- Slides available

- http://galaxy3.sb-roscoff.fr

- Login:
  - login@sb-roscoff.fr
  - *********

- Introduction

- Data import

- Tools

- Dataset

- History

- Workflow

- Share

- Dataset collections

- Introduction
- Data import
- Tools
- Dataset
- History
- Workflow
- Share
- Dataset collections

INTRODUCTION / PROBLEMATIC

- In biomedical research, high-throughput technologies produce **large datasets**.

- How to perform analyses of these data **without bioinformatics skills** ?

  o Assemble transcript sequences de novo

  o Determine the gene expression

  o Build a phylogenetic tree

  o Predict subcellular targeting for proteins

  o Identify and quantify metabolites detected by LC-MS

  o …

- **Graphical interface** click-button tools within windows

  + very ergonomic

  – too ergonomic → lack of flexibility

  – few

  – paying for it!
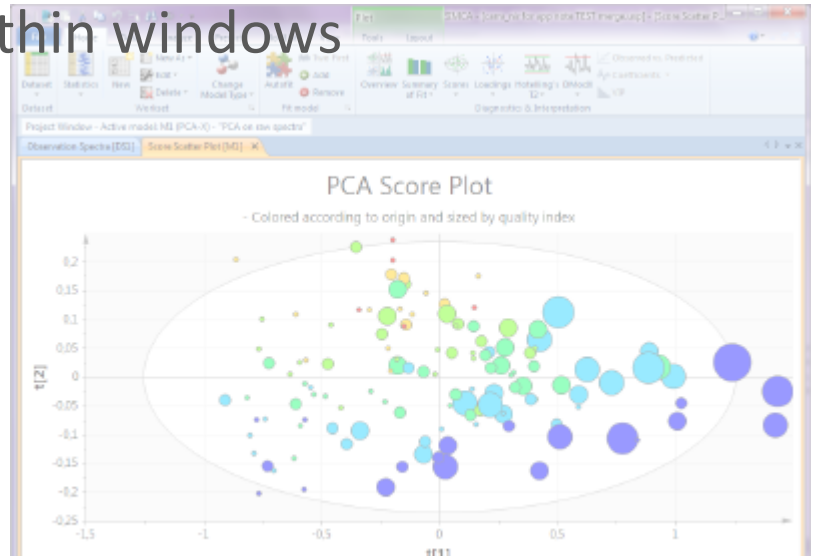
- Tools available on the **internet**

  + very ergonomic

  – too ergonomic → lack of flexibility

  – A small part of the available tools

  – the submission size / storage is often limited

  – must not be paranoid

```
library(xcms)
loaddata()
polar  "Po
noise=250000
xset <- xcmsSet(cdffiles,ppm=ppm, mzdiff=mzwid, peakwidth=peakwidth, noise=noise, snthresh=snth, method="centWave", fitgauss=TRUE, nSlaves=8)
xset2<-retco
dev.copy2pdf(device = 2, file = paste(pathResult, "/Ret_cor-Graph",expe,"_",polar,".pdf",sep=""), paper="a4", height=9, width=14)
xset3<-group(xset2, minfrac = 0.2, bw = bw, minsamp = 1, mzwid = mzwid, max = 50, sleep = 0)
xset5<-fillPeaks(xset3)

# rapport final avec statistiques de différences entre les deux classes
reporttab <- diffreport(xset5, filebase =paste(pathResult,"/Rapport_",expe,"_",polar, sep=""), mzdec=4, eicmax=5000, metlin = metlin, classeic=levels(xset5@phenoDa

#écriture du fichier Excel
dir.create(paste(pathResult,"/Rapport_",expe,"_",polar,"_diffreport/", sep=""), showWarnings = FALSE)
write.table(reporttab,paste(pathResult,"/Rapport_",expe,"_",polar,"_diffreport/resultat_",expe,"_",polar,".xls", sep=""),sep="\t")

library(CAMERA)
#annotation version rapide?
an<-annotate(xs                                                                       =3, maxiso=4, minfrac=0.5,
   ppm=15, mzabs=0.015, quick=FALSE, psg_list=NULL, rules=NULL,
   polarity=polarity)
diffreport1<-getPeaklist(an)

#diffreport <- annotateDiffreport(xsg,pval_th=0.05,fc=0.1, nSlaves=8,  calcIso=TRUE, calcCaS=FALSE, maxcharge=3, maxiso=4, minfrac=0.5,
#   ppm=15, mzabs=0.015, quick=FALSE, psg_list=NULL, rules=NULL,
#   polarity=polarity, sortpval=FALSE)
diffreport<-cbind(reporttab,diffreport1[,c("isotopes", "adduct","pcgroup")])
write.table(diffreport, file=paste(pathResult,"/result_",expe,"_",polar,"_CAMERA_diffreport-fast.xls",sep=""), row.names=FALSE, sep="\t")

library(FactoMineR)
pca3<-PCA(t(matacp), axes=c(1,2))
pca3<-PCA(t(matacp), axes=c(1,3))
pca3<-PCA(t(matacp), axes=c(2,3))
pca4<-PCA(t(matacplog2))

# -- output png --
# Percentage of variance
png("percentage_of_variance.png", width =800, height = 400);
barplot(resPCA$eig$per,xlab="Components",ylab="percentage of variance");
dev.off()

png("eigenvalue.png", width =800, height = 400);
barplot(resPCA$eig$eig,xlab="Components",ylab="eigenvalue");
dev.off()

library(ctc)
# -- Normalization: logratio --
if (normalization) {
    data=t(scale(t(data)))
```

