









27/01/2014

Metabolomics



Initiation

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INTRODUCTION / PROBLÉMATIQUE



Sélectionner votre niveau :



Level 1



"Je veux savoir quels métabolites diffèrent entre mes deux conditions"



Level 2



"Je veux savoir quels métabolites diffèrent entre mes deux conditions" "Je sais que je dois importer mes fichiers puis annoter mes pics. Et finalement, je veux une ACP"







"Je veux lancer les outils xcms pour importer et aligner mes mzXML, puis CAMERA pour l'annotation de mes adduits et un outil de corrélation pour réduire mon jeu de données avant l'ACP"



Level 4



"Je veux un espace projet avec 1To car je pense faire du ssh pour lancer mes scripts R et les packages xcms et CAMERA en multi-thread

Je pense interroger ensuite HMDB

Sinon, pas besoin de vous : P"







"J'ai un tas de scripts et outils sympas ! Mais je suis le seul à pouvoir les lancer.

Des commentaires ?"



Pourquoi?

```
library(xcms)
loaddata()
polar<-"Pos"</pre>
```

noise=250000

xset <- xcmsSet(cdffiles,ppm=ppm, mzdiff=mzwid, peakwidth=peakwidth, noise=noise, snthresh=snth, method="centWave", fitgauss=TRUE, nSlaves=8)
xset2<-retcor(xset, method="obiwarp", plottype="deviation")
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)</pre>

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=</pre>

#écriture du fichier Excel

data=t(scale(t(data)))

```
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(xsg,pval=0.05, 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)
diffreport1<-getPeaklist(an)</pre>
```

```
#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))</pre>
pca3<-PCA(t(matacp), axes=c(1,3))</pre>
pca3<-PCA(t(matacp), axes=c(2,3))</pre>
pca4<-PCA(t(matacplog2))</pre>
# -- 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) {
```

3

library(xcms)
loaddata()
polar<-"Pos"</pre>

noise=250000

xset <- xcmsSet(cdffiles,ppm=ppm, mzdiff=mzwid, peakwidth=peakwidth, noise=noise, snthresh=snth, method="centWave", fitgauss=TRUE, nSlaves=8)</pre>

xset2<-retcor(xset, method="obiwarp" dev.copy2pdf(device = 2, file = paste xset3<-group(xset2, minfrac = 0.2, bv xset5<-fillPeaks(xset3)</pre>

rapport final avec statistiques de
reporttab <- diffreport(xset5, fileba</pre>

#écriture du fichier Excel dir.create(paste(pathResult,"/Rappor write.table(reporttab,paste(pathResult))

library(CAMERA)
#annotation version rapide?
an<-annotate(xsg,pval=0.05, nSlaves=
ppm=15, mzabs=0.015, quick=FALSE, polarity=polarity)
diffreport1<-getPeaklist(an)</pre>

#diffreport <- annotateDiffreport(xs; # ppm=15, mzabs=0.015, quick=FALSE, # polarity=polarity, sortpval=FALSE; diffreport<-cbind(reporttab,diffreport write.table(diffreport, file=paste(paste))

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))</pre>

-- output png -# Percentage of variance
png("percentage_of_variance.png", wid
barplot(resPCA\$eig\$per,xlab="Componendev.off()

png("eigenvalue.png", width =800, he. barplot(resPCA\$eig\$eig,xlab="Componen dev.off()

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





- . Les outils avec interface graphique click bouton sous windows
 - + très ergonomique
 - trop ergonomique \rightarrow manque de souplesse
 - faut pas rêver ! Vous avez déjà vu un thésard trouver le temps pour faire de beaux boutons verts ?

MetaboAnalyst 2.

PCA Score Plot

- payant ?
- . Les outils en ligne sur Internet
 - + très ergonomique
 - trop ergonomique \rightarrow manque de souplesse
 - une infime part des outils disponibles
 - réparti un peu partout sur les différents sites universitaires
 - souvent limité en terme de taille de soumission
 - il ne faut pas être parano





- Le projet Worflow4Metabolomics
 - outils et workflows pour l'analyse en métabolomique
- V0(06/2012): Preuve de concept
 - Stage d'une étudiante (1 mois)
 - L'intégration du package XCMS
- V1(2012/2013)
 - Collaboration entre MetaboMER (Roscoff) & PFEM (Clermont Ferrand)
 - Développement collaboratif
- V2(2013/2014)
 - Collaboration entre MetaboMER (Roscoff), P2M2 (Rennes) et ABIMS (Roscoff)
 - Développement collaboratif autour du workflow









INTRODUCTION / GALAXY



- . Setup TP
 - http://galaxy.sb-roscoff.fr
 - . Compte
 - login@sb-roscoff.fr
 - _ *******

• Support de cours :

http://application.sb-roscoff.fr/download/fr2424/abims/lecorguille/cours/galaxy-init-metabo.pdf

Tools sendth bools Sendth bools Sendth bools Cell Black Vigblack Elis from your computer Subject database/sequence(s): Lituman_protein fas_: Subject database/sequence(s): Ext Data Subject database/sequence(s): Subj	– Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%	
Get Data • Uplad Elik ten ony vor compute Answist vor KNA-seq untit reference by Marking	Tools	NCBI BLAST+ blastx (version 0.0.17)	Â	History	00	,
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	<u>Get Data</u>	1: human_protein.fas		5.3 MB	47 🖻	2
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Workfore RNA-seque in reference by ABIMS ABIMS ABIMS Morkfore RAS-seque interference by ABIMS ABIMS TOOLS Primet RNASseq Interfast Minifestial Statistics Utils Protein FASTA file to use as database: Internal protein fast Query genetic code: Internal protein fast Query genetic code: Interfast Doin Utils Statistics Utils Protein fASTA file to use as database: Internal protein fast Query genetic code: Internal code: Int	ABIMS WORKFLOWS	FASTA file from your history (see warning note below)		<u>1: human_protein.fas</u>	@0%	3
Workhow RNA-Seq utilitreference by RAMSB Mamily More RNA-Seq utilitreference by RamsB More A Metabolomics ABIMS TOOLS Primer RNASeq Mont Stools Set expectation value cutoff: 0001 Output format: Satistics Utilis Phylogenetics Debug COMMON TOOLS Fert Manipulation Join, Subtract and Group Filter and Sort NCBIBLAST+ blacks Bearch nucleotide duery sequence(s) • NCBIBLAST+ blacks Bearch nucleotide query sequence(s) • NCBIBLAST+ blacks Bearch protein database with protein database with reference by reprivation adtabase by reprivation adtabase by reprinverse satablacks drul nucleotide query sequence(s) <td>Workflow RNA-seq de novo by ABiMS</td> <td>Protein FASTA file to use as database:</td> <td></td> <td></td> <td></td> <td></td>	Workflow RNA-seq de novo by ABiMS	Protein FASTA file to use as database:				
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Filter and Sort NCBI BLAST+ • NCBI BLAST+ • NCBI BLAST+ blastn Search nucleotide database with nucleotide query sequence(s) • NCBI BLAST+ blastp Search protein database with protein query sequence(s) • NCBI BLAST+ blastn Search nucleotide query sequence(s) • NCBI BLAST+ blastn Search protein database with protein query sequence(s) • NCBI BLAST+ blastn Search protein database with protein database with translated nucleotide query, using the NCBI BLAST+ blastx command line tool. • NCBI BLAST+ blastn Search protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool. • NCBI BLAST+ blastn Search protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool. • NCBI BLAST+ blastn Search protein database using a translated nucleotide query, using the NCBI BLAST+ blast Search protein database with translated nucleotide query sequence(s) • NCBI BLAST+ blastn Search protein database using a translated nucleotide query sequence(s) • NCBI BLAST+ blastn Search protein database using a translated nucleotide query sequence(s) • NCBI BLAST+ blastn Search protein database using a translated nucleotide query of this tool is tabular. The standard BLAST+ tabular output • Output format Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output • CotumpletiCB transe • Cotumpletice trabul	Join, Subtract and Group					
NCBI BLAST+ Image: processing. • NCBI BLAST+ blastn Search nucleotide database with nucleotide query sequence(s) What it does • NCBI BLAST+ blastn Search protein database with protein query sequence(s) Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool. • NCBI BLAST+ blastn Search protein database with protein query sequence(s) You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significiant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that. • NCBI BLAST+ blastn Search protein database using a translated nucleotide query sequence(s) Output format • NCBI BLAST+ blastn Search nucleotide query sequence(s) Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:	Filter and Sort	A Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight				
 NCBI BLAST+ blastn Search nucleotide database with nucleotide database with nucleotide query sequence(s) NCBI BLAST+ blastn Search protein database using a <i>translated nucleotide query</i>, using the NCBI BLAST+ blastx command line tool. NCBI BLAST+ blastn Search protein database using a <i>translated nucleotide query</i>, using the NCBI BLAST+ blastx command line tool. NCBI BLAST+ blastn Search protein database using a <i>translated nucleotide query</i>, using the NCBI BLAST+ blastx command line tool. NCBI BLAST+ blastn Search nucleotide query sequence(s) NCBI BLAST+ blastn Search protein database with translated nucleotide query sequence(s) NCBI BLAST+ blastn Search nucleotide query sequence(s) NCBI BLAST+ blastn Search protein database on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns: 	NCBI BLAST+	processing.				
Nucleotide database with nucleotide query sequence(s) What it does NCBI BLAST+ blastp Search protein database with protein query sequence(s) Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool. NCBI BLAST+ blasts Search protein database with translated nucleotide query sequence(s) You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significiant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that. NCBI BLAST+ tblastn Search protein database with translated nucleotide query sequence(s) Output format Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns: Image: Column (CBI pame Description)	<u>NCBI BLAST+ blastn</u> Search					
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 NCBI BLAST+ blastn Search vill search against a FASTA file of subject protein sequences. This is <i>not</i> advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significiant). In most cases you should instead turn the other FASTA file into a database first using <i>makeblastdb</i> and search against that. NCBI BLAST+ blastn Search protein database with translated nucleotide query sequence(s) NCBI BLAST+ tblastn Search contains 12 columns: ColumnalNCRI name Description 	NCPI PLAST+ blasta Soarch	Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool.				
query sequence(s) used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that. • NCBI BLAST+ blastx Search protein database with translated nucleotide query sequence(s) • Output format • NCBI BLAST+ tblastn Search contains 12 columns: • Output format • ColumnolNCBI protein database • Description	protein database with protein	A You can also search against a FASTA file of subject protein sequences. This is <i>not</i> advised because it is slower (only one CPU is				
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NCBI BLAST+ tblastn Search Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns: ColumnINCEL name Description	protein database with translated nucleotide guery seguence(s)	Output format				
Column NCRI name Description	NCBI BLAST+ tblastn Search	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output				
Column NCPI name Description		contains 12 columns:			•	5
		Column NCRI name Description	•			



- Galaxy c'est ...
 - Plus besoin de lancer une ligne de commande dans un terminal
 - Plus besoin de connaître la programmation ou le scripting
 - Des jobs soumis de manière transparente sur un cluster de calcul
 - Un gestionnaire d'historique et de données sécurisées
 - Un système de partage de données ou de protocoles
 - Des boîtes à outils dans plusieurs domaines de la bioinformatique
 - NGS Chimie
 - Métabolomique Etc ...
 - Statistique

- Analyse d'image
- Une interface web







Size of dot indicates flexibility/power



- Pourquoi Galaxy ?
 - Accessibilité
 - Accès à des outils de bioinformatique sans connaissance en informatique
 - Ergonomie à géométrie variable
 - Modularité
 - Reproductibilité
 - Traçabilité des paramètres
 - Transparence
 - Partage des données et protocoles



Monsieur GEEK





-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 login]\$ cd 13-07-29-panda/t [login@n0 mapping]\$ cat tophat.qsub #!/bin/bash #\$ -S /bin/bash #\$ -M login@sb-roscoff.fr #\$ -m bea #\$ -v

- #\$ awd
- . S –o asub.ou
- \$ -e asub.er

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







Station Biologique

Roscoff



Station Biologique Roscoff

Introduction

[lecorguille@n0 ~]\$ e-PCR --help e-PCR: invalid option -- usage: [-hV] [posix-options] stsfile [fasta ...] [compat-options] where posix-options are: Margin (default 50) -m ## -w ## Wordsize (default 7) Max mismatches allowed (default 0) -n ## Max indels allowed (default 0) -g ## Use ## discontiguos words, slow if -f ## ##>1 Set output file -0 ## Set output format: -t ## 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) Turn hits postprocess on/off -p +-Verbosity flags -v ## Use presize alignmens (only if -a a f qaps>0), slow a - Allways or f - as Fallback Use 5'-end lowercase masking of -x +primers (default -) Uppercase all primers (default -) -u +-

🔽 Galaxy / ABiMS

e-PCR (version 1.0.0)

STS file:

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

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):



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):

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):

Set maximal number of gaps allowed in primer-to-sequence alignment (per primer!).

