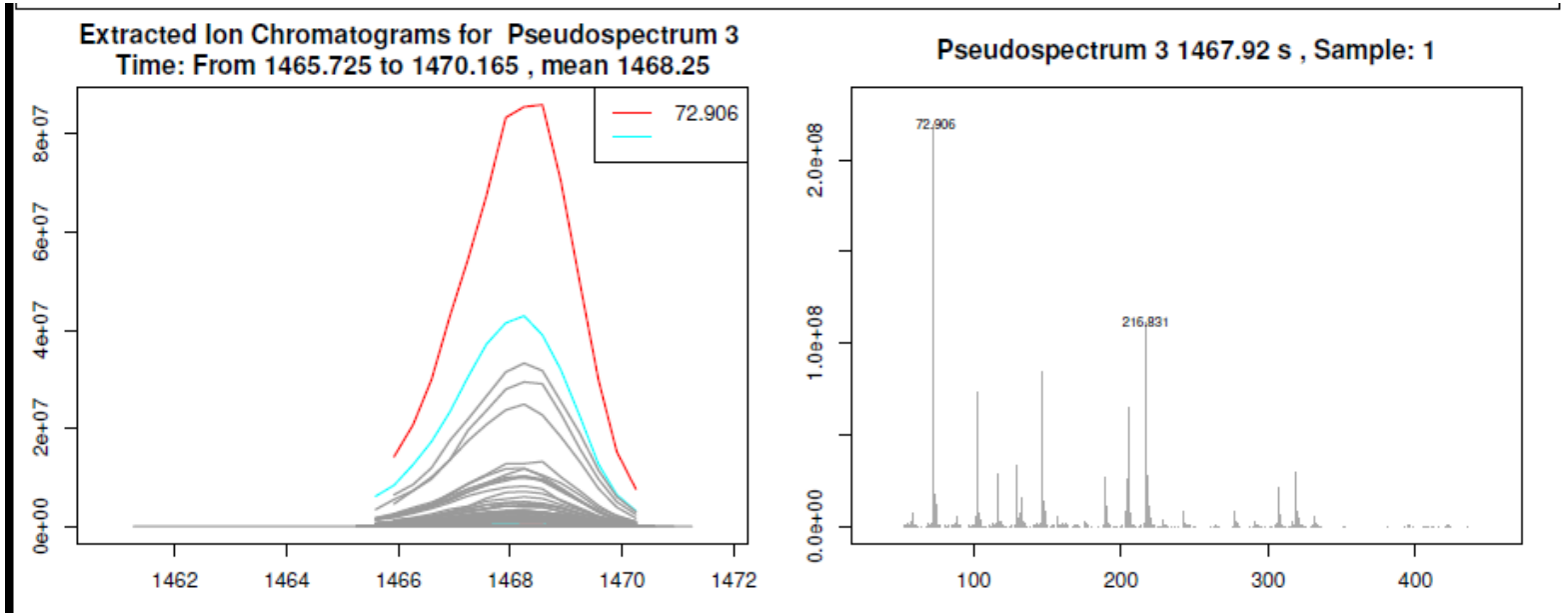
- with adapted parameters and dedicated outputs

1: GCMS_Idealq_FWS_SWS.zip
2: peaktable.tsv
3: sampleMetadata.tsv
4: variableMetadata.tsv
5: dataMatrix.tsv
6: peakspectra.msp
7: TICs_raw.pdf
8: BPCs_raw.pdf
9: GCMS_EIC.pdf
10: rungc.RData
11: rungc.log.txt
12: rungc.zip
20: GolmResult.html



