4 Wm Workflow4metabolomics

ifb INSTITUT FRANÇAIS DE BIOINFORMATIQUE

METABOHUB

MS data processing

GC/MS data processing

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v 1.0.0

cnrs

UPMC SORBONNE UNIVERSITÉS

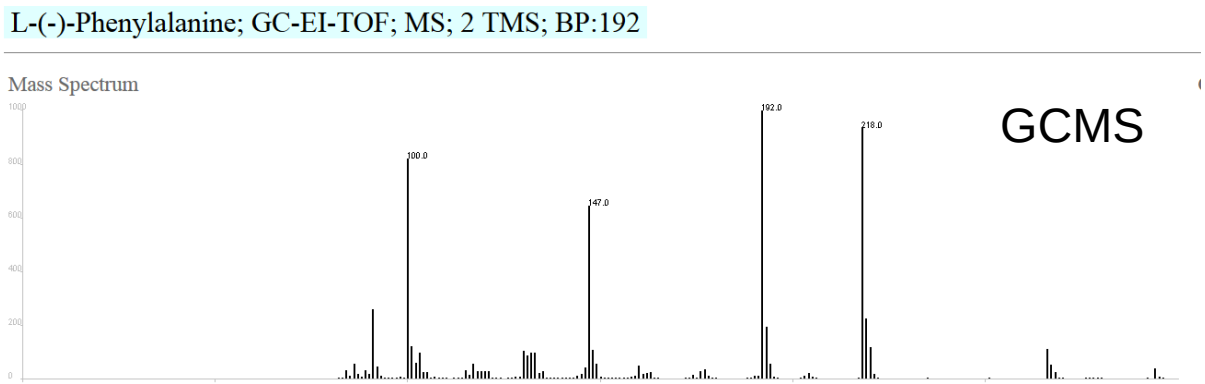
INRA SCIENCE & IMPACT