Set output format (T):

tabular

Output formats

Execute

>

[...]



findPeaks.matchedFilter(object, fwhm = 30, sigma = f

Arguments

object	xcmsRaw object
fwhm	full width at half maximum of matched filtration gaussian model p used to calculate the actual sigma, see below.
sigma	standard deviation (width) of matched filtration model peak
max	maximum number of peaks per extracted ion chromatogram
snthresh	signal to noise ratio cutoff
step	step size to use for profile generation
steps	number of steps to merge prior to filtration
mzdiff	minimum difference in m/z for peaks with overlapping retention tim
index	return indicies instead of values for m/z and retention times
sleep	number of seconds to pause between plotting peak finding cycles
scanrange	scan range to process

Galaxy / ABIMS Analyze Data Workflow Shared Data - Visualization

xcms.xcmsSet (version 20131212)

library directory name:

The name of your library directory in /projet/sbr/galaxy/import/user/username@sb-roscoff.fr/

Method:

matchedFilter 🔻

Choose the method used for finding peaks

step:

0.01

the peak detection algorithm creates extracted ion base peak chromatograms (EIBPC) on a fixed

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:



the peak identification algorithm combines a given number of EIBPCs prior to filtration and peak

Execute

Authors Colin A. Smith <u>csmith@scripps.edu</u>, Ralf Tautenhahn <u>rtautenh@gmail.com</u>, Steffen Notes <u>rtautenh@gmail.com</u>, Steffen Notes <u>rtautenh@gmail.com</u>, Steffen Notes <u>rtautenh@gmail.com</u>, Steffen Notes <u>rtautenh@gmail.com</u>

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Usi <mark>ng 41%</mark>
Tools	NCBI BLAST+ blastx (version 0.0.17)	Â	History	0 0
search tools	Nucleotide query sequence(s):		Human protein study 5.3 MB	47 🖻
<u>Upload File</u> from your computer	1: human_protein.fas		2: chr22 check.gff3	• / ×
ABIMS WORKFLOWS	FASTA file from your history (see warning note below)		<u>1: human_protein.fas</u>	• / ×
Workflow RNA-seq de novo by ABIMS Workflow RNA-seq with reference by ABIMS Workflow 4 Metabolomics	Protein FASTA file to use as database: 1: human_protein.fas	Ξ		
ABIMS TOOLS	Query genetic code:			
Primer RNASeq	Set expectation value cutoff: 0.001			
Statistics	Output format:			
Utils Phylogenetics	Tabular (extended 24 columns)	4		
Debug	Advanced Options:			
Text Manipulation	Execute			
Join, Subtract and Group Filter and Sort NCBI BLAST+	Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.			
 <u>NCBI BLAST+ blastn</u> Search nucleotide database with nucleotide query sequence(s) 	What it does			
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool. You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significiant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that.			
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Output format			
<u>NCBI BLAST+ tblastn</u> Search	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:			
	Columa NCRI name Description	-		>

le menu

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -		Using 41%
Tools	NCBLBLAST+ blasty (version 0.0.17)	History	C 0
search tools	Nucleotide query sequence(s):	Human protein study 5.3 MB	ı 27 🖻
 <u>Upload File</u> from your computer 	1: human_protein.fas	2: chr22 check.gff3	• / ×
ABIMS WORKFLOWS	FASTA file from your history (see warning note below)	<u>1: human_protein.fas</u>	• • / ×
Workflow RNA-seq de novo by ABIMS Workflow RNA-seq with reference by ABIMS Workflow 4 Metabolomics	Protein FASTA file to use as database: 1: human_protein.fas Query genetic code:		
ABIMS TOOLS	1. Standard		
<u>Primer</u> <u>RNASeq</u> InterEsil	Set expectation value cutoff: 0.001		
<u>Statistics</u> Utils	Output format:		
Phylogenetics Debug COMMON TOOLS	Advanced Options:		
Text Manipulation	Execute		
Join, Subtract and Group Filter and Sort NCBI BLAST+	A Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.		
 <u>NCBI BLAST+ blastn</u> Search nucleotide database with nucleotide query sequence(s) 	What it does		
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool. You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makehastdb and search against that		
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Output format		
<u>NCBI BLAST+ tblastn</u> Search	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:		
	Columa NCPL name Description		2

la liste des outils

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%	
Tools	NCBI BLAST+ blastx (version 0.0.17)	6	History	0 0	•
search tools	Nucleotide query sequence(s):		Human protein study 5.3 MB	0	
Get Data Upload File from your computer	1: human_protein.fas		2: chr22 check.gff3	@ () \$	3
ABIMS WORKFLOWS	FASTA file from your history (see warning note below)		<u>1: human_protein.fas</u>	@ { }	3
Workflow RNA-seq de novo by ABIMS Workflow RNA-seq with reference by ABIMS Workflow 4 Metabolomics	Protein FASTA file to use as database: 1: human_protein.fas	Ξ			
ABIMS TOOLS	Query genetic code: 1. Standard Set expectation value cutoff:				
RNASeq InterEsil Statistics	0.001 Output format:				
<u>Utils</u> Phylogenetics Debug	Tabular (extended 24 columns) Advanced Options:				
COMMON TOOLS Text Manipulation	Hide Advanced Options				
FASTA manipulation Join, Subtract and Group Filter and Sort NCBI BLAST+	Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.				
<u>NCBI BLAST+ blastn</u> Search nucleotide database with nucleotide query sequence(s)	What it does Search a <i>protein database</i> using a <i>translated nucleotide query</i> , using the NCBI BLAST+ blastx command line tool.				
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that.				
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Output format				
NCBI BLAST+ tblastn Search	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:				
	Columa NCRI name Description	-			

formulaire / visualisation / information diverse

Galaxy / ABiMS Analyze Data Workflow Shared Data - Visualization - Help - User -		Using 41%
Tools NCBI BLAST+ blastx (version 0.0.17)	History	00
search tools Nucleotide query sequence(s):	Human protein study	
Get Data 1: human_protein.fas 🛊	5.3 MB	~ E
Upload File from your computer Subject database/sequences:	2: chr22 check.gff3	• / ×
ABIMS WORKFLOWS FASTA file from your history (see warning note below)	1: human protein.fas	• / ×
Workflow RNA-seq de novo by ABiMS		
Workflow RNA-seq with reference by Protein FASTA file to use as database: ABIMS 1: human_protein.fas ‡	8	
Workflow 4 Metabolomics Query genetic code:		
ABIMS TOOLS 1. Standard		
Primer Esterna time share the set of the set		
RNASeq Set expectation value cutor:		
InterEsil		
Statistics Output format:		
Utils Tabular (extended 24 columns) 🛊		
Phylogenetics Advanced Options:		
Debug Hide Advanced Options.		
COMMON TOOLS		
Text Manipulation Execute		
FASTA manipulation		
Join, Subtract and Group		
Filter and Sort A Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight		
NCBIBLAST+		
<u>NCBI BLAST+ blastn</u> Search		
nucleotide database with What it does		
Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool.		
NCBI BLAS I + Diastip Search protein database with protein query sequence(s) You can also search against a FASTA file of subject protein sequences. This is <i>not</i> advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using <i>makeblastdb</i> and search against that.		
NCBI BLAST+ blastx Search		
protein database with translated		
nucleotide query sequence(s) Output format		
NCBI BLAST+ tblastn Search Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:		
		>

l'historique

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -		Using 41%
Tools	NCBLBLAST+ blastx (version 0.0.17)	History	0 0
Search tools	Nucleotide query sequence(s):	Human protein study 5.3 MB	47 🖻
 <u>Upload File</u> from your computer 		2: chr22 check.gff3	• / ×
ABIMS WORKFLOWS	FASTA file from your history (see warning note below)	1: human protein fas	@ / %
Workflow RNA-seq de novo by ABiMS	TASTA life from your history (see warning note below)	<u>1. numur proteinings</u>	• • • ~
Workflow RNA-seq with reference by ABIMS	Protein FASTA file to use as database:	Ξ	
Workflow 4 Metabolomics	Query genetic code:		
ABIMS TOOLS	1. Standard		
Primer	Set expectation value cutoff:		
RNASeq	0.001		
InterEsil	Output formati		
Statistics	Tabular (ortanded 24 columns)		
Dhylogenetics	Tabular (extended 24 columns)	4	
Debug	Advanced Options:		
	Hide Advanced Options ț		
Text Manipulation			
FASTA manipulation	Execute		
Join, Subtract and Group			
Filter and Sort	A Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight		
NCBIBLAST+	processing.		
<u>NCBI BLAST+ blastn</u> Search			
nucleotide database with nucleotide query sequence(s)	What it does		
NCPI PLAST+ blasta Soarch	Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool.		
protein database with protein query sequence(s)	You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that.		
<u>NCBIBLAST+ blastx</u> Search	· · · · · · · · · · · · · · · · · · ·		
protein database with translated	Output format		
 NCBI BLAST+ tblastn Search 	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output		
	contains 12 columns:		>
		- III	



IMPORT DES DONNÉES



Si fichier < 2 Go IMPORT DES DONNÉES

🗧 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 42%	
Tools	Upload File (version 1.1.3)	9	History	0	0
search tools	File Format:		Unnamed history		
Get Data	Auto dotect		0 bytes	<i>\\</i>	2
<u>Upload File</u> from your computer	Which format? See help below	Ξ	Your history is en	pty. Click 'Get Data	a'
ABIMS WORKFLOWS	File:				
Workflow RNA-seg de novo by ABIMS	/home/lecorguille/tmp/chr22_cl Browse				
Workflow RNA-seq with reference by ABIMS	TIP: Due to browser limitations, uploading files larger than 2GB is guaranteed to fail. To upload large files, use the URL method (below) or FTP (if enabled by the site administrator).				
Workflow 4 Metabolomics	URL/Text:				
ARIMS TOOLS					
Drimer					
PNASog					
InterFeil					
Statistics					
	Here you may specify a list of URLs (one per line) or paste the contents of a file.				
Dhylogenetics	Convert spaces to tabs:				
Dobug	□ Yes				
Debug	Use this option if you are entering intervals by hand.				
COMMON TOOLS	Genome:				
Text Manipulation	unspecified (?)				
FASTA manipulation					
Join, Subtract and Group	Execute 3				
Filter and Sort					
NCBI BLAST+					
NGS: QC and manipulation	Auto-detect				
NGS: RNA Analysis	The system will attempt to detect Axt, Fasta, Fastqsolexa, Gff, Gff3, Html, Lav, Maf, Tabular, Wiggle, Bed and Interval (Bed with headers)				
NGS: Mapping	formats. If your file is not detected properly as one of the known formats, it most likely means that it has some format problems (e.g., different number of columns on different rows). You can still coerce the system to set your data to the format you think it should be. You				
NGS: Picard (beta)	can also upload compressed files, which will automatically be decompressed.				
NGS: SAM Tools					
SVDetect					
VarScan	ADT				
Workflows	A binary sequence file in 'ab1' format with a '.ab1' file extension. You must manually select this 'File Format' when uploading the file.				
All workflows					
	Axt				~
	hlastz najnvisa alimmant format. Fach alimmant hlock in an avt fila contains three lines: a summany line and 2 semuance lines. Blocks	•			-

Import par copier/coller dans la zone de texte

Il est aussi possible d'y recopier une url ftp d'un fichier en ligne zippé (zip, tgz, gz) ex : ftp://ftp.ncbi.nih.gov/blast/db/FASTA/mito.aa.gz Mais attention à la taille !

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data → Visualization → Help → User →	Using 42%	٥
Tools	Upload File (version 1.1.3)	History 2 H	>
search tools		Unnamed history	
Got Data	File Format:	0 bytes 🖉	2
<u>Upload File</u> from your computer	Auto-detect Which format? See help below	Your history is empty. Click 'Get Data	ľ
ABIMS WORKFLOWS	File:		
Workflow RNA-seq de novo by ABIMS	Browse		
Workflow RNA-seq with reference by ABIMS	TIP: Due to browser limitations, uploading files larger than 2GB is guaranteed to fail. To upload large files, use the URL method (below) or FTP (if enabled by the site administrator).	4	
Workflow 4 Metabolomics	URL/Text: 2		
ABIMS TOOLS	>gij225735562:5001-89734 Homo sapiens insulin-like growth factor 1 (somatomedin C) (IGF1), RefSegGene on chromosome 12		
Primer			
RNASeq	ATTCAGAGCAGATAGAGCCTGCGCAATGGAATAAAGTCCTCAAAATTGAAATGGACATTGCTCTCAACA		
InterEsil	TCAGAAGCAATGGGAAAAATCAGCAGTCTTCCAACCCAATTATTTAAGTGCTGCTTTTGTGATTTCTTGA		
Statistics	AGGTAAATATTTCTTACTCTTTGAAGTCATTGGGGAATTCTATTTAAATTGTGTACTGTTTGCTTCTGCC		
<u>Utils</u>	TAGAACTGTTCTTCACTTTAAAATTTTCATTGTTTCGGAACCGAGAGTTATTTAT		
Phylogenetics	ACTATTGCAAGGTACTTATGCTAAATCCTCCCACTTCTGCAGGGGCTTCCGTGGTGTCATTACAGAAGAA		
Debug			
COMMON TOOLS	CAGGTGCAGATGTTTTATTTTTAAGACCATGTTCTTTTGCATGTGTGTG		
Text Manipulation			
FASTA manipulation	Convert spaces to tabs:		
Join, Subtract and Group	Use this option if you are entering intervals by hand.		
Filter and Sort	Conome:		
NCBI BLAST+			
NGS: QC and manipulation			
NGS: RNA Analysis			
NGS: Mapping	Execute		
NGS: Picard (beta)			
NGS: SAM Tools	Auto-detect		
<u>SVDetect</u>	The system will attempt to detect Axt. Easta Eastasolexa, Gff, Gff3, Html, Lay, Maf, Tabular, Wingle, Bed and Interval (Bed with headers)		
VarScan	formats. If your file is not detected properly as one of the known formats, it most likely means that it has some format problems (e.g.,		
Workflows	different number of columns on different rows). You can still coerce the system to set your data to the format you think it should be. You		
All workflows	can also upload compressed files, which will automatically be decompressed.		
	Abl	·	2



-ex:

 Les outils filtrent les données d'entrée suivant leurs formats

NCBI BLAST+ blastx (version 0.0.17)	ŕ	History		0.0
Nucleotide query sequence(s):		Human prote	in study	
1: human_protein.fas		5.3 MB		27 E
Subject database/sequences:		2: chr22 che	<u>ck.gff3</u>	• / ×
FASTA file from your history (see warning note below)		<u>1: human pr</u>	otein.fas	•0
Drotein EASTA file to use as database.				

