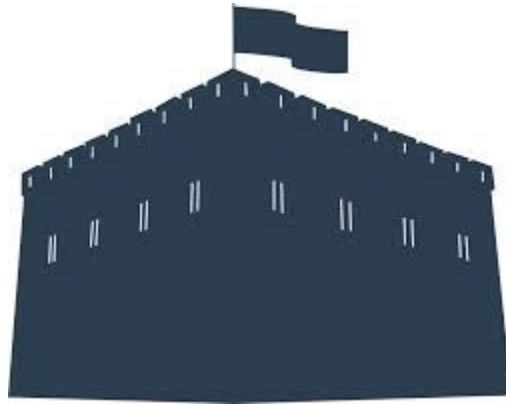


Mass Spectrometry-based Proteomics Data Analysis using Galaxy-P



The Galaxy-P Project



- Extending Galaxy for MS-based proteomics data analysis applications



UNIVERSITY OF MINNESOTA
SUPERCOMPUTING
INSTITUTE



James Johnson (JJ)



Pratik Jagtap



Tim Griffin

Documentation: z.umn.edu/gcc2015gp

Documentation and Infrastructure Support
Kevin Murray

Ray Sajulga

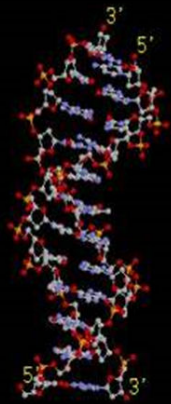
Thomas McGowan



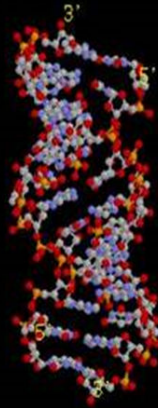
Objectives for workshop

- Basics of data analysis for proteomics/proteogenomics
- Learn about tools available in Galaxy for proteomics
- Learn how to build some workflows and use tools

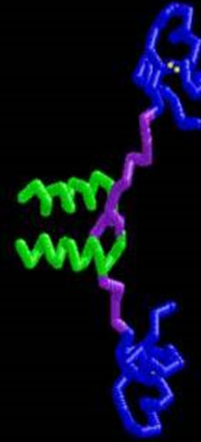
'Omic technologies and the molecular biology paradigm



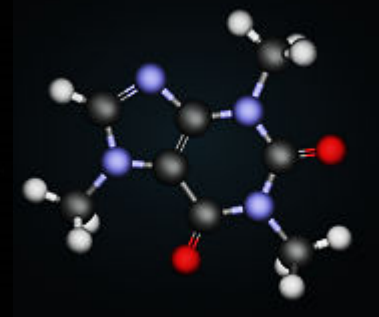
DNA
Genome



RNA
Transcriptome



Protein
Proteome



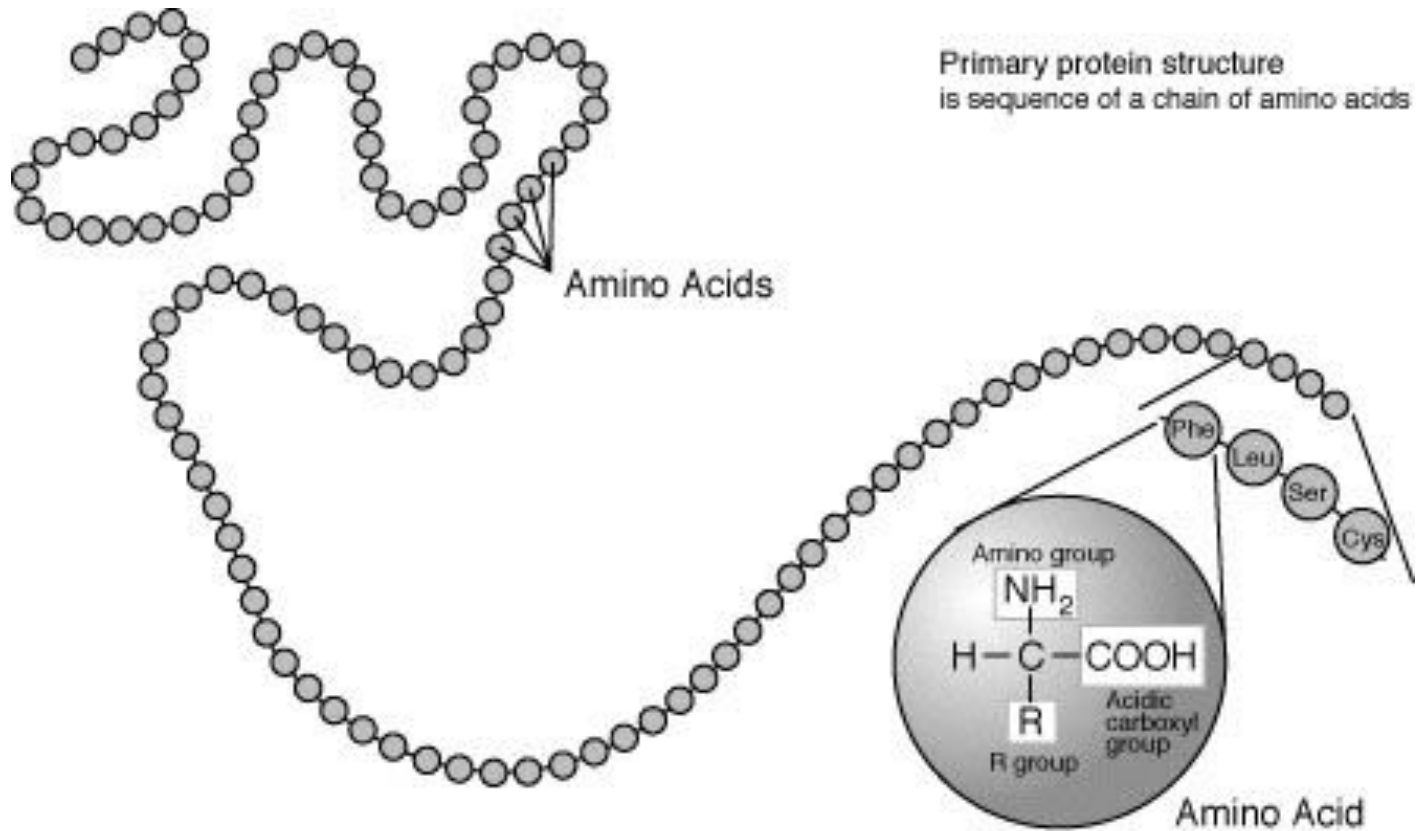
Metabolite
Metabolome

High throughput sequencing technologies

Biological Mass Spectrometry

- Proteomics complements genomics/transcriptomics
- Direct information on molecular “effectors” of cell functions (enzymes, transporters etc.)
- Properties not predicted by genes/transcripts (PTMs, protein complexes etc.)

Quick reminder: primary protein structure



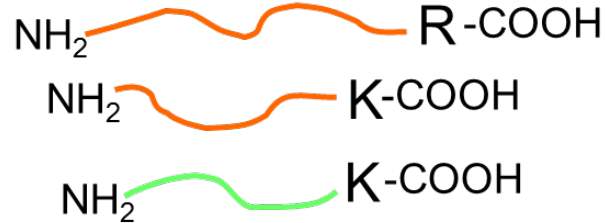
(20 naturally occurring)

Measuring masses of proteins and peptides

1. Protein, MW = 10,000 +  “Top down proteomics”

digest into peptides (enzymatic, chemical)

2. Peptides,
MW < 4,000



Trypsin

N-THK_↑NCPHIVVGTPGR_↑IPD-C

cleaves c-terminal side of
arginine (R) and lysine (K)

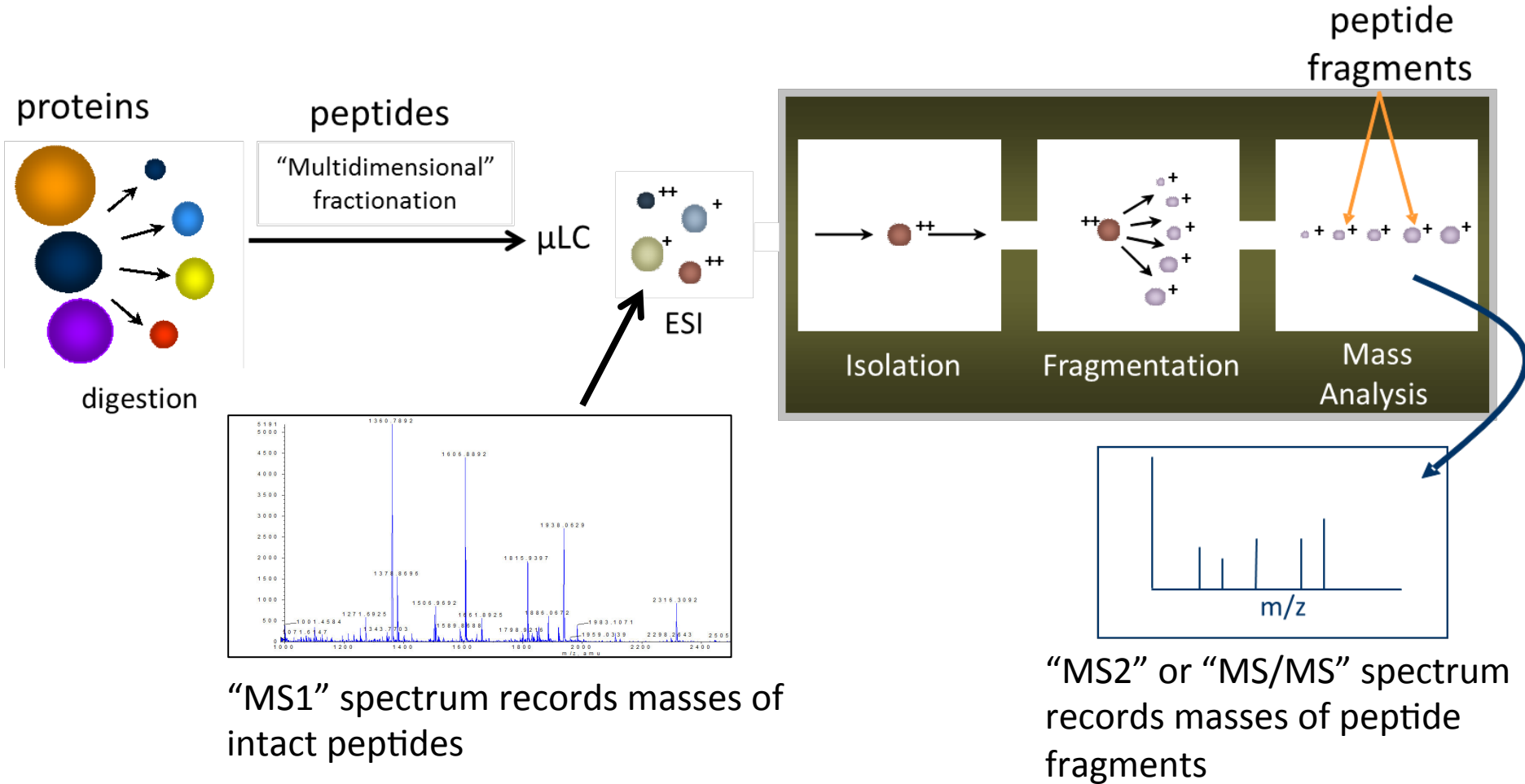
3. Peptide
fragments



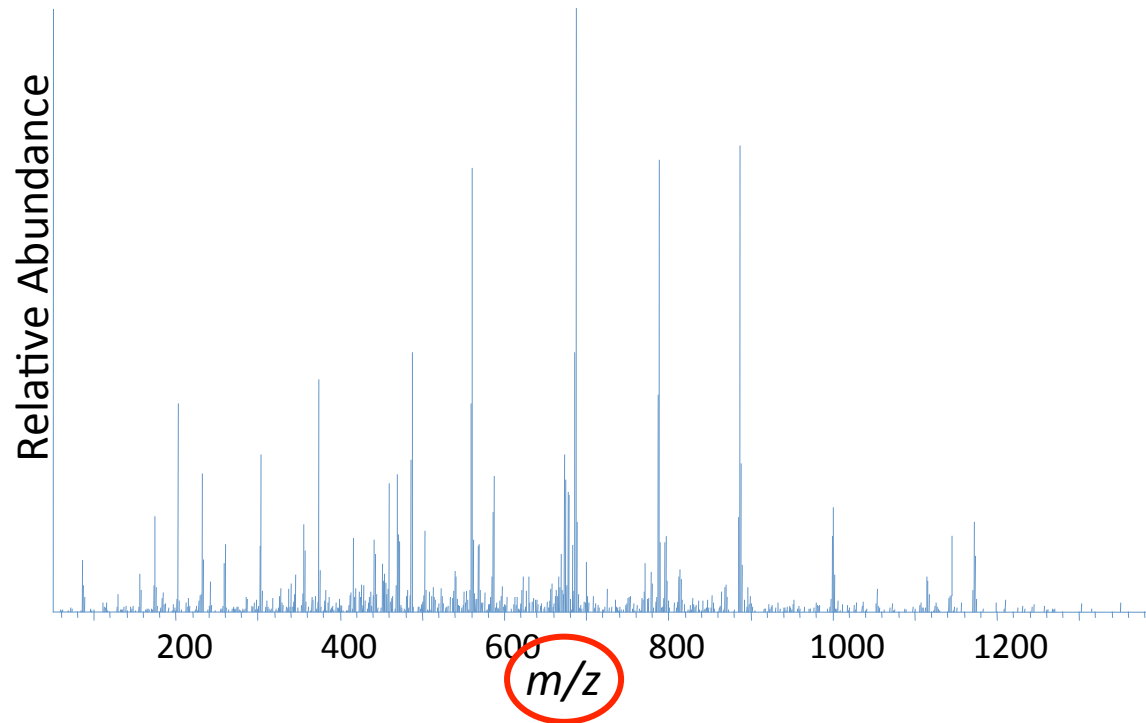
“Bottom up proteomics”

High throughput protein identification by MS

Peptide fractionation coupled to tandem mass spectrometry (MS/MS)



Information “currency” of MS: mass spectra



Common mass spectrometry terms

m/z = mass-to-charge = mass of analyte/number of retained charges

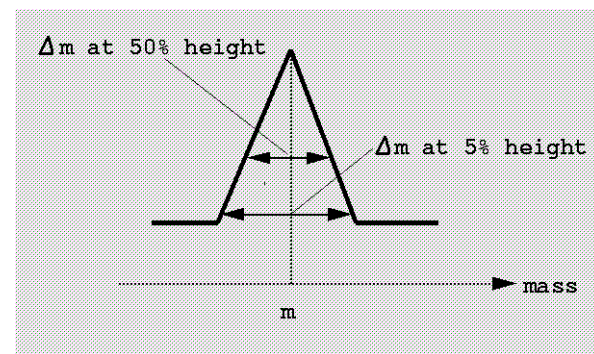
Mass accuracy (ppm) = $[(\text{measured } m/z - \text{actual } m/z)/(\text{actual } m/z)] * 10^6$

- Mass accuracy is usually expressed in units of parts per million (ppm)
- Generally a lower mass accuracy in ppm is preferred

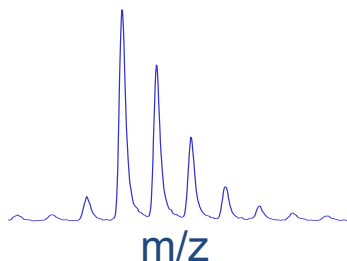
Mass resolution = $m/\Delta m$

where m = analyte mass

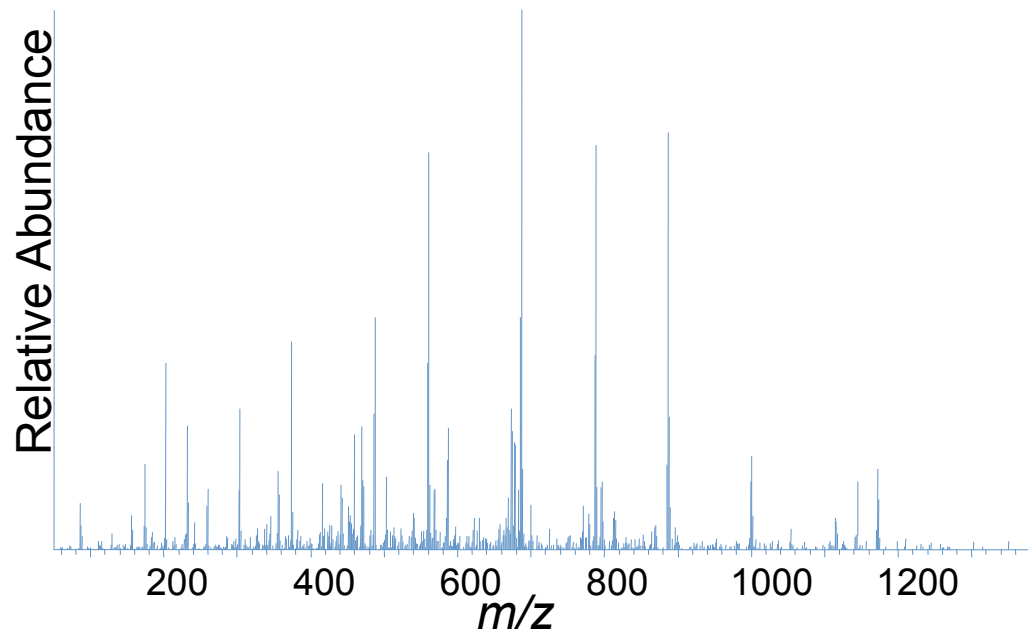
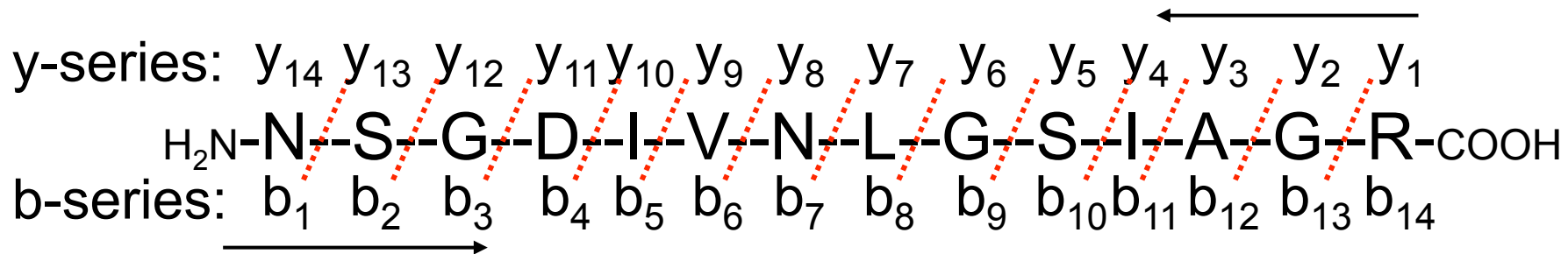
Δm = width of peak, generally at 50% of peak height (also called full-width half-max, or FWHM)



- Generally higher mass resolution is preferred



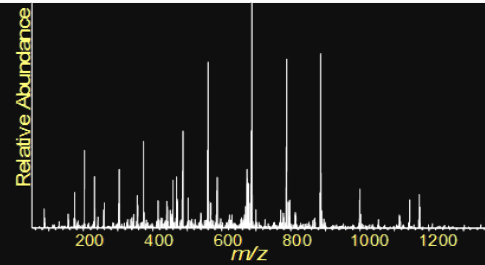
Tandem mass spectrometry and peptide sequence



