Analysis in Bioinformatics and Informatics for Marine Science

Plate-Forme EXPLORATION du METABOLISME
des gènes aux métabolites

METABOMER

Workflow4Metabo

Galaxy and the metabolomics analysis Universe

GCC2013 – Olso 2013 – Gildas Le Corguillé
JOBIM – Toulouse 2013 – Pierre Pericard

What was our choice until now ?

```
Console /projet/fr2424/informatique/ppericard/Galaxy/tmp/mzXML_copper_stress.mz/
> library(xcms)
> setwd("~/projet/Galaxy/tmp/mzXML_copper_stress.mz")
> xset <- xcmsSet()
25014H: 100:56 150:194 200:351 250:530 300:719 350:868 400:982 450:1025 500:1072 550:1159 600:1189 650:1191 700:1197
25018H: 100:47 150:183 200:346 250:523 300:706 350:867 400:984 450:1039 500:1093 550:1185 600:1214 650:1217 700:1223
25024H: 100:53 150:182 200:337 250:504 300:684 350:832 400:931 450:965 500:1015 550:1096 600:1127 650:1130 700:1135
25028H: 100:52 150:189 200:330 250:494 300:658 350:799 400:908 450:951 500:1000 550:1081 600:1111 650:1119 700:1128
25034H: 100:49 150:178 200:337 250:503 300:677 350:843 400:952 450:999 500:1049 550:1125 600:1156 650:1163 700:1168
25038H: 100:60 150:203 200:362 250:544 300:729 350:882 400:1005 450:1049 500:1092 550:1158 600:1179 650:1182 700:1189
25044H: 100:55 150:188 200:344 250:510 300:696 350:844 400:943 450:986 500:1033 550:1105 600:1123 650:1127 700:1131
25048H: 100:50 150:185 200:351 250:533 300:730 350:896 400:1019 450:1068 500:1115 550:1196 600:1214 650:1220 700:1226
C14H: 100:48 150:168 200:307 250:469 300:644 350:790 400:895 450:939 500:994 550:1084 600:1121 650:1134 700:1142
C18H: 100:53 150:182 200:337 250:493 300:689 350:866 400:983 450:1038 500:1089 550:1176 600:1200 650:1208 700:1217
C24H: 100:52 150:181 200:331 250:495 300:684 350:848 400:960 450:1011 500:1064 550:1158 600:1188 650:1197 700:1206
C28H: 100:50 150:175 200:322 250:477 300:6
C34H: 100:45 150:163 200:301 250:436 300:6
C38H: 100:50 150:181 200:332 250:495 300:6
C44H: 100:41 150:166 200:310 250:464 300:6
C48H: 100:53 150:180 200:332 250:492 300:6
> xset
An "xcmsSet" object with 16 samples

Time range: 6.8-1528.4 seconds (0.1-25.5 m
Mass range: 53.0167-699.356 m/z
Peaks: 8941 (about 559 per sample)
Peak Groups: 0
Sample classes: ref, sample

Profile settings: method = bin
                  step = 0.1

Memory usage: 1.56 MB
> xset <- group(xset)
115 178 240 303 365 428 490 553 615 678
>
```

ERGONOMICS
PARAMETER COMPLETENESS
MODULARITY
DATA & WORKFLOW SHARING

USERS **Newbies metabo analysts**
Advanced metabo analysts
Additional tools developers

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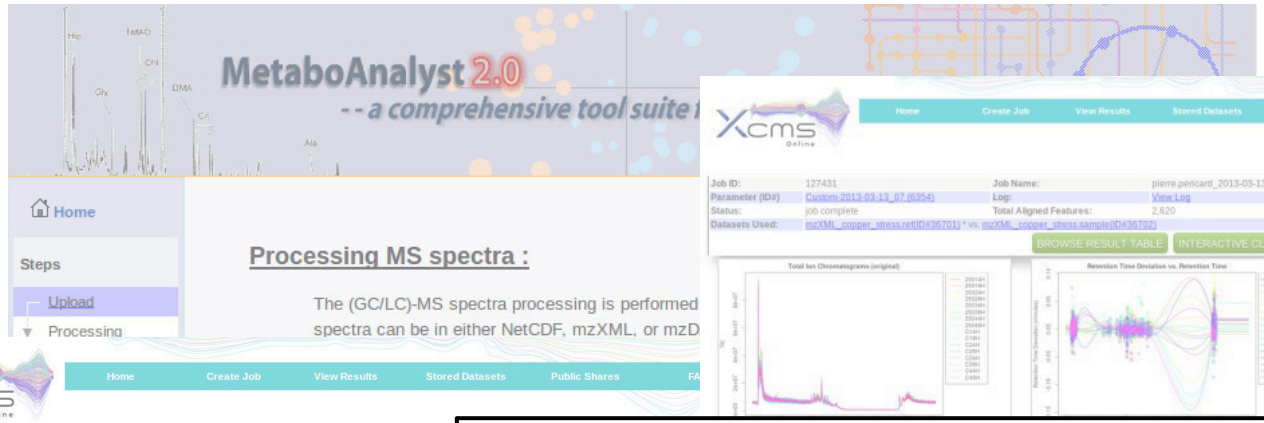