• Si le format n'est pas correctement détecté

text	\leftrightarrow	tabular
fastq	\leftrightarrow	fastqsanger
tabular	\leftrightarrow	gtf
gtf	\leftrightarrow	gff3
gff3	\leftrightarrow	gff2
Si la détection automatique du format échoue ou pour forcer un format :

- tabular \rightarrow gff
- fastq → fastqsanger
- $xml \rightarrow blastxml$





Si fichier > 2 Go IMPORT DES DONNÉES



- Création d'une librairie
 - L'import des fichiers supérieurs à 2 Go doivent être déposés sur le serveur via le protocole FTP (File Transfert Protocol)





• Les programmes de FTP





- Les paramètres
 - serveur / host
 - protocol
 - port
 - user / login
 - password

- --> ssh.sb-roscoff.fr
 - --> SFTP ou SCP

--> 22 --> **Abims**

<u>S</u> électionnez une entrée :	Général	Avancé	Para	mètres de transfert	Jeu de caractères	
 Mes Sites guest@n0 n0 ssh.sb-roscoff.fr 	<u>H</u> ôte : Pro <u>t</u> ocol	e :		ssh.sb-roscoff.fr Port : SFTP - SSH File Transfer Protocol \$		
	Type d'au	uthentifica	tion :	Demander le mot d	e passe	
	<u>M</u> ot de p C <u>o</u> mpte :	asse :				
	Co <u>m</u> men	taires :				
Nouveau Site Nouveau Dossier						
Nouveau Fa <u>v</u> ori <u>R</u> enommer						
Supprimer Copier						



🛛 😣 🔿 💿 🛛 ssh.sb-roscoff.fr - sftp://lecorguille@ssh.sb-roscoff.fr - FileZilla		
Hôte : ssh.sb-roscoff.f Identifiant : lecorguille Mot de passe : ••••••• Port : 22 Connexio	n rapide 🔻	
Statut : Transfert de fichier réussi, 12,3 Mo transférés en 1 seconde Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML" "C14H.mzXML" Commande : put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML" "C14H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML => remote:/proj Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML => remote:/proj Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Commande : put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML => remote:/proj Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML => remote:/proj Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML => remote:/proj Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C24H.mzXML" Commande : put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C24H.mzXML" "C24H.mzXML"	ML et/sbr/galaxy/ii ML et/sbr/galaxy/ii ML	۱port/user/lecorguille@sb-roscoff.fr/cooper_stress/sample/C14H.mzXML nport/user/lecorguille@sb-roscoff.fr/cooper_stress/sample/C44H.mzXML
Site local : /home/lecorguille/tmp/mzXML_copper_stress/	Site distant	<pre>/projet/sbr/galaxy/import/user/lecorguille@sb-roscoff.fr/cooper_stress</pre>
 tmp Intersection_DESeqedgeRacp Intersection_DESeqedgeRhclust annotateDiffreport mzXML_copper_stress ref sample 		<pre>2 keiglmeier@sb-roscoff.fr 2 kgazengel@sb-roscoff.fr 2 lamar@sb-roscoff.fr v</pre>
Nom de fichier ^ Taille de fic Type de fichier Dernière modific	Nom de fich	er ^ Taille de fi: Type de ficl Dernière modi Droits d'ac Propriétair
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Hôte: ssh.sb-roscoff.f Identifiant: lecorguille Mot de passe: Port.22	tres de connexion
Statut : Transfert de fichier réussi, 12,3 Mo transférés en 1 seconde Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML" Commande : put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML" "C14H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML => remote:/projet Statut : Transfert de fichier réussi, 12,4 Mo transférés en 1 seconde Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML Commande : put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Commande : put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" Statut : local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML => remote:/projet Statut : Iocal:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML => remote:/projet Statut : Transfert de fichier réussi, 11,8 Mo transférés en 2 secondes Statut : Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C24H.mzXML" Commande : put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C24H.mzXML" Commande : put "/home	L t/sbr/galaxy/import/user/lecorguille@sb-roscoff.fr/cooper_stress/sample/C14H.mzXML L t/sbr/galaxy/import/user/lecorguille@sb-roscoff.fr/cooper_stress/sample/C44H.mzXML L
Site local : /home/lecorguille/tmp/mzXML_copper_stress/	Site distant : /projet/sbr/galaxy/import/user/lecorguille@sb-roscoff.fr/cooper_stress
 tmp Intersection_DESeqedgeRacp Intersection_DESeqedgeRhclust annotateDiffreport mzXML_copper_stress ref sample 	<pre>% keiglmeier@sb-roscoff.fr % kgazengel@sb-roscoff.fr % lamar@sb-roscoff.fr % lecorguille@sb-roscoff.fr % lecorguille@sb-roscoff.fr % lecorguille@sb-roscoff.fr % lecorguille@sb-roscoff.fr % lecorguille@sb-roscoff.fr % sample</pre>
Nom de fichier ^ Taille de fic Type de fichier Dernière modific	Nom de fichier ^ Taille de fi ⁱ Type de ficl Dernière modi Droits d'ac Propriétair
Image: marked state Dossier 14/06/2012 09: Image: marked state Dossier 14/06/2012 09:	pref Dossier sample Dossier
	₿
Sélection de 2 dossiers.	2 dossiers
Serveur / Fichier local Directio Fichier distant Taille Priorité Statut	
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– Galaxy / ABiMS	Analyze Data Workflow	Shared Data -	Visualization -	Admin	Help -	User -	Using 42%
Data Libraries							
search dataset name, info, message, dbkey							
Advanced Search	a						
Data library name	ata library description						
lecorguille							
RNA-seq de-novo D	ataset for RNA-seq de-novo, re	-ingeneered - pper	icard				
RNA-seq reference D	ataset for RNA-seq with referen	ice genome - acorr	nier				



Galaxy / ABiMS	Analyze Data	Workflow	Shared Data -	Visualization -	Admin	Help -	User -		Using 42%
Upload files to a data library								Browset	this data library
Upload a directory of files									
Upload option: Upload directory of files	tory).								
File Format: Auto-detect									

Server Directory

	-	-	 -		
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			 .	_	

Upload all files in a sub-directory of /projet/sbr/galaxy/import/user/lecorguille@sb-roscoff.fr on the Galaxy server.

Copy data into Galaxy?



Normally data uploaded with this tool is copied into Galaxy's configured "file_path" location where Galaxy has a form of control over the data files. However, this may not be desired (especially for large NGS datasets), so using the option labeled "Link to files without copying into Galaxy" will force Galaxy to always read the data from its original path. Any symlinks encountered in the uploaded directory will be dereferenced once. That is, Galaxy will point directly to the file that is linked, but no other symlinks further down the line will be dereferenced.

Convert spaces to tabs:

Yes

Use this option if you are entering intervals by hand.

Genome:

unspecified (?)

Message:

This information will be displayed in the "Message" column for this dataset in the data library browser

Restrict dataset access to specific roles:

lecorguille@sb-roscoff.fr

Multi-select list - hold the appropriate key while clicking to select multiple roles. More restrictions can be applied after the upload is complete. Selecting no roles makes a dataset public.





– Galaxy / ABiMS	Analyze Data	Workflow	Shared Data -	Visualization -	Admin	Help -	User -	Using 42%
Data Library "lecorguille"								Add datasets Add folder Library Actions
Added 4 datasets to the library 'lecorguille' (each is selected).								

Name	Message	Data type	Date uploaded	File size
✓ BlueLight.sample.paired.1.cleaned.fastq ▼	This job is running	auto	2013-09-12	125.6 MB
BlueLight.sample.paired.2.cleaned.fastq -	This job is running	auto	2013-09-12	124.3 MB
✓ Dark.sample.paired.1.cleaned.fastq ▼	This job is running	auto	2013-09-12	90.9 MB
☑ Dark.sample.paired.2.cleaned.fastq ▼	This job is running	auto	2013-09-12	89.5 MB
For selected datasets: Import to current history				

() TIP: You can download individual library datasets by selecting "Download this dataset" from the context menu (triangle) next to each dataset's name.

(i) TIP: Several compression options are available for downloading multiple library datasets simultaneously:

· gzip: Recommended for fast network connections

- bzip2: Recommended for slower network connections (smaller size but takes longer to compress)
- · zip: Not recommended but is provided as an option for those who cannot open the above formats



Si vous souhaitez utiliser xcms.xcmsSet IMPORT DES DONNÉES



😣 🔿 🗊 ssh.sb-roscoff.fr - sftp://lecorguille@ssh.sb-roscoff.fr - FileZilla			
Hôte: ssh.sb-roscoff.f Identifiant: lecorguille Mot de passe: ••••••• Port: 22 Conn	exion	on rapide 💌	
Statut: Iransfert de lichier reussi, 12,3 Mo transferes en 1 seconde Statut: Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML Commande: put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML" C14H.mzXML Statut: local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C14H.mzXML => remote:/ Statut: Transfert de fichier réussi, 12,4 Mo transférés en 1 seconde Statut: Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML Commande: put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" C44H.mzXML Statut: Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML" "C44H.mzXML" Statut: local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML => remote:/ Statut: local:/home/lecorguille/tmp/mzXML_copper_stress/sample/C44H.mzXML => remote:/ Statut: Transfert de fichier réussi, 11,8 Mo transférés en 2 secondes Statut: Démarrage de l'envoi de /home/lecorguille/tmp/mzXML_copper_stress/sample/C24H.mzXML" Commande: put "/home/lecorguille/tmp/mzXML_copper_stress/sample/C24H.mzXML"	mzXM ML" projel mzXM ML" projel mzXM ML"	ML et/sbr/galaxy/import/user/lecorguille@sb-roscoff ML et/sbr/galaxy/import/user/lecorguille@sb-roscoff ML	f.fr/cooper_stress/sample/C14H.mzXML f.fr/cooper_stress/sample/C44H.mzXML
Site local : /home/lecorguille/tmp/mzXML_copper_stress/		Site distant : /projet/sbr/galaxy/import/user/	'lecorguille@sb-roscoff.fr/cooper_stress
 tmp Intersection_DESeqedgeRacp Intersection_DESeqedgeRhclust annotateDiffreport mzXML_copper_stress ref sample 		 2 keiglmeier@sb-roscoff.fr 2 kgazengel@sb-roscoff.fr 2 lamar@sb-roscoff.fr 2 lamar@sb-roscoff.fr 2 lamar@sb-roscoff.fr 2 lamar@sb-roscoff.fr 2 lamar@sb-roscoff.fr 2 lamar@sb-roscoff.fr 3 lamar@sb-roscoff.fr 4 lamar@sb-roscoff.fr 4 lamar@sb-roscoff.fr 5 lamar@sb-roscoff.fr	3
Nom de fichier ^ Taille de fic Type de fichier Dernière modific		Nom de fichier 🔨	Taille de fie Type de ficl Dernière modi Droits d'ac Propriétair
 ref Dossier 14/06/2012 09: Sample Dossier 14/06/2012 09: 	4	 ref sample	Dossier Dossier
Sélection de 2 dossiers.		2 dossiers	
Serveur / Fichier local Directio Fichier distant Taille Priorité Statut sftp://lecorguille@s /home/lecorguille/t ->> /projet/sbr/galaxy/imp 12,5 Mo Norm Transfert en cours /home/lecorguille/t ->> /projet/sbr/galaxy/imp 12,7 Mo Norm Transfert en cours	rs rs		



Si les ressources sont conséquentes et publiques

IMPORT DES DONNÉES



Pour les ressources conséquentes et publiques ex : swissprot au format blast chromosome 11 du génome humain au format bowtie2

Faire une demande à support.abims@sb-roscoff.fr

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -		Using 42%
Tools	NCBI BLAST+ blastn (version 0.0.17)	Â	History 2 🔹
search tools			Unnamed history
Get Data	Nucleotide query sequence(s):		0 bytes 🖉 🖻
Upload File from your computer	× v		3 Your history is empty. Click 'Get Data'
,	Subject database/sequences:		on the left pane to start
ABIMS WORKFLOWS	BLAST Database ‡		
Workflow RNA-seq de novo by ABIMS	Nucleotide BLAST database:		
ABIMS	nt 🔺	Ξ	
Workflow 4 Metabolomics			
ABIMS TOOLS	nt		
Primer	genhank		
RNASeq	genbank acterial		
InterEsil	genbark Environmental sampling		
Statistics	genbark Environmental sampling		
Utils	genbank EST (expressed sequence tag)	4	
Phylogenetics	genbank GSS (genome survey sequence)		
Debug	genbank HTC (high throughput cDNA sequencing)		
COMMON TOOLS	genbank HTGS (high throughput genomic sequencing)		
Text Manipulation	Hide Advanced Options		
FASTA manipulation			
Join, Subtract and Group	Execute		
Filter and Sort			
NCBIBLAST+	A Nete Detabase searches may take a substantial amount of time. For large input detects it is advisable to allow everyight		
NCBI BLAST+ blastn Search publication databases with	processing.		
nucleotide query sequence(s)	• •		
NCBI BLAST+ blastp Search	What it does		
protein database with protein	Search a nucleotide database using a nucleotide query using the NCBLRLAST+ blasts command line tool. Algorithms include blasts		
query sequence(s)	megablast, and discontiguous megablast.		
NCBI BLAST+ blastx Search	A You can also search against a FASTA file of subject nucleotide sequences. This is not advised because it is slower (only one CPU is		
nucleotide query sequence(s)	used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most		
NCBI BI AST+ thiastn Search	cases you should instead turn the other FASTA file into a database first using <i>makeblastab</i> and search against that.		
	Output format	-	



- Résumé
 - Si ressource locale :
 - Si < 2 Go :
 - . Import depuis Get Data
 - . Copier/Coller dans la zone de texte
 - Si > 2 Go :
 - . Import via le protocol FTP
 - Si ressource distante :
 - Si < 2 Go :
 - Copier/Coller de l'adresse ftp://
 - Si ressource type banque publique (brute ou reformatée)
 - Demande à <u>support.abims@sb-roscoff.fr</u> pour mise à disposition

IMPORT

ТΡ





- Import des données
 - local
 - z:\formation\metabo-20140128\
 - distant
 - software : WinSCP
 - protocole : sftp
 - host : ssh.sb-roscoff.fr
 - path : /projet/sbr/galaxy/import/user/login@sb-roscoff.fr