- **Command line** tools
  - + represent almost the majority of scientific tools
  - + good parameters completeness
  - + can be executed on high performance computers
  - + automatable, workflowsable, ...
  - − minimum linux knowledge is required
  - − cruel lack of ergonomics

```
login@sbr4-l042:~$ ssh -Y login@bioinfo.sb-roscoff.fr
[...]
[login@n0 ~]$ cdprojet
[login@n0 login]$ cd 13-07-29-panda/tmp/mapping
[login@n0 mapping]$ cat tophat.qsub
#!/bin/bash
#$ -S /bin/bash
#$ -M login@sb-roscoff.fr
#$ -m bea
#$ -V
#$ -cwd
#$ -o qsub.out
#$ -e qsub.err

tophat2 panda_v121029 ../input/IllR1-1.fq ../input/IllR1-2.fq
-GTF ../input/panda_v121029.gtf --b2-sensitive -r 100
–num-threads 8

[login@n0 mapping]$ qsub -q long.q -pe thread 8 tophat.qsub
Your job 5338969 ("tophat.qsub") has been submitted
[login@n0 mapping]$ ls
accepted_hits.bam  junctions.bed      qsub.err   unmapped.bam
deletions.bed      logs               qsub.out
insertions.bed     prep_reads.info    tmp
[login@n0 mapping]$ cd ..
[login@n0 mapping]$ mkdir cufflinks
```
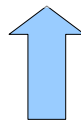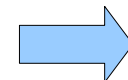
```
login@sbr4-l042:~$ ssh -Y login@bioinfo.sb-roscoff.fr
[...]
[login@n0 ~]$ cdprojet
[login@n0 login]$
[login@n0 mapping
#!/bin/bash
#$ -S /bin/bash
#$ -M login@sb-ro
#$ -m bea
#$ -V
#$ -cwd
#$ -o qsub.out
#$ -e qsub.err

tophat2 panda_v12                                    R1-2.fq
-GTF ../input/pa
-num-threads 8

[login@n0 mapping                                    .qsub
Your job 5338969
[login@n0 mapping
accepted_hits.bam                                    l.bam
deletions.bed                        qsub.out
insertions.bed        prep_reads.info    tmp
[login@n0 mapping]$ cd ..
[login@n0 mapping]$ mkdir cufflinks
```


NOOOOOOOO!

DOOM
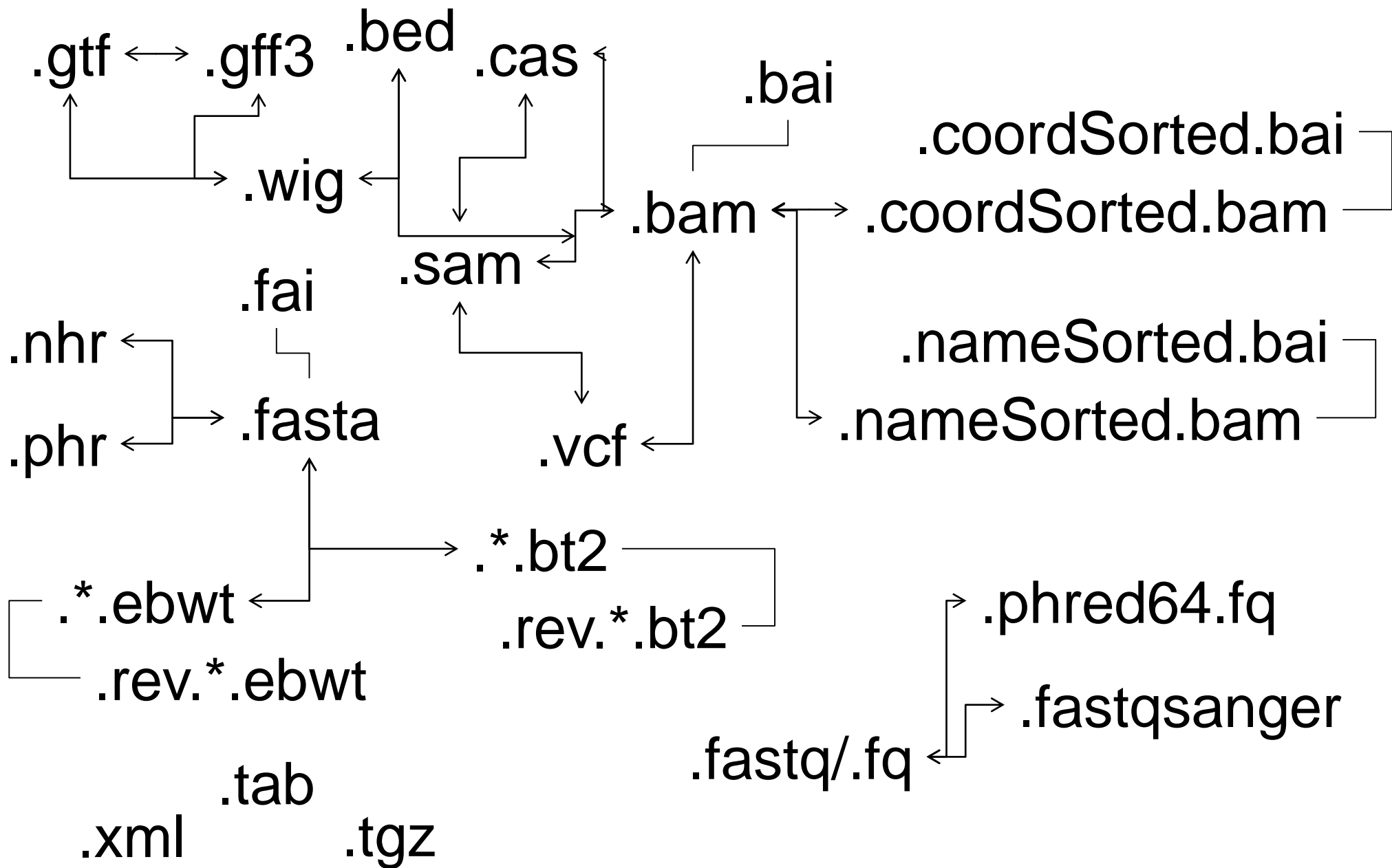
Select your level:

Level 1

« I want to know the gene expression »

Level 2

« I want to map my reads on a reference genome and count them »

Level 3

« I want to launch the tools tophat2 and cufflinks.

I have fastq files and my genome in fasta and gtf. »

Level 4

« I want 1TB for my project. I will launch tophat2 through SSH on the cluster in multi-thread mode.

Next I want to submit the bam file to my genome with cufflinks.

Except that, I will manage :P"

Level 5

« I have a bunch of cool tools!
But I'm the only one who can launch them.

Comments? »

Tools

search tools

Upload File from your computer

Export Data

LC-MS

Format Conversion

Preprocessing

Normalisation

Quality Control

Statistical Analysis

Annotation

GC-MS

Preprocessing

Normalisation

Quality Control

Statistical Analysis

Annotation

NMR

Preprocessing

Normalisation

Quality Control

Statistical Analysis

COMMON TOOLS

Data Handling

Text Manipulation

Filter and Sort

Join, Subtract and Group

---

xcms.xcmsSet   version 2.0.1

Choose your inputs method:

Zip file from your history containing your chromatograms

Zip file:

1: sacuri.zip

Extraction method for peaks detection:

matchedFilter

[method] See the help section below

Step size to use for profile generation:

0.01

[step] The peak detection algorithm creates extracted ion base peak chromatograms (EIBPC) on a fixed step size

Full width at half maximum of matched filtration gaussian model peak:

30

[fwhm] Only used to calculate the actual sigma

Advanced options:

hide

Execute

Authors Colin A. Smith csmith@scripps.edu, Ralf Tautenhahn rtautenh@gmail.com, Steffen Neumann sneumann@ipb-halle.de, Paul Benton hpaul.benton08@imperial.ac.uk and Christopher Conley cjconley@ucdavis.edu

If you use this tool, please cite: Smith,C.A. et al.(2006). XCMS: processing mass spectrometry data for metabolite profiling using nonlinear peak alignment, matching, and identification. Anal. Chem., 78, 779–787.
For details about this tool, please go to http://www.bioconductor.org/packages/release/bioc/html/xcms.html

Galaxy integration ABIMS TEAM, Station biologique de Roscoff.