Processing GC-MS data in Galaxy

9: GCMS_EIC.pdf

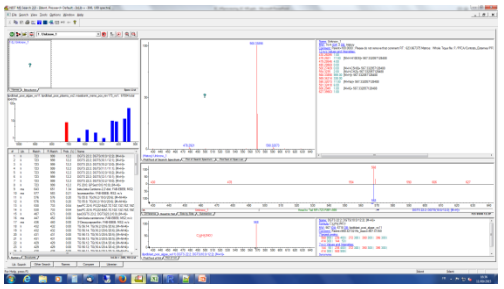


Peakpicking/grouping quality control

Processing GC-MS data in Galaxy

6: peakspectra.msp

A MSP export of pseudospectras readable by NIST or Golm Metabolome



NIST MSsearch

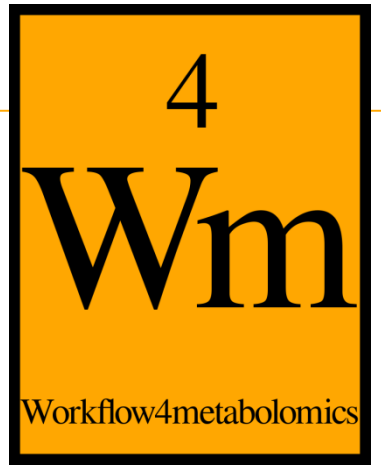
20: GolmResult.html

cname	analyteName	ri	DotproductDistance	EuclideanDistance	HammingDistance	JaccardDistance	s12GowerLegendr
Unknown 1	Citric acid (4TMS)	1803.92065	0.01	0.01	15	0.28	0.4
	Isocitric acid (4TMS)	1805.39966	0.04	0.01	109	0.74	0.71
	Gluconic acid (6TMS)	1984.52283	0.11	0.02	85	0.82	0.82
	Malic acid, 3-oxalo- (1MEOX) (4TMS) BP	2200	0.12	0.02	868	0.96	0.89
	Galactaric acid (6TMS)	2030.46814	0.12	0.02	461	0.92	0.85
	Arabinoheptulosonic acid enol, 3-deoxy- (5TMS) MP	1926.63843	0.11	0.02	499	0.92	0.85
	Malic acid, 3-oxalo- (1MEOX) (4TMS) MP	2190.4812	0.12	0.02	478	0.93	0.87
	myo-Inositol-1-phosphate (7TMS)	2414.291	0.12	0.02	403	0.92	0.85

http://web11.sb-roscoff.fr/download/w4m/howto/w4m_HowToUseNIST_V01.pdf

Processing GC-MS data in Galaxy

- Then go to other databases with the .MSP file
- Or go to statistical analysis with