- An MS/MS spectrum contains a mixture of b and y ions

High throughput identification of proteins

Raw MS/MS spectrum

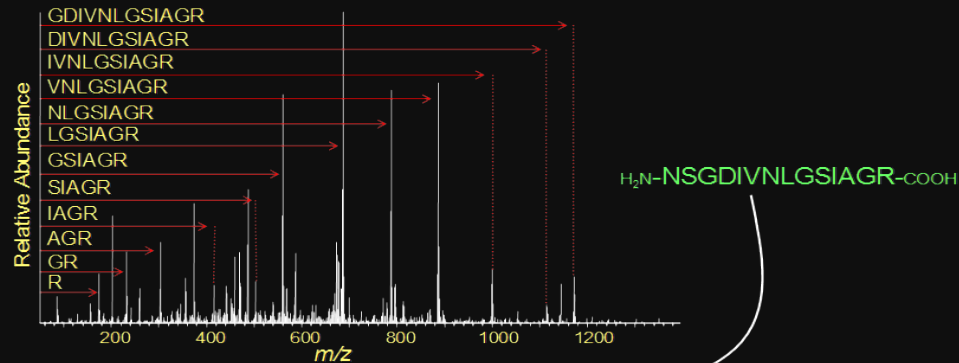


Protein sequence and/or DNA
sequence database search



Direct identification of 1000s
proteins from complex mixtures

Peptide sequence match

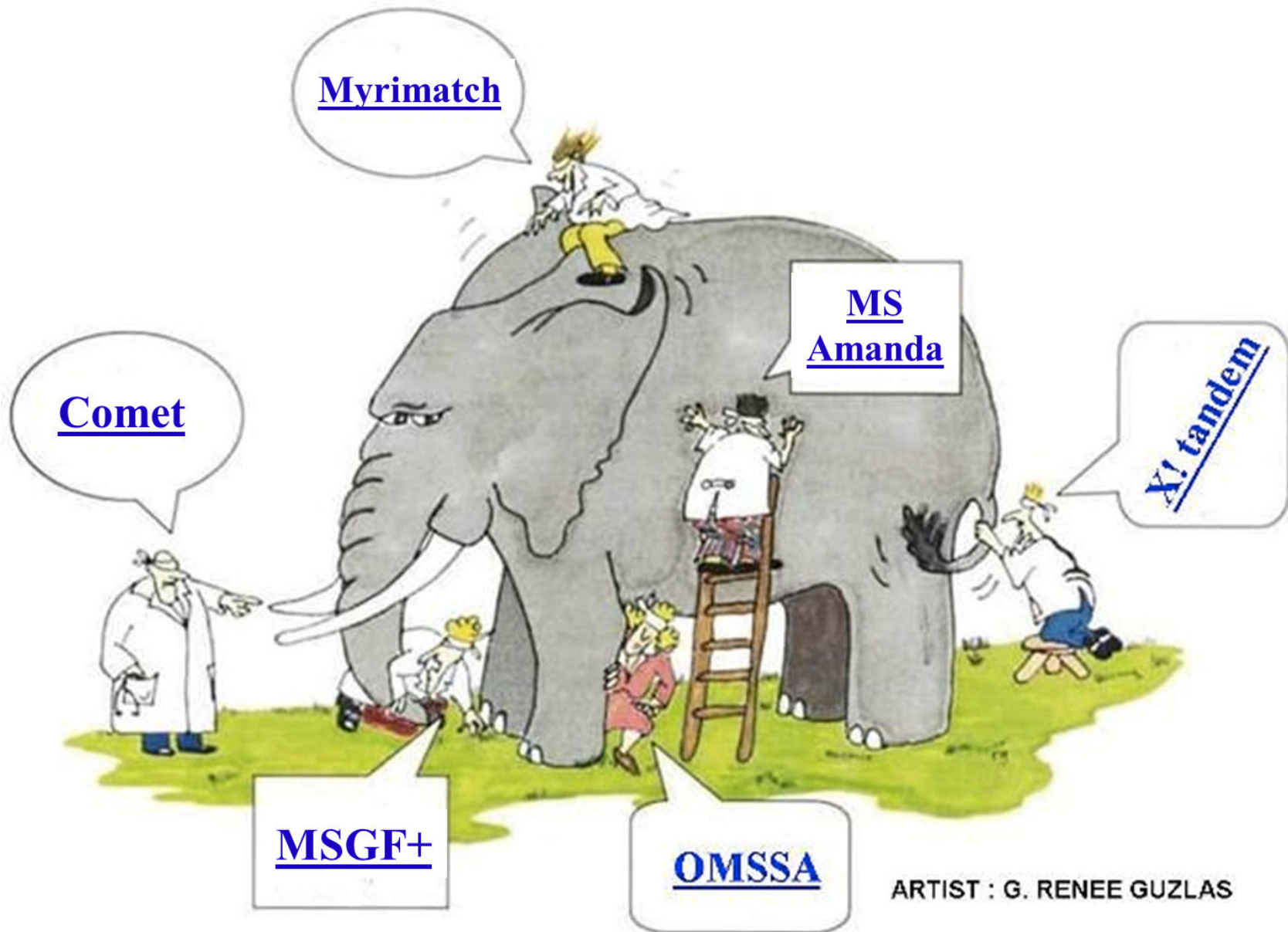


Protein identification

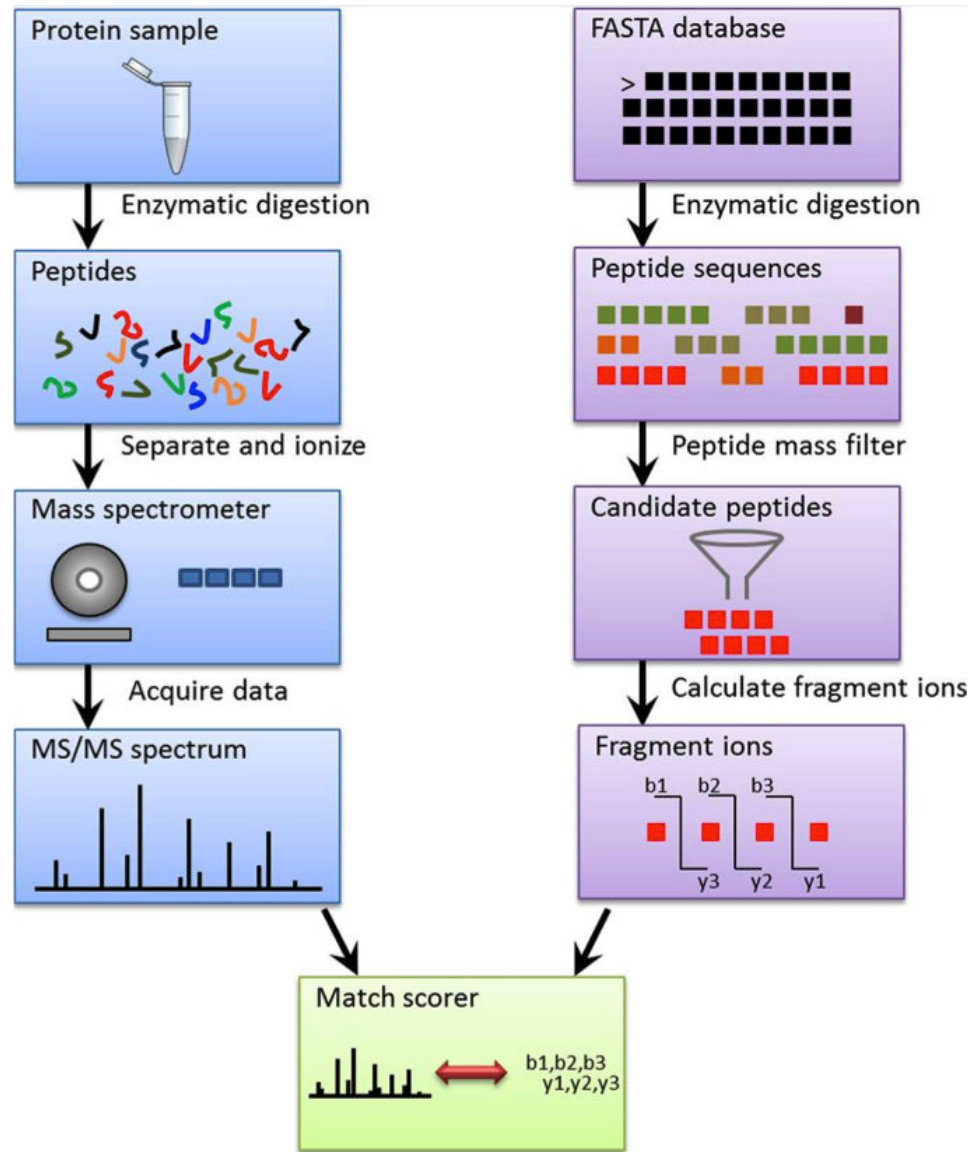


GalaxyP

Different choices for sequence database searching

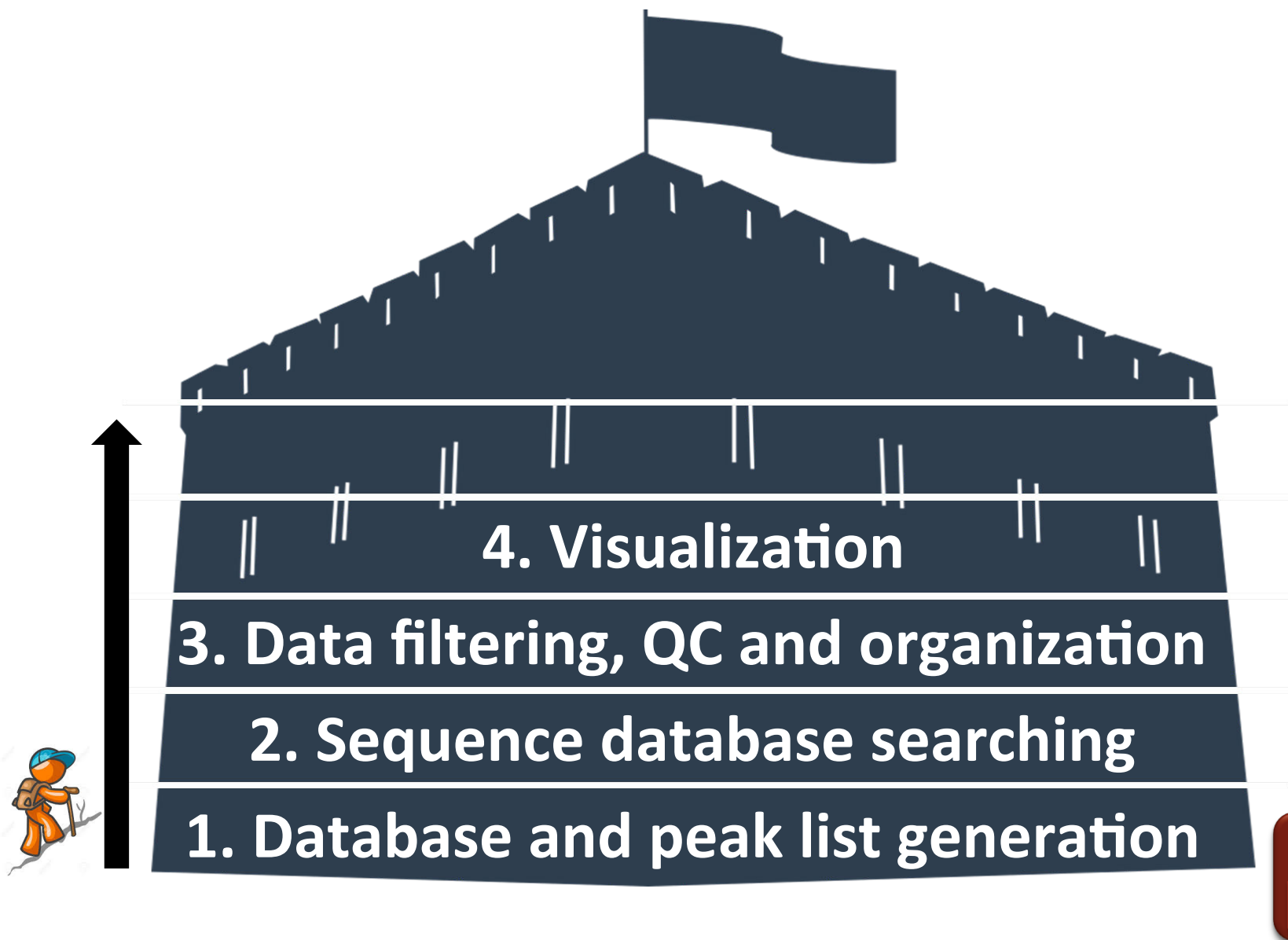


Experimental workflow in MS-based proteomics

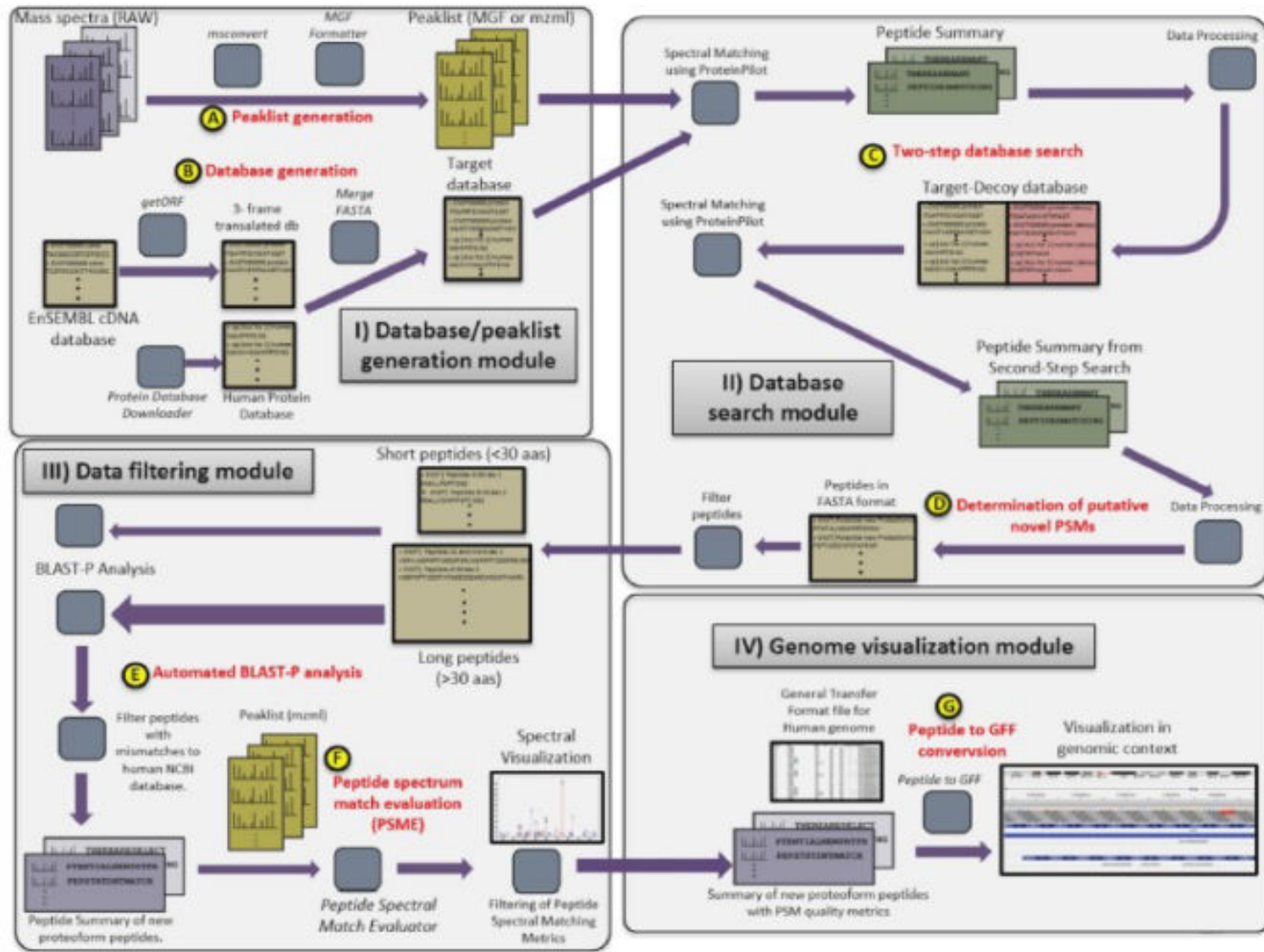


Eng et al 2011
Mol Cell Proteomics. 10(11): R111.009522.

Data analysis modules for protein identification



Why use Galaxy for proteomics data analysis?



J Proteome Res. 2014 13:5898-908

Proteomics tools accessible via the Tool Shed

<https://toolshed.g2.bx.psu.edu/>

Galaxy Tool Shed

RepositoriesHelpUser

3374 valid tools on Jul 04, 2015

Search

- [Search for valid tools](#)
- [Search for workflows](#)

Valid Galaxy Utilities

- [Tools](#)
- [Custom datatypes](#)
- [Repository dependency definitions](#)
- [Tool dependency definitions](#)

All Repositories

- [Browse by category](#)

Available Actions

- [Login to create a repository](#)

Repositories in Category Proteomics

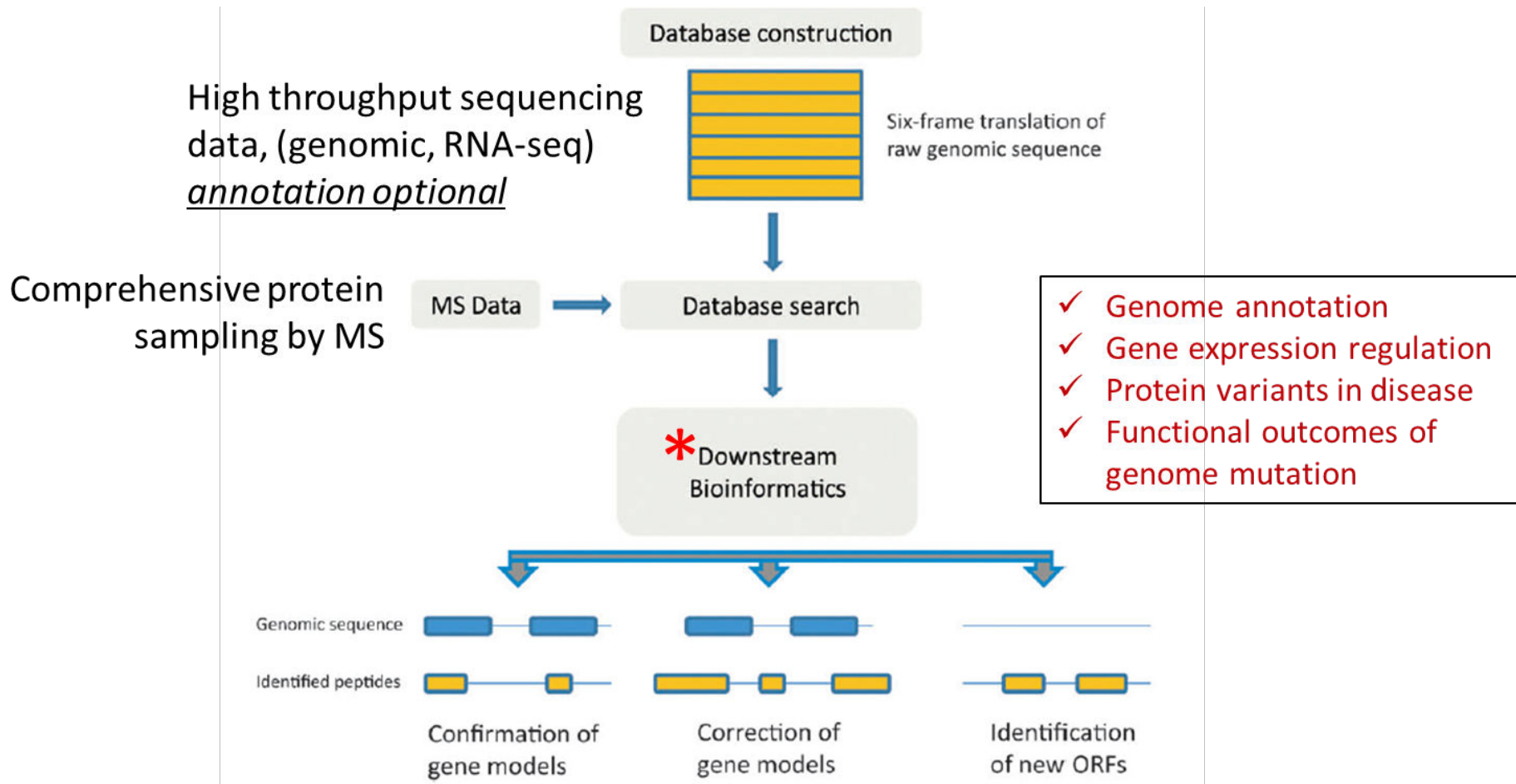
search repository name, description

Name	Synopsis	Type	Metadata Revisions	Tools or Package Verified	Owner
appendfdr	Add false discovery rate to tabular data.	Unrestricted	0 (2013-05-10)	no	galaxy
blast_plus_remote_blastp	NCBI BLAST+ remote blastp	Unrestricted	4 (2015-05-04)	no	galaxy
blastxml_to_tabular_selectable	Converts blast xml file to a tabular with options for unmatched queries, and number of hits to convert	Unrestricted	1 (2014-10-08)	no	galaxy
databases	This tool allows users to download protein databases from common sources.	Unrestricted	4 (2014-09-26)	no	galaxy
decoyfasta	Galaxy tool wrapper for the transproteomic pipeline decoyFASTA tool.	Unrestricted	6 (2014-10-08)	n/a	galaxy
directag_and_tagrecon	Bumbershoot DirectTag and TagRecon	Unrestricted	0 (2014-09-26)	no	galaxy
fasta_merge_files_and_filter_unique_sequences	Merge FASTA files, keeping only unique sequences	Unrestricted	0 (2014-09-26)	no	galaxy
feature_alignment	Feature Alignment of peakgroups below a FDR	Unrestricted		n/a	galaxy
filter_by_fasta_ids	Extract sequences from a FASTA file based on a list of IDs	Unrestricted	0 (2014-09-26)	no	galaxy
gcms_lcms_analysis	GCMS and LCMS workflows	Unrestricted	0 (2015-05-15)	n/a	proteomic
idqconvert	Bumbershoot idqConvert, a part of Bumbershoot IDPicker.	Unrestricted	2 (2014-09-30)	no	galaxy
lq_quant_cli	iQuant is a tool that performs tag based isobaric quantification	Unrestricted	0 (2014-09-26)	no	galaxy
make_protein_decoys	Generate a decoy database from an input set of protein sequences	Unrestricted	1 (2015-03-26)	no	iracooke
mascot	Mascot MS/MS Search	Unrestricted	9 (2015-03-29)	no	iracooke
mgf_formatter	This repository contains a tool wrapper for the TINT MGF formatter.	Unrestricted	1 (2014-09-26)	no	galaxy
msconvert	Tool wrappers for the msconvert application distributed as part of Proteowizard.	Unrestricted	8 (2014-09-26)	no	galaxy
ms_data_converter	AB SCIEX MS Data Converter	Unrestricted	1 (2015-03-11)	no	galaxy
msgfplus	MSGF+ Galaxy Wrapper	Unrestricted	15 (2015-03-26)	no	iracooke
ms_wiff_loader	Loads AB Sciex wiff files from URLs	Unrestricted	0 (2015-03-10)	no	galaxy
myrimatch	Bumbershoot MyriMatch	Unrestricted	0 (2014-09-26)	no	galaxy