OUTILS

L'interface de Galaxy

la liste des outils

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%	
Tools	NCBI BLAST+ blastx (version 0.0.17)	Â	History	00	
search tools	Nucleotide query sequence(s):		Human protein study 5.3 MB	0 🖻	
<u>Upload File</u> from your computer	1: human_protein.fas		2: chr22 check.gff3	@ (/ X	3
ABIMS WORKFLOWS	FASTA file from your history (see warning note below)		1: human protein.fas	• / ×	3
Workflow RNA-seq de novo by ABIMS	Protein FASTA file to use as database:				
Workflow RNA-seq with reference by ABIMS	1: human_protein.fas 🍦				
Workflow 4 Metabolomics	Query genetic code:				
ABIMS TOOLS	1. Standard				
Primer PNA Sor	Set expectation value cutoff:				
<u>RNASeq</u> InterEsil	0.001				
Statistics	Output format:				
Utils	Tabular (extended 24 columns)				
Phylogenetics	Advanced Options:				
Debug	Hide Advanced Options				
COMMON TOOLS					
Text Manipulation	Execute				
FASTA manipulation					
Filter and Sort NCBI BLAST+	A Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.				
<u>NCBI BLAST+ blastn</u> Search nucleotide database with nucleotide guery sequence(s)	What it does				
	Search a protein database using a translated nucleotide query, using the NCBI BLAST+ blastx command line tool.				
 <u>NCBIBLAS1+ biasp</u> Search protein database with protein query sequence(s) 	You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastic and search against that.				
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Output format				
<u>NCBI BLAST+ tblastn</u> Search	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output				
<)	>

L'interface de Galaxy

la liste des outils

🚾 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -		Usi <mark>ng 41%</mark>
Tools	Online	History	0 0
		Human protein study 5.3 MB	47 🖻
<u>NCBI BLAST+ blastn</u> Search nucleotide database with nucleotide	 07-06-13: Metabolomic : Workflow 4 Metabolomics, updated to version 2.1.0 (2013_06_07) 30-04-13: RNASeq : DESeq is now available for RNASeq expression data with reference (with gtf input). 26-04-13: RNASeg : DESeg is now available for denovo RNASeg expression data (without gtf input). 	2: chr22_check.gff3	• 0 ×
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	 26-04-13: RNASeq : sam2counts is now available to count the reads coverage by transcrit. It's also a requirement for DESeq denovo. 26-04-13: Metabolomic : Workflow Metabolomic by ABiMS, updated to version 2.0.0 (2013_04_18) 	<u>1: human_protein.fas</u>	• 0 %
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 			
 <u>NCBI BLAST+ tblastn</u> Search translated nucleotide database with protein query sequence(s) 			
 <u>NCBI BLAST+ tblastx</u> Search translated nucleotide database with translated nucleotide query sequence(s) 			
BLAST XML to tabular Convert BLAST XML output to tabular	Analyses and Bioinformatics for Marine Science		
Workflows All workflows	CNRS UPMC Station Biologique Roscoff		
	Information For any question or request for tools or account, send an email at support.abims 'AT' sb-roscoff.fr		
	<u>Galaxy</u> is an open, web-based platform for data intensive biomedical research. The <u>Galaxy team</u> is a part of <u>BX</u> at <u>Penn State</u> , and the <u>Biology</u> and <u>Mathematics and Computer Science</u> departments at <u>Emory University</u> . The <u>Galaxy Project</u> is supported in part by <u>NHGRI, NSF</u> , <u>The Huck Institutes of the Life Sciences</u> , <u>The Institute for CyberScience at Penn State</u> , and <u>Emory University</u> .		

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Exemple de formulaire :
Sélection du fichier d'entrée – filtre sur le type de fichier (ici : fichier fasta)

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%
Tools	NCBI BLAST+ blasto (version 0.0.17)	6	History	C 0
blast NCBI BLAST+	Protein query sequence(s):		Human protein study 5.3 MB	47 🖻
 NCBI BLAST+ blastn Search nucleotide database with nucleotide 	Subject database/sequences:		2: chr22 check.gff3	• () ×
query sequence(s)	BLAST Database		<u>1: human protein.fas</u>	• / ×
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	Protein BLAST database:	Ξ		
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Type of BLAST: blastp blastp blastp-short			
 <u>NCBI BLAST+ tblastn</u> Search translated nucleotide database with protein query sequence(s) 	Set expectation value cutoff: 0.001			
 <u>NCBI BLAST+ tblastx</u> Search translated nucleotide database with translated nucleotide query sequence(s) 	Output format: Tabular (extended 24 columns)			
 <u>BLAST XML to tabular</u> Convert BLAST XML output to tabular 	Advanced Options:			
Workflows All workflows	Execute			
	Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.			
	What it does			
	Search a protein database using a protein query, using the NCBI BLAST+ blastp command line tool.			
	You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that.			
	Output format			
1	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:			
		-		>

Exemple de formulaire : . Aide sur l'outil

Dans la limite des stocks disponibles

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%
Tools	NCBI BLAST+ blastp (version 0.0.17)	6	History	00
blast (3) NCBI BLAST+	Protein query sequence(s):		Human protein study 5.3 MB	47 🖻
 <u>NCBI BLAST+ blastn</u> Search nucleotide database with nucleotide 	Subject database/sequences:		2: chr22 check.gff3	• 0 %
query sequence(s)	BLAST Database		<u>1: human protein.fas</u>	• 0 %
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	Protein BLAST database:	Ξ		
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Type of BLAST: S blastp blastp-short			
 <u>NCBI BLAST+ tblastn</u> Search translated nucleotide database with protein query sequence(s) 	Set expectation value cutoff: 0.001			
 <u>NCBI BLAST+ tblastx</u> Search translated nucleotide database with translated nucleotide query sequence(s) 	Output format: Tabular (extended 24 columns)			
 <u>BLAST XML to tabular</u> Convert BLAST XML output to tabular 	Hide Advanced Options			
Workflows = <u>All workflows</u>	Execute			
	Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.			
	What it does			
	Search a protein database using a protein query, using the NCBI BLAST+ blastp command line tool.			
	You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that.			
	Output format			
1	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:			
		-		/

Exemple de formulaire :
Ici : possibilité de choisir une banque personnelle dans l'historique ... mais j'en ai pas !

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%
Tools	NCBI BLAST+ blastp (version 0.0.17)	Â	History	C 0
blast NCBI BLAST+	Protein query sequence(s):		Human protein study 5.3 MB	4) 📄
 NCBI BLAST+ blastn Search nucleotide database with nucleotide 	Subject database/sequences:		2: chr22 check.gff3	• / ×
query sequence(s)	BLAST database from your history		<u>1: human_protein.fas</u>	• / X
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	Protein BLAST database:	Ξ		
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Type of BLAST:			
 <u>NCBI BLAST+ tblastn</u> Search translated nucleotide database with protein query sequence(s) 	Set expectation value cutoff: 0.001			
 <u>NCBI BLAST+ tblastx</u> Search translated nucleotide database with translated nucleotide query sequence(s) 	Output format: Tabular (extended 24 columns)			
 <u>BLAST XML to tabular</u> Convert BLAST XML output to tabular 	Hide Advanced Options			
Workflows All workflows	Execute			
	Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.			
	What it does			
	Search a protein database using a protein query, using the NCBI BLAST+ blastp command line tool.			
	You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that.			
	Output format			
	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output			
<	contains 12 columns.	¥		>

65

Exemple de formulaire :Possibilité de choisir le format du fichier de sortie

Dans la limite des stocks disponibles

🗕 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%
Tools	NCBI BLAST+ blastp (version 0.0.17)	Â	History	00
blast O	Protein query sequence(s):		Human protein study 5.3 MB	0 🖻
 NCBI BLAST+ blastn Search nucleotide database with nucleotide 	Subject database/sequences:		2: chr22 check.gff3	• / %
query sequence(s)	BLAST Database		1: human protein.fas	• / X
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	Protein BLAST database:	Ξ		
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Type of BLAST: blastp blastp blastp-short			
 <u>NCBI BLAST+ tblastn</u> Search translated nucleotide database with protein query sequence(s) 	Set expectation value cutoff: 0.001			
 <u>NCBI BLAST+ tblastx</u> Search translated nucleotide database with translated nucleotide query sequence(s) 	Output format: Tabular (extended 24 columns)			
 <u>BLAST XML to tabular</u> Convert BLAST XML output to tabular 	Hide Advanced Options			
Workflows All workflows	Execute			
	Note. Database searches may take a substantial amount of time. For large input datasets it is advisable to allow overnight processing.			
	What it does			
	Search a protein database using a protein query, using the NCBI BLAST+ blastp command line tool.			
	You can also search against a FASTA file of subject protein sequences. This is not advised because it is slower (only one CPU is used), but more importantly gives e-values for pairwise searches (very small e-values which will look overly significant). In most cases you should instead turn the other FASTA file into a database first using makeblastdb and search against that.			
	Output format			
	Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:			
		-		>

Exemple de formulaire :

Possibilité d'accéder à des options avancées = accessibilité / ergonomie

Dans la limite des stocks disponibles

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Help - User -			Using 41%
Tools	NCBI BLAST+ blastp (version 0.0.17)	-	History	0 0
blast S	Protein query sequence(s):		Human protein study 5.3 MB	47 🖻
 <u>NCBI BLAST+ blastn</u> Search nucleotide database with nucleotide 	Subject database/sequences:		2: chr22 check.gff3	• (X
query sequence(s)	BLAST Database		<u>1: human protein.fas</u>	• (X
 <u>NCBI BLAST+ blastp</u> Search protein database with protein query sequence(s) 	Protein BLAST database:	=		
 <u>NCBI BLAST+ blastx</u> Search protein database with translated nucleotide query sequence(s) 	Type of BLAST:			
 <u>NCBI BLAST+ tblastn</u> Search translated nucleotide database with protein query sequence(s) 	Set expectation value cutoff: 0.001			
 <u>NCBI BLAST+ tblastx</u> Search translated nucleotide database with translated nucleotide query 	Output format: Tabular (extended 24 columns)			
 <u>BLAST XML to tabular</u> Convert BLAST XML output to tabular 	Advanced Options:			
Workflows	Filter out low complexity regions (with SEG):			
 <u>All workflows</u> 	Scoring matrix: BLOSUM62 (default)			
	Maximum hits to show: 0 Use zero for default limits			
	Word size for wordfinder algorithm: 0 Use zero for default, otherwise minimum 2.			
	Should the query and subject defline(s) be parsed?: This affects the formatting of the query/subject ID strings			
<	Execute	Ţ		>



TP

• Lancement de xcmsSet

Outils

Station Biologique Roscoff

bims

E Star

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Admin Help - User -		Using 6%
Collaxy / ABIMS Cols Conset Co	Andrage without Varied base <td>History Unnamed history 0 bytes Your history is em on the left pane to</td> <td>Using 6%</td>	History Unnamed history 0 bytes Your history is em on the left pane to	Using 6%
	Prefilter step for the first phase. Separate by coma k,I. Mass traces are only retained if they contain at least 'k' peaks with intensity >= 'I' noise filter: 5000 potional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity smaller than 'noise' are omitted from ROI detection Execute Authors Colin A. Smith csmith@scripps.edu, Ralf Tautenhahn rtautenh@gmail.com, Steffen Neumann@ipb-halle.de, Paul Benton hpaul.benton08@imperial.ac.uk, Christopher Conley cjconley@ucdavis.edu		
<	Variation of the second s	_	2

Nama yana Cat





Job en attente de soumission

= le job est dans la « queue » de l'ordonnanceur

La durée de ce statut dépend du nombre de jobs actuellement en attente et du nombre de cpu demandé





Job en cours d'exécution

- = le job tourne actuellement sur le cluster de calcul
- La durée de ce status dépend complètement de la nature du job et de la puissance de calcul allouée
- Certains programmes vont pouvoir tourner sur plusieurs processeurs et disposer de 4, 8 ou 16 Go de RAM. Et d'autres sont mono-CPU.





Job terminé

Son statut est OK mais des warnings ou des erreurs peuvent se cacher derrière. Ah hum !





Job terminé mais en erreur

= le programme renvoie une erreur

Un programme s'il est bien développé renvoie un code d'erreur :

- = 0 si tout s'est bien terminé
- > 0 s'il a rencontré une erreur

Le programme explique souvent d'où vient l'erreur et parfois ... pas.


Les statuts



Job terminé mais en erreur

Les sources d'erreur :

– L'utilisateur :P

- Mauvaise utilisation : fichier d'entrée ou format ou option
- Mauvais portage du programme sous Galaxy ... désolé :/
- Plantage non anticipé du programme

Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Admin Help - User -	Using 19.1 GB
Tools	Online	History C 🕈
search tools		Copper Stress v3 133.9 MB
ABIMS WORKFLOWS Norkflow RNA-seq de novo by ABIMS Norkflow RNA-seq with reference by ABIMS	 07-06-13: Metabolomic : Workflow 4 Metabolomics, updated to version 2.1.0 (2013_06_07) . 30-04-13: RNASeq : DESeq is now available for RNASeq expression data with reference (with gtf input). 26-04-13: RNASeq : DESeq is now available for denovo RNASeq expression data (without gtf input). 26-04-13: RNASeq : sam2counts is now available to count the reads coverage by transcrit. It's also a requirement for DESeq denovo. 26-04-13: Motabolomic : Workflow Metabolomic by ABIMS_ updated to version 2.0.0 (2013_04_18). 	Oracle Oracle mzXML copper stress.group.retcor.group.retcor.group.fillPeaks.annotateDiffreport.data matrix.tsv anova pvalue.tabular
Norkflow 4 Metabolomics ABIMS TOOLS	• 20-04-15. Metaboloffic . Worknow Metaboloffic by AbiM5, updated to version 2.0.0 (2015_04_16)	<u>6:</u> ● Ø X mzXML copper_stress.group.retcor.gro up.fillPeaks.annotateDiffreport.Rdata
Primer RNASeq nterEsil	A 4	<u>5:</u>
Statistics Jtils Phylogenetics	ADINS	<u>4:</u>
COMMON TOOLS	Analyses and Bioinformatics for Marine Science	3: mzXML copper stress.RData 3: complete tob
ASTA manipulation Join, Subtract and Group Filter and Sort	CNRS UPMC Station Biologique	1: ● Ø ⋈ mzXML copper stress.ms.zip
Graphics NCBI BLAST+ NGS: QC and manipulation	Roscoff	\$
IGS: RNA Analysis IGS: Mapping IGS: Picard (beta) IGS: SAM Tools	Information For any question or request for tools or account, send an email at support.abims 'AT' sb-roscoff.fr	
IGS: GATK Tools (beta) SVDetect /arScan Searching sequence tools	s an open, web-based platform for data intensive biomedical research. The <u>Galaxy team</u> is a part of <u>BX</u> at <u>Penn State,</u> and the and <u>Mathematics and Computer Science</u> departments at <u>Emory University</u> . The <u>Galaxy Project</u> is supported in part by <u>NHGRI, NSF,</u> <u>k Institutes of the Life Sciences, The Institute for CyberScience at Penn State</u> , and <u>Emory University</u> .	