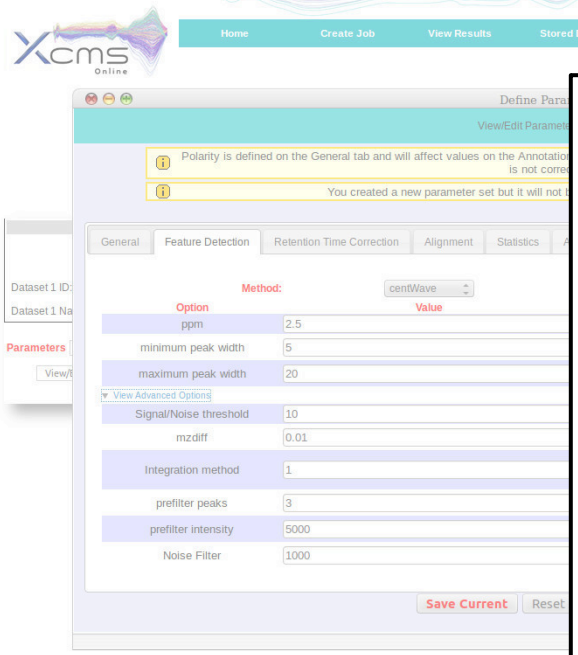

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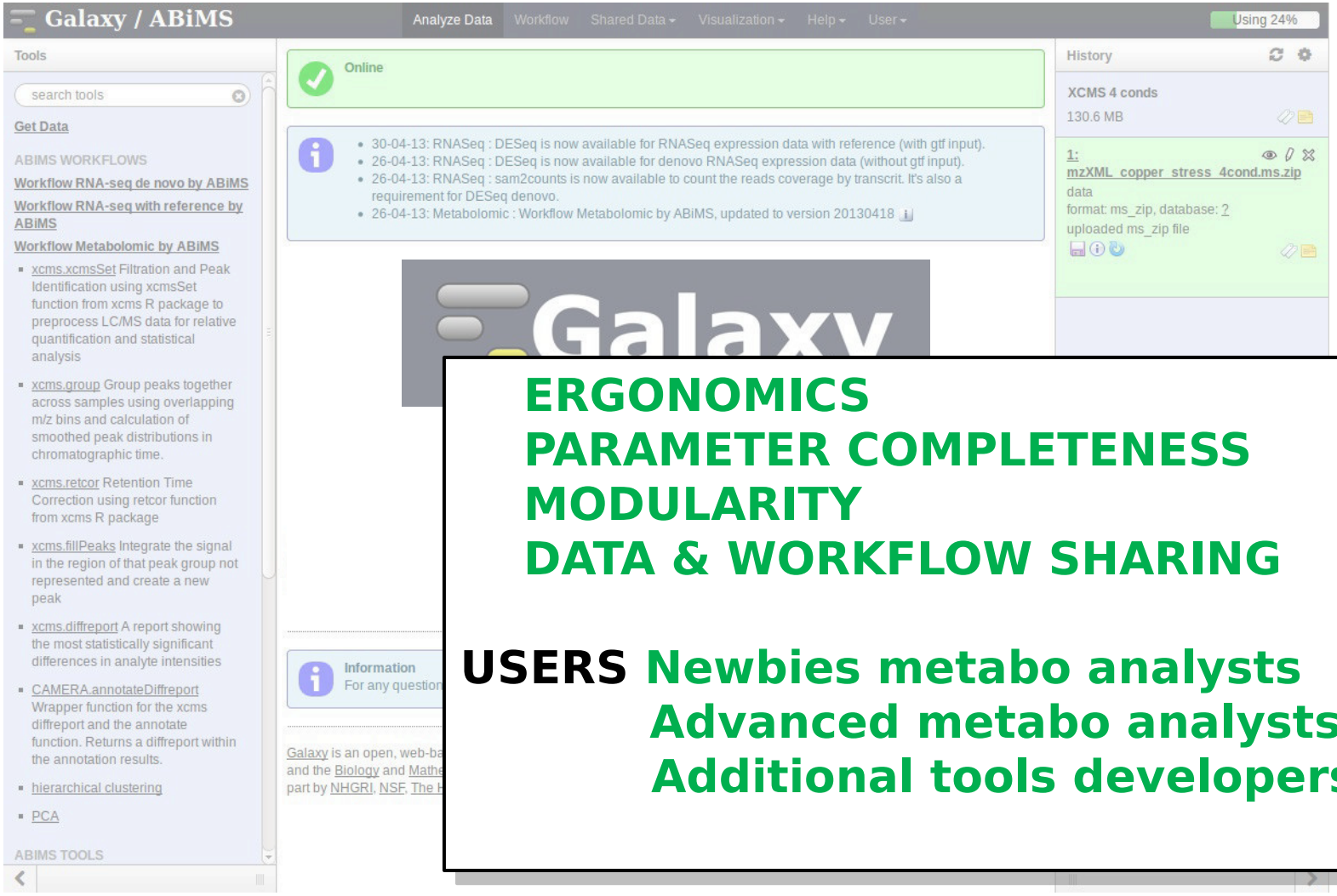
Our Solution