<https://github.com/galaxyproteomics/tools-galaxy>

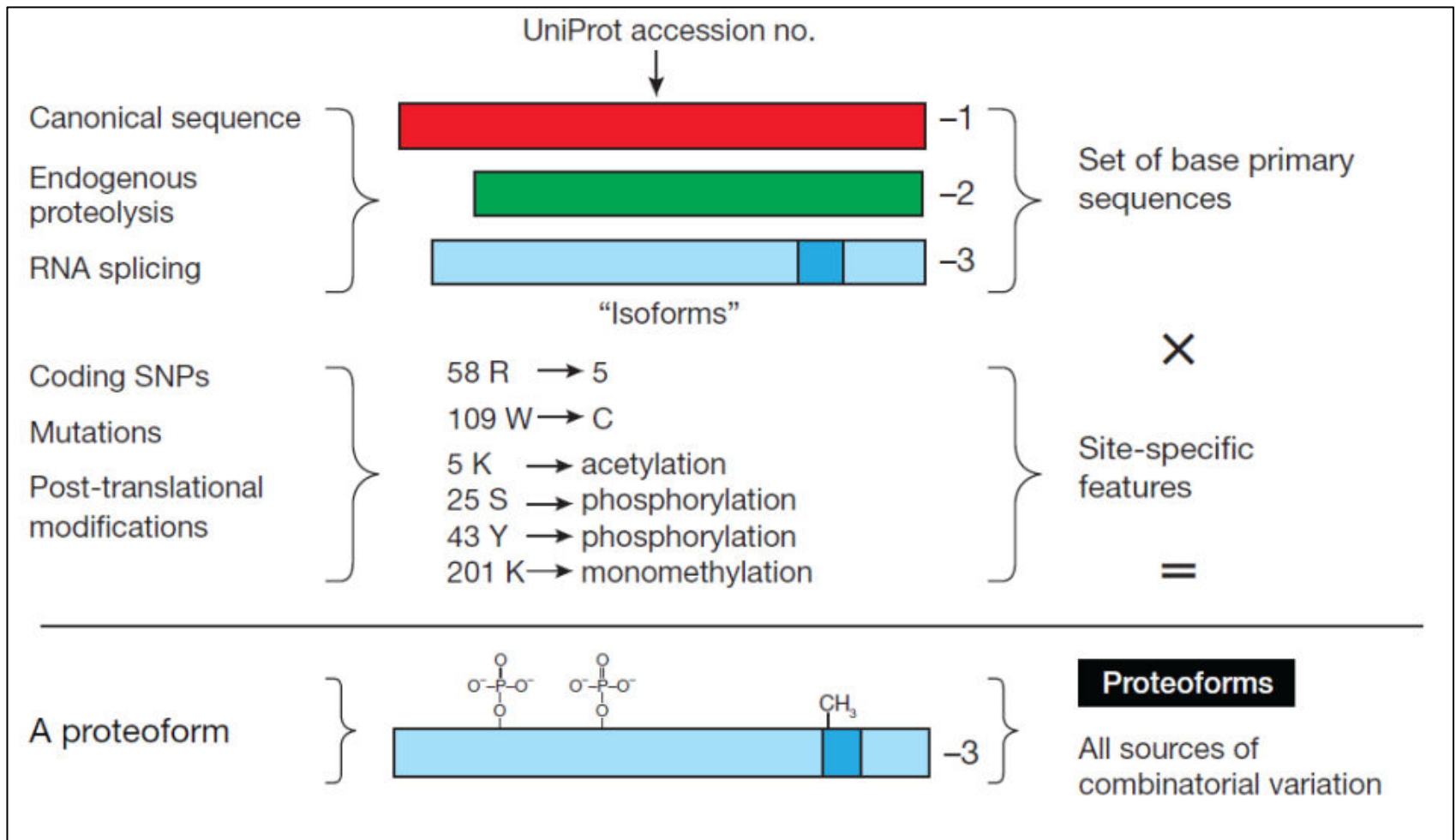


Basics of proteogenomics



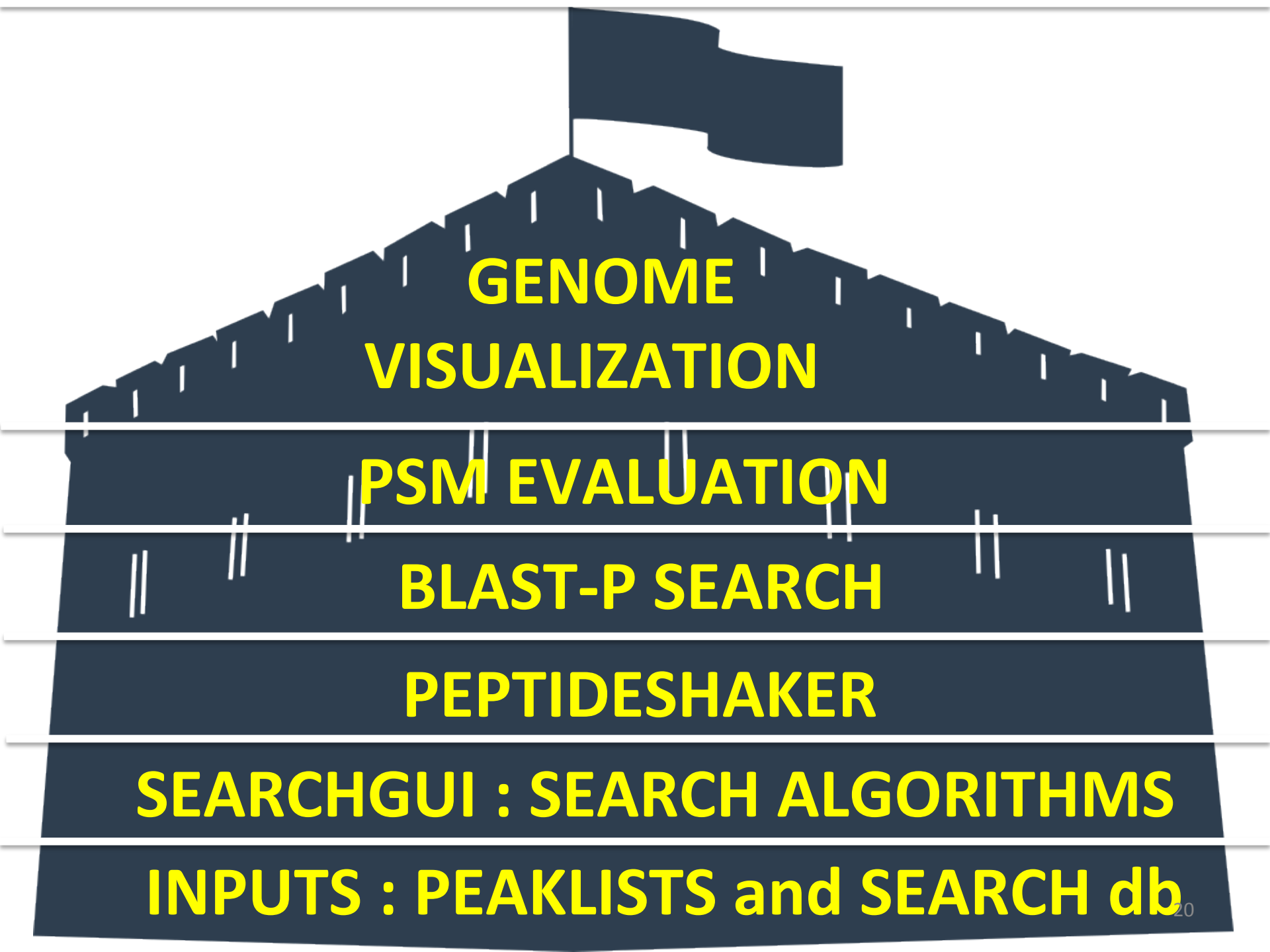
Mol. BioSyst., 2011, 7, 284–291

Peptide sequence variants and “proteoforms”



What will this workshop cover?

- Basics of MS-based proteomic data analysis, with a showcasing of proteogenomic workflows in Galaxy.
- The first workflow module for merging search databases will be actually ‘run’ while others we will ‘pretend run’ – to avoid slow down on the cloud.
- The different modules can be run as a complete workflow – for the sake of a tutorial we will run modules separately.
- We have included documentation for each portion of this workshop for reference.



**GENOME
VISUALIZATION**

PSM EVALUATION

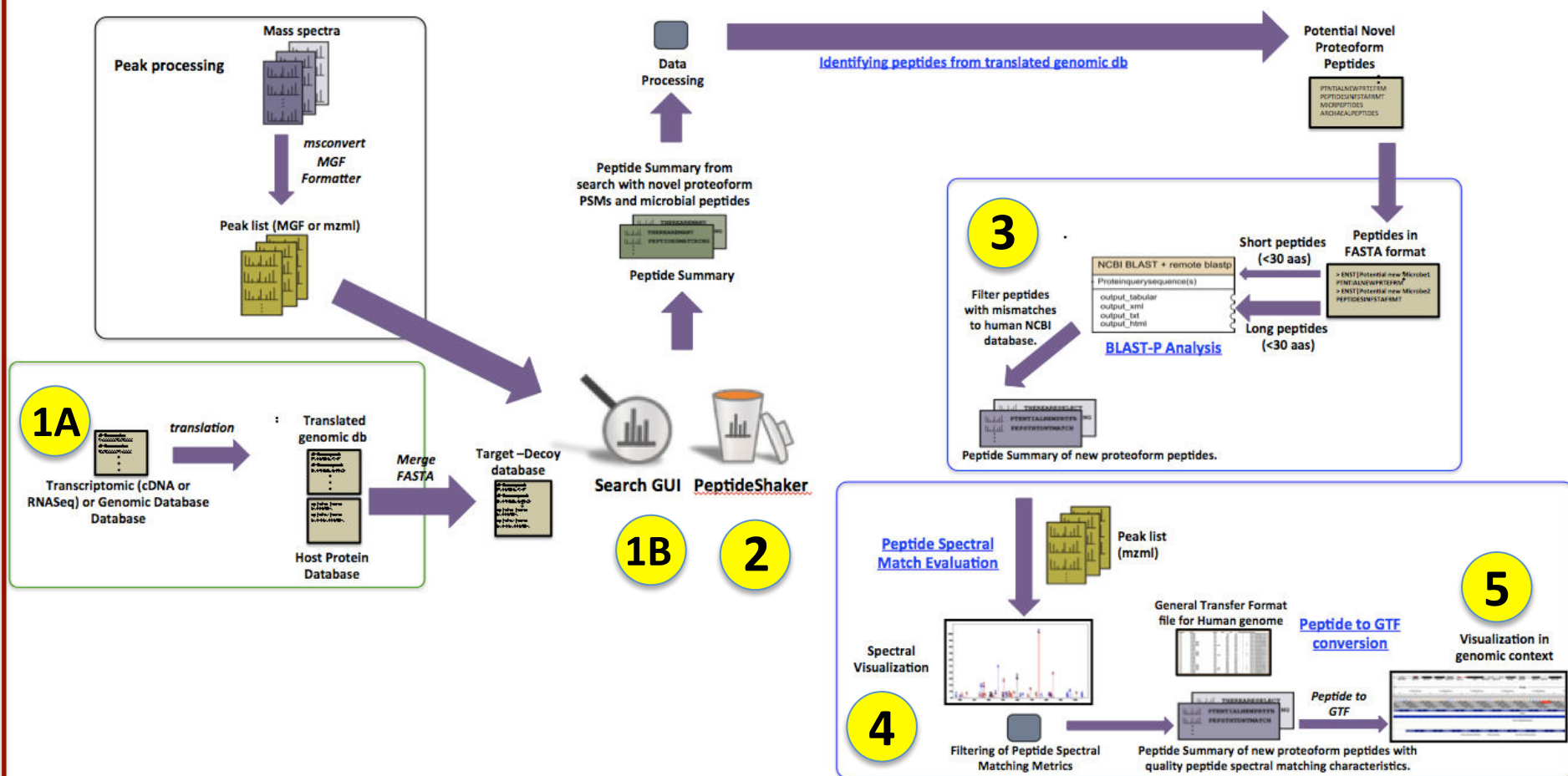
BLAST-P SEARCH

PEPTIDESHAKER

SEARCHGUI : SEARCH ALGORITHMS

INPUTS : PEAKLISTS and SEARCH db

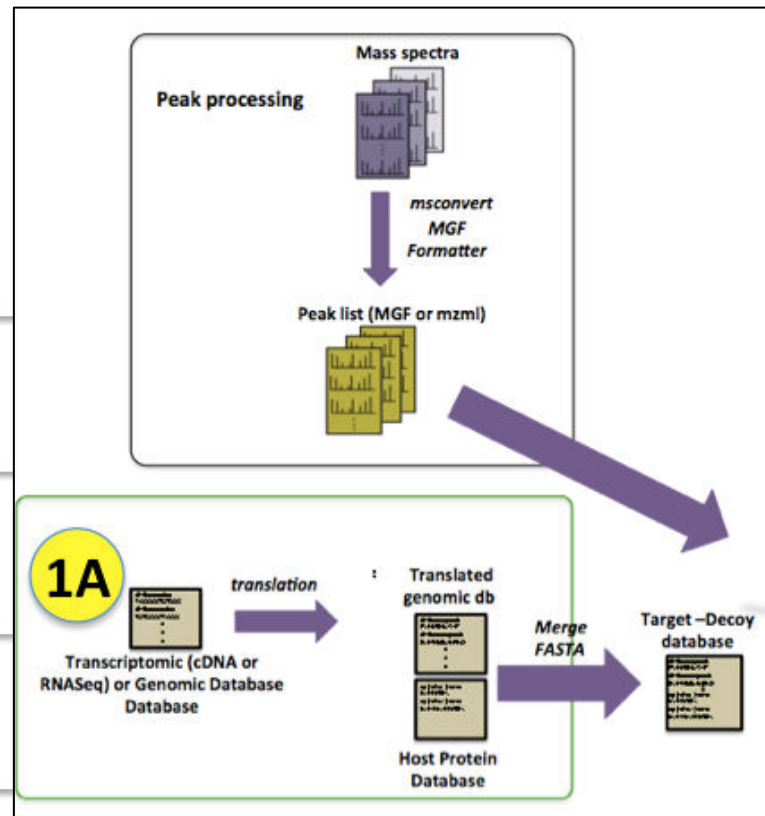
PROTEOGENOMICS WORKFLOW



July 8th 2015: Session 7 : 2:05 PM: Extending Galaxy's reach: recent progress towards complete multi-omic data analysis workflows.

Timothy J Griffin

GalaxyP



INPUTS : PEAKLISTS and SEARCH db

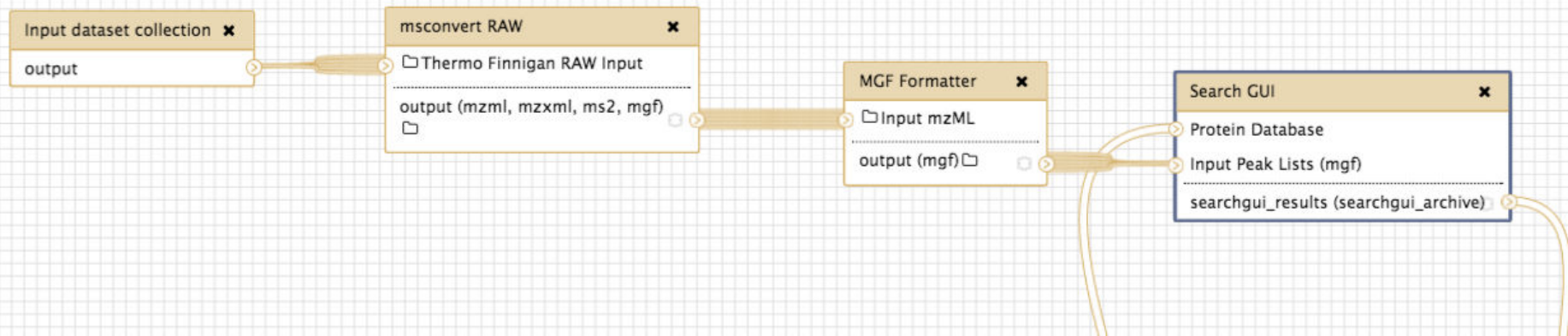
INPUTS : PEAKLISTS and SEARCH db

GALAXY TOOLS AND WORKFLOWS

INPUT

WORKFLOW

OUTPUT



*Software tools can be used in a sequential manner to generate **analytical workflows** that can be reused, shared and creatively modified for multiple studies.*

Getting Started GCC2015 GalaxyP Tutorial

Open a web browser and navigate to the GalaxyP cloud instance –

<http://54.205.17.20/>

At the top of the screen select User and Register and Log in for your Cloud username (your email) and password.

2.2 Getting Started GCC2015 GalaxyP Tutorial

A. Open a web browser and navigate to the GalaxyP cloud instance - <http://54.205.17.20/>

B. At the top of the screen select User and Register and **Log in** for your Cloud username (your email) and password.

C. At the top of the screen select **Shared Data** then migrate to **Published Histories** .

D. Select **History 1** from the list of published histories.

E. Select Import history to add the selected history to your user histories.

F. On the confirmation screen select **start using this history** to navigate to this history in the Galaxy view.

G. At the top of the screen select Shared Data then migrate to **Published Workflows** .

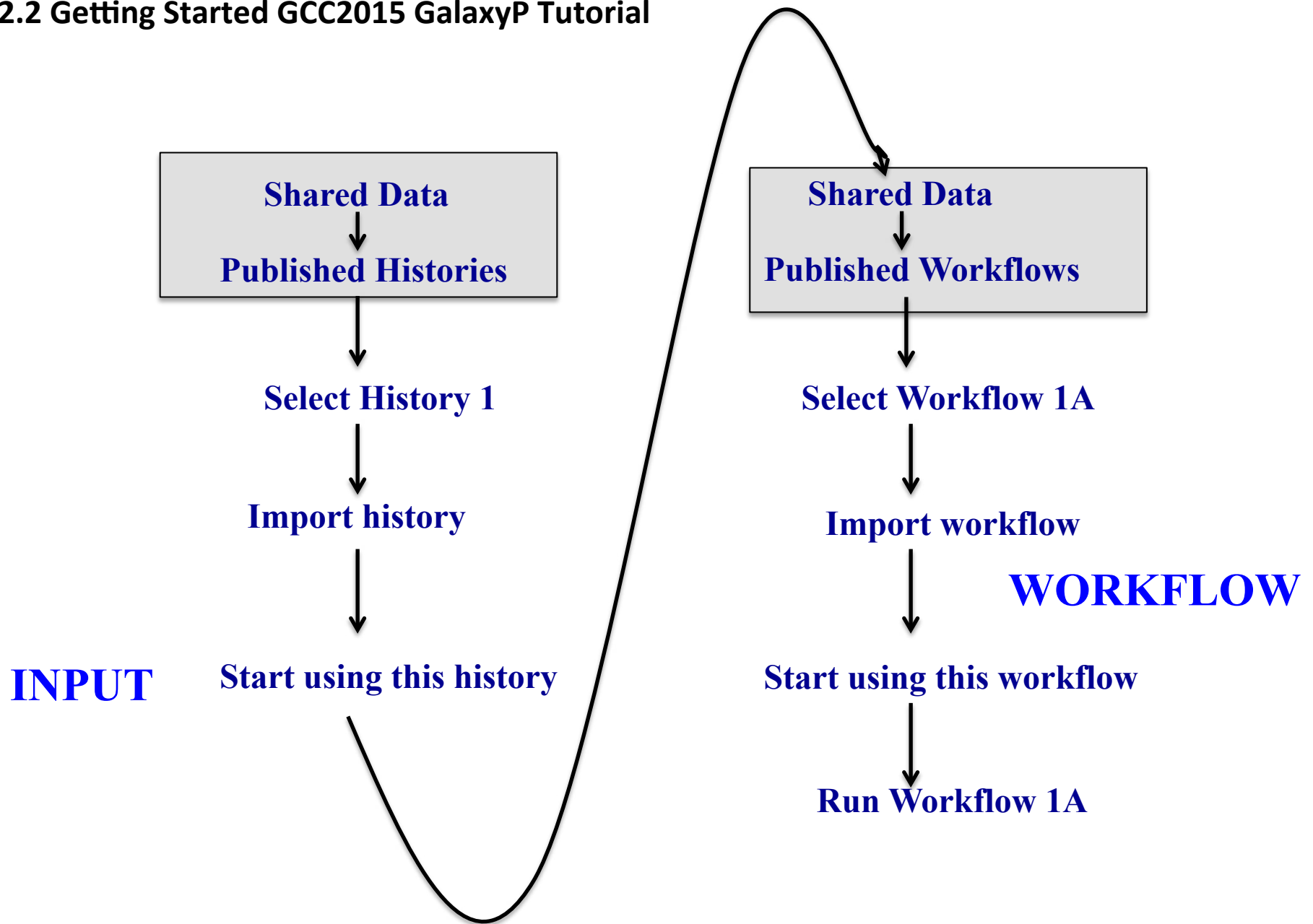
H. Select **Workflow 1A: Workflow for History 1** from the list of published workflows and choose import to copy the workflow into your user workflows.

I. On the confirmation screen, select **start using this workflow** to navigate to your user workflows.

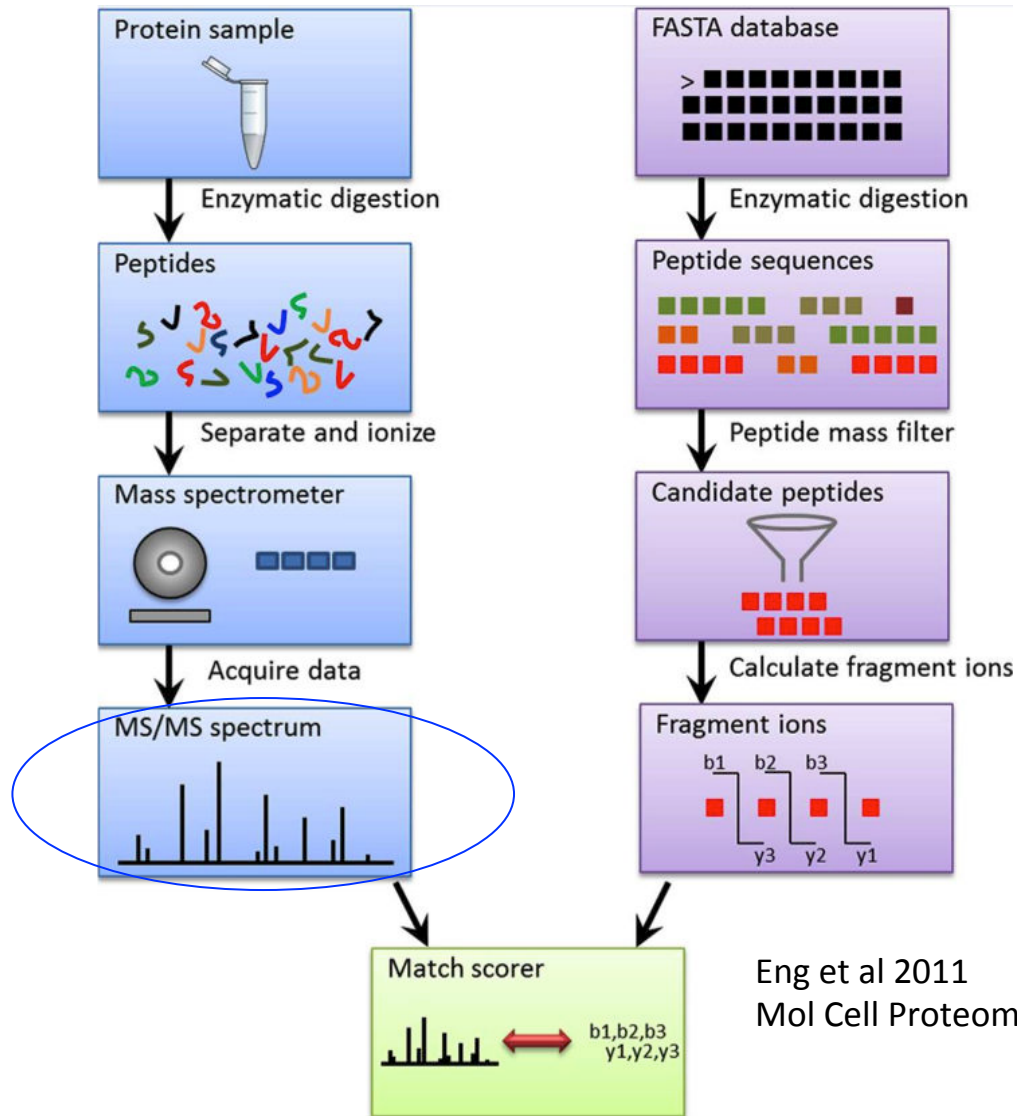
J. In the workflows menu select **Run Workflow 1A: Workflow for History 1** from the drop down menu.

K. Appropriately assign each input database from History 1 to the corresponding input or the workflow.

2.2 Getting Started GCC2015 GalaxyP Tutorial



PROTEOMICS WORKFLOW



Eng et al 2011
Mol Cell Proteomics. 10(11): R111.009522.