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🗕 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Admin Help - User -	Using 19.1 GB
Tools	Online	History 2 🌣
Search tools		Copper Stress v3 133.9 MB
ABIMS WORKFLOWS Workflow RNA-seq de novo by ABIMS Workflow RNA-seq with reference by ABIMS Workflow 4 Metabolomics ABIMS TOOLS Primer RNASeq InterEsil	 07-06-13: Metabolomic : Workflow 4 Metabolomics, updated to version 2.1.0 (2013_06_07) 1 30-04-13: RNASeq : DESeq is now available for RNASeq expression data with reference (with gff input). 26-04-13: RNASeq : DESeq is now available for denovo RNASeq expression data (without gff input). 26-04-13: RNASeq : sam2counts is now available to count the reads coverage by transcrit. It's also a requirement for DESeq denovo. 26-04-13: Metabolomic : Workflow Metabolomic by ABiMS, updated to version 2.0.0 (2013_04_18) 1 	
Statistics Utils Phylogenetics Debug COMMON TOOLS Text Manipulation	Analyses and Bioinformatics for Marine Science	NA ★ ① ② 6: ● Ø ⊗ mzXML copper stress.group.retcor.gro up.fillPeaks.annotateDiffreport.Rdata 5: ● Ø ⊗ mzXML copper stress group retcor gro
FASTA manipulation Join, Subtract and Group Filter and Sort Graphics NCBI BLAST+ NGS: QC and manipulation	CNRS UPMC Station Biologique Roscoff	4: ● Ø ⊗ mzXML copper stress.group.retcor.gro up.RData 3: ● Ø ⊗ mzXML copper stress.RData
NGS: Mapping NGS: Picard (beta) NGS: SAM Tools NGS: GATK Tools (beta)	Information For any question or request for tools or account, send an email at support.abims 'AT' sb-roscoff.fr	2: sampleInfo.tab ● Ø ※ 1: mzXML copper stress.ms.zip ● Ø ※
<u>Svbetect</u> <u>VarScan</u> <u>Searching sequence tools</u>	Biology and Mathematics and Computer Science departments at Emory University. The Galaxy tream is a part of BX at Penn State, and the <u>Biology</u> and <u>Mathematics and Computer Science</u> departments at <u>Emory University</u> . The <u>Galaxy Project</u> is supported in part by <u>NHGRI, NSF</u> , <u>The Huck Institutes of the Life Sciences</u> , <u>The Institute for CyberScience at Penn State</u> , and <u>Emory University</u> .	

- Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Admin Help - User -	Using 19.1 GB
Tools	Dataset generation errors	History
search tools	Dataset 7: mzXML_copper_stress.group.retcor.group.fillPeaks.annotateDiffreport.data_matrix.tsv_anova_pvalue.tabular	Copper Stress v3
Get Data	Tool execution generated the following error message:	133.9 MB 🖉 🖻
Get DataABIMS WORKFLOWSWorkflow RNA-seq de novo by ABIMSWorkflow RNA-seq with reference by ABIMSWorkflow 4 MetabolomicsABIMS TOOLSPrimerRNASeqInterEsilStatisticsUtilsPhylogeneticsDebugCOMMON TOOLSText ManipulationFASTA manipulationJoin, Subtract and GroupFilter and SortGraphicsNCBI BLAST+NGS: RNA Analysis	Fatal error: Exit code 10 () ERROR: There is a problem with the group of condition (presence of NA). You may need to use change the mo Current groups : NA NA NA NA NA NA NA NA	Item of the second stress of the second
NGS: Mapping	NA NA NA NA NA	2: sampleInfo.tab
NGS: SAM Tools NGS: GATK Tools (beta)	NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA	<u>1:</u>
VarScan	NA NA NA NA NA NA NA NA NA NA	
Searching sequence tools	NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA	

🗕 Galaxy / ABiMS		Analyze Data	Workflow S	hared Data -	Visualization -	Admin Help -	User -		Using 18.1 GE	в
Tools	NA NA NA NA NA							Ê	History 2 4	•
search tools	NA NA NA NA NA NA NA NA NA NA NA NA NA NA NA								Copper Stress v3	Â
Get Data	NA NA NA NA NA								133.9 MB 🖉 🖻	
ABIMS WORKFLOWS	NA NA NA NA NA NA NA NA NA NA								<u>⊗7:</u>	
Workflow RNA-seq de novo by ABiMS	NA NA NA NA NA								mzXML copper stress.group.retcor.g roup.fillPeaks.annotateDiffreport.data	
Workflow RNA-seq with reference by	NA NA NA NA NA								matrix.tsv anova pvalue.tabular	
ABIMS	NA NA NA NA NA								error An error eccurred with this detect:	
worknow 4 metabolomics	NA NA NA NA NA NA NA NA NA NA								Fatal error: Exit code 10 () ERROR:	
ABIMS TOOLS	NA NA NA NA NA								There is a problem with the group of	
Primer	NA NA NA NA NA								condition (presence of NA). You may need to use change the mode	
RNASeq	NA NA NA NA NA								(column/row) Current groups : NA NA	
InterEsil	NA NA								NA	
Statistics	4 (C			111))))		NA NA NA NA NA	
Ottis Divioranatios	Report this er	ror to the G	alaxy Tea	m					🕡 🚯 🕑	
Debug									e	Ξ
a	ne Galaxy team regu Is what vou were trvin	ariy reviews erro a to do when the	error occurred	the application.) and a contact e	-mail address. we	will be better able	e additional information (such e to investigate vour problem		mzXML copper stress.group.retcor.g	
COMMON TOOLS a	nd get back to you.	5	,				5 7 1		roup.fillPeaks.annotateDiffreport.Rdat	
Text Manipulation	Error Doport								<u>a</u>	
FASTA manipulation	Епог кероп								<u>5:</u> • 0 %	
Join, Subtract and Group	Your email							\sim	mzXML copper stress.group.retcor.g	
Graphics	lecorguille@sb-ros	coff.fr					N		Toup.mireaks.RData	
NCBI BLAST+	Message						3		<u>4:</u> ● Ø ※	
NGS: OC and manipulation									mzXML copper stress.group.retcor.g	
NGS: RNA Analysis										
NGS: Mapping									<u>3:</u> ● ℓ ×	
NGS: Picard (beta)								Ξ	mzxwil copper stress.kData	
NGS: SAM Tools									2: sampleInfo.tab	
NGS: GATK Tools (beta)									1	
SVDetect									mzXML copper stress.ms.zip	
VarScan									data	
Muscle								-	format: ms_zip, database: ?	
RAXML	Report								uploaded ms_zip lile	
								-		1



HISTORIQUE

L'interface de Galaxy : l'historique

Contient aussi bien les entrées que les sorties

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data - Visualization - Admin Help - User -		Using 18.0 GB
Tools	Opline	History	C 0
Search tools		Human chr22 proteome 19.1 MB	study 🖉 🗎
ABIMS WORKFLOWS	07-06-13: Metabolomic : Workflow 4 Metabolomics, updated to version 2.1.0 (2013_06_07) . . 30-04-13: RNASeg : DESeg is now available for RNASeg expression data with reference (with off input).	3: blastp on db	• / ×
Workflow RNA-seq de novo by ABIMS	26-04-13: RNASeq : DESeq is now available for denovo RNASeq expression data (without gtf input).	2: chr22 check.aff3	• / ×
Workflow RNA-seq with reference by ABIMS	 26-04-13: RNASeq : sam2counts is now available to count the reads coverage by transcrit. It's also a requirement for DESeq denovo. 26-04-13: Metabolomic : Workflow Metabolomic by ABiMS, updated to version 2.0.0 (2013) 04 (18) 11 	<u>1: human_protein.fas</u>	• / ×
Workflow 4 Metabolomics			
ABIMS TOOLS			
Primer			
RNASeq			
InterEsII			\$
Litils			
Phylogenetics			
Debug			
COMMON TOOLS			
Text Manipulation	Analyses and Bioinformatics for Marine Science		
FASTA manipulation			
Join, Subtract and Group			
Filter and Sort	Station Dialogique		
Graphics	Station biologique		
NCBIBLAST+	Koscoff		
NGS: QC and manipulation			
NGS: RNA Analysis			
NGS: Mapping	Information		
NGS: Picard (beta)	For any question or request for tools or account, send an email at support.abims 'AT' sb-roscoff.fr		
NGS: SAM Tools			
SVDetect	Galaxy is an open web-based platform for data intensive biomedical research. The Galaxy team is a part of RY at Denn State, and the		
VarScan	Biology and Mathematics and Computer Science departments at Emory University. The Galaxy Project is supported in part by NHGRI, NSF,		
Muscle	The Huck Institutes of the Life Sciences, The Institute for CyberScience at Penn State, and Emory University.		
Searching sequence tools			
<			>

Historique

Renommer, tagger et annoter

History	C 🕈
Unnamed history 19.1 MB	47 🖻
3: blastp on db	@ / X
2: chr22 check.gff3	@ / X
<u>1: human_protein.fas</u>	• / X
	>

History	0.0
Human chr22 proteome study	
19.1 MB	47 🖻
3: blastp on db	• / ¤
2: chr22 check.gff3	• / %
<u>1: human_protein.fas</u>	• / ×

>



Information sur l'objet :

- Code erreur
- Sorties standard / error

🗧 Galaxy / ABiMS		Analyze Data							U	sing 18.0 GB
Tool: NCBI BLAST+ blastp								History		0 0
Name:	blastp on db							 		
Created:	Aug 09, 2013							Human chr22 proteome	study	
Filesize:	13.9 MB							19.1 MB		47 🖻
Dbkey:	?									- 0.44
Format:	tabular							3: blastp on db		● (/ X
Galaxy Tool Version:	0.0.17							21,550 IIRes format: tabular, database: "	2	
Tool Version:	blastp: 2.2.27+ Package: b	last 2.2.27, build	d Sep 11 2012	2 10:14:26					<u>.</u>	\mathcal{D}
Tool Standard Output:	stdout									
Tool Standard Error:	stderr							1 2 3	4 5	6
Tool Exit Code:	0							SD P31946 1433B_HUMAN	SD A4K2U9 1433B PONAB	100.00 246
API ID:	8a4a8f9f3df4a393									
Full Path:	/w/galaxy/dev/galaxy-dist/d	latabase/files/00)1/dataset_15	34.dat				RTESEVASODNKUTTVSNSQQAT	VERLEISKKENVEINLIKLOLAL	NESVETTEILNSE
								DNKQTTVSNSQQAYQEAFEISKK	EMQPTHPIRLGLALNFSVFYYEI	LNSPEKACSLAKT
Input Parameter	Valu	e			No	ote for reru	in	 sp P31946 1433B_HUMAN	sp Q4R572 1433B_MACFA	100.00 246
Protein query sequence(s)	1: hu	iman_protein.fa	S					 RYLSEVASGDNKQTTVSNSQQAY	QEAFEISKKEMQPTHPIRLGLAL	NFSVFYYEILNSF
Subject database/sequences	db							 DNKQTTVSNSQQAYQEAFEISKK	EMQPTHPIRLGLALNFSVFYYEI	LNSPEKACSLAKT
Protein BLAST database	unipi	rot_swissprot						 (())))
histdb										
subject								 2: chr22_check.aff3		@ / %
Type of BLAST	blast	tp						 		
Set expectation value cutoff	0.00	01						 <u>1: human protein.fas</u>		• 0 ×
Output format	Tabu	llar (extended 24	4 columns)							
Advanced Options	basio	C								
Inheritance Chain										
		blastp o	n db							
		1								
		blastp on db	'in Blastp							

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Visualisation de l'objet • Tableau