Contact support@workflow4metabolomics.org for any questions or concerns about the Galaxy implementation of this tool.

History

search datasets

Sacuri Zip
19 shown

289.7 MB

19:
xset.group.retcor.group.fillPeaks.annotate.variableMetadata.tsv (Xdiffreport)

18:
xset.group.retcor.group.fillPeaks.annotate.negative.Rdata

17:
xset.group.retcor.group.fillPeaks.annotate.dataMatrix.tsv

16:
xset.group.retcor.group.fillPeaks.annotate.variableMetadata.tsv

15:
xset.group.retcor.group.fillPeaks.RData

14:
xset.group.retcor.group.Rplots.pdf

13:
xset.group.retcor.group.RData
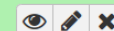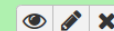
12:
xset.group.retcor.BPCs_corrected.pdf

11:
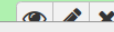
INTRODUCTION / GALAXY

Why Galaxy ?

- Accessibility

- Reproductibility

- Transparency

- ## Galaxy it's …
  - A web-based interface
  - No need to execute a command line through a terminal
  - Programming or scripting skills are not required
  - Submission of jobs is transparent through a high performance computer cluster
  - Secure histories and data manager
  - A data and protocols sharing system
  - Tool-boxes of several bioinformatics fields
    - NGS
    - Metabolomics
    - Statistics
    - Chemistry
    - Image analysis
    - Etc …

```
[login@n0 ~]$ cdprojet
[login@n0 login]$ cd 13-07-29-panda/tmp/mapping
[login@n0 mapping]$ cat tophat.qsub
#!/bin/bash
#$ -S /bin/bash
#$ -M login@sb-roscoff.fr
#$ -m bea
#$ -V
#$ -cwd
#$ -o qsub.out
#$ -e qsub.err

tophat2 panda_v121029 ../input/I11R1-1.fq ../input/I11R1-2.fq
-GTF ../input/panda_v121029.gtf --b2-sensitive -r 100
-num-threads 8

[login@n0 mapping]$ qsub -q long.q -pe thread 8 tophat.qsub
Your job 5338969 ("tophat.qsub") has been submitted
```

```
[login@n0 ~]$ cdprojet
[login@n0 login]$ cd 13-07-29-panda/tmp/mapping
[login@n0 mapping]$ cat tophat.qsub
#!/bin/bash
#$ -S /bin/bash
#$ -M login@sb-roscoff.fr
#$ -m bea
#$ -V
#$ -cwd
#$ -o qsub.out
#$ -e qsub.err

tophat2 panda_v121029 ../input/I11R1-1.fq ../input/I11R1-2.fq
-GTF ../input/panda_v121029.gtf --b2-sensitive -r 100
-num-threads 8

[login@n0 mapping]$ qsub -q long.q -pe thread 8 tophat.qsub
Your job 5338969 ("tophat.qsub") has been submitted
```

MR. HAPPY
by Roger Hargreaves

```
[lecorguille@n0 ~]$ e-PCR --help
e-PCR: invalid option -- -
usage: [-hV] [posix-options] stsfile [fasta ...]
[compat-options]
where posix-options are:
          -m ##      Margin (default 50)
          -w ##      Wordsize   (default 7)
          -n ##      Max mismatches allowed (default 0)
          -g ##      Max indels allowed (default 0)
          -f ##      Use ## discontiguos words, slow if
                            ##>1
          -o ##      Set output file
          -t ##      Set output format:
                     1 - classic, range (pos1..pos2)
                     2 - classic, midpoint
                     3 - tabular
                     4 - tabular with alignment in
comments
                            (slow)
          -d##-##    Set default size range
                            (default 100-350)
          -p +-      Turn hits postprocess on/off
          -v ##      Verbosity flags
          -a a|f     Use presize alignmens (only if
                            gaps>0), slow
                      a - Allways or f - as Fallback
          -x +-      Use 5'-end lowercase masking of
                            primers (default -)
          -u +-      Uppercase all primers (default -)

[...]
```

Galaxy / ABiMS

e-PCR (version 1.0.0)

STS file:
100: (as tabular) Trinity on data 9..Transcripts
format : tabular

Fasta file:
100: Trinity on data 9..Transcripts
format : fasta

Wordsize (W):
7
Set word size for primers hash (nucleotide positions). Longer word size decreases hash collision rate, but increases memory usage. Also no mismatches are allowed within word size near 'inner' boundary of primers unless one uses discontiguous words, and no gaps are ever allowed in that region.

Use ## discontinuos words (F):
1
Set discontiguous word count for primers hash (1 means 'use contiguous words'). Discontiguous words increase number of hash tables and decrease 'effective' word size (thus increasing hash collision rate), so make search significantly slower, but increase sencitivity by allowing mismatches within word size. Reasonable values are 1 (contiguous words) and 3.

Margin (M):
50
Set maximal allowed deviation of hit product size from expected STS size.

Set default sts lower size (D):
100
Set ddefault STS size range - values used for STSs that have no size associated in file.

Set default sts higher size (D):
400
Set ddefault STS size range - values used for STSs that have no size associated in file.

Max mismatches allowed (N):
0
Set maximal number of mismatches allowed in primer-to-sequence alignment (per primer!).

Max indels allowed (G):
0
Set maximal number of gaps allowed in primer-to-sequence alignment (per primer!).