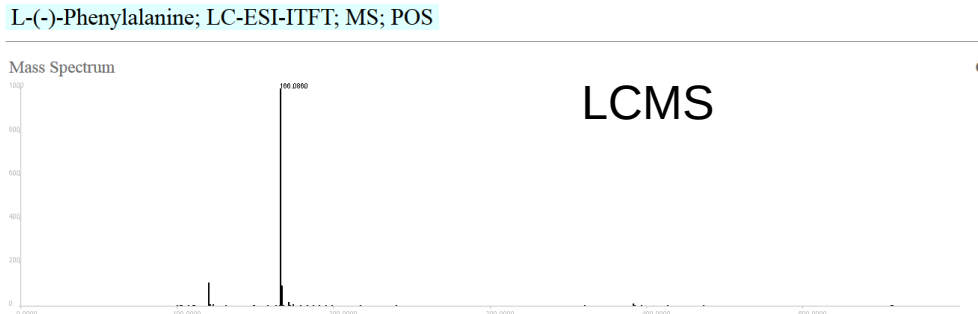
cea

LABERCA

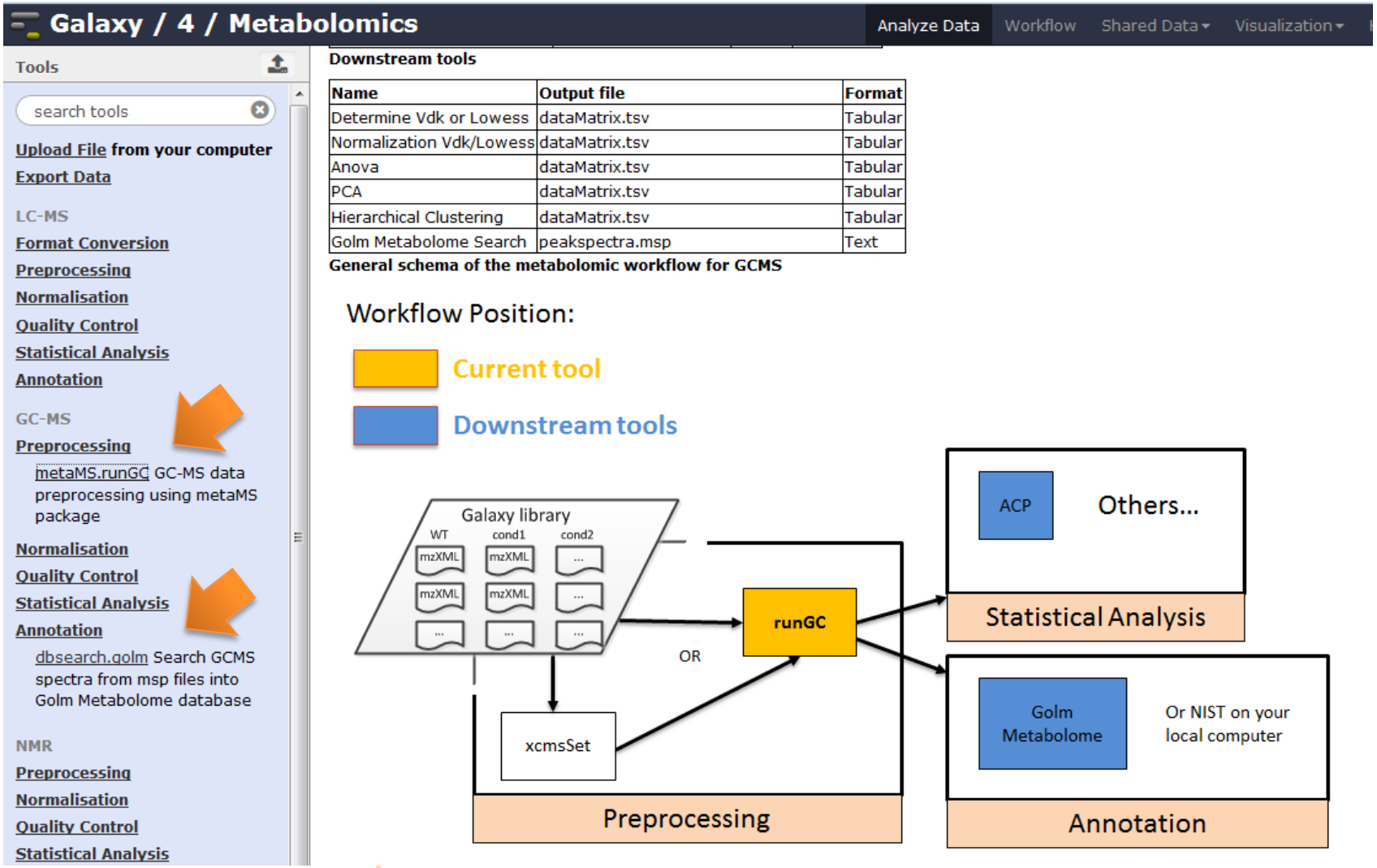
Processing GC-MS data in Galaxy

- 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



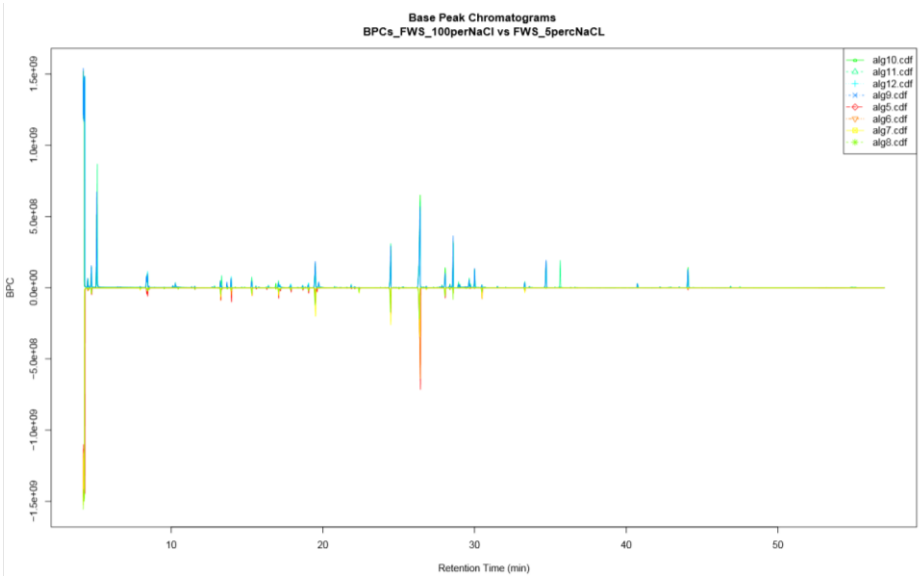
Processing GC-MS data in Galaxy

- *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.