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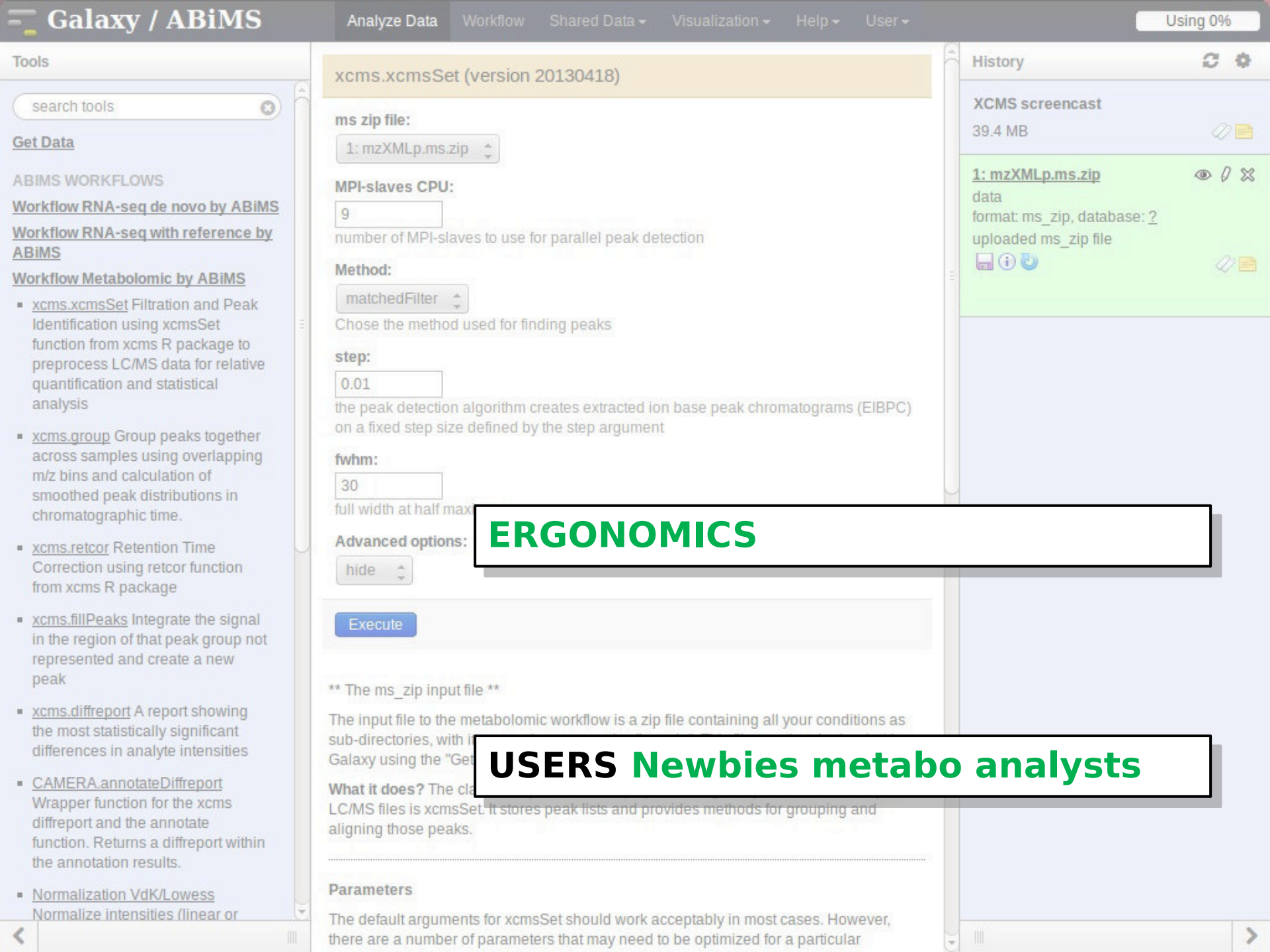
Galaxy / ABiMS
Analyze Data
Workflow
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Normalization VdK/Lowess
Normalize intensities (linear or
xcms.xcmsSet (version 20130418)
ms zip file:
1: mzXMLp.ms.zip
MPI-slaves CPU:
9
number of MPI-slaves to use for parallel peak detection
Method:
matchedFilter
Chose the method used for finding peaks
step:
0.01
the peak detection algorithm creates extracted ion base peak chromatograms (EIBPC) on a fixed step size defined by the step argument
fwhm:
30
full width at half max
Advanced options:
hide
Execute
** The ms_zip input file **
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History
XCMS screencast
39.4 MB
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data
format: ms_zip, database: ?
uploaded ms_zip file
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search tools

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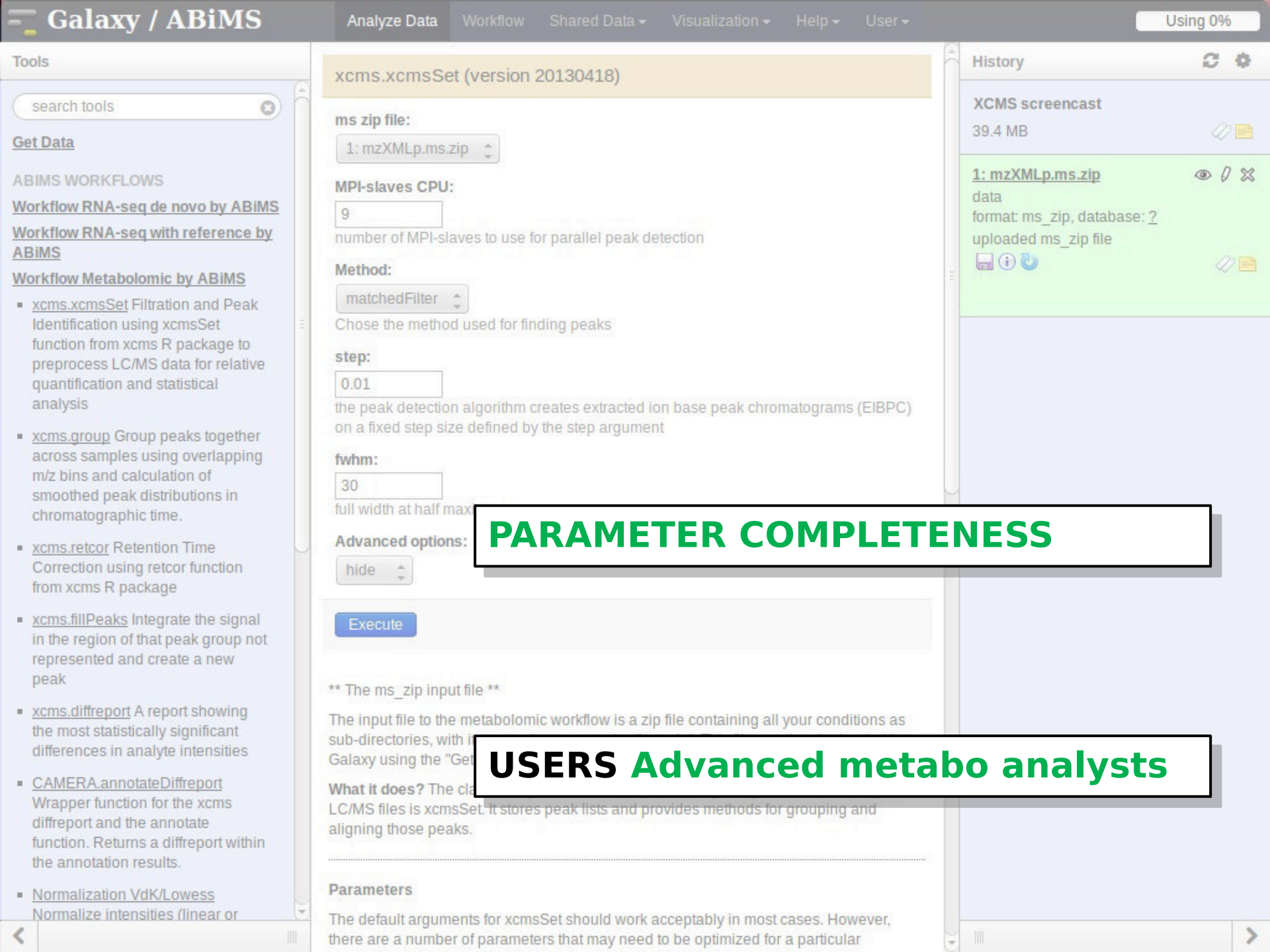
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matchedFilter