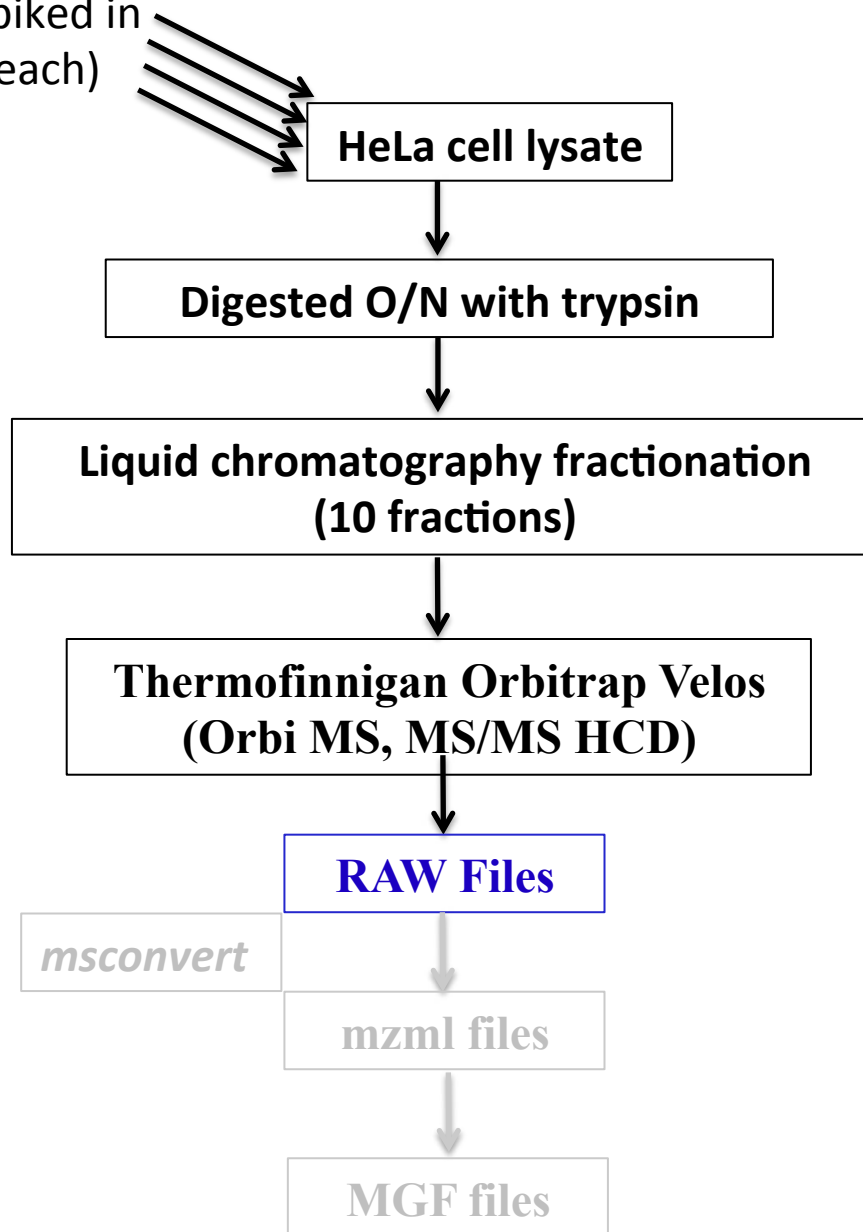
INPUTS : PEAKLISTS and SEARCH db

GalaxyP



INPUTS : MASS SPECTRAL DATA AND SEARCH DATABASE.

4 proteins spiked in
(10 fmols each)



The dataset will be searched against FASTA database with human proteins, contaminant proteins, spiked in proteins and a subset of 3-frame translated cDNA database from EnSEMBL.

INPUTS: a) *MGF formatter MGF files. (dataset collection)*

b) ABRF-Spike4: FASTA sequences of 4 spiked in proteins.

c) FASTA File from EnSEMBL

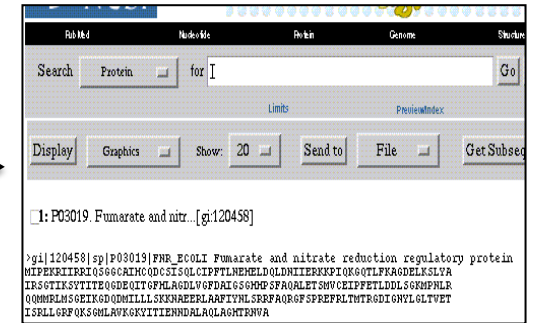
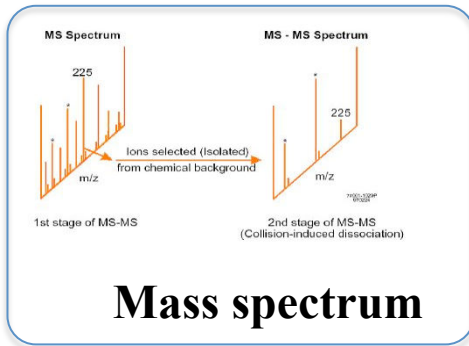
Searches: Subset of 3-frame translated cDNA database from EnSEMBL (our template for identifying novel proteoforms).

d) Human UniProt FASTA file + contaminant proteins.

INPUTS : PEAKLISTS and SEARCH db

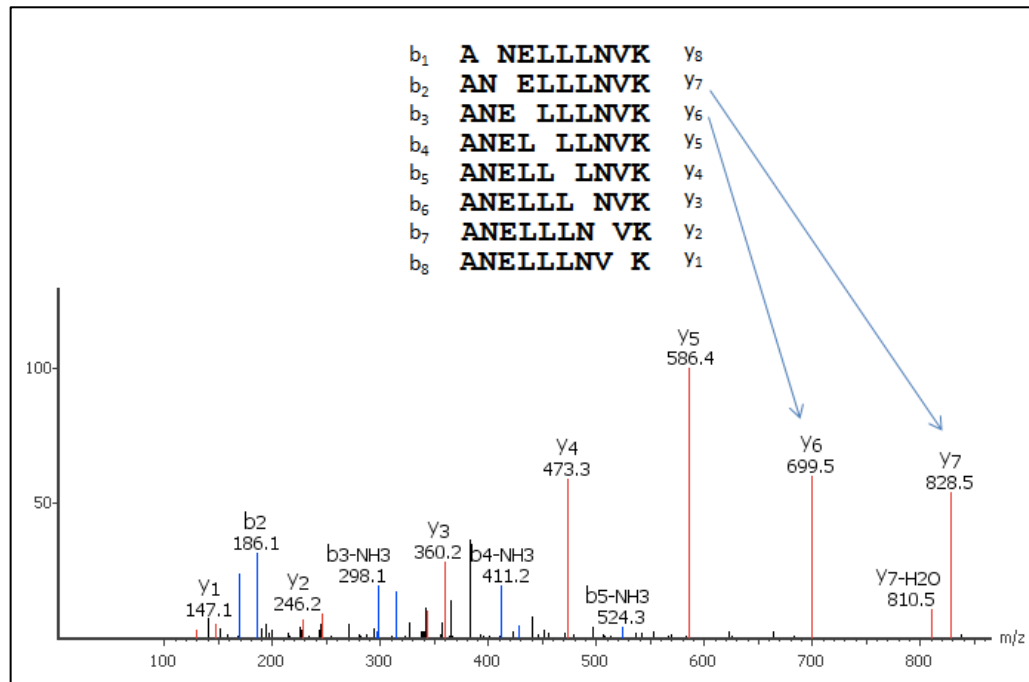
GalaxyP

SEARCH DATABASES



**Reference Protein Database
from genomic annotation**

Peptide Spectral Match



INPUTS : PEAKLISTS and SEARCH db

PROTEOMIC DATABASES

Swiss-Prot is the manually annotated and reviewed section of the UniProt Knowledgebase (UniProtKB).

It is a high quality annotated and non-redundant protein sequence database, which brings together experimental results, computed features and scientific conclusions.

<http://en.wikipedia.org/wiki/Swiss-Prot>

TrEMBL contains high-quality computationally analyzed records, which are enriched with automatic annotation.

The translations of annotated coding sequences in the EMBL-Bank/GenBank/DBJ nucleotide sequence database are automatically processed and entered in TrEMBL.

<http://en.wikipedia.org/wiki/TrEMBL>

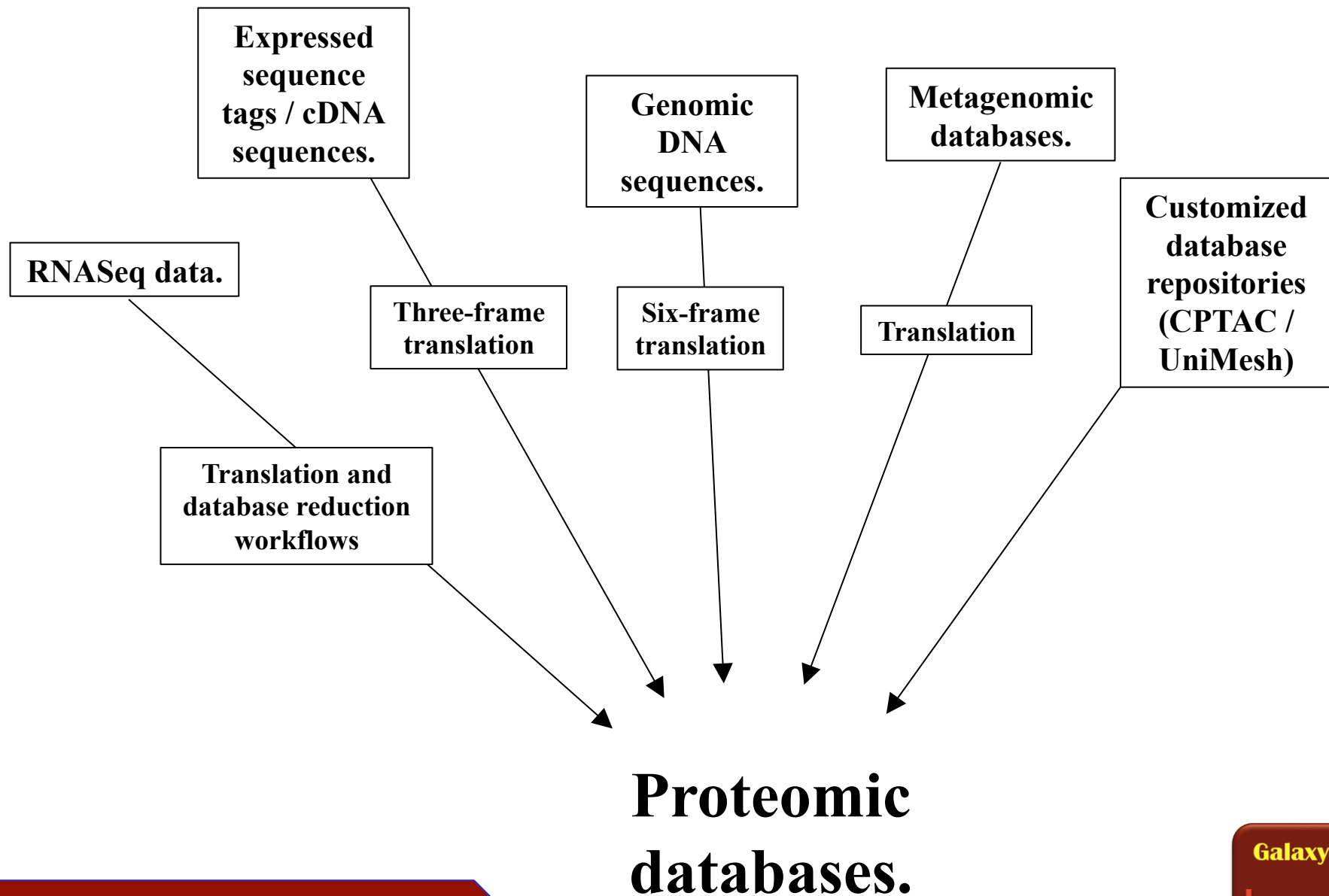


INPUTS : PEAKLISTS and SEARCH db

GalaxyP

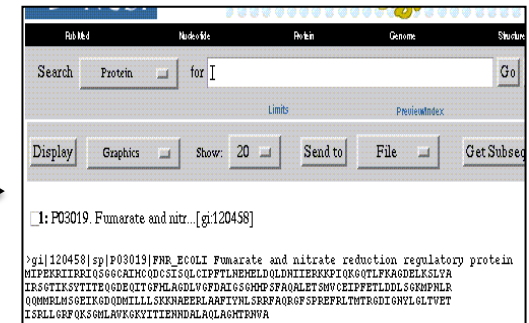
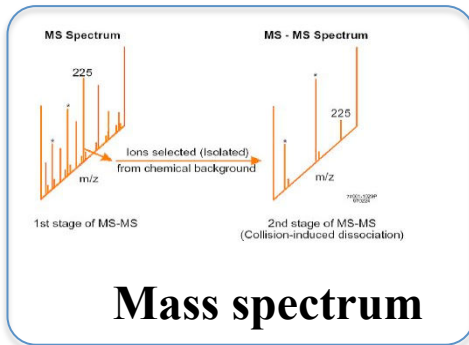


CUSTOMIZED PROTEOMIC DATABASES



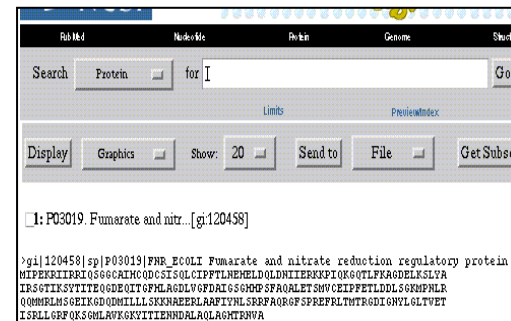
INPUTS : PEAKLISTS and SEARCH db

LOOKING BEYOND THE KNOWN PROTEOME



**Reference Protein Database
from genomic annotation**

**Identification of
peptides
corresponding
to novel proteoforms.**



**6-frame DNA
sequences.
3-frame cDNA
sequences.**

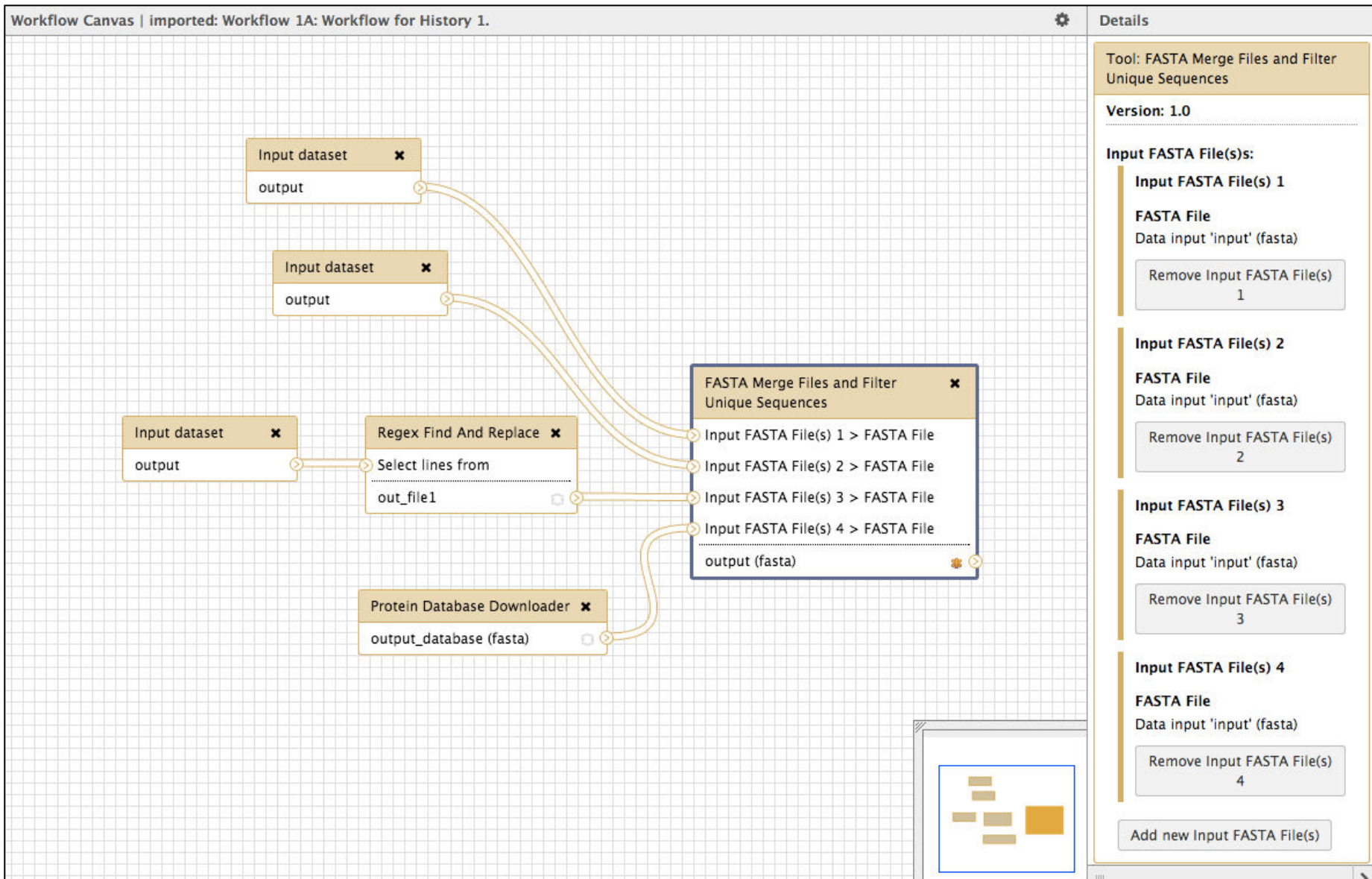
**Cancer / Disease related
Databases such as COSMIC,
IARC p53, OMIM...**

**Deep genome sequencing data
from ICGC, TCGA and CPTAC**

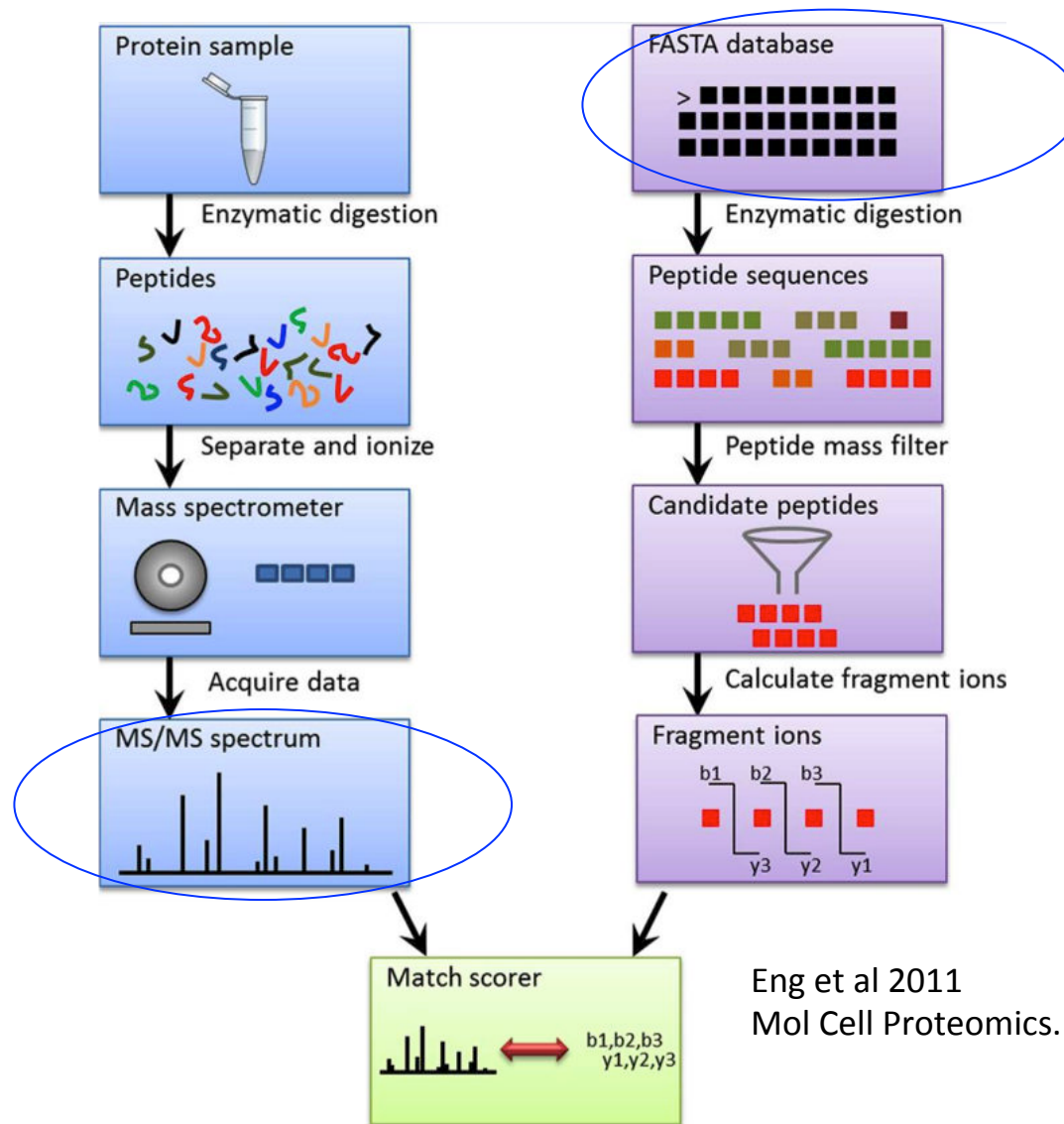
**RNASeq data
(Customized OR
Combined)**

INPUTS : PEAKLISTS and SEARCH db

WORKFLOW 1A



PROTEOMICS WORKFLOW



Eng et al 2011

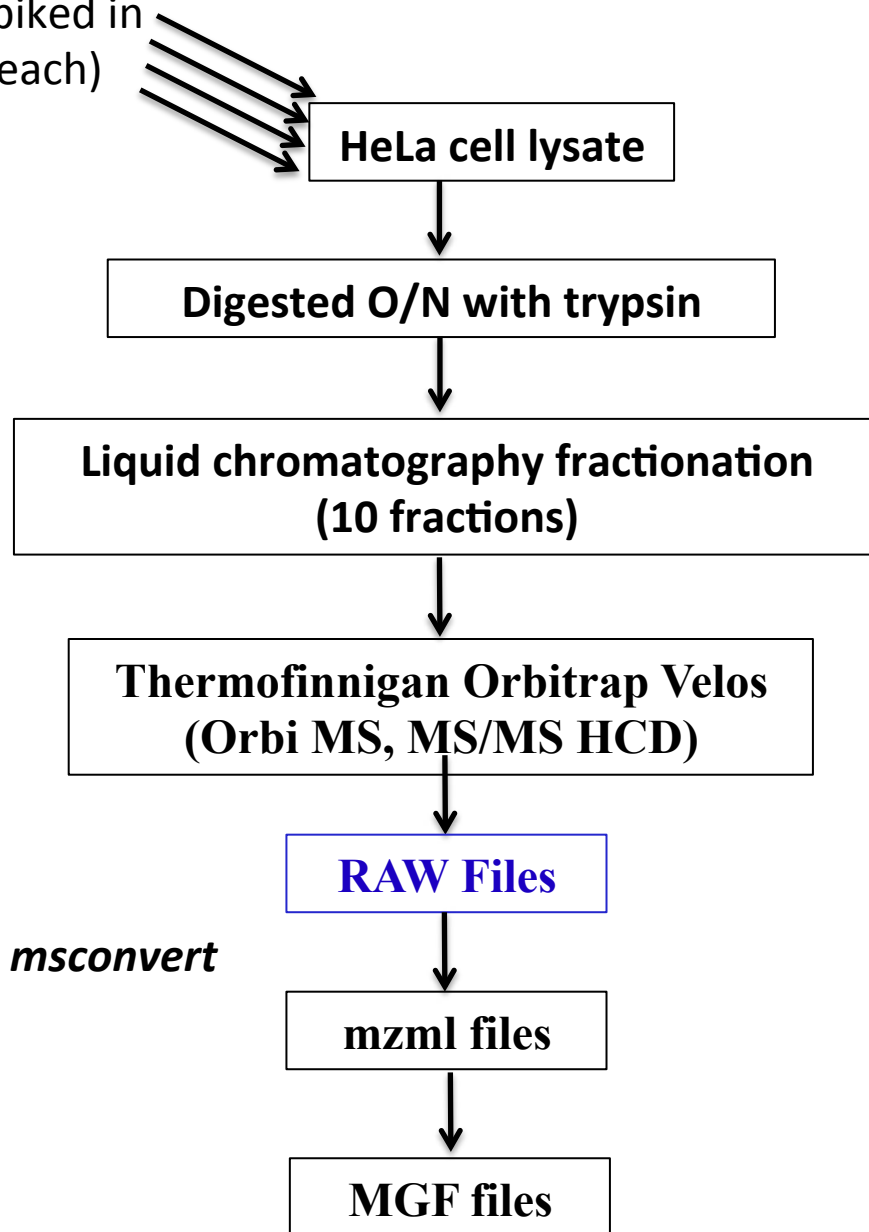
Mol Cell Proteomics. 10(11): R111.009522.