Processing GC-MS data in Galaxy

HOW TO

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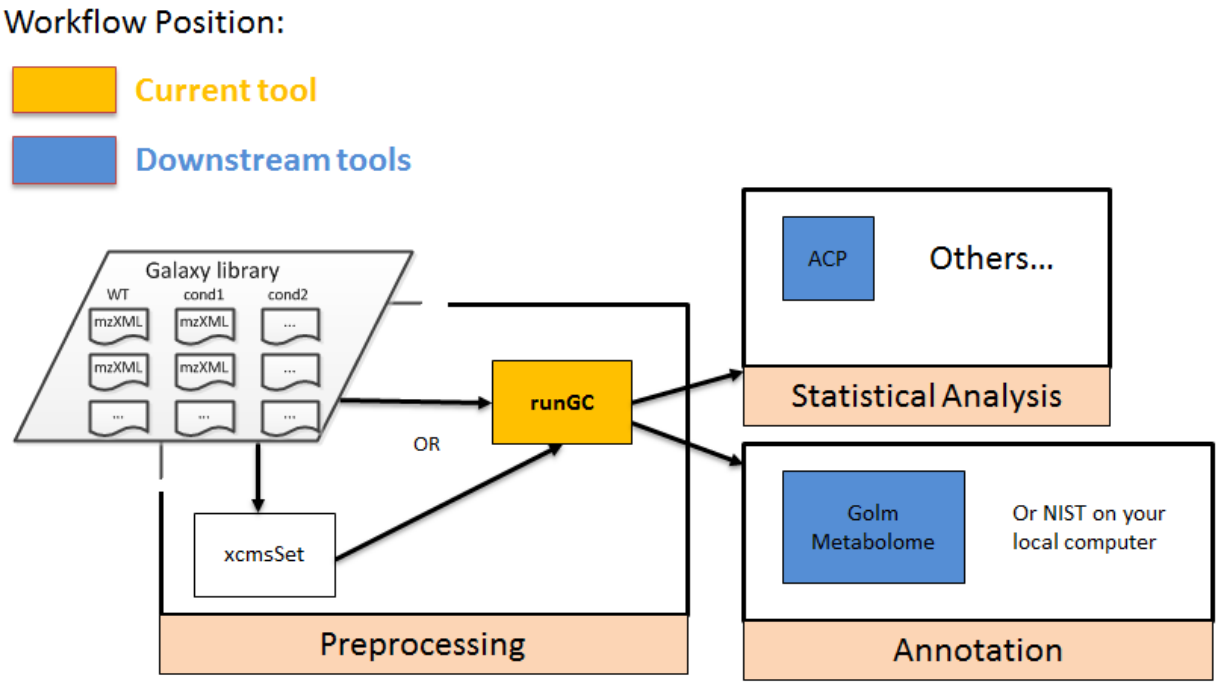
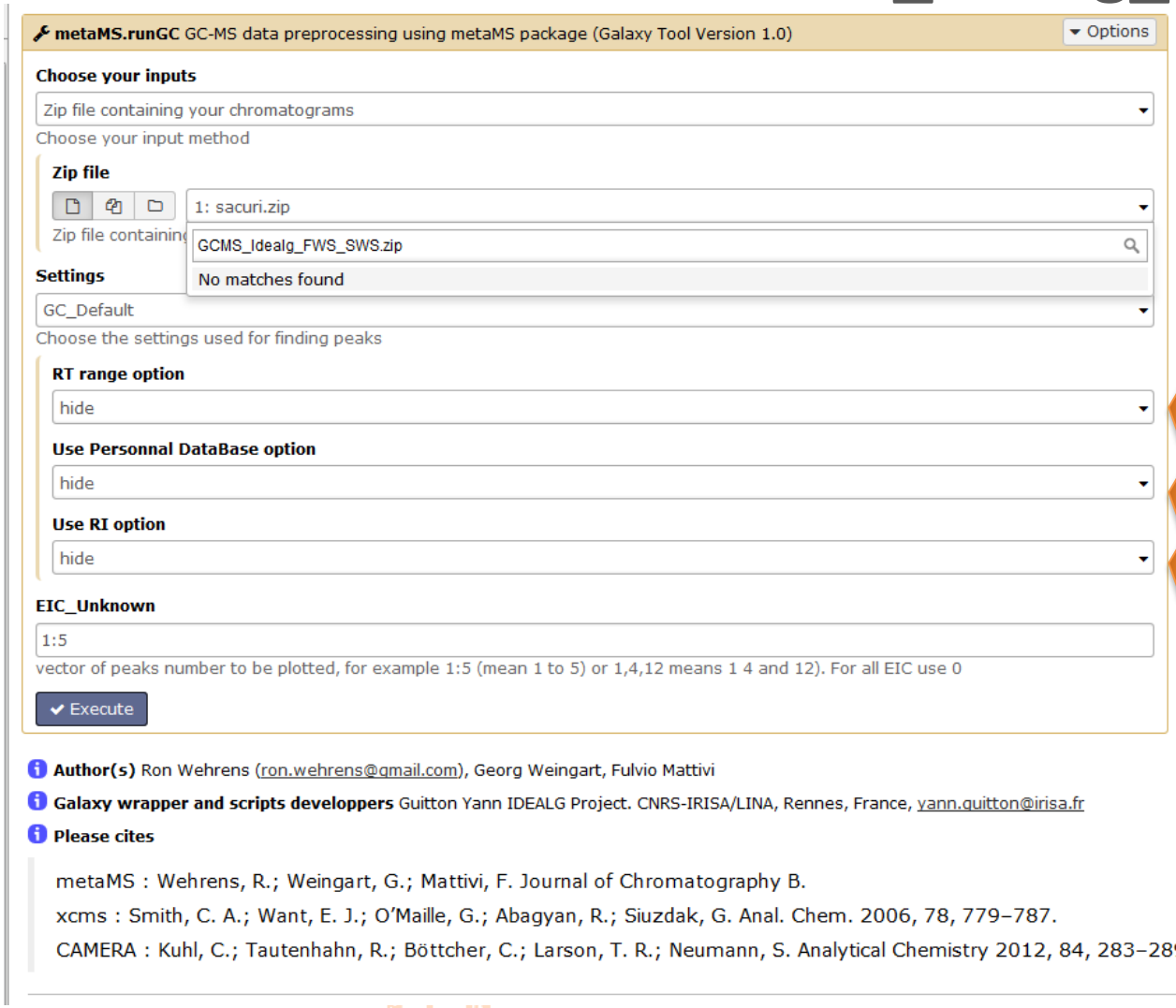


How to : Processing GC-MS data in Galaxy

- Can be tested with GCMS_Idealg_FWS_SWS.zip



Input your data as zip, or as library (data should be in CDF, mzXML or mzData) and organised in sub folders

GC default settings, give it a try

RT range: cut a part of your chromatogramme

Can import a DB in MSP format

Calculate Ris need a file with alcane RT

Only the five first EIC by default use 0 to draw all

How to : Processing GC-MS data in Galaxy

Settings

User_Defined

Choose the settings used for finding peaks

FWHM

5

The FWHM of your peaks (matchedFilter method is used)

RT range option

hide

RT_Diff

0.05

The allowed RT shift between same molecule in different sample

Min_Features

5

The minimum number of ion in a mass spectra to consider it a molecule

similarity_threshold

0.7

The minimum similarity allowed between peaks mass spectra to be considered as equal

min.class.fract

0.5

The fraction of samples in which a pseudospectrum is present before it is regarded as an unknown

