

## Galaxy Overview



Matt Gitzendanner  
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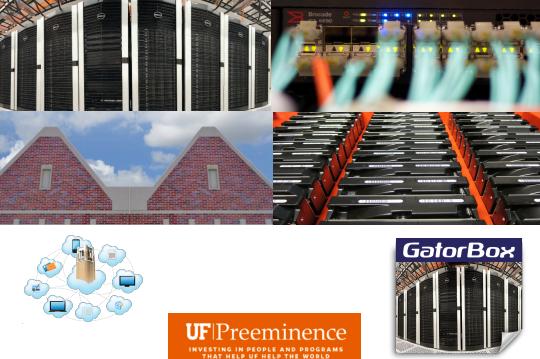
10/1/15

**UF** Research Computing  
Information Technology  
Home of High-Performance Computing and **HiPerGator**

**UF** Information Technology [www.it.ufl.edu](http://www.it.ufl.edu)

UNIVERSITY OF FLORIDA'S 2015-2020  
**STRATEGIC GOALS FOR IT**  
One IT for the GatorGood

- Research Computing Strategic Goals
  - Expand HPC, data storage and research network capacity, performance and usability
  - Enhance and expand services that use HPC, data storage and network resources
  - Improve faculty awareness and access to use of Research Computing services



**UF** Preeminence  
INVESTING IN PEOPLE AND PROGRAMS THAT HELP THE WORLD

**GatorBox**

**UF** Information Technology [www.it.ufl.edu](http://www.it.ufl.edu)



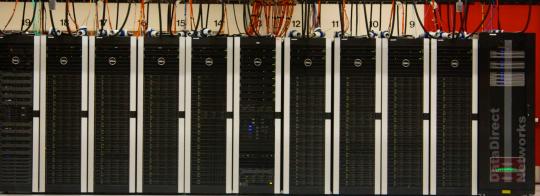
**HiPerGator 2.0**  
The University of Florida Supercomputer for Research

**UF** Information Technology [www.it.ufl.edu](http://www.it.ufl.edu)

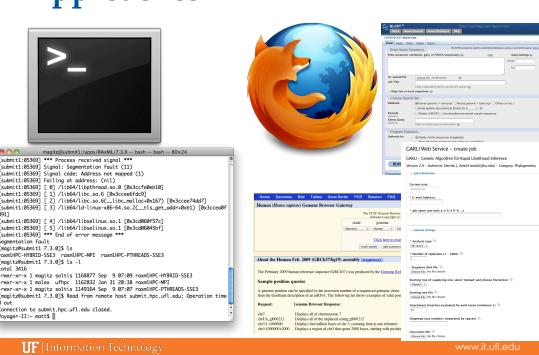
# HiPerGator

The University of Florida Supercomputer for Research

- 16,384 cores—**total of about 21,000 cores today**
- Infiniband interconnect
- >3PB fast, high-availability, storage
- GPGPUs**
- Large memory (**512GB to 1TB of RAM**) nodes



## Approaches



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UNIVERSITY OF FLORIDA | High-Performance Computing

# HiPerGator

The University of Florida Supercomputer for Research

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## Cluster basics

- User interaction
  - Galaxy
  - Login node (Head node)
- Scheduler
  - Tell the scheduler what you want to do
- Compute resources
  - Your job runs on the cluster

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## What is Galaxy?

**Bio-IT World** BONUS EDITION: Open Source

Galaxy Provides Life Support for NGS Exploration

powered by Galaxy

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## Galaxy: Data intensive biology for everyone

- Accessible, reproducible, transparent computational biology
- galaxy.rc.ufl.edu
  - Local instance of Galaxy
    - Faster access to storage, easier upload
    - Local compute resources
    - Local control

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## Galaxy Analysis Workspace

Galaxy / UF HPC

Tools Options

MACS

Treatment file: 3 hg19.chr10.bam

Input file: 31:Summary\_Statistics.an

Format: Auto

Effective Genome Size: Human (hg18) 13530955

Tag size (Optional): 15

P-value: 1e-05

Keep duplicate tags at the exact same location?  Keep All  Keep Minimal  Keep Single

Use Model: True

small fold enrichment for model building: 10

large fold: 30

Advanced Options:

Analyze Data Workflow Shared Data Admin Help User

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Advanced Options:

Analyze Data Workflow Shared Data Admin Help User

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The screenshot shows the Galaxy interface with the following details:

- Treatment file:** 3-hg19.chr10.bam
- Input file:** Selection is Optional
- Format:** Auto
- Effective Genome Size:** Human (hg18) 3.5 Gb
- Tag size (Optional):** 25
- P-Value:** 1e-05
- Keep duplicate tags at the exact same location?**  Keep ALL
- Output:**  By Binomial
- Use Model:** True
- small fold enrichment for model building:** 10
- large fold:** 30
- Advanced Options:** No
- Diagnosis Report:** No

**History:**

- 0915 Macs Exercise 5.3 Gb
- 35: Summary Statistics on hg19.chr10.bam
- 33: UCSC Main on Human hg18
- 31: MACS job log on hg19.chr9.bam
- 30: MACS wiggle on hg19.chr9.bam
- 29: MACS xis on hg19.chr9.bam
- 28: MACS summits on hg19.chr9.bam
- 27: MACS peaks on hg19.chr9.bam
- 26: BAM-to-SAM on data hg19.chr9.bam
- 25: converted SAM
- 23: hg19.chr9.bam

**MACS** Treatment file: 3-hg19.chr10.bam  
Input file: Selection is Optional  
Format: Auto  
Effective Genome Size: Human (hg18) 3.5 Gb  
Tag size (Optional): 25  
P-Value: 1e-05  
Keep duplicate tags at the exact same location?:  Keep ALL  
Output:  By Binomial  
Use Model: True  
small fold enrichment for model building: 10  
large fold: 30  
Advanced Options: No  
Diagnosis Report: No

The screenshot shows the Galaxy interface with the following details:

- Treatment file:** 3-hg19.chr9.bam
- Input file:** Selection is Optional
- Format:** Auto
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**History:**

- 0915 Macs Exercise 5.3 Gb
- 35: Summary Statistics on hg19.chr9.bam
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- 27: MACS peaks on hg19.chr9.bam
- 26: BAM-to-SAM on data hg19.chr9.bam
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- 23: hg19.chr9.bam

**MACS** Treatment file: 3-hg19.chr9.bam  
Input file: Selection is Optional  
Format: Auto  
Effective Genome Size: Human (hg18) 3.5 Gb  
Tag size (Optional): 25  
P-Value: 1e-05  
Keep duplicate tags at the exact same location?:  Keep ALL  
Output:  By Binomial  
Use Model: True  
small fold enrichment for model building: 10  
large fold: 30  
Advanced Options: No  
Diagnosis Report: No

The screenshot shows the Galaxy interface with the following details:

- Treatment file:** LANA ChIP peaks on hg19
- Input file:** Selection is Optional
- Format:** Auto
- Effective Genome Size:** hg19
- Tag size (Optional):** 25
- P-Value:** 1e-05
- Keep duplicate tags at the exact same location?**  Keep ALL
- Output:**  By Binomial
- Use Model:** True
- small fold enrichment for model building:** 10
- large fold:** 30
- Advanced Options:** No
- Diagnosis Report:** No

**History:**

- 27: MACS peaks on hg19.chr9.bam
- 236 regions
- format: bed, database: Z

**Tags:**

- LANA x chip x hg19 x
- peaks x chr9 x

**Annotation / Notes:**

Peak calling on LANA ChIP-seq data using Human chromosome 9 from hg19 build

**Metadata** Treatment file: LANA ChIP peaks on hg19  
Input file: Selection is Optional  
Format: Auto  
Effective Genome Size: hg19  
Tag size (Optional): 25  
P-Value: 1e-05  
Keep duplicate tags at the exact same location?:  Keep ALL  
Output:  By Binomial  
Use Model: True  
small fold enrichment for model building: 10  
large fold: 30  
Advanced Options: No  
Diagnosis Report: No

## Getting Data into Galaxy

- Upload a file from your computer
  - Direct upload (<2GB)
  - For large files: scp or copy files to HPC
    - Load from within Galaxy
    - [http://wiki.hpc.ufi.edu/index.php/Galaxy\\_Data\\_Import](http://wiki.hpc.ufi.edu/index.php/Galaxy_Data_Import)
- External data
  - UCSC table browser
  - Biomart
  - interMine / modMine
  - EuPathDB
  - EncodeDB
  - EpiGRAPH
  - FlyMine
  - GrameneMart...

**Getting Data into Galaxy**

Upload a file from your computer

- Direct upload (<2GB)
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External data

- UCSC table browser
- Biomart
- interMine / modMine
- EuPathDB
- EncodeDB
- EpiGRAPH
- FlyMine
- GrameneMart...