INPUTS : PEAKLISTS and SEARCH db

GalaxyP

INPUTS : MASS SPECTRAL DATA AND SEARCH DATABASE.

4 proteins spiked in
(10 fmols each)



The dataset will be searched against FASTA database with human proteins, contaminant proteins, spiked in proteins and a subset of 3-frame translated cDNA database from EnSEMBL.

INPUTS: a) MGF formatter MGF files. (dataset collection)

b) ABRF-Spike4: FASTA sequences of 4 spiked in proteins.

c) FASTA File from EnSEMBL

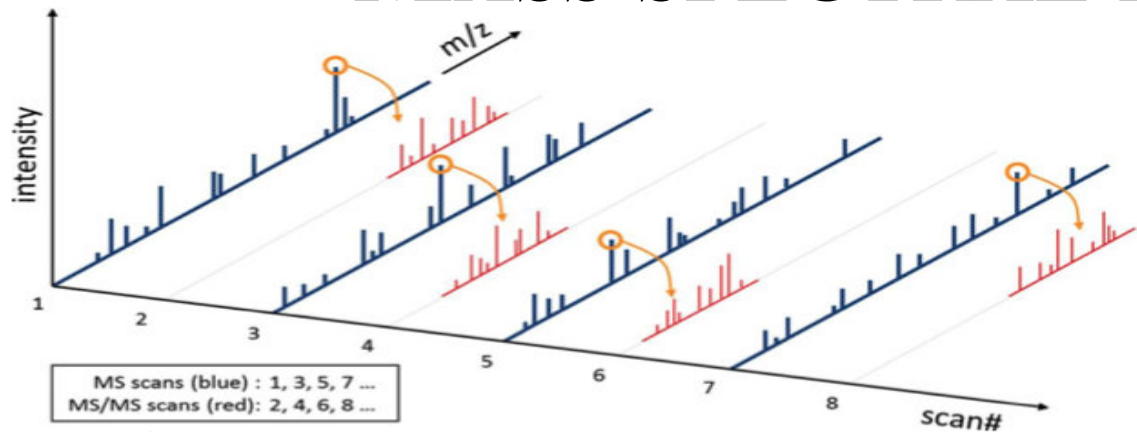
Searches: Subset of 3-frame translated cDNA database from EnSEMBL (our template for identifying novel proteoforms).

d) Human UniProt FASTA file + contaminant proteins.

INPUTS : PEAKLISTS and SEARCH db

GalaxyP

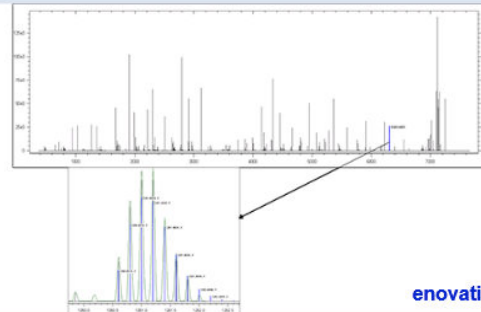
MASS SPECTRAL DATA



Eng et al 2011

Mol Cell Proteomics. 10(11): R111.009522.

RAW DATA AND PEAKLIST



Rat9_SILAC (MaxQuant generated mgf)

```

BEGIN IONS
PEPMASS=990.346560756
CHARGE=2+
TITLE=RawFile: ms1002_sam010_01108_1TMSMS_mgf1 raw ProteomicScanNumber: 26_img_
216.1748 56.6722
252.15672 5948105
281.0481 9841784
287.02904 1163825
288.06392 6392027
311.0520 1138603
344.28992 1787929
356.3282 1979669
370.2976 2853645
370.28174 2053854
374.38409 2378725
415.22412 2911907
440.2218 9653118
461.29526 1269172
484.80181 3863349
486.27486 1987223
502.1441 5236445
503.46969 1620232
563.8878 5023445
571.18756 2784028
572.47089 3694262
END IONS
    
```

- Peak detection
- Noise removal
- Baseline correction
- Monoisotoping
- Charge state

Raw Data

Peaks with wider distribution
(Area under curve)

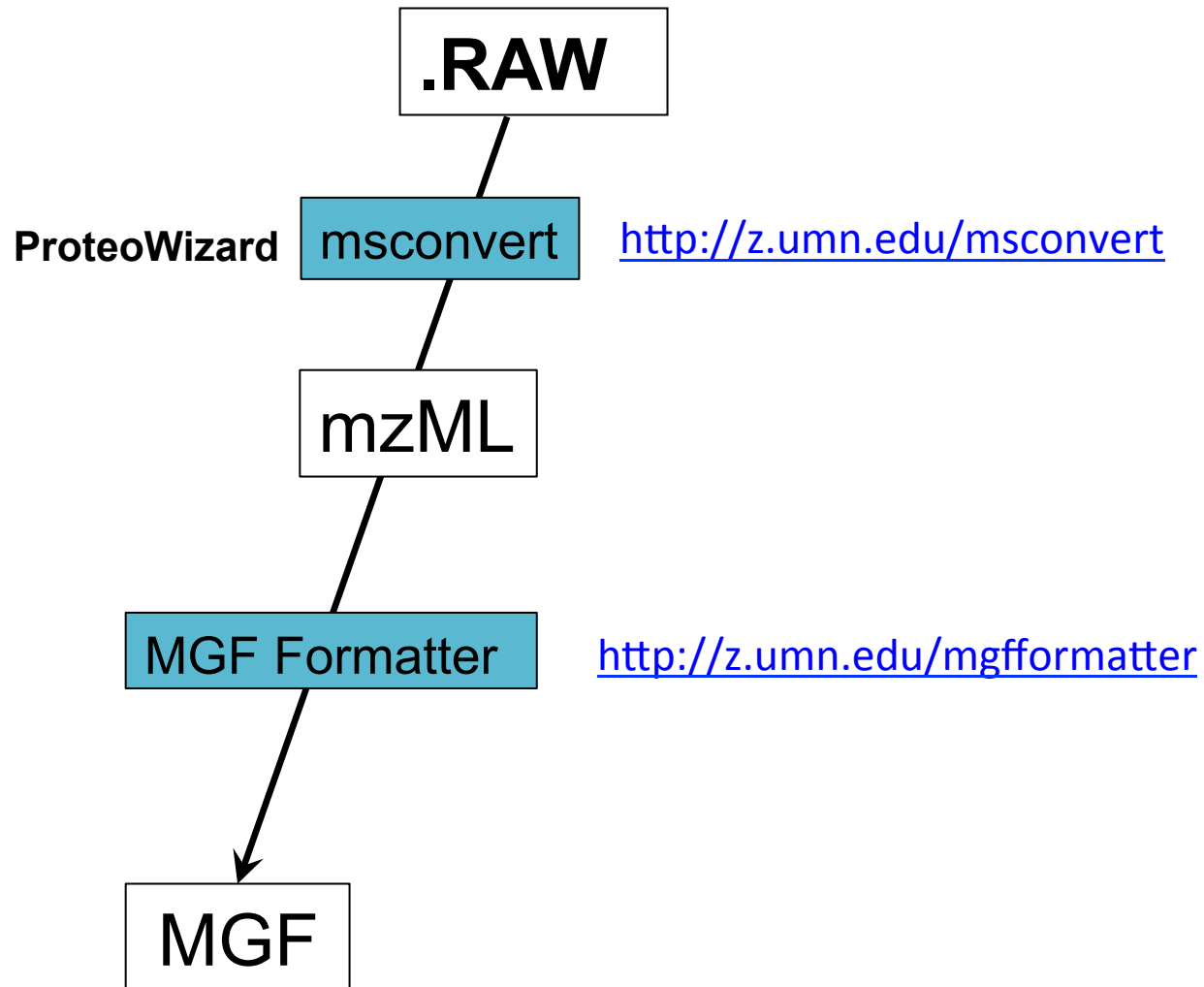
Additional information
(Noise Peaks)

PeakList (Processed)

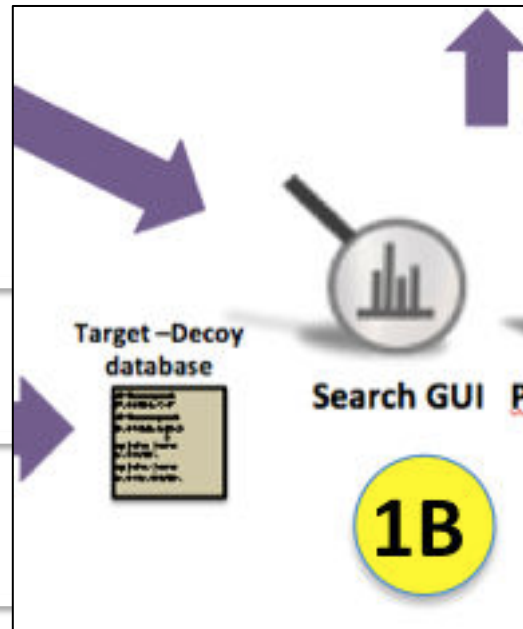
Peaks (centroid) with
intensity values.

Removal of **noise** peaks.

RAW DATA CONVERSION TOOL



INPUTS : PEAKLISTS and SEARCH db

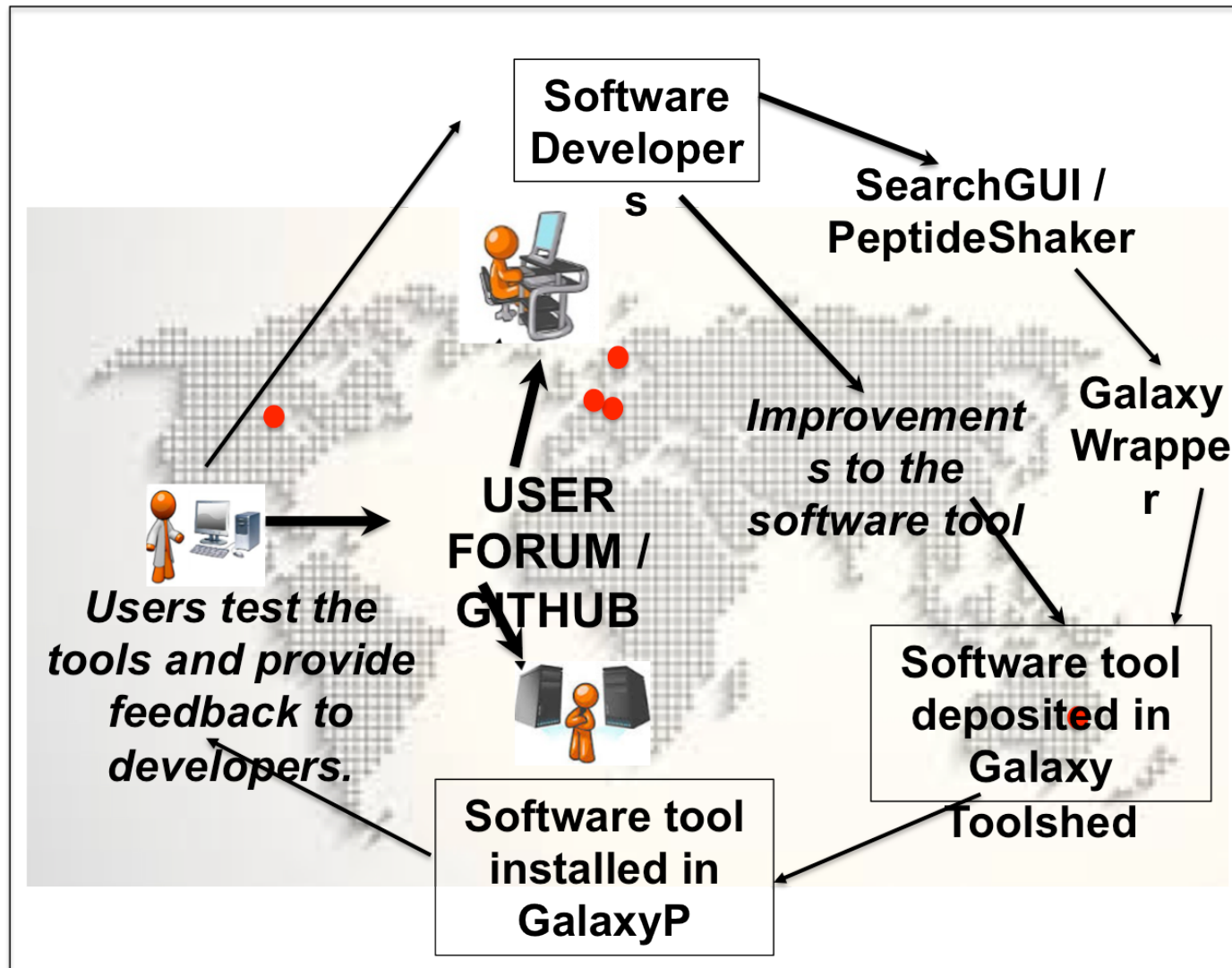


INPUTS : PEAKLISTS and SEARCH db → SEARCHGUI

SEARCHGUI : SEARCH ALGORITHMS

INPUTS : PEAKLISTS and SEARCH db

COMMUNITY-BASED SOFTWARE DEVELOPMENT

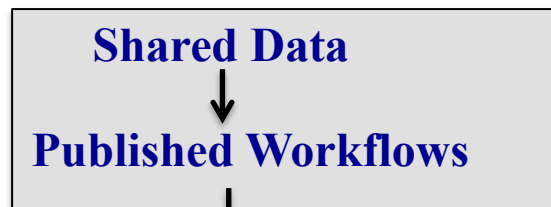


INPUTS : PEAKLISTS and SEARCH db → SEARCHGUI

3.2 SearchGUI in GalaxyP

- From Published Workflows, import Workflow 1B: Workflow for History 1 to History 2.
- On the confirmation screen, select start using this workflow to navigate to your user workflows.
- Run Workflow 1B on your current history (History 1).
- Appropriately select each dataset from History 1 that corresponds to input within the workflow.
- In Step 3: SearchGUI some parameters must be set at run time:
- Choose to run X!Tandem, MyriMatch, MS-GF+, OMSSA, and Comet
- Change the Fragment Tolerance to 0.01 Daltons
- Select the box Send results to a new history named: and enter History 2 into the field provided.
- Select Run and navigate to History 2 in the normal Galaxy view. For the purposes of this tutorial, a completed History 2 may be imported from Published Histories.

3.2 SearchGUI in GalaxyP



Select Workflow 1B

Import workflow

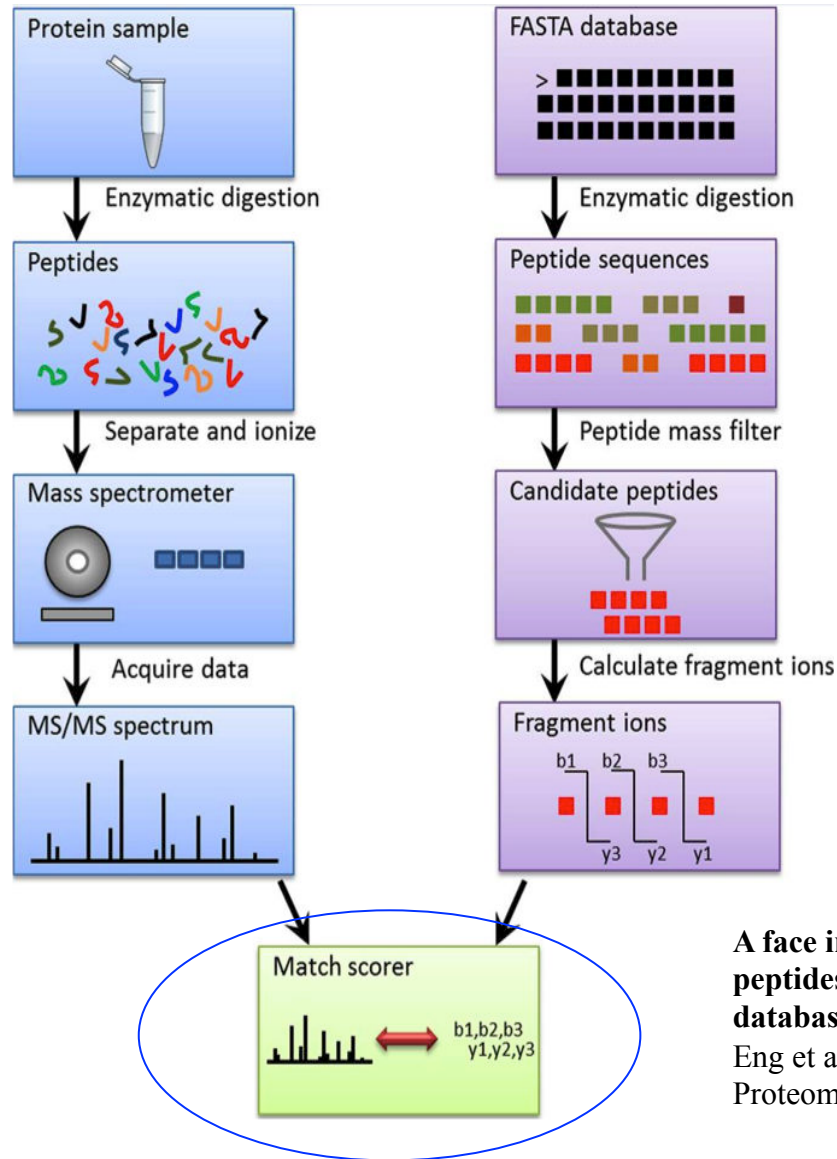
Start using this workflow

Run Workflow 1B

WORKFLOW

INPUTS : PEAKLISTS and SEARCH db **SEARCHGUI**

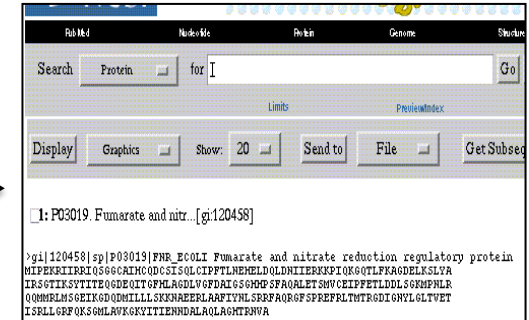
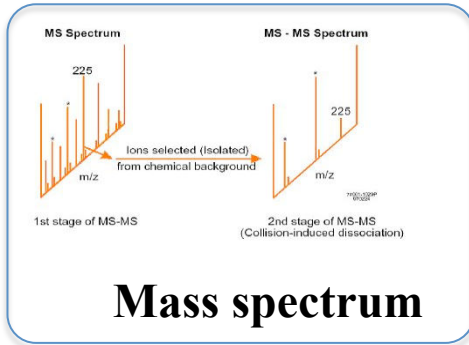
PROTEOMICS WORKFLOW



A face in the crowd: recognizing peptides through database search.