- ٠
- lmage HTML \bullet

Ξ	🗧 Galaxy / ABiMS	S	Analy	ze Data	W	orkflow	1 5	Shared I	Data -	- Vis	sualization -	- Adr	min Help - User -	Using 18.0 GB
	sp P31946 1433B_HUMAN	sp A4K2U9 1433B_PONAB	100.00	246	0	0	1	246	1	246	0.0	508	sp A4K2U9 1433B_P0	History 2 🔅
	sp P31946 1433B_HUMAN	sp Q4R572 1433B_MACFA	100.00	246	0	0	1	246	1	246	0.0	508	sp Q4R572 1433B_MA	Users also 22 materies at the
	sp P31946 1433B_HUMAN	sp P31946 1433B_HUMAN	100.00	246	0	0	1	246	1	246	0.0	508	sp P31946 1433B_HU	Human chrzz proteome study
	sp P31946 1433B_HUMAN	sp P68250 1433B_BOVIN	99.59	246	1	0	1	246	1	246	0.0	506	sp P68250 1433B_BO	19.1 MB
	sp P31946 1433B_HUMAN	sp Q9CQV8 1433B_MOUSE	98.78	246	3	0	1	246	1	246	3e-179	499	sp Q9CQV8 1433B_M	3: blastp op db
	sp P31946 1433B_HUMAN	sp P35213 1433B_RAT	98.37	246	4	0	1	246	1	246	2e-178	497	sp P35213 1433B_RA	21.556 lines
	sp P31946 1433B_HUMAN	sp Q5ZLQ6 1433B_CHICK	97.95	244	5	0	3	246	1	244	3e-177	494	sp Q5ZLQ6 1433B_CH	format: tabular, database: ?
	sp P31946 1433B_HUMAN	sp Q6UFZ9 143B1_ONCMY	91.80	244	20	0	3	246	1	244	1e-164	462	sp Q6UFZ9 143B1_ON	l 🖬 🖲 🖏 🏠 🖉 🖉
	sp P31946 1433B_HUMAN	sp Q5PRD0 143BA_DANRE	91.39	244	21	0	3	246	1	244	3e-164	461	sp Q5PRD0 143BA_D/	
	sp P31946 1433B_HUMAN	sp Q5XHK2 143BA_XENLA	88.11	244	29	0	3	246	1	244	2e-159	449	sp Q5XHK2 143BA_XE	1 2 3 4 5 6
	sp P31946 1433B_HUMAN	sp Q8AVQ3 143BB_XENLA	87.70	244	30	0	3	246	1	244	6e-159	447	sp Q8AVQ3 143BB_XE	sp P31946 1433B_HUMAN sp A4K2U9 1433B_PONAB 100.00 24€
	sp P31946 1433B_HUMAN	sp Q5XGC8 1433B_XENTR	88.52	244	28	0	3	246	1	244	6e-159	447	sp Q5XGC8 1433B_XE	RYLSEVASGDNKQTTVSNSQQAYQEAFEISKKEMQPTHPIRLGLALNFSVFYYEILNSF
	sp P31946 1433B_HUMAN	sp P63102 1433Z_RAT	88.02	242	29	0	3	244	1	242	2e-157	444	sp P63102 1433Z_RA1	DNKQTTVSNSQQAYQEAFEISKKEMQPTHPIRLGLALNFSVFYYEILNSPEKACSLAKT
	sp P31946 1433B_HUMAN	sp P63101 1433Z_MOUSE	88.02	242	29	0	3	244	1	242	2e-157	444	sp P63101 1433Z_MO	sp P31946 1433B_HUMAN sp Q4R572 1433B_MACFA 100.00 24€
	sp P31946 1433B_HUMAN	sp P29361 1433Z_SHEEP	87.60	242	30	0	3	244	1	242	1e-156	442	sp P29361 1433Z_SHE	RYLSEVASGDNKQTTVSNSQQAYQEAFEISKKEMQPTHPIRLGLALNFSVFYYEILNSF
	sp P31946 1433B_HUMAN	sp Q5R651 1433Z_PONAB	87.60	242	30	0	3	244	1	242	3e-156	441	sp Q5R651 1433Z_PO	DNKQTTVSNSQQAYQEAFEISKKEMQPTHPIRLGLALNFSVFYYEILNSPEKACSLAKT
	sp P31946 1433B_HUMAN	sp P63104 1433Z_HUMAN	87.60	242	30	0	3	244	1	242	3e-156	441	sp P63104 1433Z_HUI	
	sp P31946 1433B_HUMAN	sp P63103 1433Z_BOVIN	87.60	242	30	0	3	244	1	242	3e-156	441	sp P63103 1433Z_BO	
	sp P31946 1433B_HUMAN	sp Q5ZKC9 1433Z_CHICK	87.19	242	31	0	3	244	1	242	7e-156	440	sp Q5ZKC9 1433Z_CH	2: chr22_check.gff3
	sp P31946 1433B_HUMAN	sp Q7T356 143BB_DANRE	88.52	244	26	1	3	246	1	242	2e-155	439	sp Q7T356 143BB_DA	
	sp P31946 1433B_HUMAN	sp P29309 1433_XENLA	87.23	235	30	0	12	246	1	235	6e-152	429	sp P29309 1433_XENI	<u>1: human protein.fas</u> ④ ∅ 🖇
	sp P31946 1433B_HUMAN	sp Q6UFZ8 143B2_ONCMY	88.41	233	27	0	3	235	1	233	3e-150	426	sp Q6UFZ8 143B2_ON	
	sp P31946 1433B_HUMAN	sp Q6P4Z5 1433Z_XENTR	84.71	242	37	0	3	244	1	242	4e-150	426	sp Q6P4Z5 1433Z_XEI	
	sp P31946 1433B_HUMAN	sp Q91896 1433Z_XENLA	83.47	242	40	0	3	244	1	242	3e-148	421	sp Q91896 1433Z_XEI	
	sp P31946 1433B_HUMAN	sp Q5ZMD1 1433T_CHICK	82.23	242	43	0	3	244	1	242	1e-147	419	sp Q5ZMD1 1433T_CF	
	sp P31946 1433B_HUMAN	sp Q5RFJ2 1433T_PONAB	81.82	242	44	0	3	244	1	242	2e-146	416	sp Q5RFJ2 1433T_PO	
	sp P31946 1433B_HUMAN	sp P27348 1433T_HUMAN	81.82	242	44	0	3	244	1	242	2e-146	416	sp P27348 1433T_HUI	
	sp P31946 1433B_HUMAN	sp Q3SZI4 1433T_BOVIN	81.82	242	44	0	3	244	1	242	2e-146	416	sp Q3SZI4 1433T_BOV	
	sp P31946 1433B_HUMAN	sp Q52M98 1433T_XENLA	81.82	242	44	0	3	244	1	242	2e-146	416	sp Q52M98 1433T_XE	
	sp P31946 1433B_HUMAN	sp P68255 1433T_RAT	81.82	242	44	0	3	244	1	242	2e-146	416	sp P68255 1433T_RA1	
	sp P31946 1433B_HUMAN	sp Q6Q6X0 1433T_RABIT	81.82	242	44	0	3	244	1	242	2e-146	416	sp Q6Q6X0 1433T_RA	
	sp P31946 1433B_HUMAN	sp P68254 1433T_MOUSE	81.82	242	44	0	3	244	1	242	2e-146	416	sp P68254 1433T_MO	
	sp P31946 1433B_HUMAN	sp Q2F637 1433Z_BOMMO	79.92	244	49	0	1	244	1	244	3e-143	408	sp Q2F637 1433Z_BOI	
	sp P31946 1433B_HUMAN	sp P29310 1433Z_DROME	79.42	243	50	0	2	244	3	245	3e-142	405	sp P29310 1433Z_DR	
	splP31946 1433B_HUMAN	splQ1HR36 1433Z_AEDAE	78.60	243	52	0	2	244	3	245	2e-140	401	splQ1HR36 1433Z_AE	
	splP31946 1433B_HUMAN	splQ20655 14332_CAEEL	78.78	245	52	0	1	245	1	245	7e-140	399	sp Q20655 14332_CAI	
>	en P31946 1433B_HUMAN	sp P41932 14331_CAEEL	78.10	242	48	2	7	244	7	247	1e-131	378	sp P41932 14331_CAL	
-) Þ)	

Modification des attributs

- Renommer
- Annoter...



Ajout de tags et d'annotations

Galaxy / ABiMS Analyze Data Workflow Shared Data - Visualization - Admin Help - User -	Using 18.0 GB
Attributes Convert Format Datatyne Permissions	History 2 •
Edit Attributes	Human chr22 proteome study 19.1 MB
Name: blastp_vs_swissprot Info:	3: blastp vs_swissprot 21,556 lines format: tabular, database: ? a
Number of comment lines:	NKQTTVSNSQQAYQEAFEISKKEMQPTHPIRLGLALNFSVFYYEILNSF DNKQTTVSNSQQAYQEAFEISKKEMQPTHPIRLGLALNFSVFYYEILNSPEKACSLAKT
Auto-detect This will inspect the dataset and attempt to correct the above column values if they are not accurate.	2: chr22 check.gff3 ● 𝔅 X 1: human protein.fas ● 𝔅 X

>

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Modification du type de fichier

- Tabular \rightarrow gtf
- fastq \rightarrow fastqsanger (phred33)

Attitubes Datatype Permissions History Human chr22 proteome study 101MB 21,556 lines 21,556	Galaxy / ABiMS	Analyze Data Workflow Shared Data				Using 18.0 GB
Change data type New Type: indular indular rdata rdata rdata rgb sam scf sff summary_tree svg tabular tabular tabular tabular tabular stf summary_tree svg tabular tabular <t< td=""><td>Attributes Convert Format Datatype Permissions</td><th></th><td></td><td></td><td>History</td><td>C 🔶</td></t<>	Attributes Convert Format Datatype Permissions				History	C 🔶
Change data type 19.1 MB New Type: 1 1 2 1 3 1 4 2 3 4 0 3 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0					Human chr22 proteome study	
New Type: tabular aset but not modify its contents. Use this if Galaxy has incorrectly guessed the type of your dataset. rdata rgb sam scf sff summary_tree svg tabular vigo tabular 2: chr22 check.gff3 * 0 %	Change data type				19.1 MB	47 🖻
1: human protein fas	New Type: tabular data rdata rgb sam scf sff summary_tree svg tabular	lify its contents. Use this if Galaxy has incorrect	ly guessed the type of your datase	t.	3: blastp on db 21,556 lines format: tabular, database: ? im im </td <td>O X</td>	O X
				-	1: human protein.fas	

>

Conversion de type

Galaxy / ABiMS	Analyze Data					Using 18.0 GB
Attributes Convert Format Datatype Permissions					History	C 🗘
Convert to new format					 Human chr22 proteome study 19.1 MB	47 🖻
Convert GEE to BED					<u>3: blastp_vs_swissprot</u>	• / ×
This will create a new dataset with the contents of this dataset co	nverted to a new f	format.			2: chr22 check.gff3 66,141 lines, 1 comments format: gff, database: <u>?</u> uploaded gff file	• () ×
						47 🖻
					1.Seqname 2.Source3.Feature#gff-version 3	4.Start 5.End
					chr22 processed_transcript gene	42545877 42551007
					chr22 processed_transcript transcript	42548208 42550874
					chr22 processed_transcript exon	42549039 42549216
					chr22 processed_transcript exon	42550831 42550874
					<u>1: human_protein.fas</u>	• / %
					\$	

Visualisation

- Tabular \rightarrow graphique de type scatterplot
- gff/bam \rightarrow visualisation dans un système de track



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Re-ouverture du formulaire à l'origine de l'objet avec ces options pré-remplies

Galaxy / ABiMS	Analyze Data V	Vorkflow	Shared Data -	Visualization -	Admin	Help v U	ser -		U	sing 18.0 GB
NCBI BLAST+ blastp (version 0.0.17)							Â	History		0.0
Protein query sequence(s):								Human chr22 proteome 19.1 MB	study	4 🖻
Subject database/sequences: BLAST Database Protein BLAST database: uniprot_swissprot Type of BLAST: blastp							Ξ	3: blastp vs swissprot 21,556 lines format: tabular, database: ()))) Run this job again 3 sp P31946 1433B_HUMAN RYLSEVASGDNKQTTVSNSQQAN	2 4 5 sp A4K2U9 1433B_PONAB 'QEAFEISKKEMQPTHPIRLGLAL	 Ø Ø Ø 100.00 246 NFSVFYYELLNSF
 > blastp-short Set expectation value cutoff: 0.0001 Output format: Tabular (extended 24 columns) ♀ 								DNKQTTVSNSQQAYQEAFEISKK sp P31946 1433B_HUMAN RYLSEVASGDNKQTTVSNSQQAY DNKQTTVSNSQQAYQEAFEISKK	EMQPTHPIRLGLALNFSVFYYEI sp Q4R572 1433B_MACFA QEAFEISKKEMQPTHPIRLGLAL EMQPTHPIRLGLALNFSVFYYEI	LNSPEKACSLAKT 100.00 246 NFSVFYYEILNSF LNSPEKACSLAKT
Advanced Options:								2: chr22 check.gff3 1: human protein.fas		• / ×
Execute										
A Note. Database searches may take a substantial amount of tim	ne. For large input da	atasets it is	advisable to allo	v overnight proces	sing.					
What it does										
Search a protein database using a protein query, using the NCBI B	3LAST+ blastp comm	mand line to	ool.							
You can also search against a FASTA file of subject protein sea importantly gives e-values for pairwise searches (very small e- FASTA file into a database first using makeblastdb and search	quences. This is not values which will loo against that.	advised be ok overly si	cause it is slower gnficiant). In mos	(only one CPU is t cases you should	used), but m instead turr	nore n the other				
Output format										

Because Galaxy focuses on processing tabular data, the default output of this tool is tabular. The standard BLAST+ tabular output contains 12 columns:

	6	lumn	NCBI name	Description
2			qseqid	Query Seq-id (ID of your sequence)

Suppression d'un objet

Galaxy / ABiMS	Analyze Data Workflow Shared	Data - Visualization -	Admin Help -	User -		Using 18.0 GB
Tool: Upload File					History	C 0
Name: chr22_check.gff?	3					
Created: Aug 09, 2013					Human chr22 proteome study	
Filesize: 5.2 MB					19.1 MB	47 🖻
Dbkey: ?						
Format: gff					<u>3: blastp vs swissprot</u>	
Galaxy Tool Version: 1.1.3					1: human protein fas	a /x
Tool Version:						
Tool Standard Output: <u>stdout</u>						
Tool Standard Error: <u>stderr</u>						
Tool Exit Code: 0						
API ID: e3c6542f4e1089	974					
Full Path: /w/galaxy/dev/ga	laxy-dist/database/files/001/dataset_1672.dat					
Input Parameter	Value	Note for	r rerun			
File Format	auto					
async_datasets	1984					
Specify Files for Dataset (auto)	1 uploaded datasets					
Genome	unspecified (?)					
File Format	auto					
Inheritance Chain						
	chr22_check.gff3					

Suppression d'un objet Mais attention, l'objet est dans une sorte de corbeille

🗧 Galaxy / ABiMS	Analyze Data	Workflow Shared Data -	Visualization - Admin	Help + User +		Using 18.0 GB
Tool: Upload File					History	C 0
Name: chr22	2_check.gff3					HISTORY LISTS
Created: Aug	09,2013				Human chr22 proteome stud	Saved Histories
Filesize: 5.2 M	ЛВ				19.1 MB	Histories Shared with Me
Dbkey: ?					2: blasta va avrianarat	CURRENT HISTORY
Format: gff					<u>s. biastp vs swissprot</u>	Create New
Galaxy Tool Version: 1.1.3	1				A This dataset has been	Copy History
Tool Version:					undelete it or here to	Copy Datasets
Tool Standard Output: stdou	<u>t</u>				disk	
Tool Standard Error: stder	1				2: chr22_check.aff3	Share of Publish
Iool Exit Code: 0	54044-400074					Extract Workflow
APTID: e300	54214e108974	001/dataast 1670 dat			<u>1: human_protein.fas</u>	Dataset Security
Full Path: /w/ga	liaxy/dev/galaxy-dist/database/liles/	001/dataset_1672.dat				Resume Paused Jobs
Input Parameter	Value		Note for rerun			Collapse Expanded Datasets
File Format	auto					 Include Deleted Datasets
async_datasets	1984					Include Hidden Datasets
Specify Files for Dataset (auto)	1 upload	ded datasets				Unhide Hidden Datasets
Genome	unspecif	fied (?)				Delete Hidden Datasets
File Format	auto					Purne Deleted Datasets
Inheritance Chain						Show Structure
						Show Structure
	chr22_che	eck.gff3				Export to File
						Delete
						Delete Permanently
						OTHER ACTIONS
						Import from File

Suppression d'un objet

Mais attention, l'objet est dans une sorte de corbeille « Du coup, l'espace disque n'est pas libéré »

🗧 Galaxy / ABiMS		Analyze Data						Using 18.0 GB			
Tool: Upload File							History	<u>a</u> e			
Name: Created: Filesize: Dbkey:	chr22_check.gff3 Aug 09, 2013 5.2 MB ?						Human chr22 proteome stud 19.1 MB	HISTORY LISTS Saved Histories Histories Shared with Me			
Format: Galaxy Tool Version: Tool Version: Tool Standard Output: Tool Standard Error: Tool Exit Code:	gff 1.1.3 <u>stdout</u> <u>stderr</u> 0						3: blastp vs swissprot ▲ This dataset has been undelete it or <u>here</u> to disk 2: chr22_check.gff3	CORRENT HISTORY Create New Copy History Copy Datasets Share or Publish Extract Workflow			
API ID: Full Path: Input Parameter	e3c6542t4e108974 /w/galaxy/dev/galaxy-di	st/database/files/(001/dataset_	1672.dat	Note fo	r rerun	<u>1: human_protein.fas</u>	Dataset Security Resume Paused Jobs Collapse Expanded Datasets			
File Format async_datasets Specify Files for Dataset (auto) Genome File Format Inheritance Chain		auto 1984 1 upload unspecif auto	led datasets fied (?) eck.gff3					 Include Deleted Datasets Include Hidden Datasets Unhide Hidden Datasets Delete Hidden Datasets Purge Deleted Datasets Show Structure Export to File Delete Delete Permanently OTHER ACTIONS Import from File 			

Purge des objets deletés Mais attention, là, c'est pour de bon !