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0.01

the peak detection algorithm creates extracted ion base peak chromatograms (EIBPC) on a fixed step size defined by the step argument

fwhm:

30

full width at half maximum

Advanced options:

show

max:

5

maximum number of peaks per extracted ion chromatogram

snthresh:

10

signal to noise ratio cutoff

steps:

2

the peak identification algorithm combines a given number of EIBPCs prior to filtration and peak detection, as defined by the steps argument

Execute

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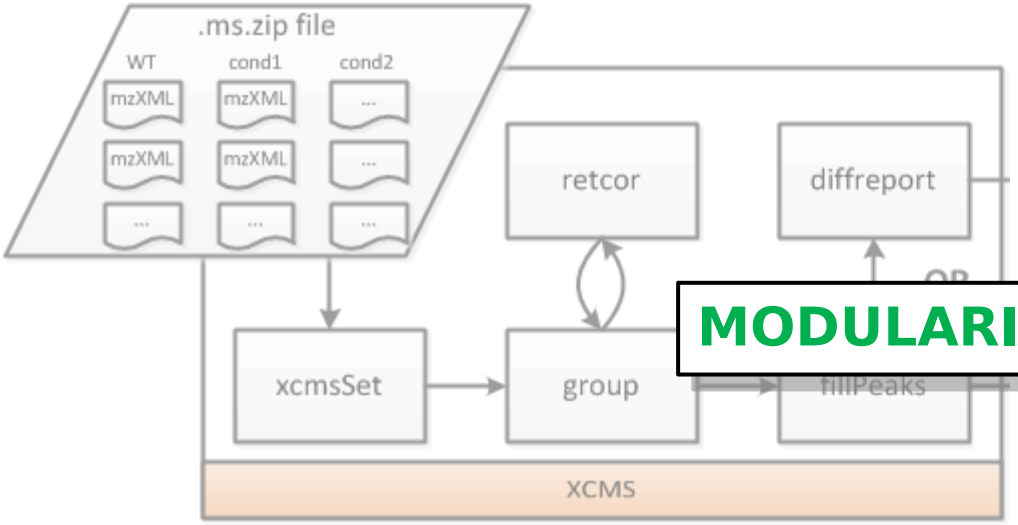
Our Pipeline (so far…)



MODULARITY

USERS **Advanced metabo analysts**
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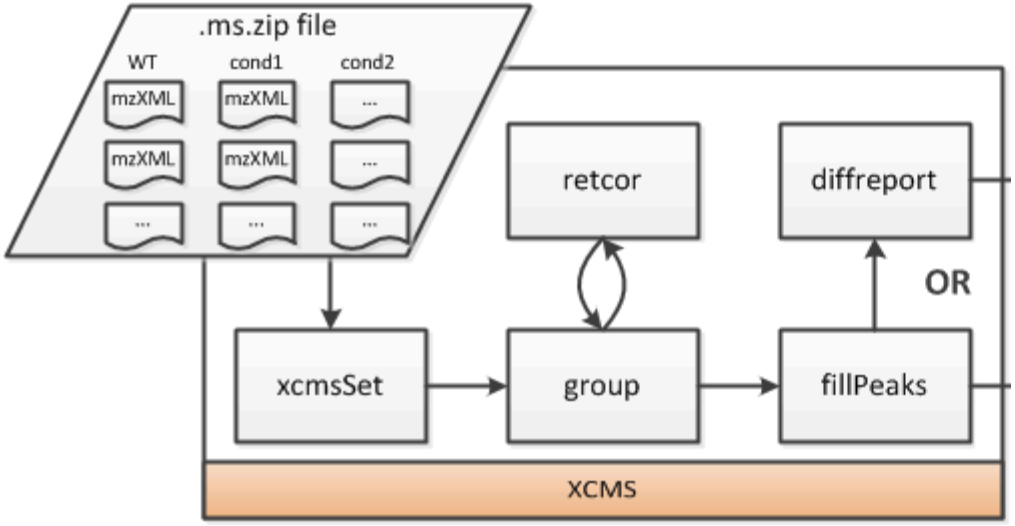