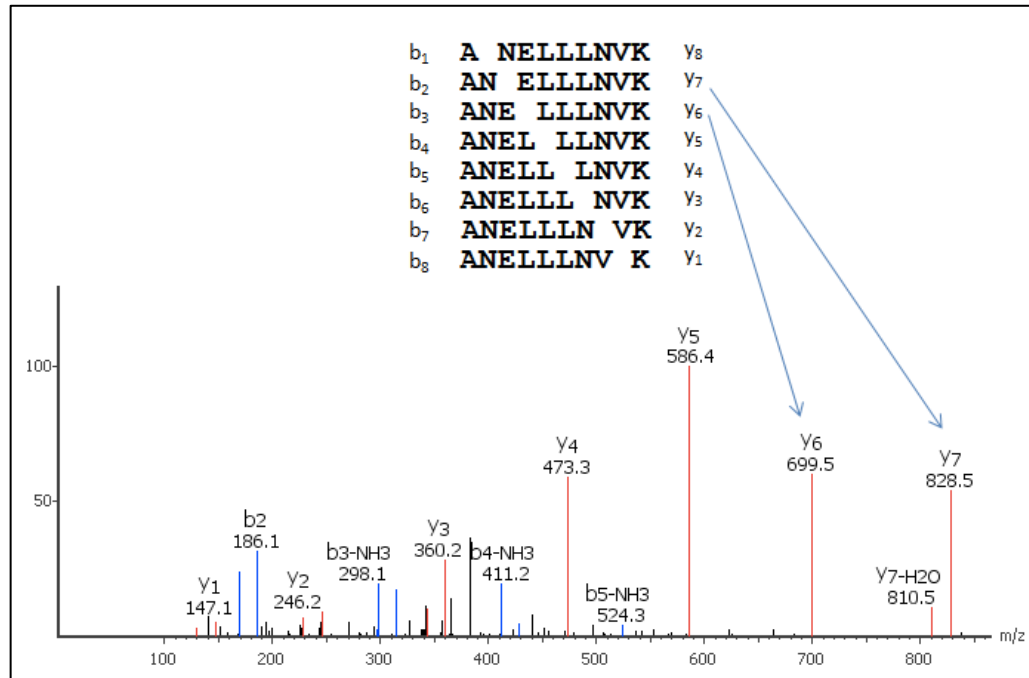
Eng et al 2011 Mol Cell Proteomics. 10(11)

DATABASE SEARCH



**Reference Protein Database
from genomic annotation**

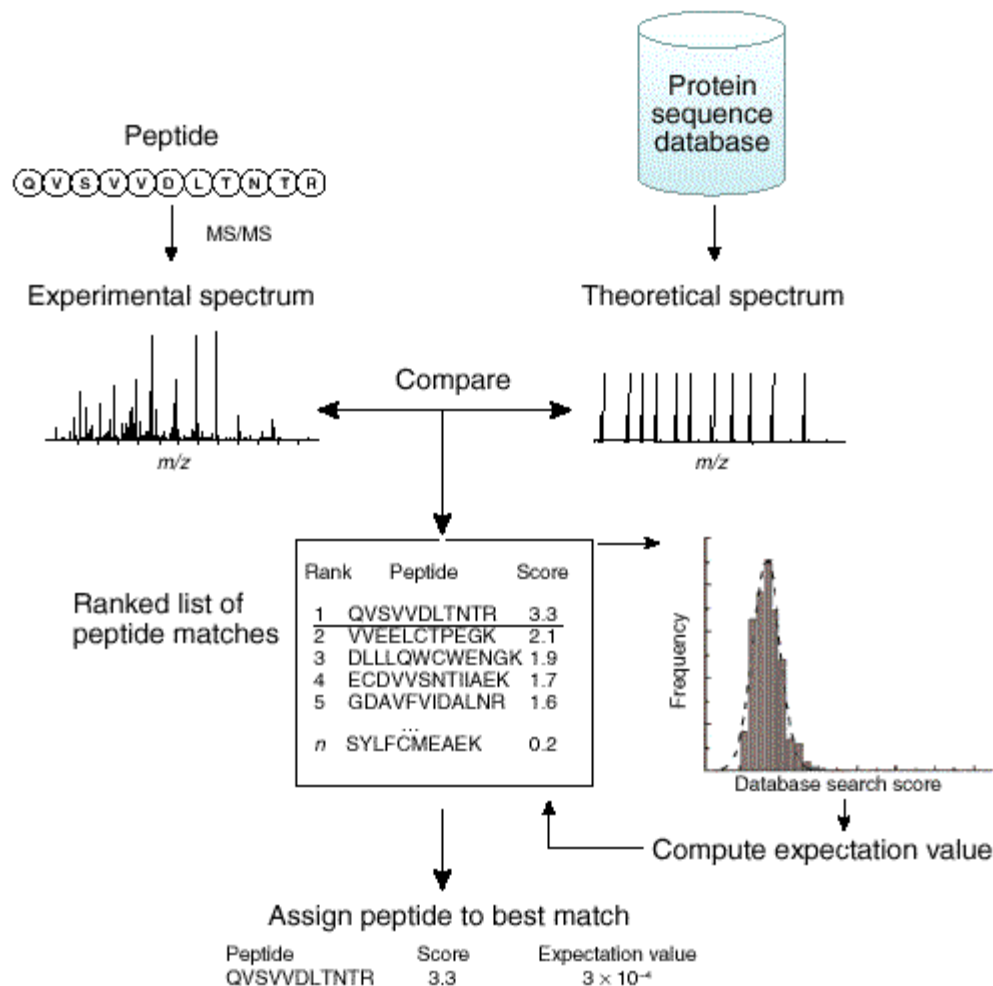
Peptide Spectral Match



INPUTS : PEAKLISTS and SEARCH db SEARCHGUI

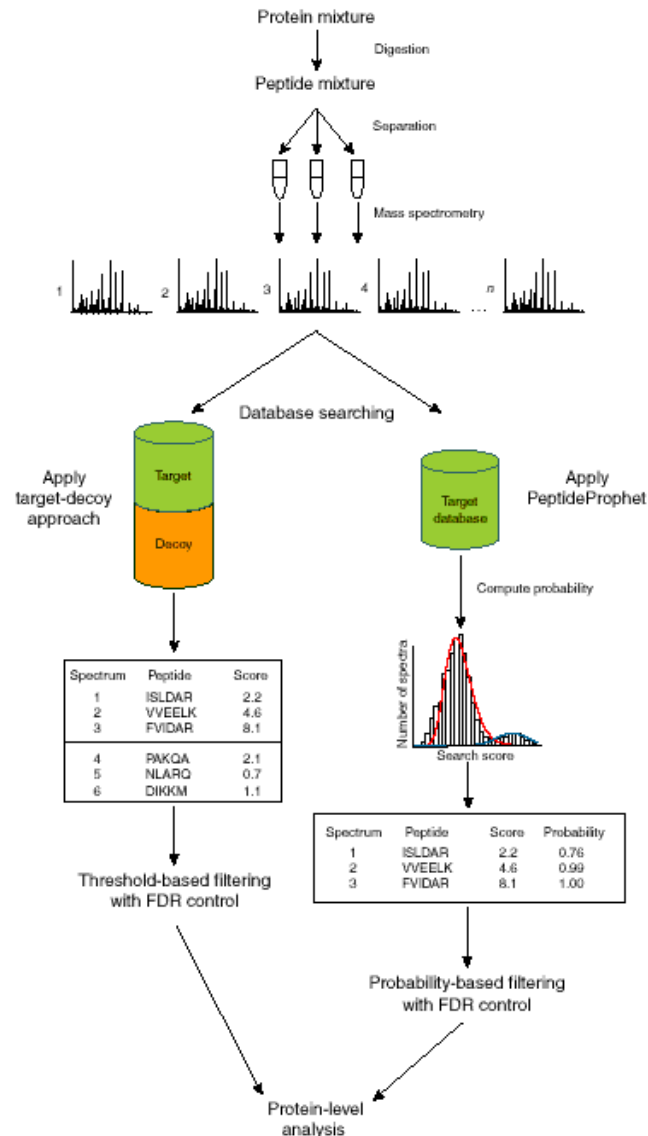
GalaxyP

DATABASE SEARCH



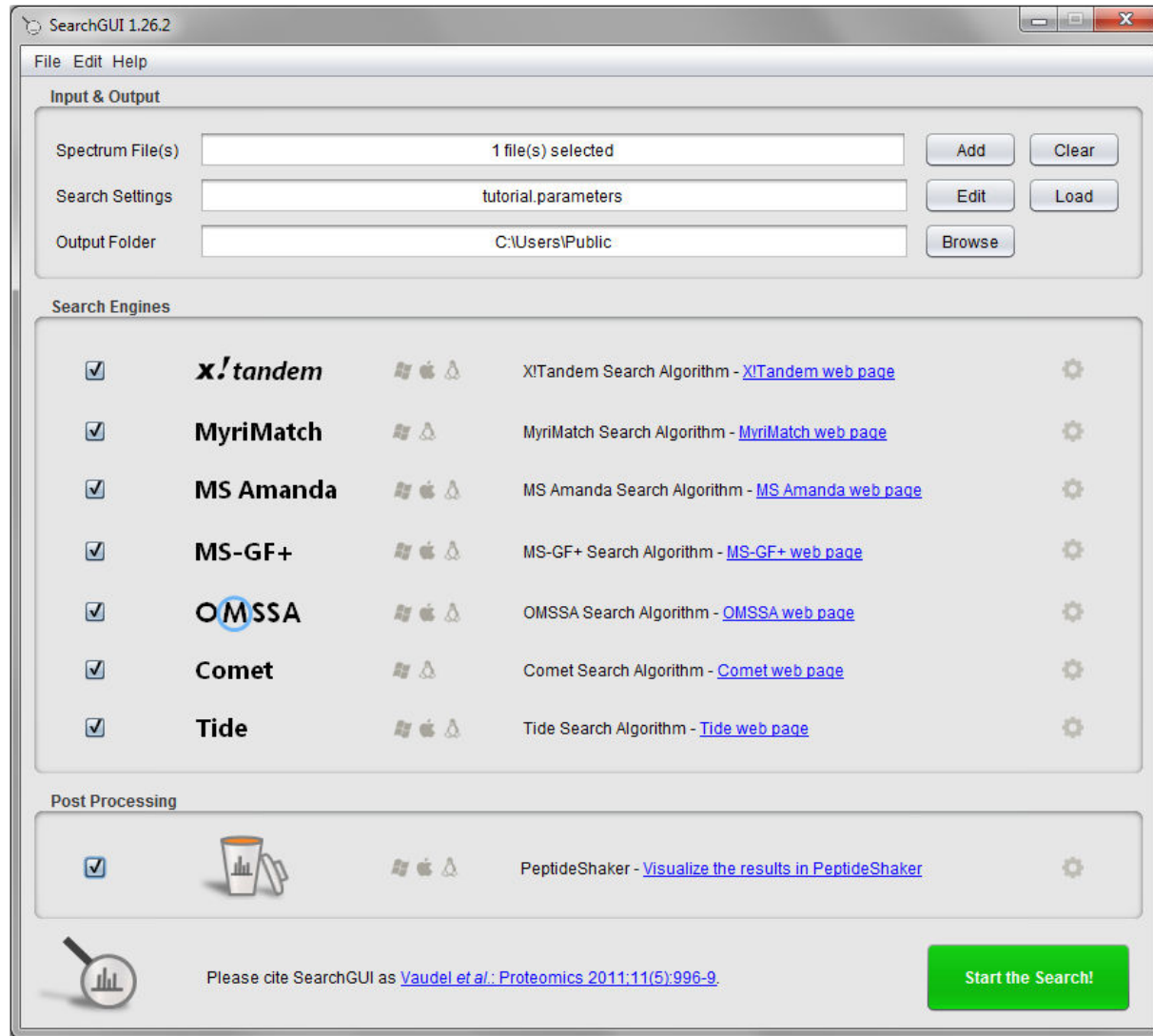
Nesvizhskii *et al* *Nature Methods* - **4**, 787 - 797 (2007)

DATABASE SEARCH



Nesvizhskii *et al*
Nature Methods - **4**, 787
 - 797 (2007)

SEARCHGUI



Vaudel M. *et al* Proteomics (2011) 11(5)

<https://code.google.com/p/searchgui/>

INPUTS : PEAKLISTS and SEARCH db → SEARCHGUI



MULTIPLE SEARCH ALGORITHMS

[Myrimatch](#)

Tabb *et al*, *J. Proteome Res.*, 2007, 6 (2)

Dorfer *et al*, *J Proteome Res.*, 2014, 13(8).

[MS
Amanda](#)

[X!tandem](#)

Craig and Beavis.
Bioinformatics.,
2004, Jun 20(9)

[Comet](#)

Eng *et al*, *Proteomics*. 2013, 13(1)

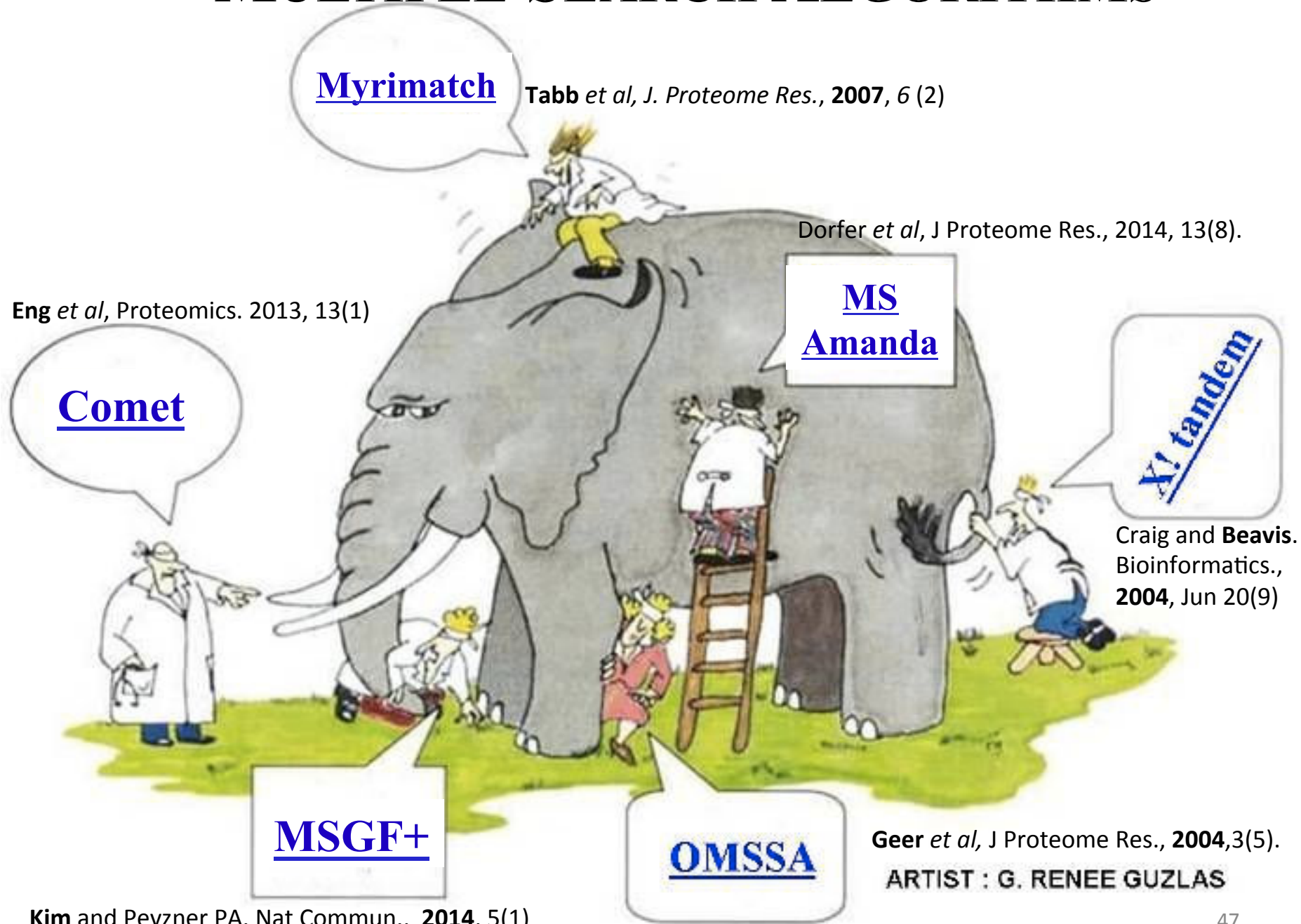
[MSGF+](#)

Kim and Pevzner PA. *Nat Commun.*, 2014, 5(1)

[OMSSA](#)

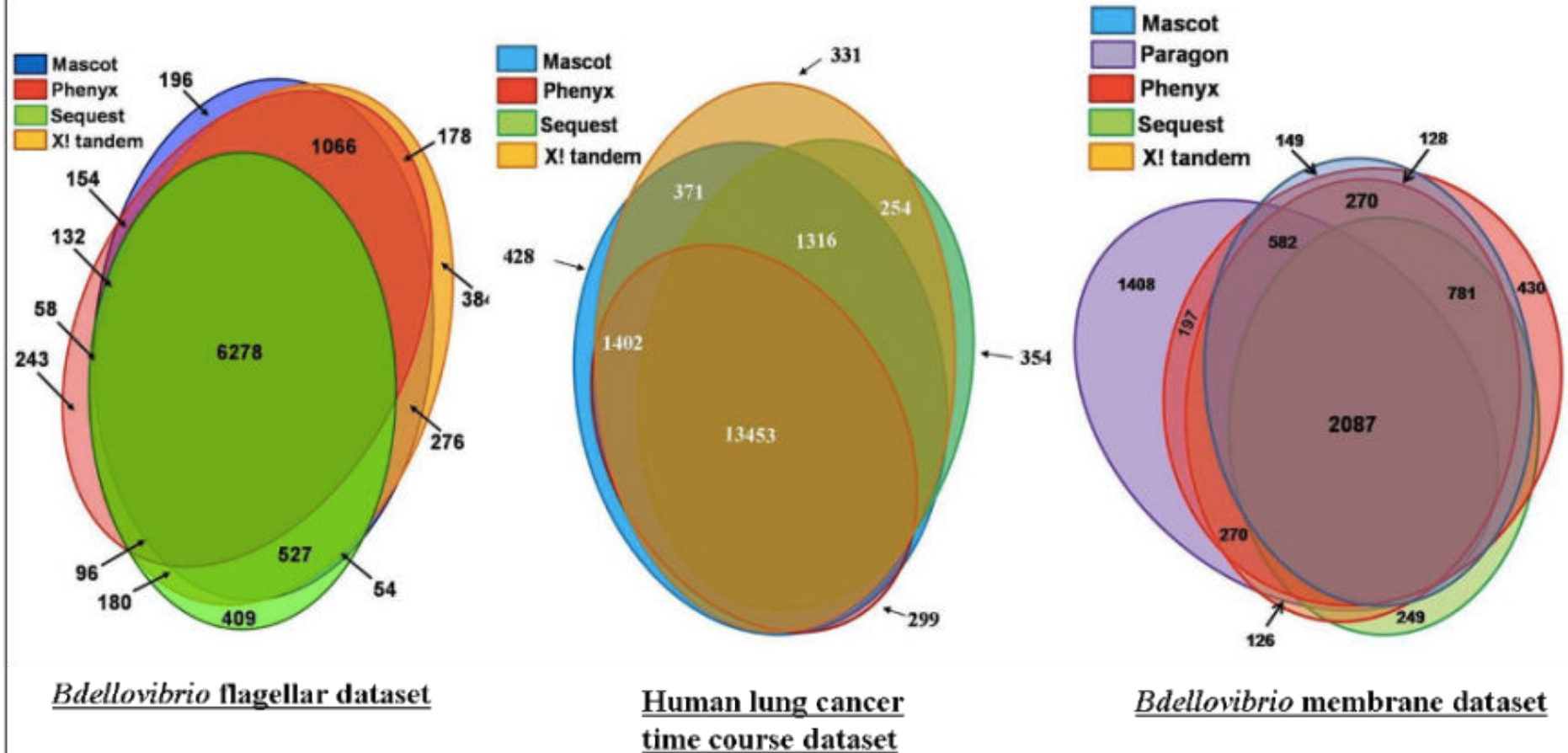
Geer *et al*, *J Proteome Res.*, 2004,3(5).

ARTIST : G. RENEE GUZLAS



MULTIPLE SEARCH ALGORITHMS

Venn Diagrams representing the distribution of peptide assignments at 1% FPR by multiple search algorithms.



Visualizing parameters for SearchGUI analysis

Merged and Filtered FASTA file 
14: Merged and Filtered FASTA from data 12, data 13, and others
type to filter

Step 2: Input dataset collection
MGF files LTQ/ Orbitrap acquired dataset.

Mascot formatted MGF Files: Input Dataset Collection (MGF Files) 
5: MGF Data Set List
type to filter

Step 3: Search GUI (version 1.28.0)

Protein Database
Output dataset 'output' from step 1
Create a concatenated target/decoy database before running PeptideShaker
True 

Input Peak Lists (mgf)
Output dataset 'output' from step 2

DB-Search Engines

☒ X!Tandem
☐ MyriMatch
☐ MS_Amanda
☒ MS-GF+
☒ OMSSA
☒ Comet
☐ Tide

Precursor Ion Tolerance Units
Parts per million (ppm) 

Precursor Ion Tolerance
10.0

Fragment Tolerance (Daltons)
0.01

History

search datasets 

imported: History 2
13 shown
384.3 MB   

15: Search GUI on data 3, data 4, and data 14   
179.4 MB
format: searchgui_archive, database: ?