Set output format (T):
tabular
Output formats

Execute

Galaxy interface

Galaxy interface

Menu

Tools

search tools

Upload File from your computer

Export Data

LC-MS

Format Conversion

Preprocessing

Normalisation

   Batch_correction Corrects intensities for signal drift and batch-effects

   Determine_batch_correction to choose between linear, lowess and loess methods

   Transformation Transforms the dataMatrix intensity values

Quality Control

Statistical Analysis

Annotation

GC-MS

Preprocessing

Normalisation

Quality Control

Statistical Analysis

Annotation

NMR

Preprocessing

Normalisation

Batch_correction (version 2.0.0)

Data Matrix file :

17: xset.group.retcor.group.fillPeaks.annotate.dataMatrix.tsv

Sample metadata file :

3: sampleMetadata.tsv

must contain at least the three following columns: 'batch' + 'injectionOrder' + 'sampleType'

Variable metadata file :

16: xset.group.retcor.group.fillPeaks.annotate.variableMetadata.tsv

Type of regression model :

linear

To select between linear or non-linear (lowess or loess) methods to be used in Van der Kloet algorithm ; when using loess, you can choose to use pools or samples to model batch effect.

Factor of interest :

batch

column name of factor of interest (often a biological factor); if none, leave 'batch'

Level of details for plots :

basic

Amount of plots in the pdf file output. See Help section for more details.

Execute

ℹ **Authors**
Jean-Francois Martin - PF MetaToul-AXIOM ; INRA ; MetaboHUB (for original version of this tool and overall development of the R script)

ℹ **Contributors**
Melanie Petera - PFEM ; INRA ; MetaboHUB (for R wrapper and R script improvement)
Etienne Thevenot - LIST/LADIS ; CEA ; MetaboHUB (for R script and wrapper concerning "all loess pool" and "all loess sample" methods)

History

search datasets

Sacuri Zip
19 shown

289.7 MB

19:
xset.group.retcor.group.fillPeaks.annotate.variableMetadata.tsv (Xdiffreport)

18:
xset.group.retcor.group.fillPeaks.annotate.negative.Rdata

17:
xset.group.retcor.group.fillPeaks.annotate.dataMatrix.tsv

16:
xset.group.retcor.group.fillPeaks.annotate.variableMetadata.tsv

15:
xset.group.retcor.group.fillPeaks.RData

14:
xset.group.retcor.group.Rplots.pdf

13:
xset.group.retcor.group.RData

12:
xset.group.retcor.BPCs_corrected.pdf

11:

Galaxy interface

Tool list

Galaxy interface

Web forms / dataset visualization / diverse information

Galaxy interface

History

GET HELP

Get help

DATA IMPORT

DATA IMPORT
< 2 GO

Data import < 2 Go

Data import < 2 Go

Data import < 2 Go

Copy / Paste data

Data import < 2 Go

From local files

From local files

Data import < 2 Go

From local files

Data import < 2 Go

From local files

Data import < 2 Go

From local files

Data import < 2 Go

From local files

Data import < 2 Go

From local files

Data import < 2 Go

From local files

Step 1: Choose a FTP Client

DATA IMPORT

> 2 GO

STEP 1: CHOOSE A FTP CLIENT

FileZilla

Cyberduck

WinSCP

STEP 1: CHOOSE A FTP CLIENT

FileZilla

Cyberduck

WinSCP

Step 2: Easy!

DATA IMPORT
> 2 GO

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

62

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

Data import > 2 Go

~~DATA IMPORT~~

~~Data import~~

For HUGE public resources: genome, databank …

--> Make a request to the support team

Hands-on
DATA IMPORT

1. Fetch the file with your internet browser (see given URL)

2. Upload this file into Galaxy

    a. First, as you want

    b. Consider that it is >2 Go

TOOLS

What tools are available?

>80 public Galaxy servers available:

https://galaxyproject.org/public-galaxy-servers

>80 public Galaxy servers available:
https://galaxyproject.org/public-galaxy-servers

RNAseq: http://galaxy3.sb-roscoff.fr
SBR tools: http://webtools.sb-roscoff.fr
Metagenomics: http://galaxy4frogs.sb-roscoff.fr

Metabolomics:
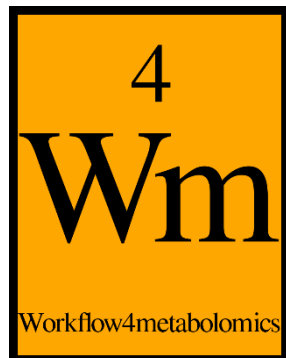
ChIP-seq:

an open and powerful Galaxy instance
for integrative Omics data analysis

Tools - panel

Tools - form

Tools - form

Tools - form

Tools can have some advanced options

Tools - form

Tools - form

2: xset.RData

Job is waiting to run

= the job is in the scheduler « queue »

Duration time of this status depends on the amount of actual queued jobs and on the requested number of processors

2: xset.RData

Job is currently running

= the job is being executed on the computing cluster

Duration time of this status depends on the job's attributes and the computing ressources allocated.

Some programs are executed with several processors (using 4, 8 or 16 Gb of RAM).

And others are mono-threaded ☹

2: xset.RData

Job is finished and status is OK

But warnings or errors can be hidden behind!

Job is finished but with an error status

= the program sends an error

The error is often explained by the program but sometimes … not.

16: xset.RData

Job is finished but with an error status

= the program sends an error

Possible causes of error :

– ~~The user~~ :P

– Bad usage : input file, format or option

– Bad integration of the program into Galaxy … sorry :/

– Non anticipated crash of the program

Tools - Handle errors

Sent to the support team

DATASET

Dataset

Both inputs and outputs

Informations

Dataset

Informations

Dataset

Download

Dataset

Re-run a job

Dataset

Dataset display : text, tabular, pdf, picture, html …

Dataset

Renaming and annotation

Dataset

Renaming and annotation

Dataset

Change the Datatype of the Dataset

Datatypes

DATASET

- Every Galaxy dataset is associated with a datatype.
- Datatype can be detected or user specified.

Dataset - Datatypes

- Every Galaxy dataset is associated with a datatype.
- Datatype can be detected or user specified.