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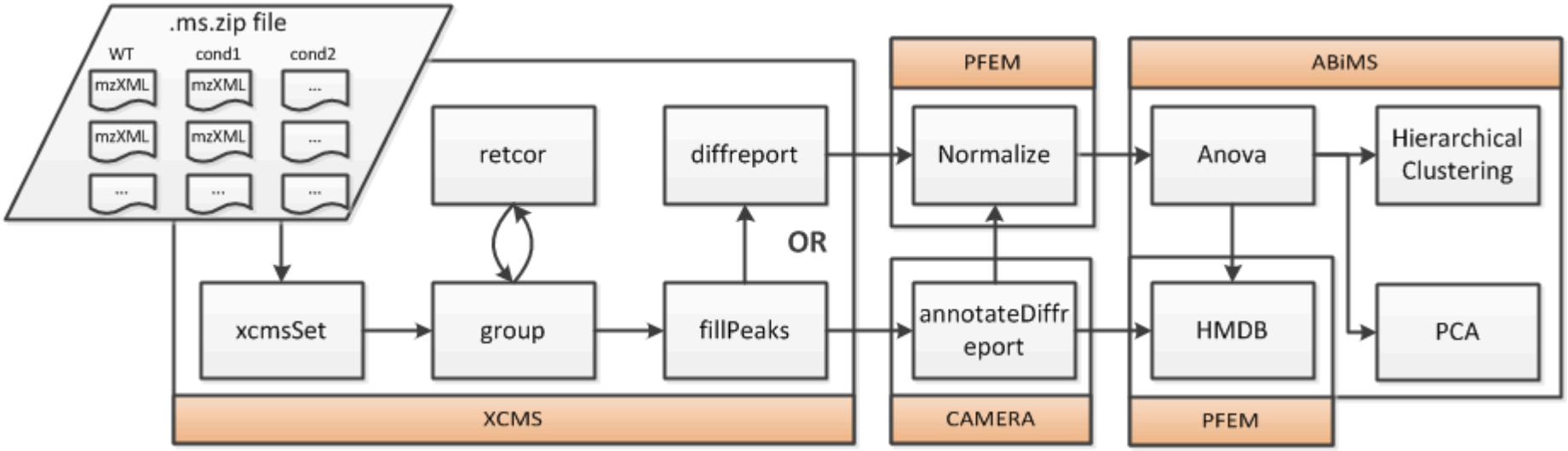

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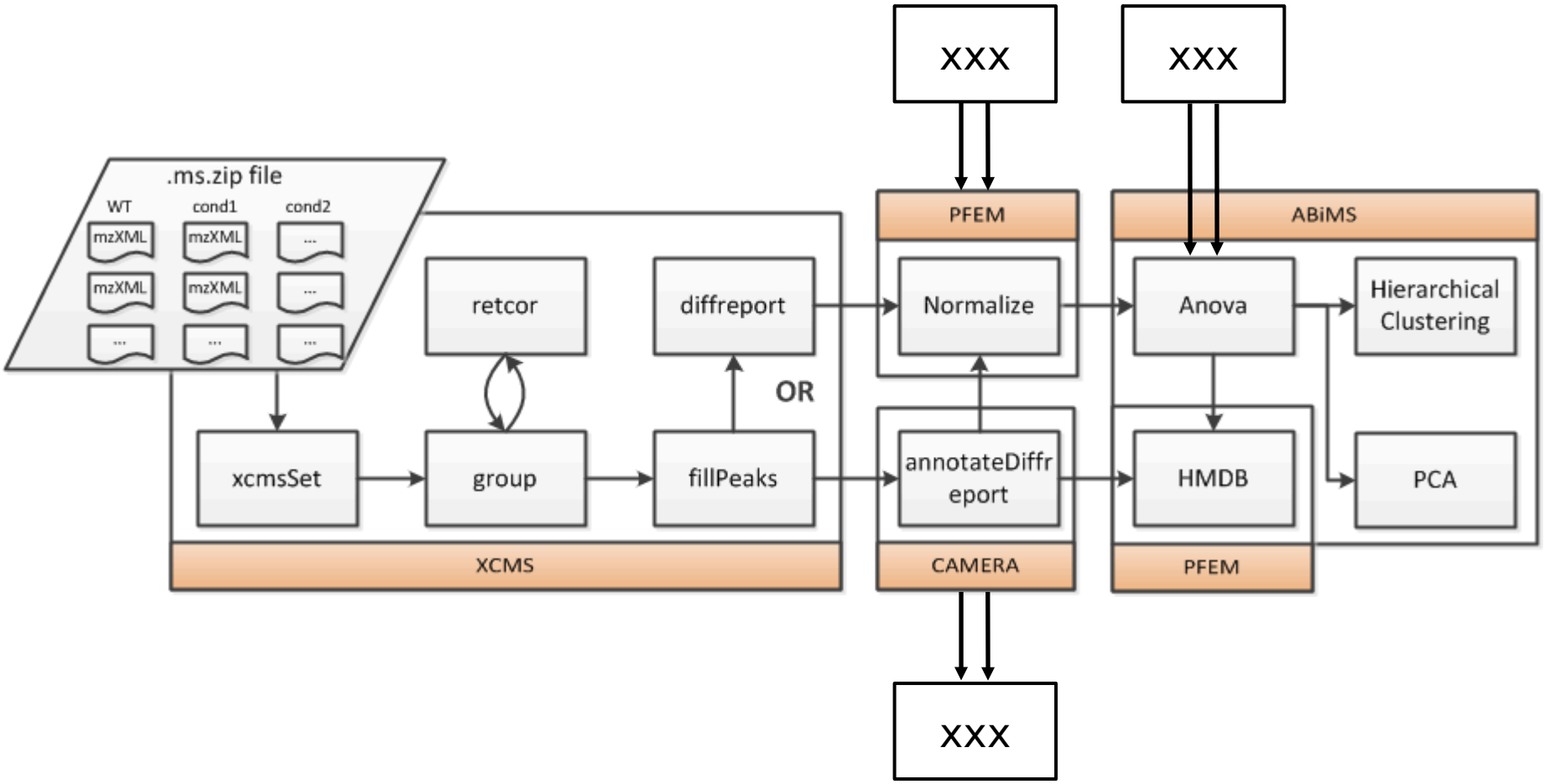