## Data libraries

Data Library "GMS 6001 MACS Exercise"

Name	Message	Uploaded By	Date	File Size
2011-10-14 7 hg19.chr10.samtoolsbam	onthispc@efi.edu	2011-09-13	1.6 Gb	
2011-10-14 7 hg19.chr10.samtoolsbam	onthispc@efi.edu	2011-09-13	1.6 Gb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	80.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	82.5 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	74.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	70.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	36.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	48.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	55.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	64.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	33.8 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	39.8 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	145.5 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	38.4 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	17.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	16.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	126.3 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	48.6 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	133.0 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	85.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	102.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	65.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	80.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	85.5 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	64.8 Mb	

For selected datasets: Import to current history | Go |

Data Library "GMS 6001 MACS Exercise"

MACS test data

Name	Message	Uploaded By	Date	File Size
2011-10-14 7 hg19.chr10.samtoolsbam	onthispc@efi.edu	2011-09-13	1.6 Gb	
2011-10-14 7 hg19.chr10.samtoolsbam	onthispc@efi.edu	2011-09-13	1.6 Gb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	80.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	82.5 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	74.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	70.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	36.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	48.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	55.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	64.1 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	33.8 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	39.8 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	145.5 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	38.4 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	17.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	16.9 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	126.3 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	48.6 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	133.0 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	85.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	102.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	65.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	80.7 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	85.5 Mb	
hg19.chr10bam	onthispc@efi.edu	2011-09-14	64.8 Mb	

For selected datasets: Import to current history | Go |

Data Library "GMS 6001 MACS Exercise"

# Data Access Control

Roles associated with new group  
HPC test ChIP-seq analyses

Groups

search Advanced Search

Name	Users	Roles
HPC	0	2
Taylor HPC Lab	2	1

For selected groups: [Delete](#) | [Undelete](#) | [Purge](#)

Users associated with new group  
om@hpc.ufl.edu  
magitz@ufl.edu

Roles

search Advanced Search

Name	Description	Type	Groups
HPC	Role for group HPC	system	1
HPC test ChIP-seq analyses	Test analyses of ChIP-seq data	admin	1

Users

search Advanced Search

Email	User Name	Groups	Roles	External	Last Login
adision@ufl.edu	adision	0	1	yes	Sep 15, 2011
bostwick@ufl.edu	bostwick	0	1	yes	Sep 15, 2011
cavriles@ufl.edu	cavriles1	0	1	yes	Sep 15, 2011
cliffrey@ufl.edu	cliffrey	0	1	yes	Sep 15, 2011
coltd3@ufl.edu	coltd3	0	1	yes	Sep 15, 2011

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# Galaxy Tool Suites

- ▶ Text Manipulation
- ▶ Format Converters
- ▶ Filtering and Sorting
- ▶ Join, Subtract, Group
- ▶ Sequence Tools
- ▶ Multi-species Alignment Tools
- ▶ Genomic Interval Operation
- ▶ Summary Statistics, graphing
- ▶ Regional Variation
- ▶ EMBOSS
- ▶ Evolution
- ▶ RNA-Seq
- ▶ ChIP-Seq
- ▶ GATK
- ▶ Phylogenetics