Dataset - Datatypes

- **Many tools will only accept input datasets with the appropriate datatype assigned.**

Common text formats:

- **txt**: plain text ('.txt')

- **tabular**: tab delimited ('.tab', '.txt', etc.)

```
                    wt_37_2   wt_37_3   wt_37_1
TR24|c0_g1_i1       90.00     67.00     85.00
TR2779|c0_g1_i1     186.00    137.00    217.00
TR127|c1_g1_i1      9.00      23.00     16.00
```

- **csv**: comma-separated values ('.csv')

```
Year,Make,Model
1997,Ford,E350
2000,Mercury,Cougar
```

- **html**: standard language for web pages

```
<!DOCTYPE html>
<html>
  <head>
    <title>This is a title</title>
  </head>
  <body>
    <p>Hello world!</p>
  </body>
</html>
```

Common binary formats:

- *data*: generic binary format

- *zip, tar*: archives

- *pdf, png, jpg, bmp, tiff, gif*: images

- *rdata*: statistical computing program R

- *bam*, **wig**, **bigwig**: sequence alignment

Sequence file formats:

- **_fasta_**: a single-line description with '>', followed by lines of sequence data ('.fasta', '.fas')

```
>sequence1
atgcgtttgcgtgcatgcgtttgcgtgcatgcgtttgcgtgcatgcgtttgcgtgc
atgcgtttgcgtgc
>sequence2
tttcgtgcgtatagtttcgtgcgtatagtttcgtgcgtatagtttcgtgcgtatag
tggcgcggt
```

- **_fastq_**: sequence + quality score ('.fastq', '.fq')

```
@SEQ_ID
GATTTGGGGTTCAAAGCAGTATCGATCAAATAGTAAATCCATTTGTTCAACTCACAGTTT
+
!''*((((***+))%%%++)(%%%).1***-+*''))**55CCF>>>>>>CCCCCCC65
@SEQ_ID2
GATTTGGGGTTCAAAGCAGTATCGATCAAATAGTAAATCCATTTGTTCAACTCACAGTTT
+
!''*((((***+))%%%++)(%%%).1***-+*''))**55CCF>>>>>>CCCCCCC65
```

Sequence file formats:

- **gff3, bed, genbank**: sequence + annotations

bed
```
track name=pairedReads description="Clone Paired Reads" useScore=1
chr22 1000 5000 cloneA 960 + 1000 5000 0 2 567,488, 0,3512
chr22 2000 6000 cloneB 900 - 2000 6000 0 2 433,399, 0,3601
```

gff3
```
##gff-version 3
ctg123  .  exon  1300  1500  .  +  .  ID=exon00001
ctg123  .  exon  1050  1500  .  +  .  ID=exon00002
ctg123  .  exon  3000  3902  .  +  .  ID=exon00003
##FASTA
>ctg123
cttctgggcgtacccgattctcggagaacttgccgcaccattccgccttg
tgttcattgctgcctgcatgttcattgtctacctcggctacgtgtggcta
…
```

Cleanup

DATASET

Dataset

Delete a dataset

Dataset

The dataset isn't really deleted. It's in the Trash

Dataset

"Empty Trash" : to free up disk space

HISTORY

History panel

Both inputs and outputs

History panel

Both inputs and outputs

History panel   renaming and annotation

History panel

History menu: Create new, Rename, Delete, Delete Permanently

Saved histories

History panel

Saved histories: Switch histories

History panel

History panel

History panel

History panel

History panel

Hands-on
TOOLS

Which coding exon has the highest number of single nucleotide polymorphisms on chromosome 22?
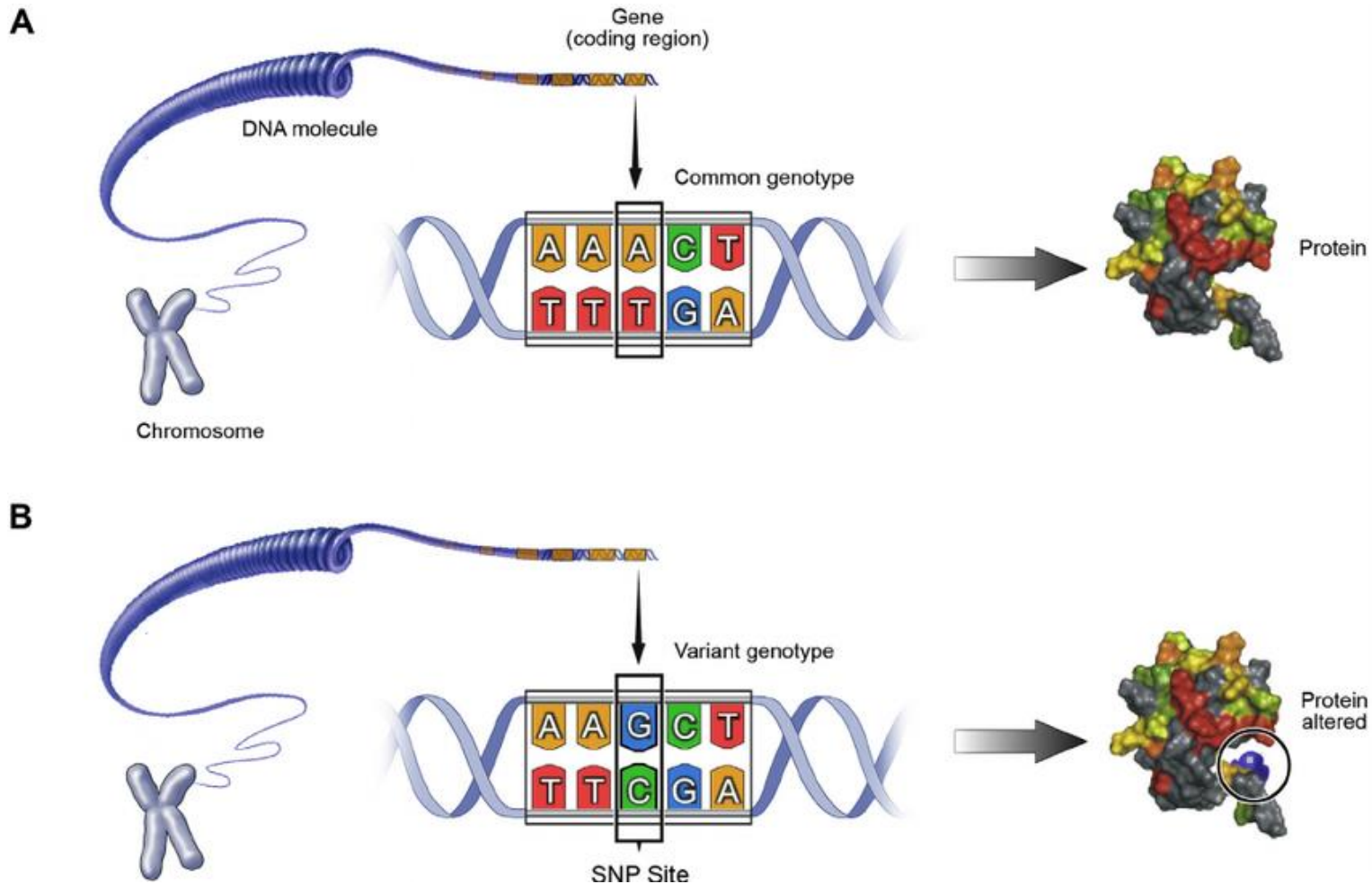
Which coding exon has the highest number of single nucleotide polymorphisms on chromosome 22?