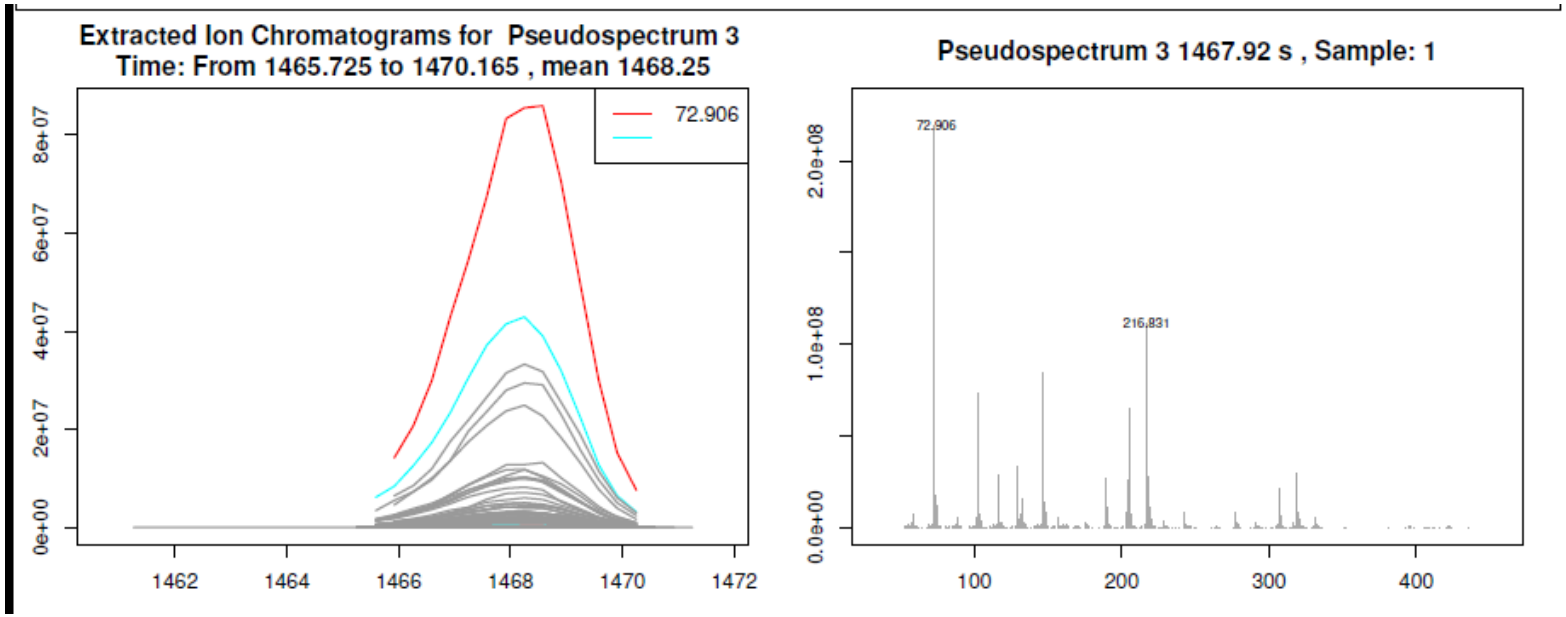
- with adapted parameters and dedicated outputs

1: GCMS_Idealg_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: runqc.RData
11: runqc.log.txt
12: runqc.zip
20: GolmResult.html