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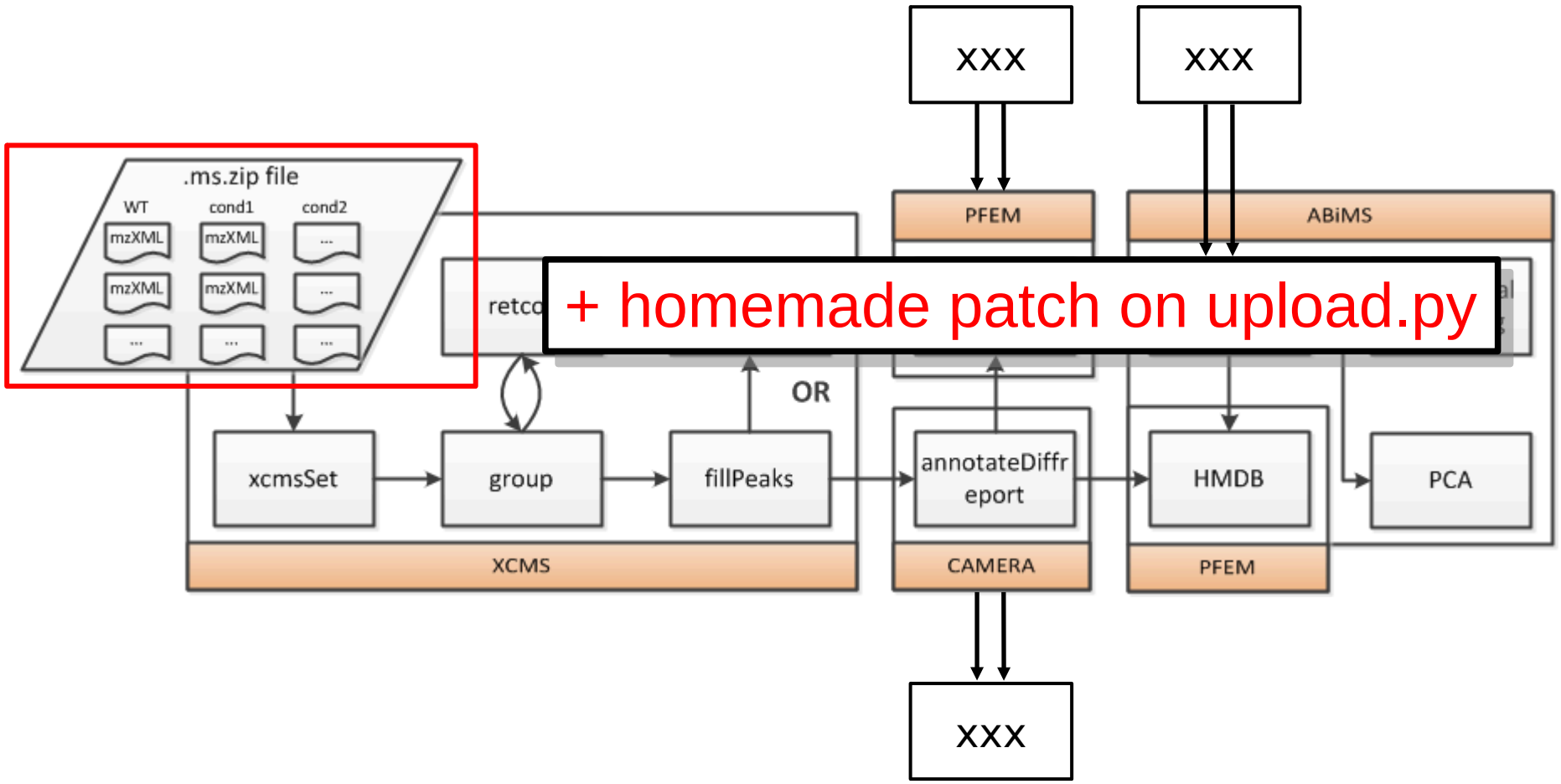