Creating decoy database.
Reindexing: input_database.fasta.
10% 20% 30% 40% 50% 60% 70% 80% 90%Input:
/mnt/galaxy/tmp/job_working_directc

Name: input_database
Version: 24.6.2015
Decoy Tag: null
Type: UniProt
Last modified:

Compressed binary file

14: Merged and Filtered FASTA from data 12, data 13, and others   

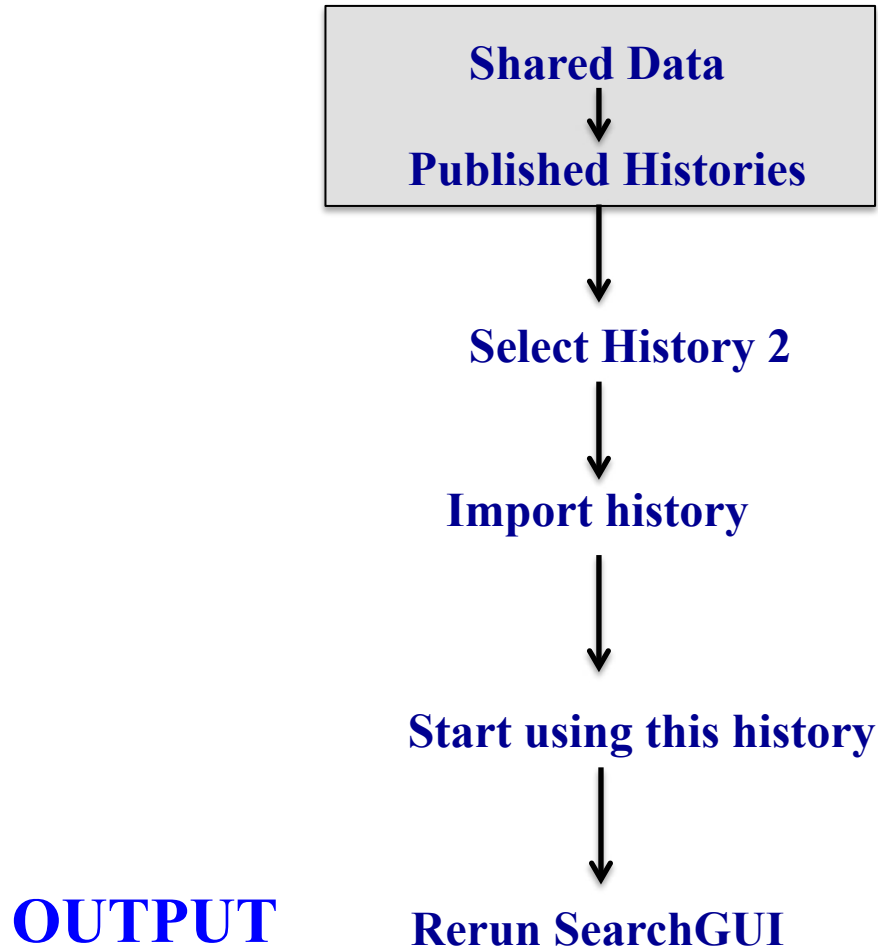
13: Regex Find And Replace on data 2   

12: Protein Database   

11: Protein Database   

8: Regex Find And Replace   

Visualizing parameters for SearchGUI analysis





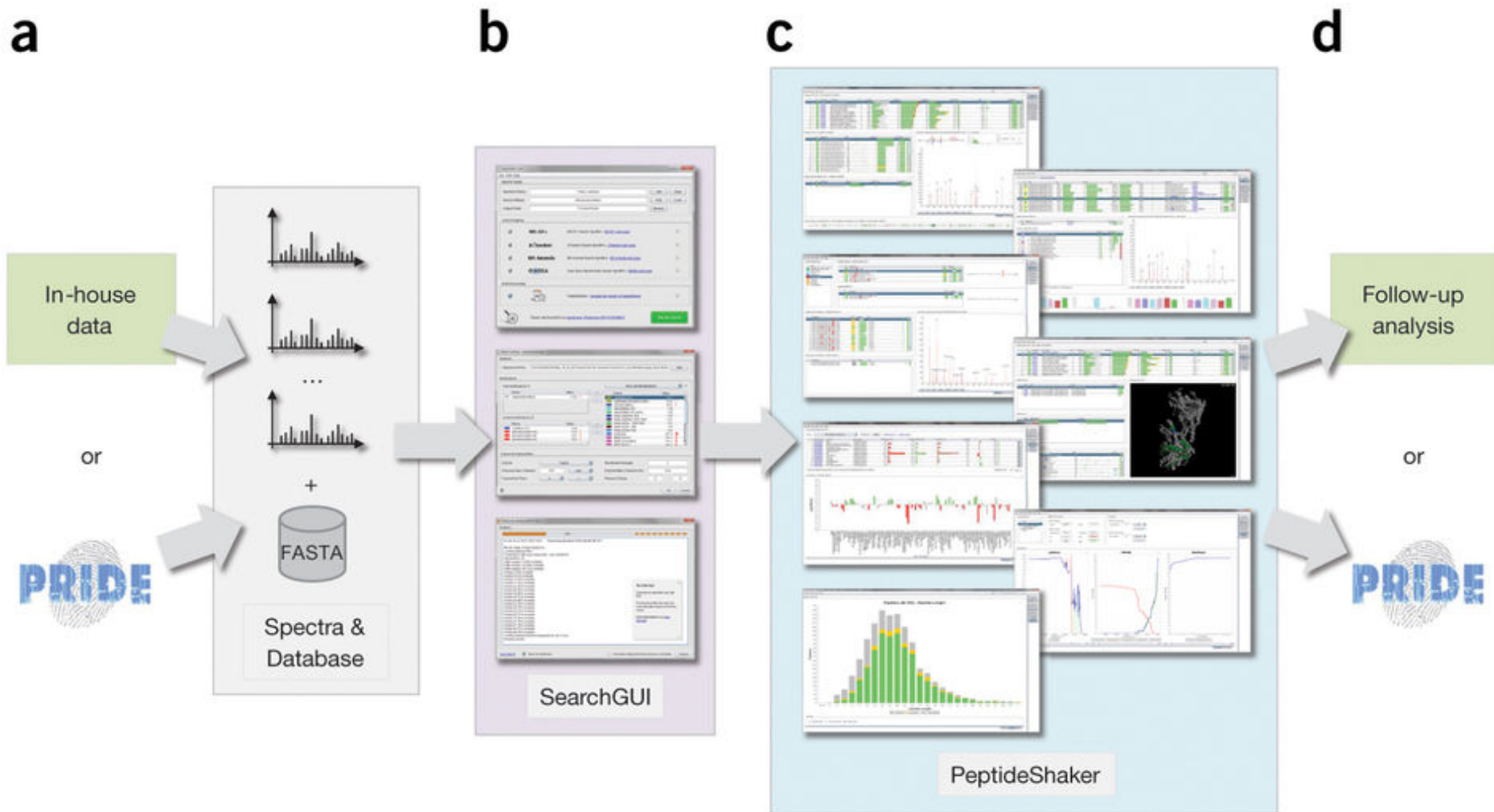
INPUTS : PEAKLISTS and SEARCH db → SEARCHGUI → PEPTIDESHAKER

PEPTIDESHAKER

SEARCHGUI : SEARCH ALGORITHMS

INPUTS : PEAKLISTS and SEARCH db

PEPTIDESHAKER



Vaudel et al *Nature Biotechnology*, 33, (2015)

<http://galaxyproteomics.github.io/peptideshaker/>

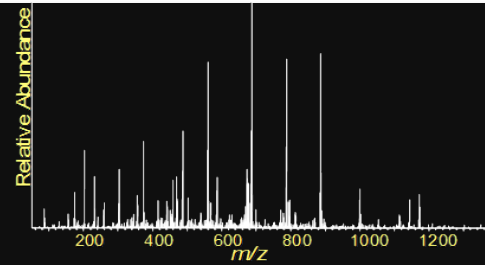
INPUTS : PEAKLISTS and SEARCH db → **SEARCHGUI** → **PEPTIDESHAKER**

GalaxyP

52

High throughput identification of proteins

Raw MS/MS spectrum

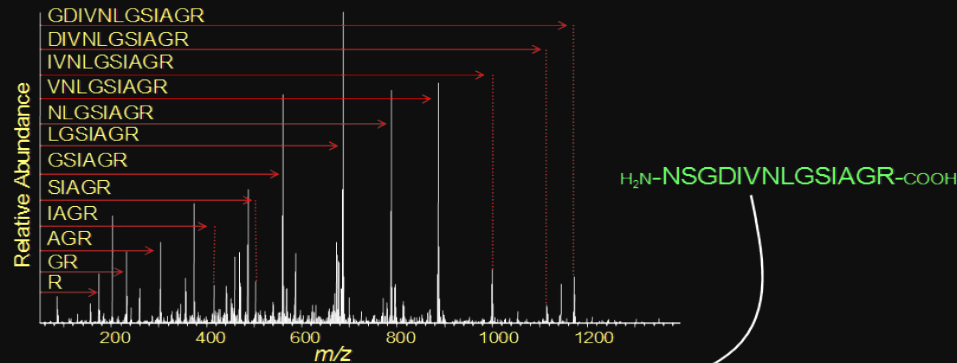


Protein sequence and/or DNA
sequence database search



Direct identification of 1000s
proteins from complex mixtures

Peptide sequence match



Protein identification



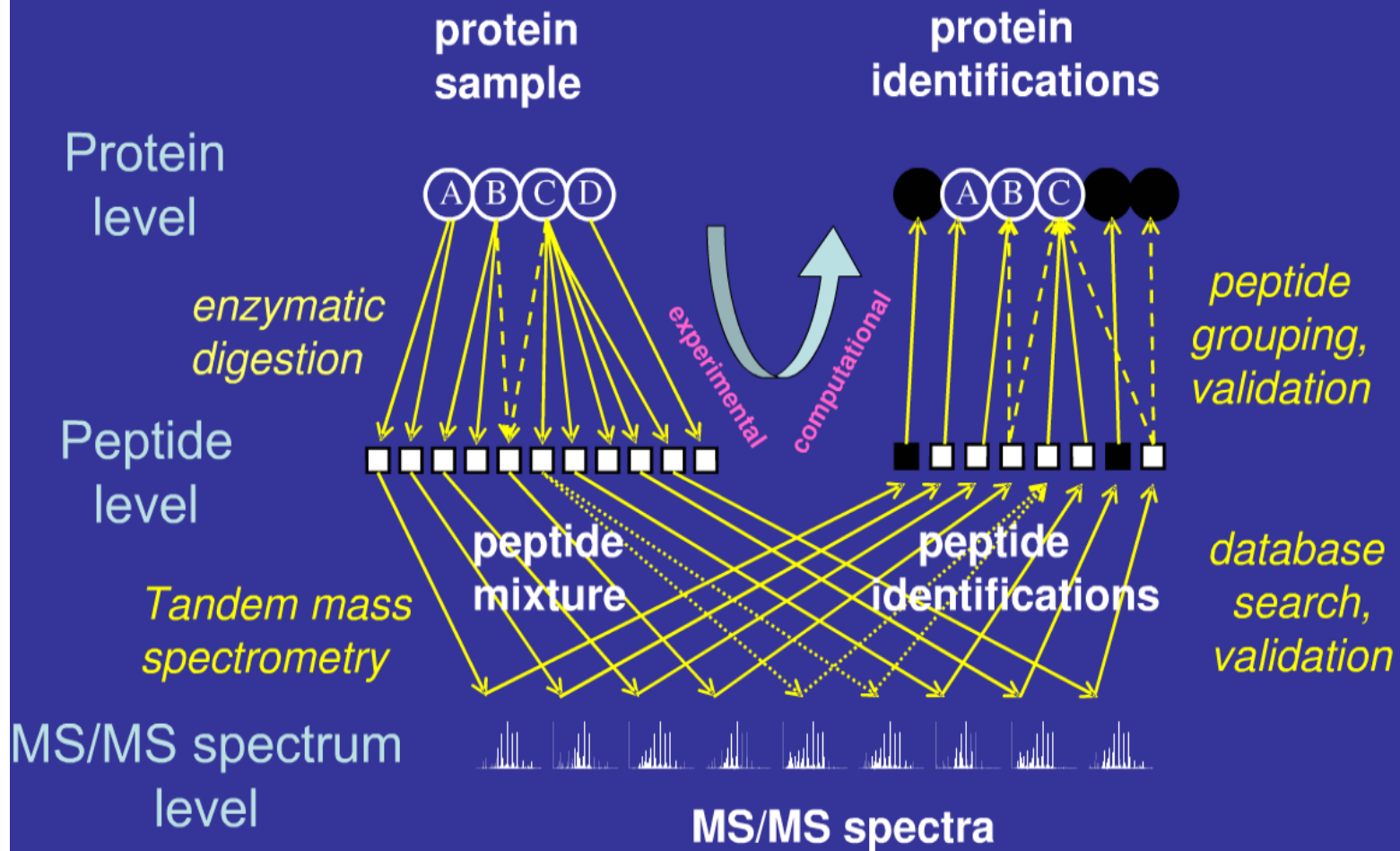
INPUTS : PEAKLISTS and SEARCH db SEARCHGUI PEPTIDESHAKER

GalaxyP



PEPTIDESHAKER : PROTEIN INFERENCE

Shotgun Protein Identification

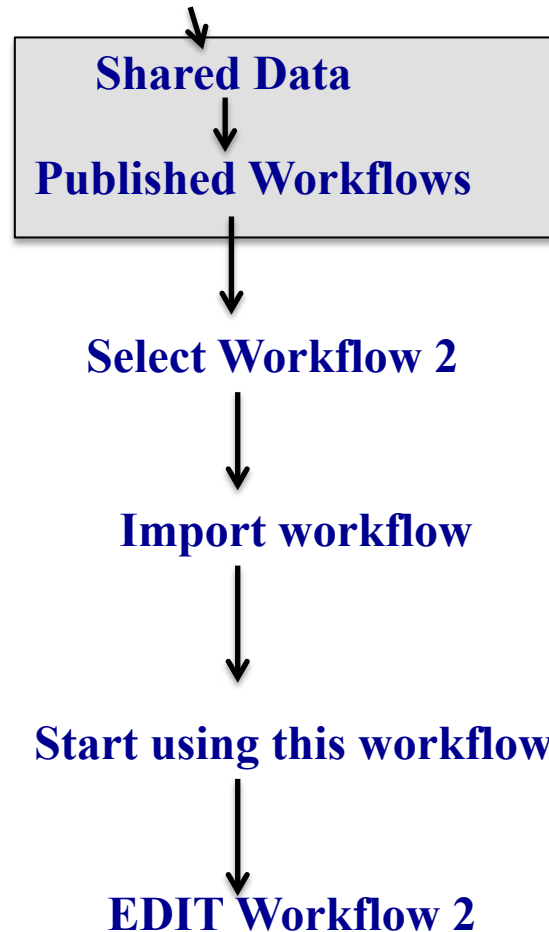


Slide from Alexey Nesvizshkii talk at <http://www.scivee.tv/node/12671>

4.3 Peptide Shaker in GalaxyP

- A. At the top of the screen, click Shared Data then select the option: Published Workflows .
- B. Click 'Workflow2: Workflow for History 2 to History 3' and choose import.
- C. Select start using this workflow.
- D. Click imported Workflow 2: Workflow for History 2 to History 3' and choose edit to open the workflow editor.
- E. To view the whole workflow (two tools*), navigate to the right and down by clicking and dragging the grid...
 - i. ...or use the minimap in the lower right corner.
 - ii. Note: Galaxy workflows are usually more complex with many more tools and Connections; for the sake of this tutorial we will start simple.
- F. Click on the PeptideShaker tool to view its details in the right panel.
- G. To run, click the cogwheel at the top right corner of the middle frame and select run from the resulting menu.
 - a. The input for this workflow under SearchGUI Results should be 8: SearchGUI On data 7 data2 and data 1 from History 3 . If this is not the case then refer to Section 2.2 on how to import a complete history.

4.3 Peptide Shaker in GalaxyP



WORKFLOW

4.3 Peptide Shaker in GalaxyP

Input dataset x

output

Peptide Shaker x

- Compressed SearchGUI results
- mzidentML (mzid)
- output_cps (peptideshaker_archive)
- output_zip (zip)
- output_certificate (txt)
- output_hierarchical (tabular)
- output_psm_phosphorylation (tabular)
- output_psm (tabular)
- output_peptides_phosphorylation (tabular)
- output_peptides (tabular)
- output_proteins_phosphorylation (tabular)
- output_proteins (tabular)

Details

Tool: Peptide Shaker

Version: 0.40.0

Compressed SearchGUI results
Data input 'searchgui_input' (searchgui_archive)

The species type to use for the gene annotation:
No species restriction

Specify Advanced PeptideShaker Processing Options:
Advanced Processing Options

FDR at the protein level: ▼
1.0

FDR at the peptide level: ▼
1.0

FDR at the PSM level: ▼
1.0

Minimum confidence required for a protein in the fraction MW plot: ▼
95.0

The PTM probabilistic score to use for PTM localization:
A-score

Specify Advanced Filtering Options:
Advanced Filtering Options

Minimum Peptide Length: ▼
6

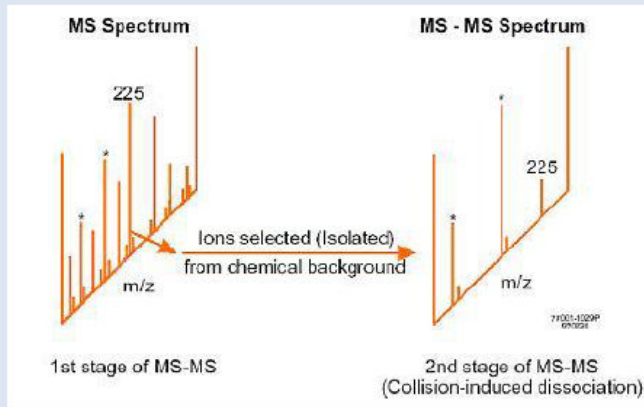
Maximum Peptide Length: ▼
40

Maximum Precursor Error: ▼
10.0

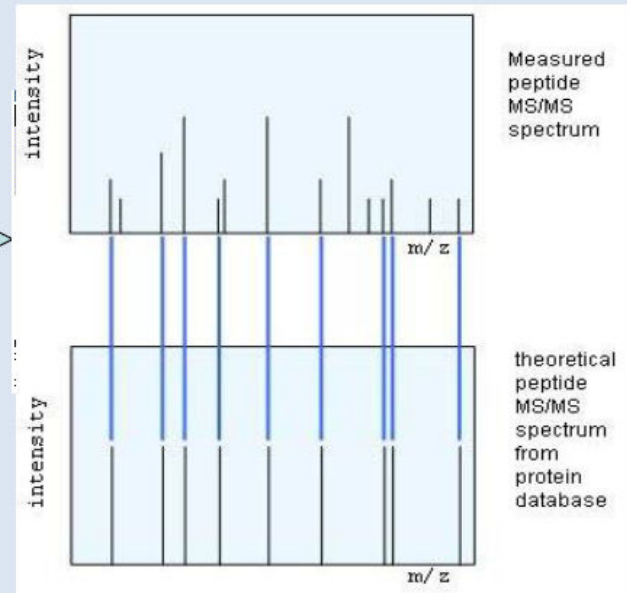
Maximum Precursor Error Type: ▼
ppm

PEPTIDESHAKER : TARGET-DECOY SEARCH

REVERSE DATABASE SEARCH



Mass spectrum



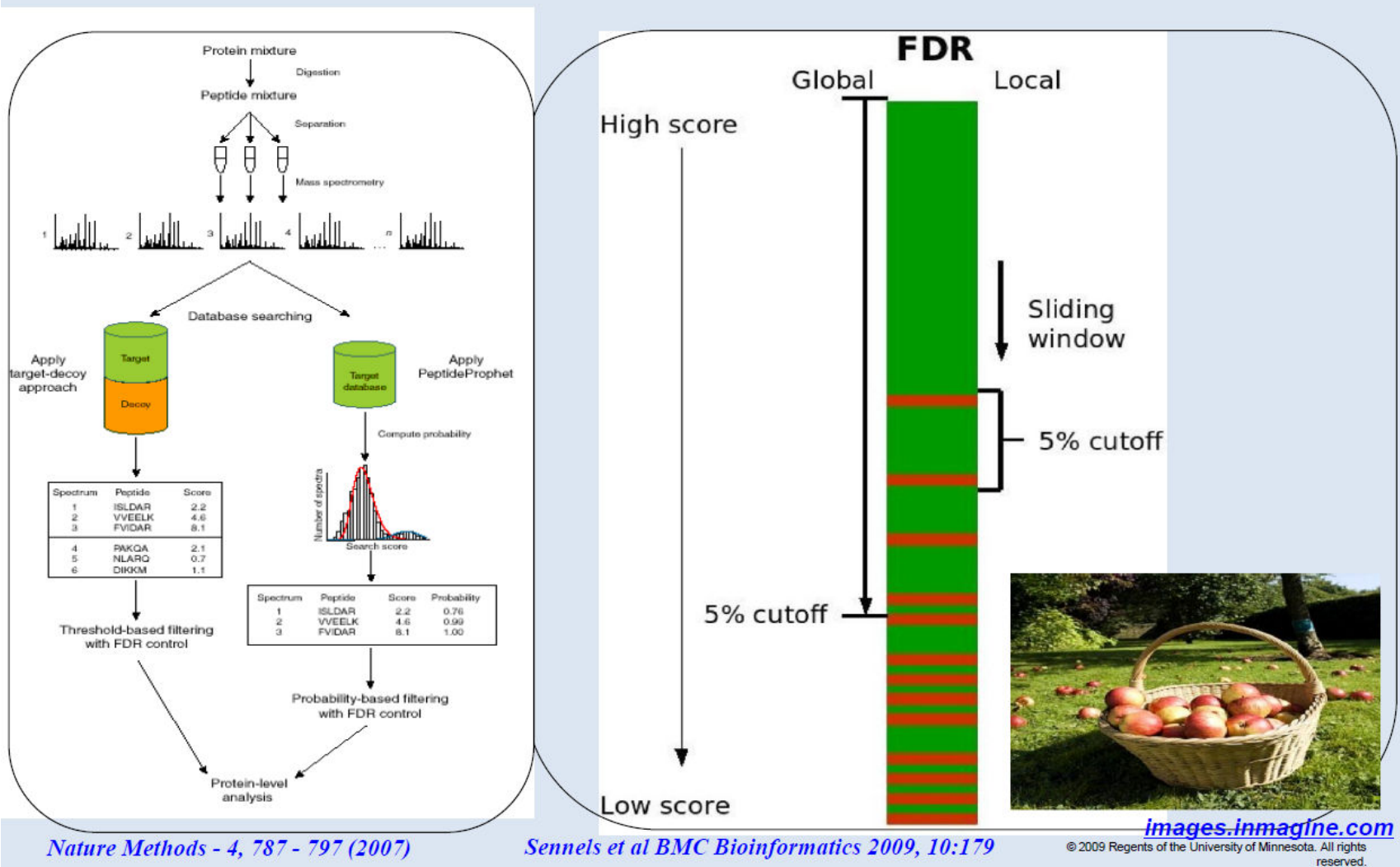
>IPI:IPI00205563.1|Gene_Symbol=Tmsbl1 thymosin beta-like protein
MSDKPDLSEVETFDKSKLKKTNTEEKNTLPSKETIQQEKEYNQRS



>IPI:**REV**_IPI00205563.1|Gene_Symbol=Tmsbl1 thymosin beta-like protein
SRQNYKEEQQITKESPLTKNEETNKKTKLKSDFTVEVESLDKPDSM

PEPTIDESHAKER : TARGET-DECOY SEARCH

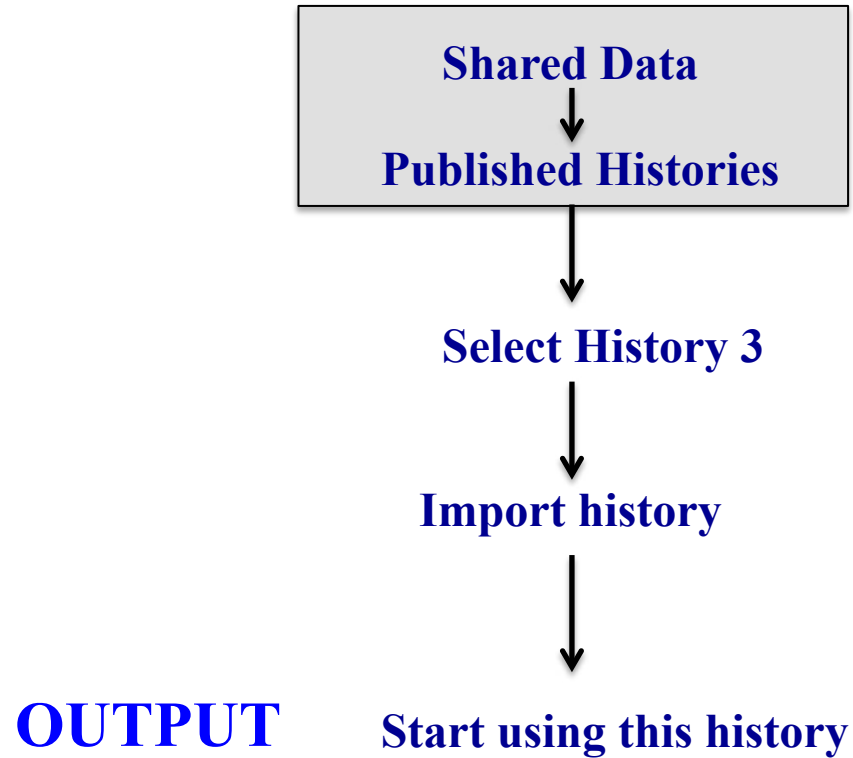
FALSE DISCOVERY RATE ANALYSIS



Nature Methods - 4, 787 - 797 (2007)

Sennels et al BMC Bioinformatics 2009, 10:179

PEPTIDESHAKER: OUTPUTS



PEPTIDESHAKER: OUTPUTS

GCC5: PeptideShaker Outputs
7 shown
359.1 MB

7: [Peptide Shaker on data 8: Protein Report](#)

6: [Peptide Shaker on data 8: Peptide Report](#)

4,372 lines
format: **tabular**, database: ?