1. Get the data in a new history
2. Join exons with SNPs
3. Count the number of SNPs per exon
4. Sort exons by SNP count
5. Select top five
6. Build a bar diagram
7. Recover exon info and display data in genome browsers

Which coding exon has the highest number of single nucleotide polymorphisms on chromosome 22?

1. Get the data in a new history

2. Join exons with SNPs *Operate on Genomics Intervals -> Join*

3. Count the number of SNPs per exon *Join, Subtract, and Group -> Group*

4. Sort exons by SNP count *Filter and Sort -> Sort*

5. Select top five *Text Manipulation -> Select First*

6. Build a bar diagram *Visualize -> Charts*

7. Recover exon info and display data in genome browsers *Join, Subtract and Group -> Compare two Datasets*

WORKFLOW

- A workflow is a sequence of tool operations and parameters

- Can match the experiment protocol

- A workflow is built to be replayed (more or less strict)

Workflow

Our workflow with Galaxy

Workflow

From history

Workflow

From history

Workflow

From history

Workflow

Workflow manager

Workflow

Workflow manager

Workflow

Edit a workflow: add tags and annotation

Workflow

Edit a workflow

Workflow

Edit a workflow: drag and drop

Workflow

Edit a workflow: delete a noodle

Workflow

Edit a workflow: delete a noodle

Workflow

Edit a workflow: add a tool

Workflow

Edit a workflow: add a noodle

Workflow

Edit a workflow: hide intermediate steps

Workflow

Edit a workflow: set or release a parameter

Workflow

Edit a workflow: set or release a parameter

Workflow

Edit a workflow: rename the outputs

Workflow

Save

Workflow

Run a workflow

Workflow

Run a workflow

Workflow

Run a workflow

Workflow

Run a workflow

Workflow

Run a workflow

Run a workflow

- ## Possible

Super-workflow

- ## Impossible (until now)

For / While

True

False

If

SHARE

biologist ↔ biologist

- **Sharing histories or datasets**
  - With or without linked workflow

bioanalyst ↔ biologist

- **Sharing workflows**
  - Pre-configured parameters
  - With or without release parameters (set at runtime)

    - According to the user-end knowledge

bioinformatician ⟷ bioinformatician

- ## Sharing tools ,scripts and wrappers
  - – Toolshed

Share

History

Share

Workflow

Share

Mode

• Get shared histories

Share

- **Get shared workflows**

- Import shared

Share

Level 5

- Share tools and descriptions in the ToolShed

Level 4

- Launch tools autonomously
- Use advanced parameters
- Use the Galaxy API
- Provide workflow for colleagues Level 1-3

Level 3

- Launch tools autonomously
- Use workflow more or less preset

Level 2

- Use preset workflow

Level 1

- Share his data to collegues Level 2-5

Hands-on
WORKFLOW

Which coding exon has the highest number of ~~single nucleotide polymorphisms~~ on chromosome 22?
  repeats

1. Extract a workflow from your history
2. Edit the workflow (hide intermediate steps, rename inputs/outputs, set parameters at runtime, save)
3. Create a new history with the input data
4. Run the workflow
5. Share your history/workflow with your neighbour

Collection
DATASET

- Problematic: you have a large numbers of datasets to send through the same analysis

- Problematic: you have a large numbers of datasets to send through the same analysis

- Solution 1: select multiple datasets as input

Dataset collection

Select multiple datasets as input

Dataset collection

Select multiple datasets as input

- Problematic: you have a large numbers of datasets to send through the same analysis

- Solution 1: select multiple datasets as input
- Solution 2: create a dataset collection

- Problematic: you have a large numbers of datasets to send through the same analysis

- Solution 1: select multiple datasets as input
- Solution 2: create a dataset collection
  - Dataset list: set of files of the same type
  - Dataset pairs: pairs of read files (forward, reverse)
  - List of dataset pairs

- Problematic: you have a large numbers of datasets to send through the same analysis

- Solution 1: select multiple datasets as input

- Solution 2: create a dataset collection
  - Dataset list: set of files of the same type
  - Dataset pairs: pairs of read files (forward, reverse)
  - List of dataset pairs

- Galaxy runs the tool automatically on each dataset in the collection using the same settings

Dataset collection

Create a dataset collection

Dataset collection

Create a dataset collection

Dataset collection

Create a dataset collection

Dataset collection

Create a dataset collection

Dataset collection

Create a dataset collection

Dataset collection

Tools for collection operations

Dataset collection

Use a collection as input

Dataset collection

Use a collection as input

Hands-on
COLLECTION

1. Create a dataset list with SNPs, repeats and exons
2. Run tool "Convert Formats -> BED-to-GFF converter" on the dataset list

END

BONUS

How are tools born?

BONUS

- How to import a tool in Galaxy?

- How to import a tool in Galaxy?

```
[lecorguille@n0 ~]$ e-PCR --help
e-PCR: invalid option -- -
usage: [-hV] [posix-options] stsfile [fasta ...]
[compat-options]
where posix-options are:
        -m ##    Margin (default 50)
        -w ##    Wordsize  (default 7)
        -n ##    Max mismatches allowed (default 0
        -g ##    Max indels allowed (default 0)
        -f ##    Use ## discontiguos words, slow i
                         ##>1
        -o ##    Set output file
        -t ##    Set output format:
                 1 - classic, range (pos1..pos2)
                 2 - classic, midpoint
                 3 - tabular
                 4 - tabular with alignment in com
                         (slow)
        -d##-##  Set default size range
                         (default 100-350)
        -p +-    Turn hits postprocess on/off
        -v ##    Verbosity flags
        -a a|f   Use presize alignmens (only if
                         gaps>0), slow
                  a - Allways or f - as Fallback
        -x +-    Use 5'-end lowercase masking of
                         primers (default -)
        -u +-    Uppercase all primers (default -)

[...]
```

Galaxy / ABiMS

e-PCR (version 1.0.0)

STS file:
100: (as tabular) Trinity on data 9..Transcripts
format : tabular

Fasta file:
100: Trinity on data 9..Transcripts
format : fasta

Wordsize (W):
7
Set word size for primers hash (nucleotide positions). Longer word size decreases hash collision rate, but increases memory usage. Also no mismatches are allowed within word size near 'inner' boundary of primers unless one uses discontiguous words, and no gaps are ever allowed in that region.

Use ## discontinuos words (F):
1
Set discontiguous word count for primers hash (1 means 'use contiguous words'). Discontiguous words increase number of hash tables and decrease 'effective' word size (thus increasing hash collision rate), so make search significantly slower, but increase sencitivity by allowing mismatches within word size. Reasonable values are 1 (contiguous words) and 3.