🗧 Galaxy / ABiMS		Analyze Data	Workflow	Shared Data -	Visualization -	Admin	Help 🗸 User 🗸		Using 18.0 GB
Tool: Upload File								History	C 8
Name:	chr22_check.gff3								HISTORY LISTS
Created:	Aug 09, 2013							Human chr22 proteome stud	Saved Histories
Filesize:	5.2 MB							19.1 MB	Histories Shared with Me
Dbkey:	?							2: blasto va avriantet	CURRENT HISTORY
Format:	gff							<u>s. biastp vs swissprot</u>	Create New
Galaxy Tool Version:	1.1.3							A This detect has been	Copy History
Tool Version:								undelete it or here to	Copy Patasata
Tool Standard Output:	<u>stdout</u>							disk	Copy Datasets
Tool Standard Error:	stderr							2: chr22, chock aff2	Share or Publish
Tool Exit Code:	0							Z. CHIZZ CHECK.ghs	Extract Workflow
API ID:	e3c6542f4e108974							1: human_protein.fas	Dataset Security
Full Path:	/w/galaxy/dev/galaxy-dis	st/database/files/0)01/dataset_	1672.dat					Resume Paused Jobs
Input Parameter		Value			Note fo	r rerun			Collapse Expanded Datasets
File Format		auto							 Include Deleted Datasets
async_datasets		1984							Include Hidden Datasets
Specify Files for Dataset (auto)		1 upload	led datasets						Unhide Hidden Datasets
Genome		unspecif	ied (?)						Delete Hidden Datasets
File Format		auto							Purgo Dolotod Datasots
Inheritance Chain									Show Swicture
									Export to File
		chr22_che	ck.gff3						Delete
									Delete
									Delete Permanently
									OTHER ACTIONS
									Import from File

Purge des objets deletés Mais attention, là, c'est pour de bon !

🗧 Galaxy / ABiMS	Analyze Data	Workflow Shared Data -	Visualization - Admin	Help 👻 User 🗸		Using 18.0 GB
Tool: Upload FileName:chr2:Created:AugFilesize:5.2 MDbkey:?Format:gffGalaxy Tool Version:1.1.3	2_check.gff3 09, 2013 MB 3				History Human chr22 proteome stur 19.1 MB <u>3: blastp_vs_swissprot</u>	HISTORY LISTS Saved Histories Histories Shared with Me CURRENT HISTORY Create New
Tool Ver Tool Sta Tool Sta Tool Sta Tool Exi API ID: Full Pat Input Pa File Forn async_c Specify	ittentio	n, là,	c'est	τροι	ur de l	DON I ets
Genome File Format	auto	ed (?)				Delete Hidden Datasets
Inheritance Chain						Show Soucture
	chr22_che	sk.gff3				Export to File Delete Delete Permanently OTHER ACTIONS Import from File



- Cycle de vie des données
 - http://abims.sb-roscoff.fr/galaxyproject
 - . Gestion par l'utilisateur de son quota
 - Suppression automatique en cours de réflexion
 - 6 mois ou 1 an

- Saved history : Renommer Supprimer [définitivement]

💳 Galaxy / ABiMS	AI	nalyze Data Work							Using 41%
Tools search tools Get Data	Saved Histories search history names and ta Advanced Search	ıgs 🔤 🔍						History Huma 20.0 N	HISTORY LISTS Saved Histories
ABIMS WORKFLOWS Workflow RNA-seq de novo by ABIMS Workflow RNA-seq with reference by ABIMS Workflow 4 Metabolomics ABIMS TOOLS Primer RNASeq InterEsil Statistics	Name Human chr22 proteo study X-Files • RNAseq de-novo • XCMS input test •	Dataset	Tags 1 Tag 0 Tags 0 Tags 0 Tags 0 Tags 0 Tags	SharingSize on Disk20.0 MB353.6 MB870.9 MB130.6 MB	Created 6 days ago Mar 25, 2013 Mar 20, 2013 Apr 02, 2013 Mar 20, 2013	Last Updated † less than a minute ago 2 minutes ago Jun 10, 2013 Apr 15, 2013	Status current history	3: blas	Create New Copy History Copy Datasets Share or Publish Extract Workflow Dataset Security Resume Paused Jobs Collapse Expanded Datasets Include Deleted Datasets
Utils Phylogenetics Debug COMMON TOOLS Text Manipulation FASTA manipulation Join, Subtract and Group Filter and Sort NCBI BLAST+	RNAseq de-novo inp For 0 selected histories Histories that have been dele	s: Rename De	0 Tags	439.6 MB	administrator(Mar 20, 2013 s) may be permanently	deleted.		Unhide Hidden Datasets Purge Deleted Datasets Show Structure Export to File Delete Delete Permanently OTHER ACTIONS Import from File
NGS: QC and manipulation NGS: RNA Analysis NGS: Mapping NGS: Picard (beta) NGS: SAM Tools SVDetect VarScan Workflows • All workflows								- 10	

Saved history :

- Renommer
- Supprimer [définitivement]

🗧 Galaxy / ABiMS	Ana	alyze Data Workf							Using 41	1%
Tools	Saved Histories								History 2	; o
search tools	search history names and tag	s Q							RNAseq de-novo	
Get Data	Advanced Search	-							870.9 MB	27 🖻
ABIMS WORKFLOWS	Name	Datas	ets Tags	Sharing	Size on Disk	Created	Last Updated †	<u>Status</u>	100: Trinity on data 98 and	0 %
Workflow RNA-seq de novo by ABIMS	Human chr22 proteom								data 31. Assembled franscripts	
Workflow RNA-seq with reference by ABIMS	study	2	<u>2 Tags</u>		20.0 MB	6 days ago	14 minutes ago		92: Dark.sample.paired.2.fastq_good.f	Ø ⊠ astq.
Workflow 4 Metabolomics	□ X-Files ▼	6	<u>0 Tags</u>		353.6 MB	Mar 25, 2013	16 minutes ago		<u>cutadapt.fastq_good.fastq.nonrrna</u> .paired.fastq	<u>.fastq</u>
ABIMS TOOLS	RNAsen de-nove		0 Та па		070.0 MD	Mar 20,	hup 10, 2012	current	<u>91:</u>	0 🛚
RNASeq		9	<u>u tags</u>		870.9 MB	2013	Jun 10, 2013	history	Dark.sample.paired.1.fastq_good.fr	astq.
InterEsil	XCMS input test	1	0 Tags		130.6 MB	Apr 02, 2013	Apr 15, 2013		.paired.fastq	LIASIQ
Statistics							•			0.44
Utils	RNAseq de-novo inpu	ts • 4	<u>0 Tags</u>		439.6 MB	Mar 20, 2013	Mar 20, 2013		88: BlueLight.sample.paired.2.fastq_g	∉/
Phylogenetics	For 0 selected histories:		Dolot	o Dormany		oto			stq.cutadapt.fastq_good.fastq.nonr	rrna.f
Debug	For o selected histories.			erennand		ele			asiq.paireu.iasiq	
COMMON TOOLS	Histories that have been delete	ed for more than a ti	me period sp	ecified by	the Galaxy adm	ninistrator(s) ma	ay be permanently	deleted.	<u>87:</u> ®	0 🛚
Text Manipulation				-	-				BlueLight.sample.paired.1.fastg_go	<u>ood.fa</u> rrna f
FASTA manipulation									astq.paired.fastq	i i i i a i i
Join, Subtract and Group										
Filter and Sort									4: Dark.sample.paired.2.fastq @	0 %
NCBI BLAST+									3: Dark.sample.paired.1.fastg @	0 %
NGS: QC and manipulation										
NGS: RNA Analysis									2: (1) Plual ight cample paired 2 factor	0 %
NGS: Mapping									BlueLight.sample.paired.z.lastq	
NGS: Picard (beta)									<u>1:</u>	0 🛚
NGS: SAM Tools									BlueLight.sample.paired.1.fastq	
SVDetect										
VarScan										
Workflows										
<u>All workflows</u>										



TP METABOLOMIQUE SUR Galaxy



La Metabolomique par Sophie



WORKFLOW



. Un workflow est un enchaînement d'outils et de paramètres

• Peut correspondre au protocole de l'expérience

 Un workflow est construit pour être rejoué (de manière plus ou moins stricte)



Notre workflow



102

Notre workflow sauce Galaxy



Création d'un workflow à partir d'un historique



Création d'un workflow à partir d'un historique · Changement du nom

- Possibilité de décocher des étapes

💳 Galaxy / ABiMS	Analyze Data Workflow	Shared D	ata			Using 14%	
Tools	The following list contains each tool that was run t	to create the (datasets in your current history. Please select those that you wish to include	9	History	0	•
search tools	In the worknow.	annatha ina	erested into a worldfau will be about in grou		Projet Cidre Misharl		Ê
Get Data	Tools which cannot be run interactively and thus o	annot be inco	corporated into a worknow will be shown in gray.		3.7 GB	42 🖻	
	Workflow name				Course to an Dalata a	H O D O	0
ABIMS WORKFLOWS	Workflow constructed from history 'Projet Cidre	Mishari			69: XSet.group.Rplots.pd	<u>II</u> (00 (/ XX	>
Workflow RNA-seq with reference	Create Workflow Check all Uncheck all				68: xset.group.RData	• () ×	ŝ
Workflow 4 Metabolomics	Tool		History items created		65: yeat group Polote p	df @ // Sd	2
Workflow 4 Pelagos			1: xset.RData		00. Abel.group.repiolo.pc		
	xcms.xcmsSet				64: xset.group.RData	• / X	S
ABIMS TOOLS	Include "xcms.xcmsSet" in workflow	•	2: sample_info.tab	Ξ	58:	• / ×	2
RNASeg			3: xset.TICs_raw.pdf		xset.group.retcor.group	.fillPeaks.anno	0
InterEsil					tateDiffreport.Rdata		
Statistics	xcms.group		4: xset.group.RData		format: rdata, database: [2	
Utils	Include "xcms group" in workflow	▶	5: yset group Rolots odf		R version 2.15.1 (2012-0	6-22)	
Phylogenetics			er veerigt eahn throethau		"Roasted Marshmallows" 2012 The R Foundation f	Copyright (C)	
Tests	C 115				Computing ISBN 3-9000	51-07-0	
COMMON TOOLS	xcms.fillPeaks		21: xset.group.fillPeaks.RData		Platform: x86_64-unknow	vn-linux-gnu	
Convert Formats	👿 Include "xcms.fillPeaks" in workflow				with ABSOLUTELY NO W	VARRANTY.	
FASTA manipulation					You are welcom		
Filter and Sort			22: xset.group.fillPeaks.diffreport.tsv			47 🖻	
Graphics	xcms diffreport		23: xset.group.fillPeaks.diffreport.data_matrix.tsv		binary data		
Join, Subtract and Group	Xonisianieport	•					
NCBI BLAST+	lnclude "xcms.diffreport" in workflow		24: xset.group.fillPeaks.diffreport.zip		57:	• / ×	3
Text Manipulation			25: xset.group.fillPeaks.diffreport.RData		xset.group.retcor.group	.fillPeaks.anno	0
NGS TOOLS					tateDiffreport.zip		
NGS: BedTools			26: xset.group.annotateDiffreport.tsv		<u>56:</u>	• / ×	S
NGS: Mapping	CAMERA.annotateDiffreport		27: xset.group.annotateDiffreport.data_matrix.tsv		xset.group.retcor.group.	<u>.fillPeaks.anno</u>	0
NGS: Picard (beta)	Ringlude "CAMERA appetete Diffeoport" in work	► Flow	20: yeat group appotato Diffragart zin			TIALOV	
NGS: QC and manipulation	Minclude CAMERA.annotateDhireport in Work	.IIUW	zo. xserigi ouplannotatennn eport.zip		<u>55:</u>	• / X	5
NGS: RNA Analysis			29: xset.group.annotateDiffreport.Rdata		tateDiffreport.tsv	.miPeaks.anno	2
NGS. SAM 10015							_
USEFUL TOOLS	xcms.retcor		21: yeat aroun rateor TICs, corrected off		54: xset group retcor group	● Ø X fillPeaks anno	\$
Control-FREEC	Include "yoms retoor" in workflow		ar vaeral onbueron uno consciention		tateDiffreport.Rdata	and outstand	-

Liste des workflows

• Possibilité de créer un workflow de zéro

Galaxy / ABiMS	Analyze Data	Workflow	Shared Data -	Admin	Help -	User •			Using 6%
Your workflows							C	Create new workflow	The second secon
Name								# of Steps	
workflow4metabo -								11	
imported: RNA-seq de-novo assembly -								13	
imported: RNA-seq de-novo cleaning -								7	
RNA-seq de-novo cleaning -								7	
RNA-seq de-novo assembly -								12	
RNASeq - DE analysis - DESeq - edgeR - Venn - HAC - ACP -								11	
Annotation and Filter -								9	
Workflow constructed from history 'X-Files' -								3	
Workflow RNAseq de-novo 💌								12	

Workflows shared with you by others

No workflows have been shared with you.