<p><b>GQ: QC and manipulation</b></p> <ul style="list-style-type: none"> <li><b>NanoPlot DATA</b></li> <li><b>FASTQ_Groomer:</b> convert between various FASTQ quality formats</li> <li><b>FASTQ_Splitter:</b> join paired end FASTQ files</li> <li><b>FASTQ_Joiner:</b> join paired end reads</li> <li><b>FASTQ_SUMMARY:</b> Statistics by contig</li> <li><b>ROCHE_454 DATA</b></li> <li><b>BamQC:</b> QC for BAM files</li> <li><b>Select_Raw_Quality:</b> Select high-quality sequences</li> <li><b>Combine_FASTA_and_QUAL_to_FASTQ</b></li> <li><b>FASTQ_SOLID</b></li> <li><b>Convex_Solid_to_FASTQ</b></li> <li><b>Compute_quality_statistics</b> for FASTQ files</li> <li><b>Display_Score_histo</b> for SOLID quality</li> <li><b>GENOME_FASTQ</b></li> <li><b>MANIPULATION</b></li> <li><b>Filter_FASTQ</b> reads by quality</li> <li><b>FASTQ_Cleaner</b></li> <li><b>FASTQ_Trimmer</b> by column</li> <li><b>FASTQ_QUALITY_Trimmer</b> by sliding window</li> </ul>	<p><b>extension</b> Metagenomic analysis Human Genome Variants</p> <p><b>NGS_TOOLS</b></p> <ul style="list-style-type: none"> <li><b>NGS_TOOLBOX_BETA</b></li> <li><b>NGS_QC_and_manipulation</b></li> <li><b>NGS_Mapping</b></li> <li><b>Map</b> with Bowtie for Illumina</li> <li><b>Map</b> with BWA for Illumina</li> <li><b>ROCHE_454</b></li> <li><b>Lazier</b> map short reads against reference sequence</li> <li><b>Mosaicist</b> compare short reads against genome, nc, and rgs databases</li> <li><b>Pairwise_Blast_XM</b> output</li> <li><b>Samtools</b></li> <li><b>Map</b> with Bowtie for SOLID</li> <li><b>NGS_Solid_Tools</b></li> <li><b>NGS_Solid_Models</b></li> <li><b>NGS_PolyA</b></li> <li><b>NGS_RNA_Analysis</b></li> </ul> <p><b>IGENETICS</b></p> <ul style="list-style-type: none"> <li><b>SNP_WGA:</b> Data Filters</li> <li><b>SNP_WGA_SAC_DNA:</b> Models</li> <li><b>SNP_WGA_Manhattan</b> Models</li> </ul>	<p><b>NGS_QC_and_manipulation</b></p> <p><b>NGS_Mapping</b></p> <p><b>NGS_SAM_Tools</b></p> <ul style="list-style-type: none"> <li><b>Estimate</b> coverage, bwa, bowtie flag values</li> <li><b>Convert</b> BAM to internal format</li> <li><b>BAM2FASTQ</b> converts BAM format to FASTQ format</li> <li><b>Merge_BAM</b> merges BAM files into one BAM file</li> <li><b>Generate_aligns</b> from BAM dataset</li> <li><b>Printcov</b> on coverage and SNPs</li> <li><b>Peiwei</b>-to-internal condenses BAM files into smaller BAM files</li> <li><b>Samtools</b> provides simple stats on BAM files</li> </ul> <p><b>NGS_PolyA</b></p> <p><b>NGS_PCA</b></p> <p><b>NGS_RNA_Analytics</b></p> <p><b>IGENETICS</b></p> <ul style="list-style-type: none"> <li><b>SNP_WGA_DNA_Filters</b></li> <li><b>SNP_WGA_QC_Lite</b>: Phase</li> <li><b>SNP_WGA_Manhattan</b> Models</li> </ul>	<p><b>NGS_SAM_Tools</b></p> <ul style="list-style-type: none"> <li><b>NGS_SAM</b> - filter tools for SAM</li> <li><b>Extract_ids</b> from SAM</li> <li><b>Index</b> Analysis</li> <li><b>NGS_Bam_Caliber</b></li> <li><b>MAQC</b> - Multi-Panel Analysis of ChIP-Seq</li> <li><b>GenTrackIndex</b> on a BED file</li> <li><b>Peak_predictor</b> on GeneTrack models</li> </ul> <p><b>NGS_RNA_Analysis</b></p> <ul style="list-style-type: none"> <li><b>RNASeq</b></li> <li><b>Find_fusion_splice_junctions</b> using RNA-seq data</li> <li><b>Cufflinks</b> transcript assembly tool, provides transcript_id for each gene_id</li> <li><b>Cufflinks</b> compare assembled transcripts</li> <li><b>Cufflinks</b> transcript assembly tool, provides transcript_id and track_id</li> <li><b>Cufflinks</b> transcripts across multiple samples</li> <li><b>Cuffdiff</b> find significant changes in expression, including splicing, and promoter use</li> </ul> <p><b>FILTERING</b></p> <ul style="list-style-type: none"> <li><b>Filter_Constituted_Transcripts</b> using tracking file</li> </ul>
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# Galaxy Workflows

**Unknown**

This tool cannot be used in workflows

---

**BAM-to-SAM**

Include "BAM-to-SAM" in workflow

---

**Convert Genomic Intervals To Strict BED6**

Include "Convert genomic intervals to strict BED6" in workflow

---

**MACS**

Include "MACS" in workflow

---

**Convert BED To GeneTrack Index**

Include "Convert BED to GeneTrack index" in workflow

- ▶ 25: hg19.chr9.bam
  - Treat as input dataset
  
- ▶ 26: BAM-to-SAM on data 2: converted SAM
  
- ▶ 27: MACS peaks on hg19.chr9.bam
  
- ▶ 27: MACS peaks on hg19.chr9.bam
- ▶ 28: MACS summits on hg19.chr9.bam
  
- ▶ 29: MACS wiggle on hg19.chr9.bam
- ▶ 30: MACS job log on hg19.chr9.bam
- ▶ 31: MACS job log on hg19.chr9.bam
  