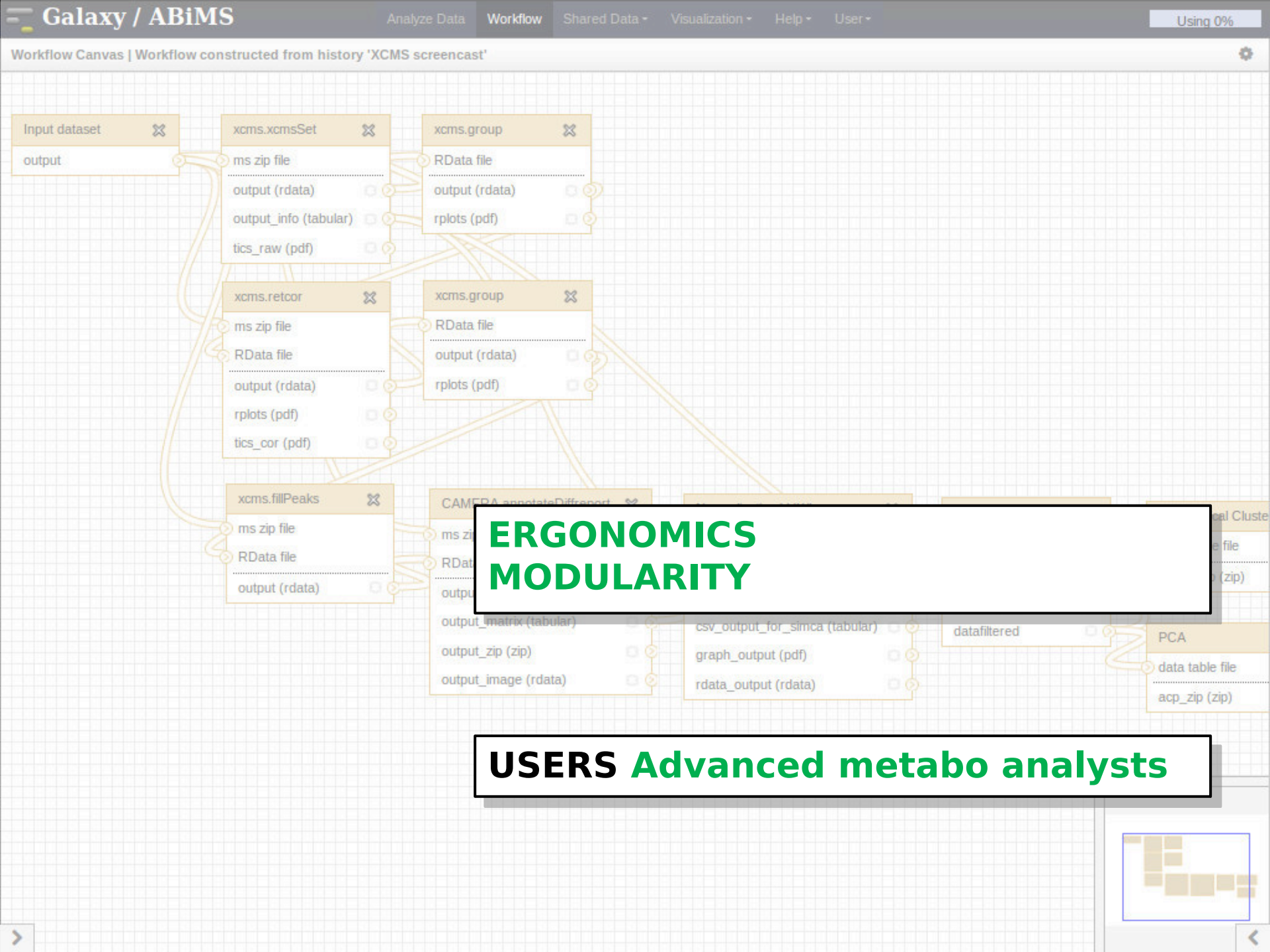
Galaxy / ABiMS
Analyze Data
Workflow
Shared Data
Visualization
Help
User
Using 0%
Workflow Canvas | Workflow constructed from history 'XCMS screencast'
Input dataset
output
xcms.xcmsSet
ms zip file
output (rdata)
output_info (tabular)
tics_raw (pdf)
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output_image (rdata)
csv_output_for_simca (tabular)
graph_output (pdf)
rdata_output (rdata)
datafiltered
PCA
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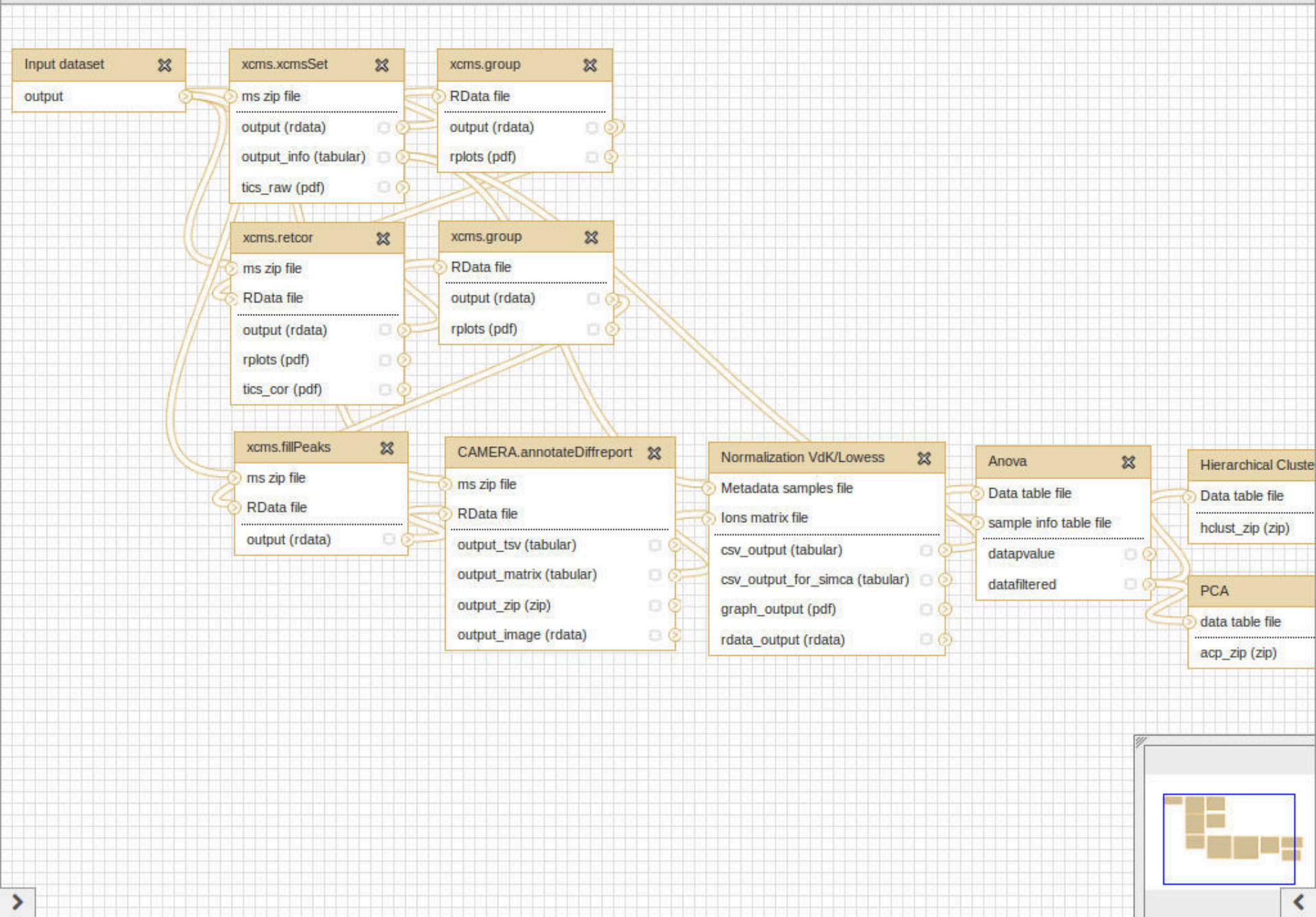