Processing GC-MS data in Galaxy

9: GCMS_EIC.pdf

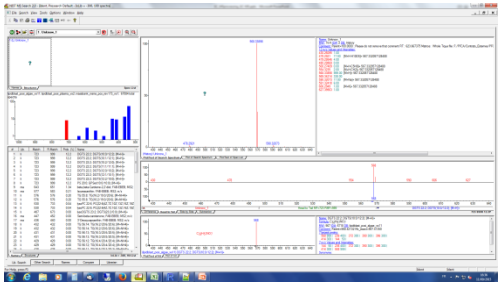


Peakpicking/grouping quality control

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

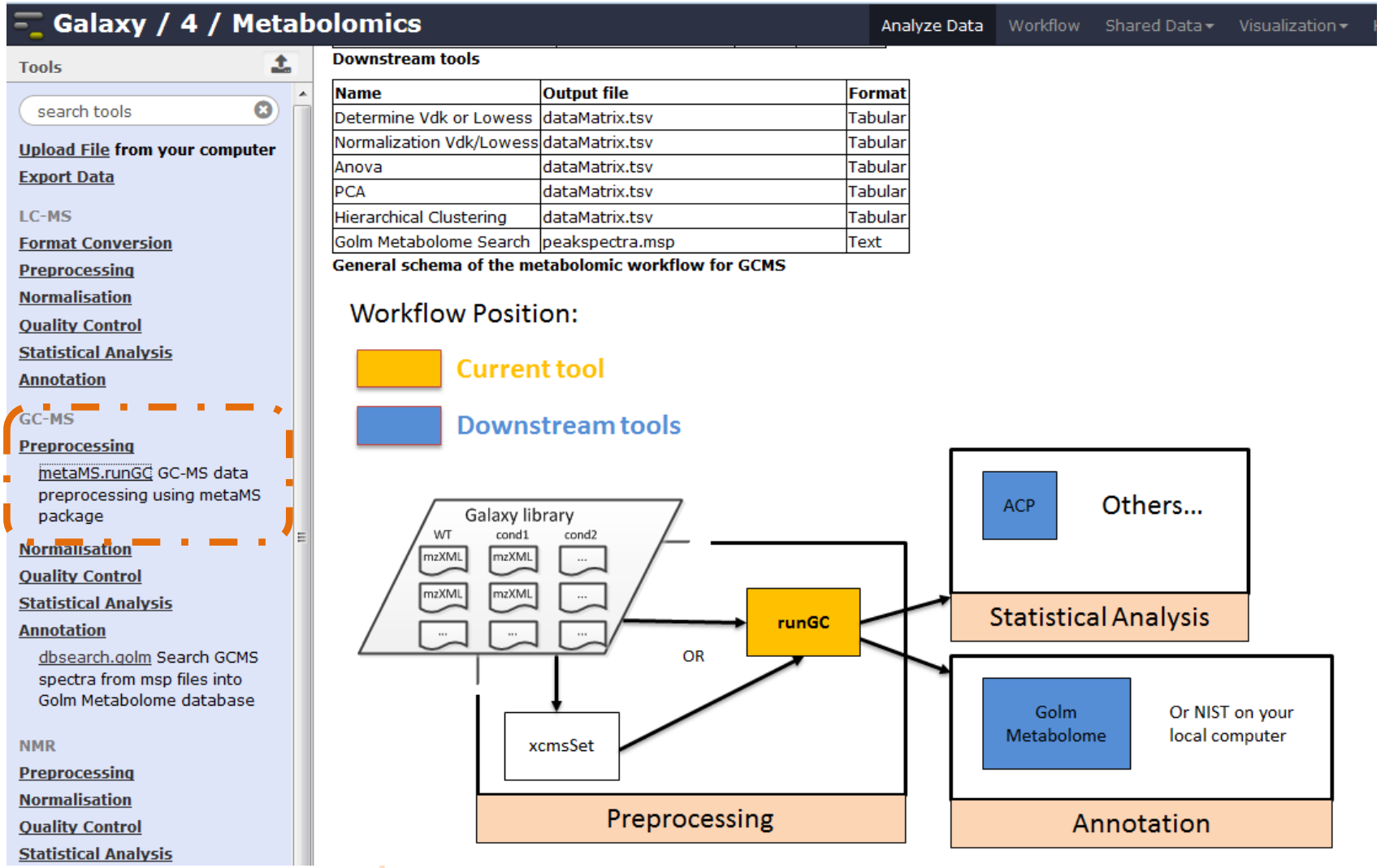
Processing GC-MS data in Galaxy

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

Processing GC-MS data in Galaxy

HOW TO

How to : Processing GC-MS data in Galaxy



How to : Processing GC-MS data in Galaxy

- Can be tested with GCMS_Idealg_FWS_SWS.zip

metaMS.runGC GC-MS data preprocessing using metaMS package (Galaxy Tool Version 1.0) — Options

Choose your inputs

Zip file containing your chromatograms

Choose your input method

Zip file

1: sacuri.zip

Zip file containing

GCMS_Idealg_FWS_SWS.zip

No matches found

Settings

GC_Default

Choose the settings used for finding peaks

RT range option

hide

Use Personnal DataBase option

hide

Use RI option

hide

EIC_Unknown

1:5

vector of peaks number to be plotted, for example 1:5 (mean 1 to 5) or 1,4,12 means 1 4 and 12). For all EIC use 0

Execute

Author(s) Ron Wehrens (ron.wehrens@gmail.com), Georg Weingart, Fulvio Mattivi

Galaxy wrapper and scripts developpers Guitton Yann IDEALG Project. CNRS-IRISA/LINA, Rennes, France, yann.guitton@irisa.fr

Please cites

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

xcms : Smith, C. A.; Want, E. J.; O'Maille, G.; Abagyan, R.; Siuzdak, G. Anal. Chem. 2006, 78, 779–787.