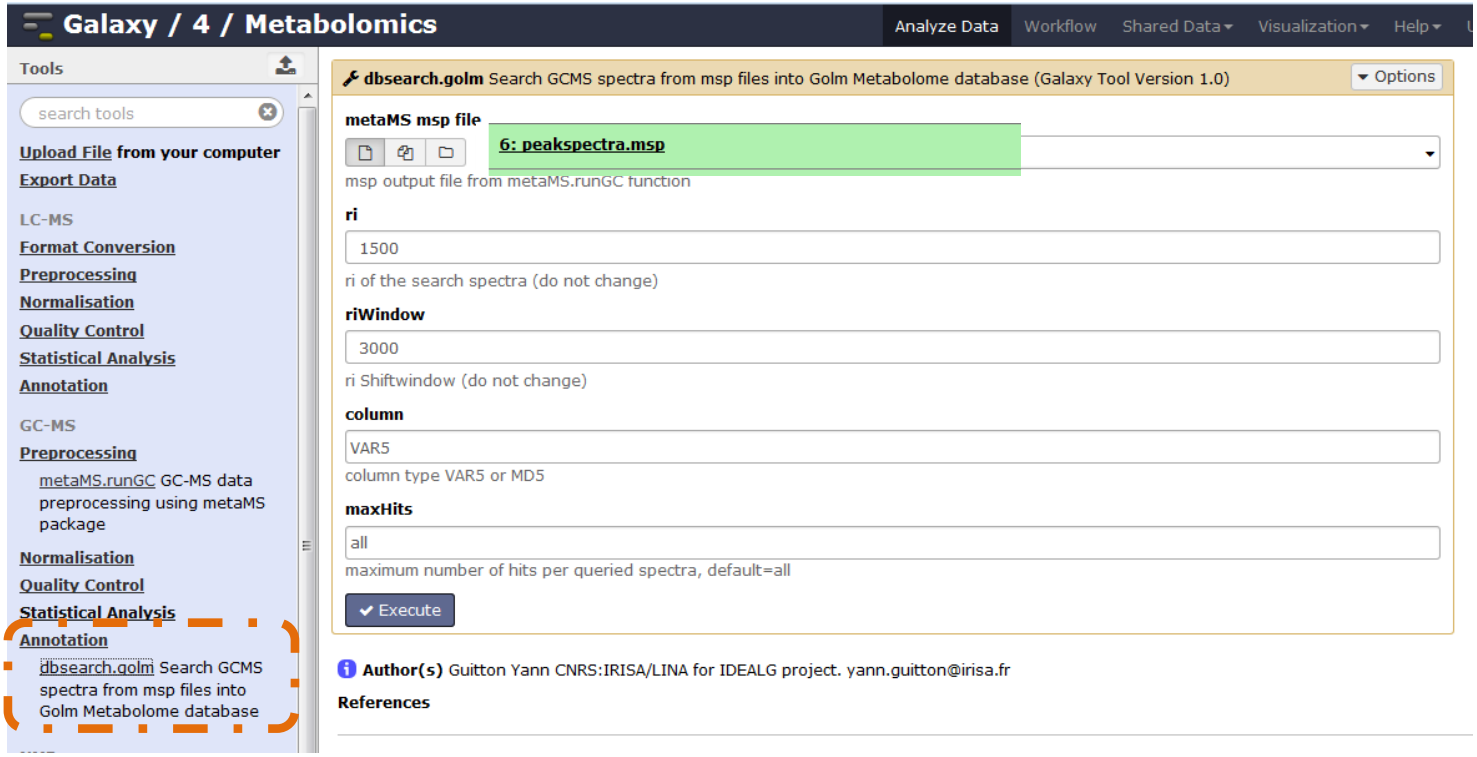
min.class.size

3

The absolute number of samples in which a pseudospectrum is present before it is regarded as an unknown

In fact all are xcms/CAMERA parameters

How to : Processing GC-MS data in Galaxy



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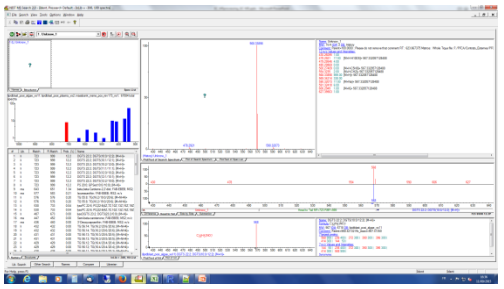

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Thanks!