- ▶ 27: MACS peaks on hg19.chr9.bam

Extract Workflow  
Dataset Security  
Show Deleted Datasets  
Show Hidden Datasets  
Show Structure  
Export to File  
Delete  
**Other Actions**  
Import from File

The screenshot shows a complex Galaxy Workflow titled "Workflow constructed from history 'LANA ChIP peaks on hg19'". The workflow consists of several steps connected by arrows:

- Input dataset** → **BAM-to-SAM** (with "Input BAM" and "Output BAM" outputs)
- Input dataset** → **MACS** (with "Treatment file", "Input file", "Bam file", "Summary statistics (bed)", "Log (txt)", and "Shardreport (rdbar)" outputs)
- Input dataset** → **Convert BED to Genomic Intervals** (with "Convert BED" and "Output BED" outputs)
- BAM-to-SAM** → **Convert BED to Genomic Intervals** (using "Output BAM" as input)
- MACS** → **Convert BED to Genomic Intervals** (using "Shardreport (rdbar)" as input)
- Convert BED to Genomic Intervals** → **Summary Statistics** (using "Output BED" as input)
- Summary Statistics** → **MACS** (using "Output BAM" as input)

The "Details" panel on the right shows the following configuration:

- Tool: MACS**
- Input BAM**: Data input type (interval or sam or bam or eland or elandmulti or bed)
- Input file**: Data input type (interval or sam or bam or eland or elandmulti or bed)
- Format:** Auto
- Effective Genome Size:** Human (hg19)
- Tag size (Optional):** 25

The "Help" section at the bottom right says "Is at the exact same place as the tool for model building: all".



# Galaxy Workflows

**Sharing and publishing**

**Share or Publish History 'LANA ChIP peaks on hg19'**

**Making History Accessible via Link and Publishing 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.

**Sharing History with Specific Users**  
You have not shared this history with any users.

**Share with a user**

[Back to Histories List](#)

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**Sharing and publishing**

**Share or Publish History 'LANA ChIP peaks on hg19'**

**Making History Accessible via Link and Publishing It**  
This history is currently accessible via link and published.  
Anyone can view and import this history by visiting the following URL:  
<http://galaxy.hpc.ufl.edu/u/moskalenko/lana-chip-peaks-on-hg19/>

**Unpublish History**  
Removes this history from Galaxy's [Published Histories](#) section so that it is not publicly listed or searchable.

**Disable Access to History via Link and Unpublish**  
Disables this history's link so that it is not accessible and removes history from Galaxy's [Published Histories](#) section so that it is not publicly listed or searchable.

**Sharing History with Specific Users**  
The following users will see this history in their history list and will be able to view, import, and run it.

<b>Email</b> magitz@ufl.edu
<b>Share with another user</b>

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**Summary**

- Analyze data without the CLI
- Visualize the results
- Publish histories, workflows, and annotated pages
- Add new tools, get support @ HPC
- Focus on your science, not minutiae
- UF Galaxy** – coming to a browser near you!

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**Demo**

**Galaxy / UF HPC /** Analyze Data Workflow Shared Data Help User

Tools Options

- Get Data
- Save Data
- ENCODE Tools
- lif|Over
- Text Manipulation
- Join, Subtract and Sort
- Join, Subtract and Group
- Convert Formats
- Extract Features
- Get Feature Scores
- Fetch Alignments
- Get Genome Scores
- Statistics
- Graph/Display Data
- Regional Variation
- Multiple regression
- Genomic Data Analysis
- Evolution
- Modif Tools
- Multiple Alignments
- Metabolic analysis
- FASTA manipulation
- NCR BLAST
- Sequence manipulation
- NCS BLAST

History Options

MACS hg19 0 bytes

Your history is empty. Click Get 'Data' on the left pane to start

UFL HPC Galaxy News:

- 2011-08-09 Prototype Galaxy Instance

An instance of Galaxy Platform for Biological Mass Spectrometry (BMS) data is available at the University of Florida High-Performance Computing Center for research and demonstration purposes. This instance is not available for public use, yet. However, you can email HPC or the Bioinformatics group at [hpc@ufl.edu](mailto:hpc@ufl.edu) to request to be notified of its general availability.

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**Galaxy demo**

**http://galaxy.rc.ufl.edu**

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