Margin (M):
50
Set maximal allowed deviation of hit product size from expected STS size.

Set default sts lower size (D):
100
Set ddefault STS size range - values used for STSs that have no size associated in file.

Set default sts higher size (D):
400
Set ddefault STS size range - values used for STSs that have no size associated in file.

Max mismatches allowed (N):
0
Set maximal number of mismatches allowed in primer-to-sequence alignment (per primer!).

Max indels allowed (G):
0
Set maximal number of gaps allowed in primer-to-sequence alignment (per primer!).

Set output format (T):
tabular
Output formats

Execute

- How to import a tool in Galaxy?

```xml
<tool id="abims_epcr" name="e-PCR">
    <!-- author : lecorguille@sb-roscoff.fr -->
    <!-- date : 11-05-12 -->
    <description>e-PCR parses stsfile in unists format, then reads nucleotide sequence data in FASTA format from files listed in commandline if
    any, or from stdin otherwise. For input sequences e-PCR finds matches and prints output in one of three formats.</description>

    <command>e-PCR -w $wordsize -f $wordcnt -m $margin -d$sts_size_lo-$sts_size_hi -n $max_mismatch -g $max_gap -t $output_format $infile_stsfile
    $infile_fasta > $output</command>

    <inputs>
        <param name="infile_stsfile" type="data" label="STS file" format="tabular" help="format : tabular" />
        <param name="infile_fasta" type="data" label="Fasta file" format="fasta" help="format : fasta" />
        <param name="wordsize" type="integer" label="Wordsize (W)" value="7" help="Set word size for primers hash (nucleotide positions).
        Longer word size decreases hash collision rate, but increases memory usage. Also no mismatches are allowed within word size near
        'inner' boundary of primers unless one uses discontiguous words, and no gaps are ever allowed in that region." />
        <param name="wordcnt" type="integer" label="Use ## discontinuos words (F)" value="1" help="Set discontiguous word count for primers
        hash (1 means 'use contiguous words'). Discontiguous words increase number of hash tables and decrease 'effective' word size (thus
        increasing hash collision rate), so make search significantly slower, but increase sencitivity by allowing mismatches within word
        size. Reasonable values are 1 (contiguous words) and 3." />
        <param name="margin" type="integer" label="Margin (M)" value="50" help="Set maximal allowed deviation of hit product size from
        expected STS size." />
        <param name="sts_size_lo" type="integer" label="Set default sts lower size (D)" value="100" help="Set ddefault STS size range - values
        used for STSs that have no size associated in file." />
        <param name="sts_size_hi" type="integer" label="Set default sts higher size (D)" value="400" help="Set ddefault STS size range -
        values used for STSs that have no size associated in file." />
        <param name="max_mismatch" type="integer" label="Max mismatches allowed (N)" value="0" help="Set maximal number of mismatches allowed
        in primer-to-sequence alignment (per primer!)." />
        <param name="max_gap" type="integer" label="Max indels allowed (G)" value="0" help="Set maximal number of gaps allowed in primer-to-
        sequence alignment (per primer!)." />
        <param name="output_format" type="select" help="Output formats">
            <label>Set output format (T)</label>
            <option value="1">classic, range (pos1..pos2)</option>
            <option value="2">classic, midpoint</option>
            <option value="3" selected="true">tabular</option>
            <option value="4">tabular with alignment in comments (slow)</option>
        </param>
    </inputs>

    <outputs>
        <data name="output" format="tabular" />
    </outputs>
```
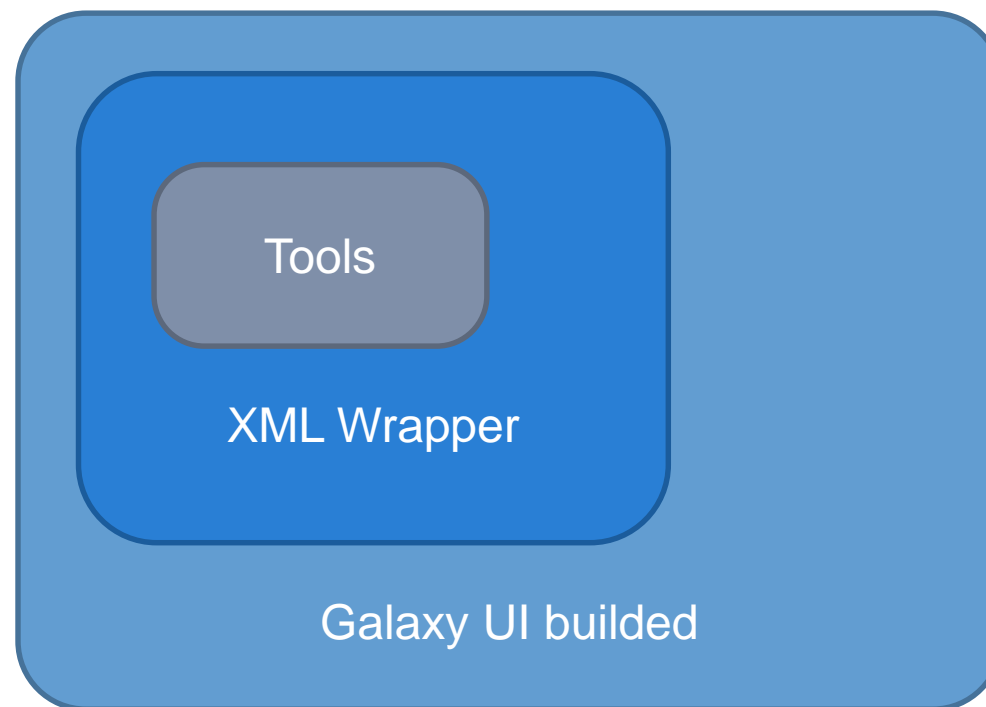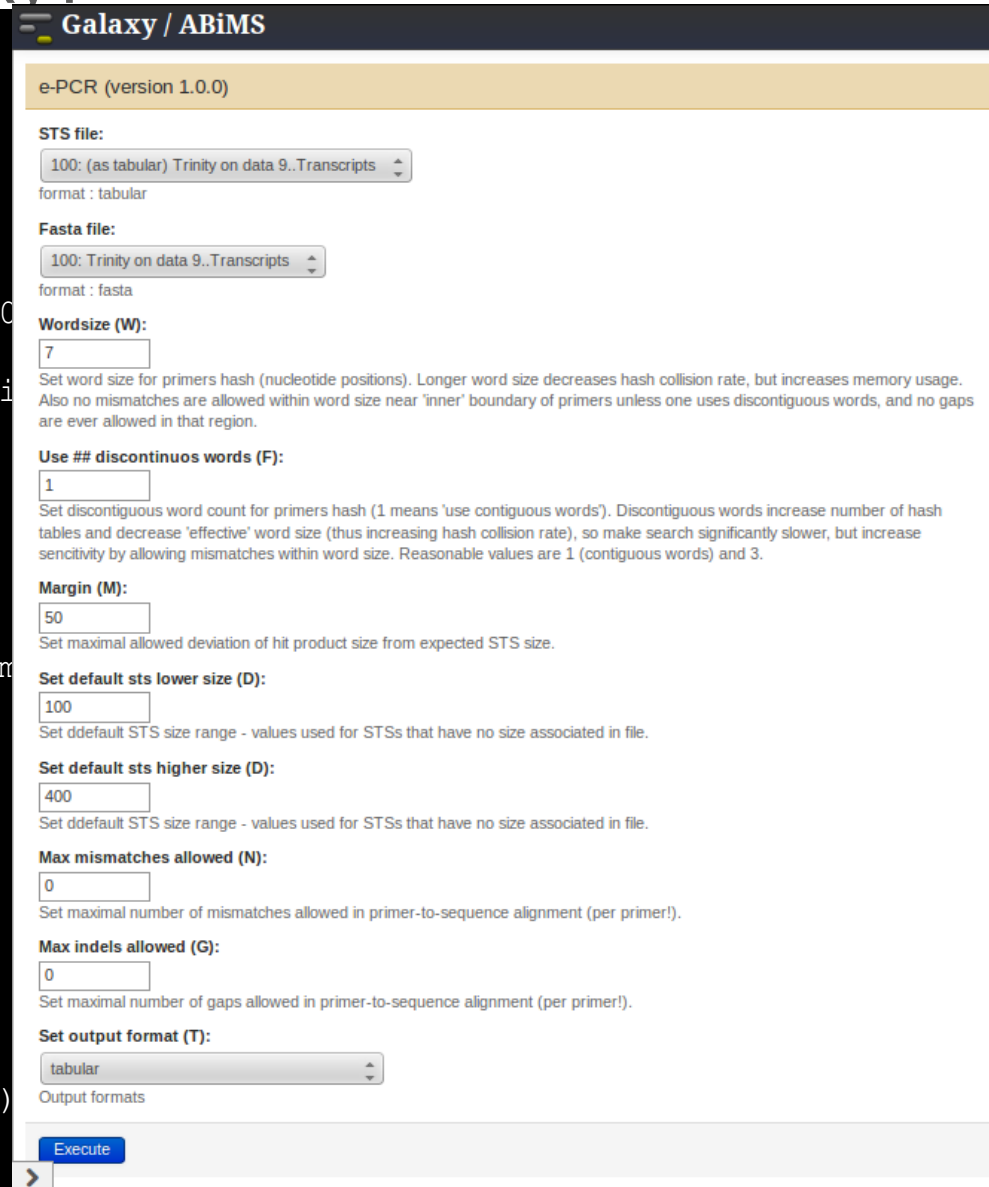
- How to import a tool in Galaxy?

```
[lecorguille@n0 ~]$ e-PCR --help
e-PCR: invalid option -- -
usage: [-hV] [posix-options] stsfile [fasta ...]
[compat-options]
where posix-options are:
        -m ##       Margin (default 50)
        -w ##       Wordsize  (default 7)
        -n ##       Max mismatches allowed (default 0
        -g ##       Max indels allowed (default 0)
        -f ##       Use ## discontiguos words, slow i
                          ##>1
        -o ##       Set output file
```