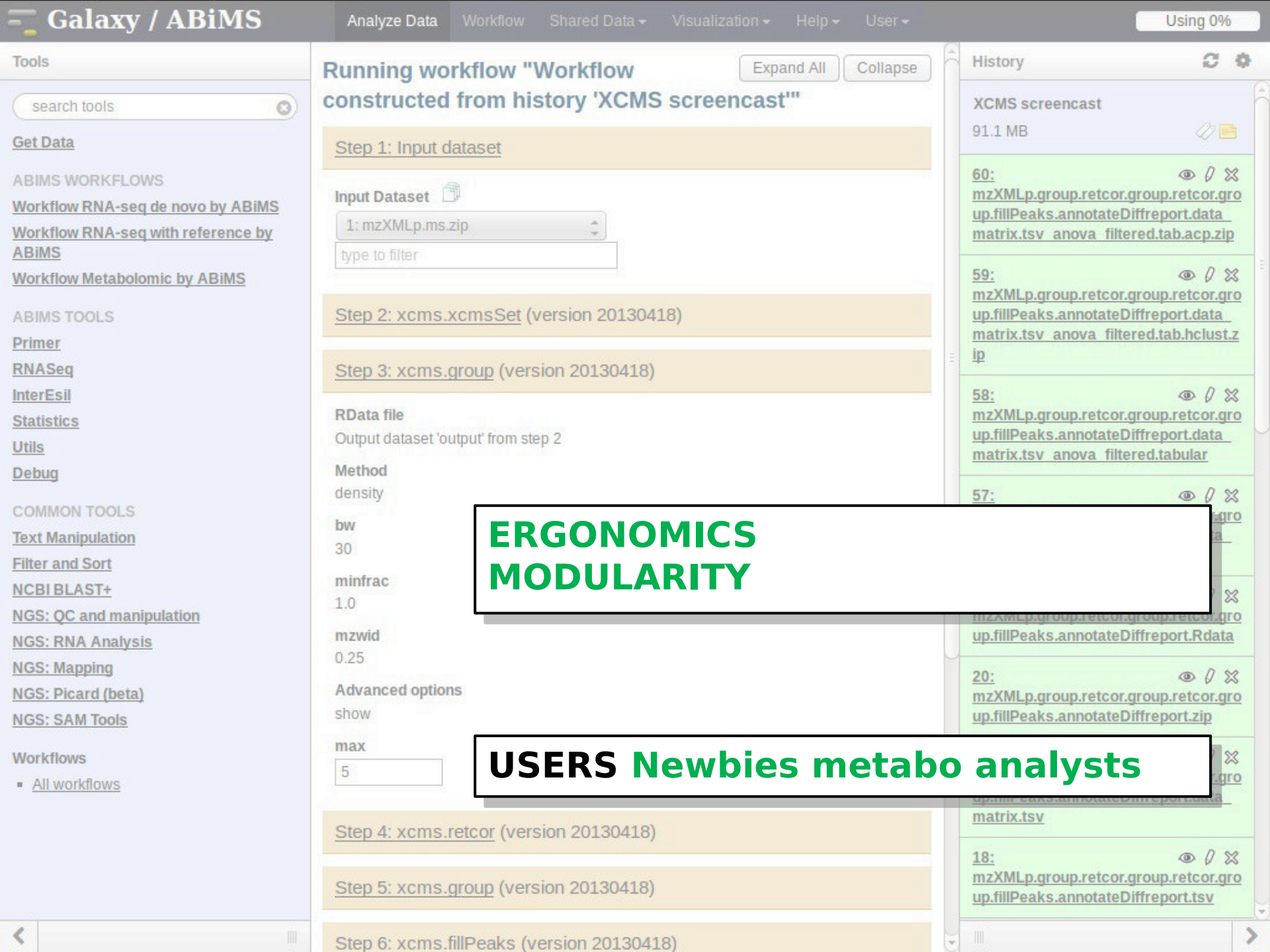
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Text Manipulation
Filter and Sort
NCBI BLAST+
NGS: QC and manipulation
NGS: RNA Analysis
NGS: Mapping
NGS: Picard (beta)
NGS: SAM Tools
Workflows
All workflows
Running workflow "Workflow constructed from history 'XCMS screencast'"
Expand All
Collapse
Step 1: Input dataset
Input Dataset
1: mzXMLp.ms.zip
type to filter
Step 2: xcms.xcmsSet (version 20130418)
Step 3: xcms.group (version 20130418)
RData file
Output dataset 'output' from step 2
Method
density
bw
30
minfrac
1.0
mzwid
0.25
Advanced options
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max
5
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InterEsil

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Workflow Metabolomic by ABiMS

ABIMS TOOLS

Primer

RNASeq

InterEsil

Statistics

Utils

Debug

COMMON TOOLS

Text Manipulation

Filter and Sort

NCBI BLAST+

NGS: QC and manipulation

NGS: RNA Analysis

NGS: Mapping

NGS: Picard (beta)

NGS: SAM Tools

Workflows

- All workflows

Running workflow "Workflow constructed from history 'XCMS screencast'"

Expand All | Collapse

Step 1: Input dataset

Input Dataset

1: mzXMLp.ms.zip

type to filter

Step 2: xcms.xcmsSet (version 20130418)

Step 3: xcms.group (version 20130418)

RData file

Output dataset 'output' from step 2

Method

density

bw

30

minfrac

1.0

mzwid

0.25

Advanced options

show

max

5

Step 4: xcms.retcor (version 20130418)

Step 5: xcms.group (version 20130418)

Step 6: xcms.fillPeaks (version 20130418)

History

XCMS screencast

91.1 MB

60: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_filtered.tab.acp.zip

59: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_filtered.tab.hclust.zip

58: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_filtered.tabular

57: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_pvalue.tabular

21: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.Rdata

20: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.zip

19: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv

18: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.tsv

Tools

search tools

Get Data

ABIMS WORKFLOWS

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59: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_filtered.tab.hclust.zip

58: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_filtered.tabular

57: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_pvalue.tabular

21: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.Rdata

20: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.zip

19: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv

18: mzXMLp.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.tsv

Data & workflows & tools sharing

- **Data**: Easy sharing of Galaxy histories, even between distant instances
- **Workflow**: Advanced users can share pre-configured workflows (eg. high or medium resolution MS)
- **Tools**: Galaxy tools and pipelines can be shared through Toolsheds

Who's who

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