CAMERA : Kuhl, C.; Tautenhahn, R.; Böttcher, C.; Larson, T. R.; Neumann, S. Analytical Chemistry 2012, 84, 283–289.

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

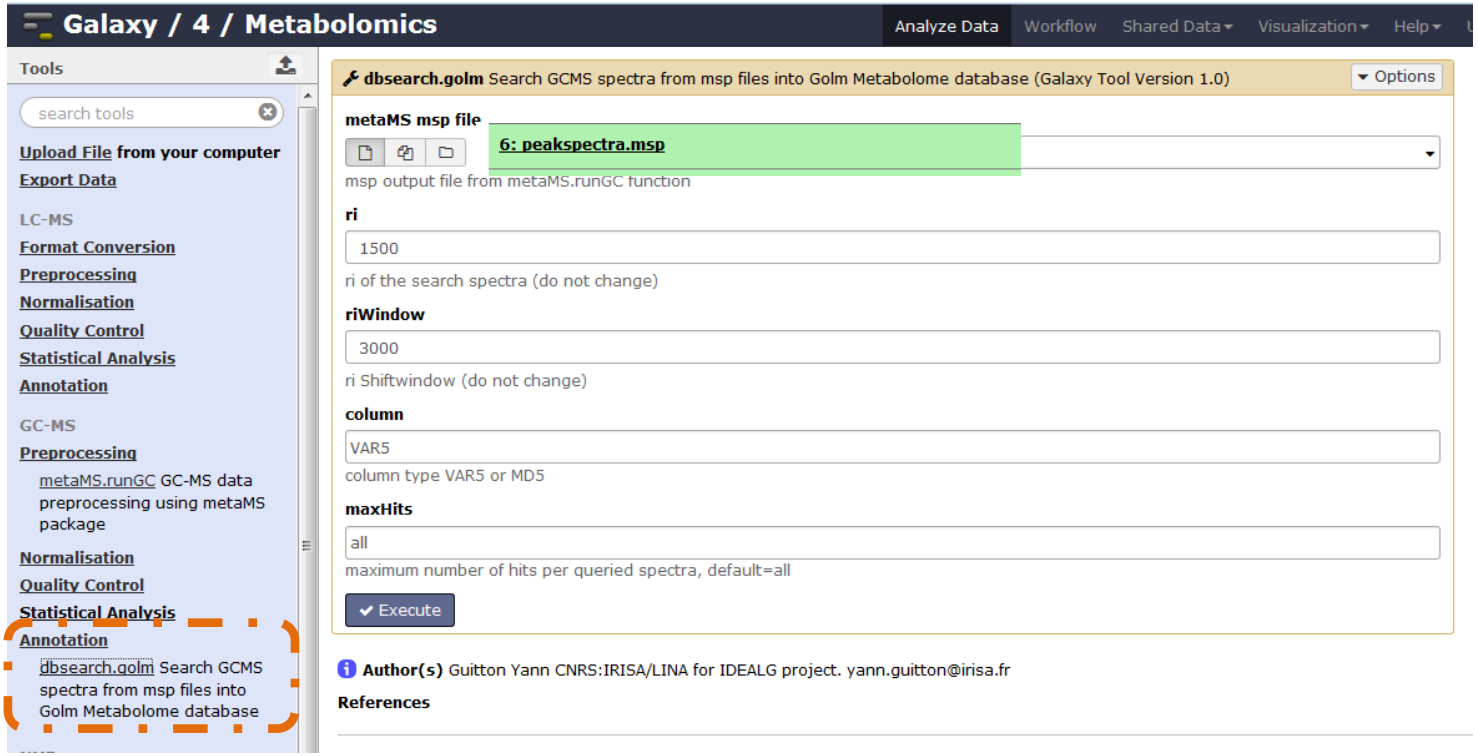
min.class.size

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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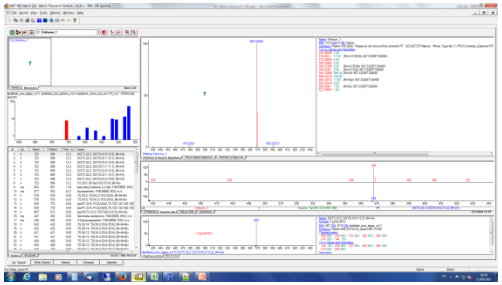

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Thanks!