Galaxy / ABiMS

e-PCR (version 1.0.0)

STS file:
100: (as tabular) Trinity on data 9..Transcripts
format : tabular

Fasta file:
100: Trinity on data 9..Transcripts
format : fasta

Wordsize (W):
7

Set word size for primers hash (nucleotide positions). Longer word size decreases hash collision rate, but increases memory usage. Also no mismatches are allowed within word size near 'inner' boundary of primers unless one uses discontiguous words, and no gaps are ever allowed in that region.

Use ## discontinuos words (F):
1

```xml
<tool id="abims_epcr" name="e-PCR">
»       <!-- author : lecorguille@sb-roscoff.fr -->
»       <!-- date : 11-05-12 -->
»
»       <description>e-PCR parses stsfile in unists format, then reads nucleotide sequence data in FASTA format from files listed in commandline if
        any, or from stdin otherwise. For input sequences e-PCR finds matches and prints output in one of three formats.</description>
»
»
»       <command>e-PCR -w $wordsize -f $wordcnt -m $margin -d$sts_size_lo-$sts_size_hi -n $max_mismatch -g $max_gap -t $output_format $infile_stsfile
        $infile_fasta > $output</command>
»
»       <inputs>
»       »       <param name="infile_stsfile" type="data" label="STS file" format="tabular" help="format : tabular" />
»       »       <param name="infile_fasta" type="data" label="Fasta file" format="fasta" help="format : fasta" />
»       »       <param name="wordsize" type="integer" label="Wordsize (W)" value="7" help="Set word size for primers hash (nucleotide positions).
        Longer word size decreases hash collision rate, but increases memory usage. Also no mismatches are allowed within word size near
        'inner' boundary of primers unless one uses discontiguous words, and no gaps are ever allowed in that region." />
»       »       <param name="wordcnt" type="integer" label="Use ## discontinuos words (F)" value="1" help="Set discontiguous word count for primers
        hash (1 means 'use contiguous words'). Discontiguous words increase number of hash tables and decrease 'effective' word size (thus
        increasing hash collision rate), so make search significantly slower, but increase sencitivity by allowing mismatches within word
        size. Reasonable values are 1 (contiguous words) and 3." />
»       »       <param name="margin" type="integer" label="Margin (M)" value="50" help="Set maximal allowed deviation of hit product size from
        expected STS size." />
»       »       <param name="sts_size_lo" type="integer" label="Set default sts lower size (D)" value="100" help="Set ddefault STS size range - values
        used for STSs that have no size associated in file." />
»       »       <param name="sts_size_hi" type="integer" label="Set default sts higher size (D)" value="400" help="Set ddefault STS size range -
        values used for STSs that have no size associated in file." />
»       »       <param name="max_mismatch" type="integer" label="Max mismatches allowed (N)" value="0" help="Set maximal number of mismatches allowed
```