Other options

Configure your workflow menu

Galaxy / ABiMS	Analyze Data			Using 6%
Your workflows				O Create new workflow
Name				# of Steps
workflow4metabo -				11
imt Edit mbly -				13
imp Share or Publish ing •				7
Download or Export				7
Copy				10
Rename				12
RN. View edgeR - Venn - HAC - ACP -				11
				9
Workflow constructed from history 'X-Files'				3
Workflow RNAseq de-novo 💌				12

Workflows shared with you by others

No workflows have been shared with you.

Other options

Configure your workflow menu

Le canevas

Glisser-Déposé



Edition d'un workflow :

ightarrow

Ajout d'un nouvel outil dans le workflow


Edition d'un workflow :

• Ajout d'un nouvel outil dans le workflow



Edition d'un workflow :

Rendre paramétrable un paramètre au moment de l'exécution



Galaxy / ABiMS	Workflow			Using 6%
Your workflows				O Create new workflow
Name				# of Steps
workflow4metabo 🕶				11
im Edit Imply •				13
im Share or Publish ning -				7
RI Download or Export				7
Copy Rt Bename				12
RN View - edgeR - Venn - HAC - ACP -				11
Anhoustand + mor				9
Workflow constructed from history 'X-Files' -				3
Workflow RNAseq de-novo 💌				12

Workflows shared with you by others

No workflows have been shared with you.

Other options

Configure your workflow menu

- Paramètres par défaut
 Paramètres à renseigner

💳 Galaxy / ABiMS	Analyze Data Workflow Shared Data + Visualization + Admin Help + User +		Using 6	6%
Tools	Running workflow "workflow4metabo"	Dĥ	History	; o
search tools	Step 1: xcms.xcmsSet (version 20131212)		Unnamed history	12 🔜
<u>Get Data</u>	library directory name		0 bytes	~
ABIMS WORKFLOWS			Your history is empty. Click 'Get I on the left pane to start	Data'
Workflow RNA-seq de novo				
Workflow RNA-seq with reference	Method			
Workflow 4 Metabolomics				
worknow 4 Pelagos	step			
ABIMS TOOLS	fullym			
Primer	30			
RNASeq	Advanced options			
InterEsil	hide			
Statistics		=		
Ours Dhylogenetics	Step 2: xcms.group (version 20131212)			
Tests		-		
	RData file			
COMMON TOOLS	Output dataset 'output' from step 1			
Convert Formats	Method			
FASTA manipulation	density			
Graphics	bw			
Join, Subtract and Group	30			
NCBI BLAST+	minfrac			
Text Manipulation	0.5			
NGS TOOLS	mzwid			
NGS: BedTools	0.25			
NGS: Mapping	Advanced options			
NGS: Picard (beta)	nide			
NGS: QC and manipulation	Step 9: years retear (version 20121212)			
NGS: RNA Analysis	Step 3: XCms.retCor (Version 20131212)			
NGS: SAM Tools	Stop 4: years group (version 20121212)			
USEFUL TOOLS	Step 4. xcms.group (version 20131212)			
Control-FREEC	Step 5: yems rateor (version 20121212)			
GATK Tools				
Muscle	Step 6: ycms group (version 20131212)			
SnpEff tools				
<	Step 7: xcms.fillPeaks (version 20131212)			>



• Ce qui est possible dans Galaxy



Ce qui n'est pas possible dans Galaxy pour le moment Super-workflow





PARTAGE



« biologiste » \leftrightarrow « biologiste »

- Partage de datasets
 - . Historique en entier
 - Avec ou sans workflow associé (Extract workflow)
 - Sous ensembles



massiste \rightarrow « biologiste »

- Partage de workflows
 - Paramètres pré-configués
 - Paramètres à configurer (Set at runtime)
 - => Suivant le niveau de l'utilisateur
- Partage de pages (voir plus loin)



$bioinformaticien \rightarrow bioinformaticien$

• Partage de descriptions d'outils et/ou de scripts

Toolshed Galaxy

Partage de datasets

– Galaxy / ABiMS	Analyze Data Workflow Shared Dat	a → Visualization → Help → User →	Using 42%
Tools	Saved Histories		History
search tools	search history names and tags		RNAseq de-novo
Get Data	Advanced Search		870.9 MB 🖉 🗎
ABIMS WORKFLOWS	Datasets Tags Sharing S	Size on Disk Created Last Updated † Status	100: Trinity on data 98 and I and a 2 X
Workflow RNA-seq de novo by ABiMS		Aug 07, less than a minute	
Workflow RNA-seq with reference by ABIMS	Switch	2013 ago	92:
Workflow 4 Metabolomics	C View 6 0 Tags 3	53.6 MB Mar 25, Aug 13, 2013	cutadapt.fastq_good.fastq.nonrrna.fastq .paired.fastq
ABIMS TOOLS	Rename 9 0 Tags #	370.9 MB Mar 20, Jun 10, 2013 current	91: • / %
Primer	Delete	2013 history	Dark.sample.paired.1.fastq_good.fastq.
InterEsil	Delete Permanently 1 <u>0 Tags</u>	130.6 MB Apr 02, 2013 Apr 15, 2013	cutadapt.fastq_good.fastq.nonrrna.fastq .paired.fastg
Statistics			
Utils	inputs	i39.6 MB 2013 Mar 20, 2013	88:
Phylogenetics		stq.cutadapt.fastq_good.fastq.nonrrna.f	
Debug	For 0 selected histories: Rename Delete Delete Perm	nanently Undelete	astq.paired.fastq
COMMON TOOLS	Histories that have been deleted for more than a time period specified	by the Galaxy administrator(s) may be permanently deleted.	<u>87:</u>
Text Manipulation			BlueLight.sample.paired.1.fastq_good.fa
FASTA manipulation			astq.paired.fastq
Join, Subtract and Group			
Filter and Sort			4: Dark.sample.paired.2.fastq @ (/ 💥
NCBIBLAST+			3: Dark.sample.paired.1.fastq @ 🖉 💥
NGS: QC and manipulation			
NGS: RNA Analysis			2:
NGS: Mapping			DreeligntSumprespaned.2.ndStd
NGS: Picard (beta)			<u>1:</u> @ 0 %
NGS: SAM Tools			BlueLight.sample.paired.1.fastq
Muscle			
<u>SVDetect</u>			
PAyM			
INA MIL			
Workflows			
<			

- <mark>-</mark> (Galaxy / ABiMS		Analyze Data	Workflow	Shared Data -	Visualization -	Admin	Help -	User -	Using 18.1 GB
You	r workflows									Create new workflow
Nam	e									# of Steps
Bla	st and Filter 👻									7
R	Edit	8								6
	Run									14
	Share or Publish	. •]								14
Mc	Download or Export	h you by others								
vvc	Сору	in you by others								
No v	Rename	/ith you.								
Otl	View									
_	Delete									
Co.	ngure your worknow menu	J								

Partage : les modes

- Via lien url
- Via les listes de la rubrique Shared Data
- Via l'identifiant d'utilisateurs (login@sb-roscoff.fr)
- → communauté restreinte
- \rightarrow tous les utilisateurs du serveur Galaxy
- → communauté restreinte

- Galaxy / ABiMS Analyze Data Workflow Shared Data Visualization - Help - User - User - Using 42%
Share or Publish History 'JohnDoe'
Make History Accessible via Link and Publish It

This history is currently restricted so that only you and the users listed below can access it. You can:

Make History Accessible via Link Generates a web link that you can share with other people so that they can view and import the history.

Make History Accessible and Publish

Makes the history accessible via link (see above) and publishes the history to Galaxy's Published Histories section, where it is publicly listed and searchable.

Share History with Individual Users

You have not shared this history with any users.

Share with a user

Back to Histories List

>



Import d'un published *

🗧 Galaxy / ABiMS	Analyze Data	Workflow	Shared Data 🗸	Visualizatior	n.+ Help.+	User -	Using 42%
Published Histories			Data Libraries		N		
search name, annotation, owner, and tags			Published Histories		3		
Advanced Search			Published Wor	kflows			
			Published Visu	alizations			
Name Annotation	<u>Owner</u>	Com	Published Pag	es	nmunity Tags	Last Updated +	
JohnDoe	lecorguille	**	***	hu	ıman blast	less than a minute ago	

. Import d'un shared history

– Galaxy / ABiMS	Analyze Data	Workflow Shared Da	.ta → Visualization → Help	v≠ User≠		Using 42%
Histories shared with you by others					History	
					RNAs	Saved Histories
□ <u>Name</u>	Datasets <u>Cre</u>	eated Las	t Updated † Sh	ared by	870.9	Histories Shared with Me
□ TestSPE positivemode	50 Apr	r 15, 2013 Jun	03.2013	@sb-roscoff.fr	100: T	CURRENT HISTORY
					data 9	Create New
For 0 selected histories: Copy Unshare					02.	Copy History
					Dark.s	Copy Datasets

Partage



Station Biologique

- Level 5
- Partage d'outils et de descriptions via le toolshed
 Level 4



- . Lancement des outils de manière autonome.
- . Utilisation des options avancées.
- . Utilisation de l'API Galaxy
- . Propose des workflows aux collègues de niveau --



- Level 3
 - · Lancement des outils de manière autonome.
 - Utilisation d'un workflow plus ou moins préconfiguré
 Level 2



Utilisation d'un workflow préconfiguré



• Partage des données avec un collègue de niveau ++



BONUS



Mécanique **BONUS**



• Comment un outil arrive dans Galaxy ?





. Comment un outil arrive dans Galaxy ?

[lecorquille@n0 ~]\$ e-PCR --help e-PCR: invalid option -- usage: [-hV] [posix-options] stsfile [fasta ...] [compat-options] where posix-options are: Margin (default 50) -m ## Wordsize (default 7) -w ## Max mismatches allowed (default -n ## Max indels allowed (default 0) -a ## Use ## discontiguos words, slow -f ## ##>1 Set output file -0 ## -t ## Set output format: 1 - classic, range (pos1..pos2) 2 - classic, midpoint 3 - tabular 4 - tabular with alignment in co (slow) -d##-## Set default size range (default 100-350) Turn hits postprocess on/off -p +-Verbosity flags -v ## -a alf Use presize alignmens (only if qaps>0), slow a - Allways or f - as Fallback Use 5'-end lowercase masking of -x +primers (default -) Uppercase all primers (default -11 +-

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):

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

0

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

Max indels allowed (G):

Set maximal number of gaps allowed in primer-to-sequence alignment (per primer!).

Set output format (T):

tabular Output formats

lats

Execute



Comment un outil arrive dans Galaxy ?

<tool id="abims_epcr" name="e-PCR">

<!-- author : lecorquille@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 format="tabular" help="format : tabular" label="STS file" name="infile_stsfile" type="data"/>
»	<param format="fasta" help="format : fasta" label="Fasta file" name="infile_fasta" type="data"/>
»	<pre><param help="Set word size for primers hash (nucleotide positions).</pre></th></tr><tr><th></th><th>Longer word size decreases hash collision rate, but increases memory usage. Also no mismatches are allowed within word size near</th></tr><tr><th></th><th>'inner' boundary of primers unless one uses discontiguous words, and no gaps are ever allowed in that region." label="Wordsize (W)" name="wordsize" type="integer" value="7"/></pre>
>	<pre><param help="Set discontiguous word count for primers</pre></th></tr><tr><th></th><th>hash (1 means 'use contiguous words'). Discontiguous words increase number of hash tables and decrease 'effective' word size (thus</th></tr><tr><th></th><th>increasing hash collision rate), so make search significantly slower, but increase sencitivity by allowing mismatches within word</th></tr><tr><th></th><th>size. Reasonable values are 1 (contiguous words) and 3." label="Use ## discontinuos words (F)" name="wordcnt" type="integer" value="1"/></pre>
>	<pre><param help="Set maximal allowed deviation of hit product size from</pre></th></tr><tr><th></th><th>expected STS size." label="Margin (M)" name="margin" type="integer" value="50"/></pre>
>	<pre><param help="Set ddefault STS size range - values</pre></th></tr><tr><th></th><th>used for STSs that have no size associated in file." label="Set default sts lower size (D)" name="sts_size_lo" type="integer" value="100"/></pre>
>	<param help="Set ddefault STS size range -</th></tr><tr><th></th><th>values used for STSs that have no size associated in file." label="Set default sts higher size (D)" name="sts_size_hi" type="integer" value="400"/>
>	<param help="Set maximal number of mismatches allowed</p></th></tr><tr><th></th><th>in primer-to-sequence alignment (per primer!)." label="Max mismatches allowed (N)" name="max_mismatch" type="integer" value="0"/>
>	<param help="Set maximal number of gaps allowed in primer-to-</th></tr><tr><th></th><th>sequence alignment (per primer!)." label="Max indels allowed (G)" name="max_gap" type="integer" value="0"/>
>	<param help="Output formats" name="output_format" type="select"/>
>	» <label>Set output format (T)</label>
»	» <pre><pre>option value="1">classic, range (pos1pos2)</pre></pre>
>	<pre>> <option value="2">classic, midpoint</option></pre>
>	<pre>> <option selected="true" value="3">tabular</option></pre>
»	<pre>> <option value="4">tabular with alignment in comments (slow)</option></pre>
>	
<th>\$></th>	\$>

<outputs>

<data name="output" format="tabular" />

</outputs>

<help>



Comment un outil arrive dans Galaxy ?



<!-- 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" />
- comparam name="infile_fasta" type="data" label="Fasta file" format="fasta" help="format : fasta" />
- <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!)." />



- Comment un outil arrive dans Galaxy ?
 - Tooshed
 - Description maison

- Une seul adresse :
 - => support.abims@sb-roscoff.fr