Path configuration completed.
Thu Jun 11 16:50:55 CDT 2015 Unzipping searchgui_input.zip.
10% 20% 30% 40% 50% 60% 70% 80% 90% 100%

Thu Jun 11 16:51:26 CDT 2015 Import process for
Galaxy_Experiment_2015061116501434059408 (Sample:
Sample_20150611165014340

1	2
Protein(s)	
1	H0YMR4; H0YN07; Q8TEX9; Q8TEX9-2
2	A0A0A0MSD5; A0A0A0MSS8; A0A0A0MT30; B4DK69; H0Y
(16)	2 2 100.0 0 Confide
3	ENST00000291565_14; FZZZY4; Q00764; Q00764-2; Q00764-
4	A0A0A0MSM0; Q92598; Q92598-2; Q92598-3; Q92598-4

5: [Peptide Shaker on data 8: PSM Report](#)

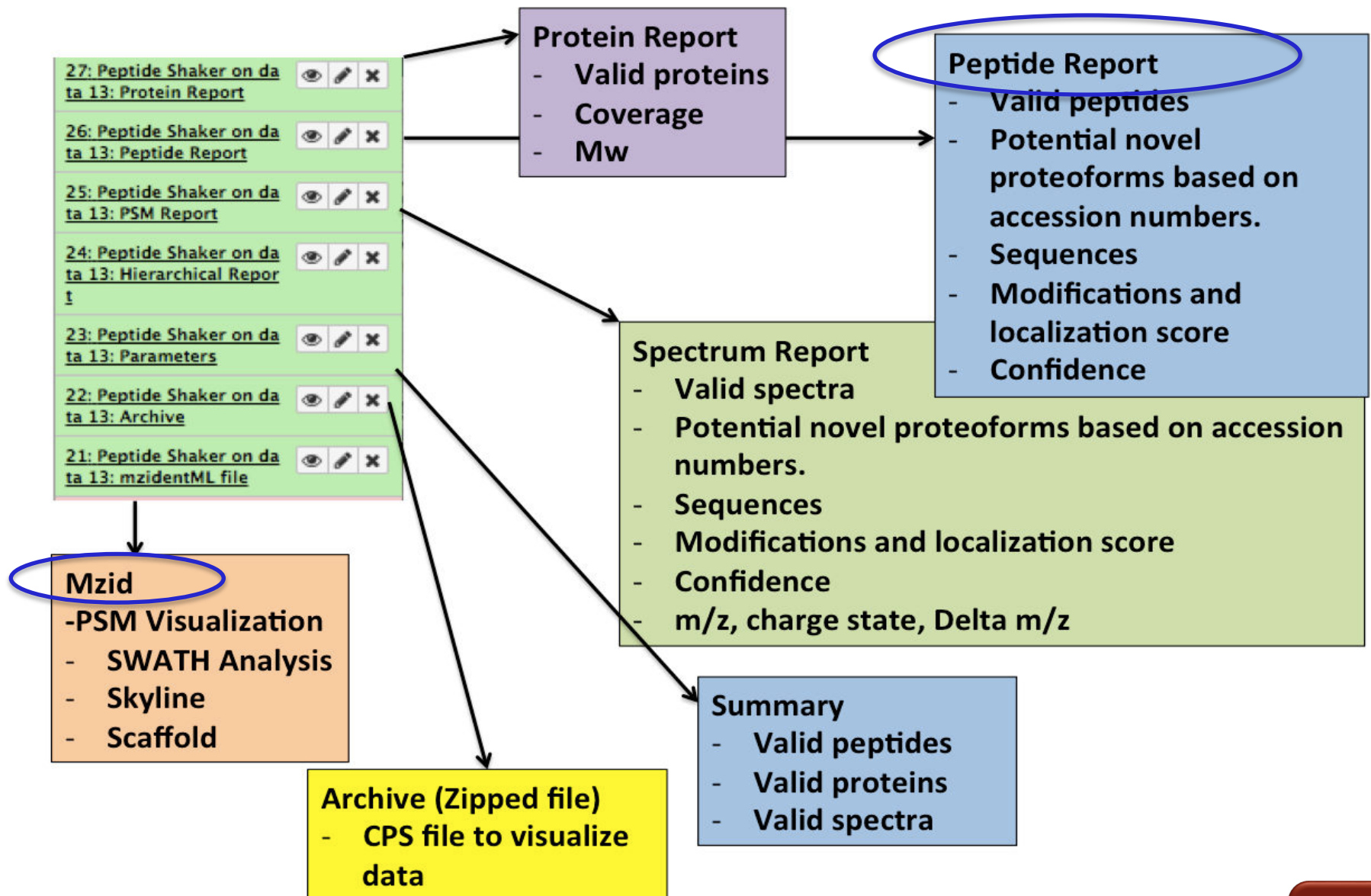
4: [Peptide Shaker on data 8: Parameters](#)

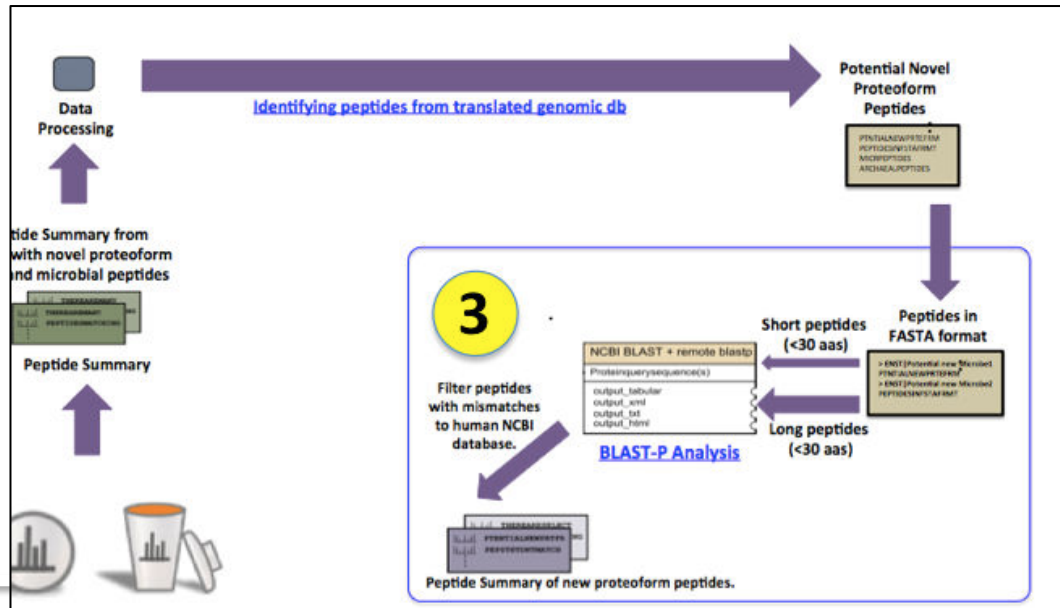
3: [Peptide Shaker on data 8: Archive](#)

2: [Peptide Shaker on data 8: mzidentML file](#)

1: [Search GUI on data 7, data 2, and data 1](#)

PEPTIDESHAKER: OUTPUTS





INPUTS → **SEARCHGUI** → **PEPTIDESHAKER** → **BLAST-P**

BLAST-P SEARCH

PEPTIDESHAKER

SEARCHGUI : SEARCH ALGORITHMS

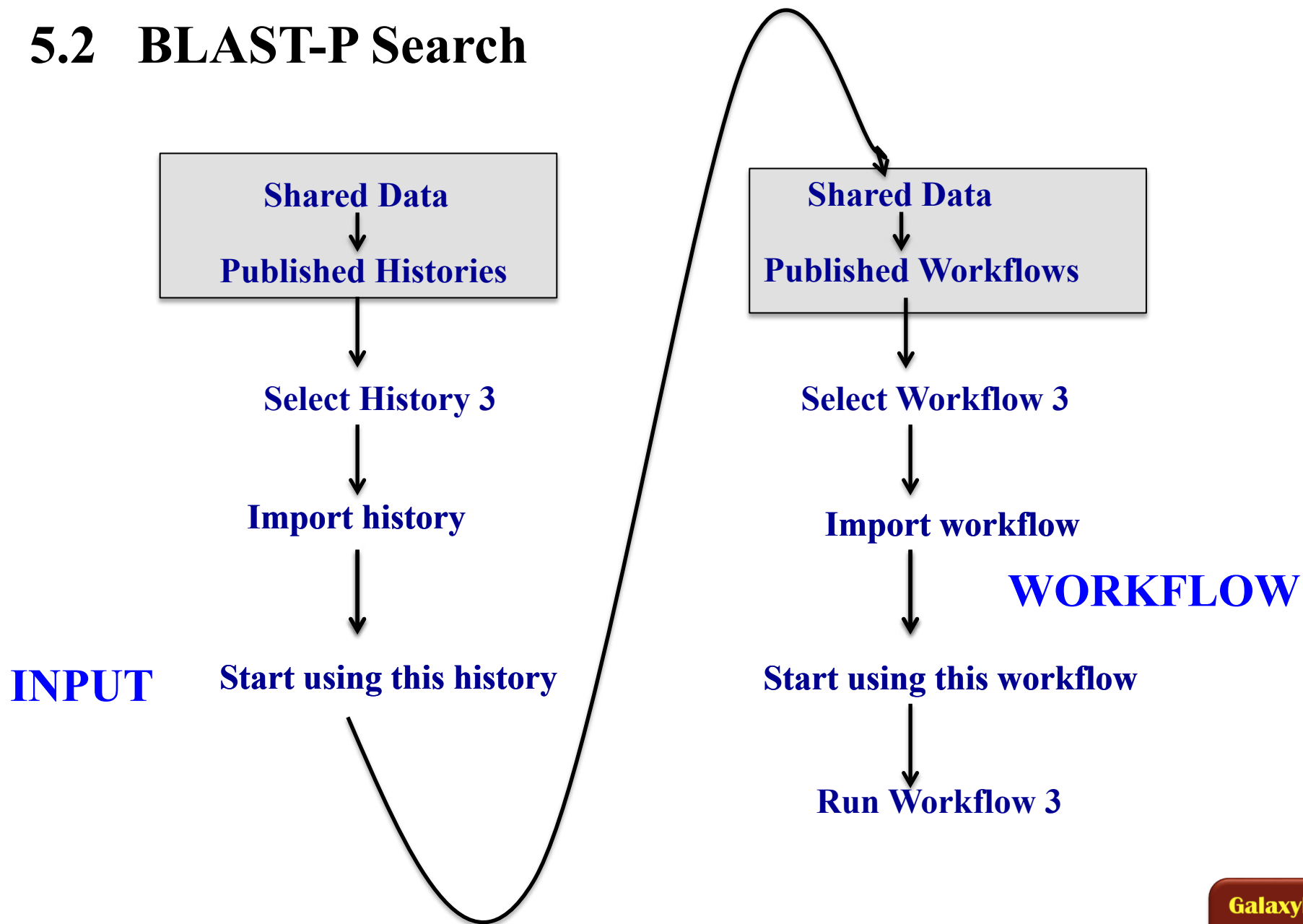
INPUTS : PEAKLISTS and SEARCH db

5.2 BLAST-P Search

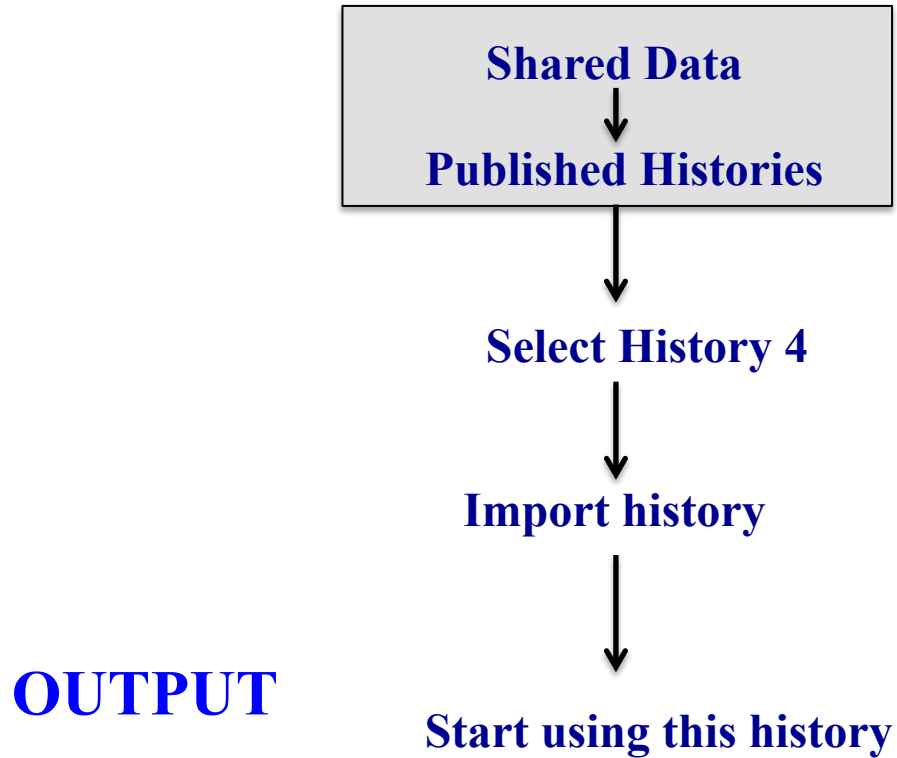
- a. At the top of the screen, click Shared Data then select the option: Published Workflows .
- b. Click Workflow 3: Workflow for History 3 to History 4 and choose import.
- c. Select start using this workflow .
- d. To run, click 'Workflow 3: Workflow from History 3 to History 4 and choose run .
- i. Change your input file to 6: Peptide Shaker on data 8: Peptide Report.
- ii. Notice the number of steps in the workflow (refer to Section 5.3 for more detail)
- iii. Check Send results to a new history at the bottom and name it History 4.



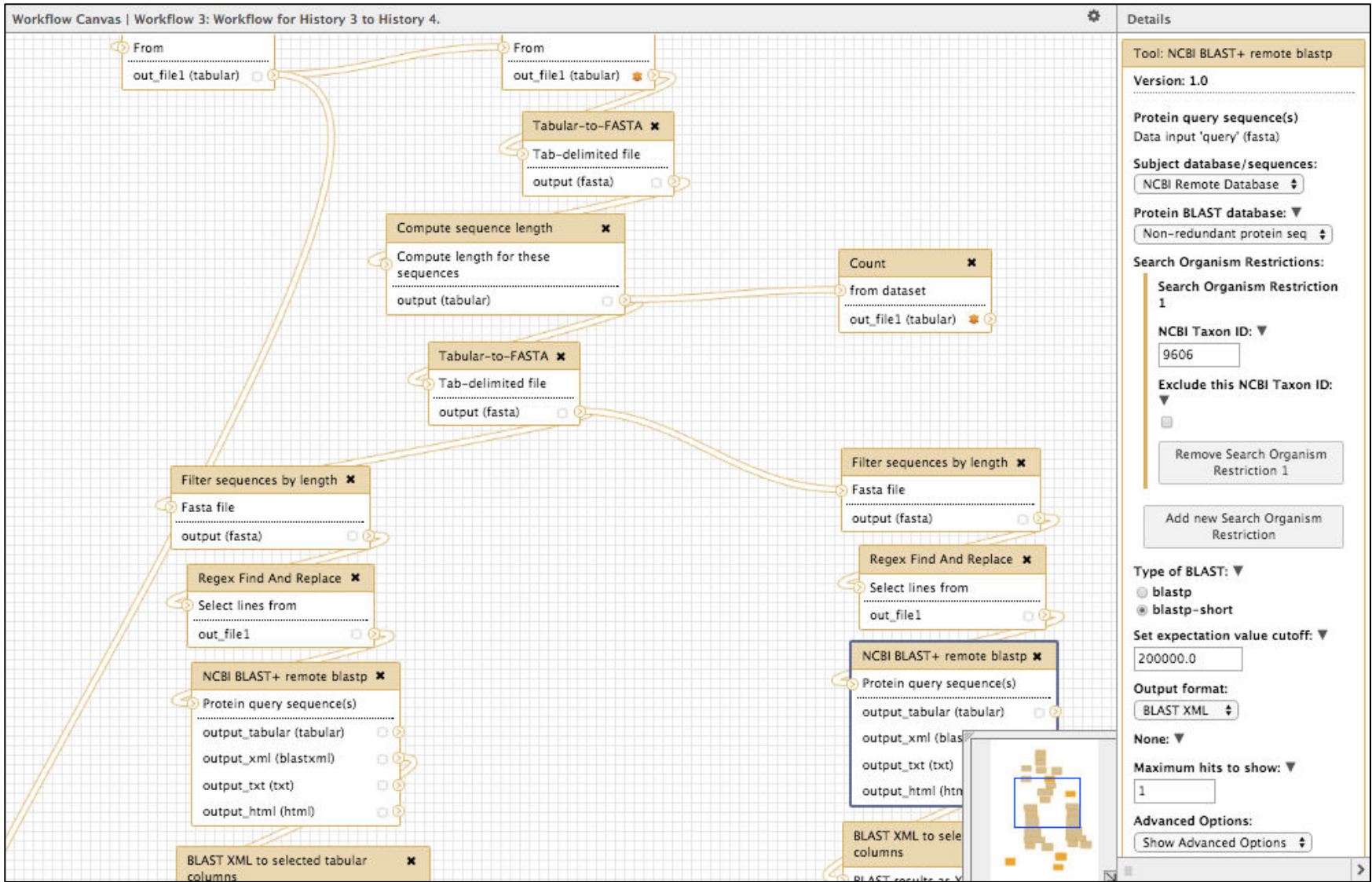
5.2 BLAST-P Search

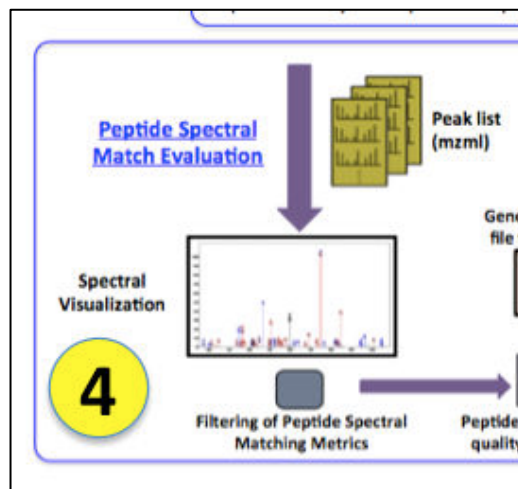


5.2 BLAST-P Search



BLAST-P SEARCH





PSM EVALUATION

BLAST-P SEARCH

PEPTIDESHAKER

SEARCHGUI : SEARCH ALGORITHMS

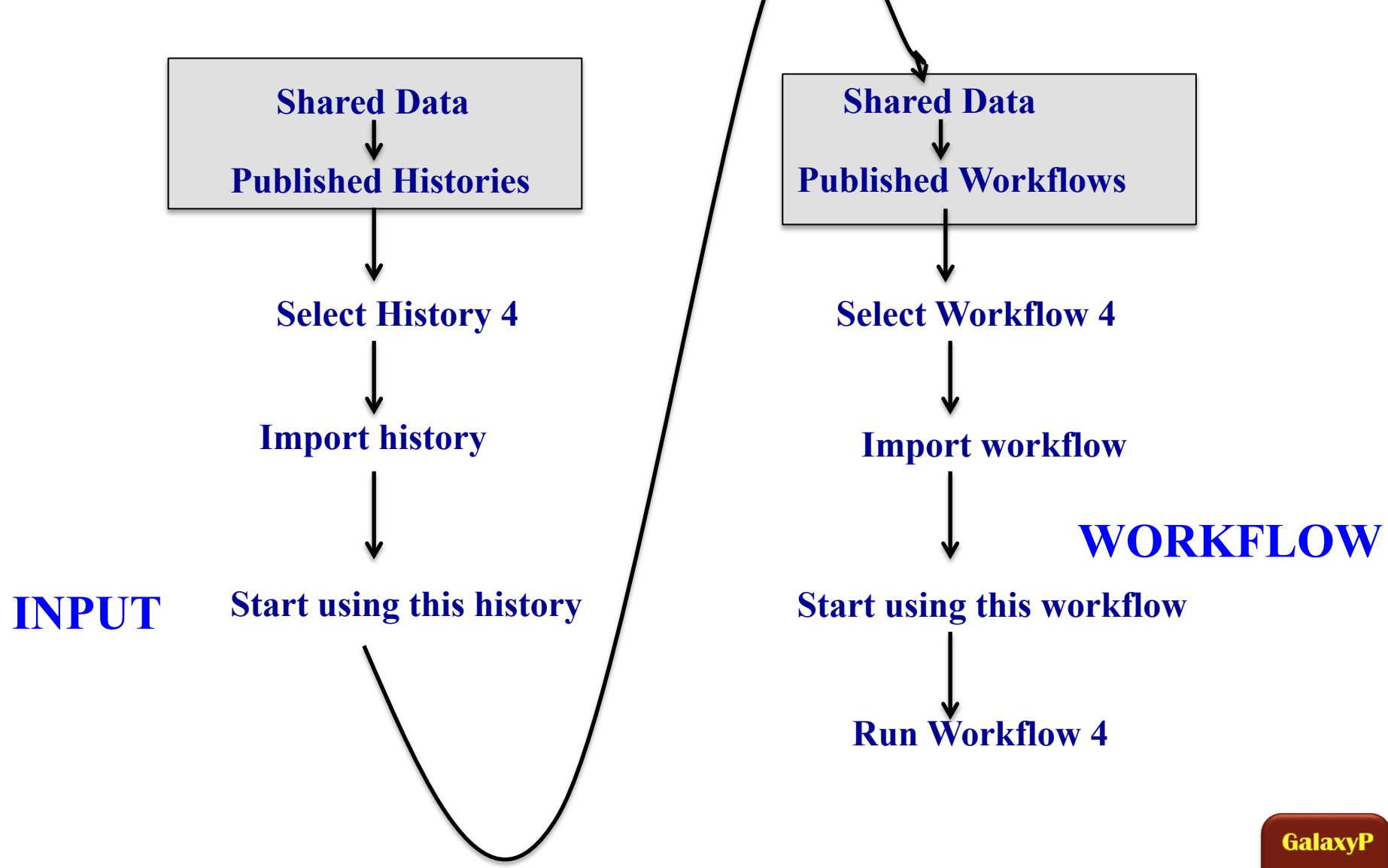
INPUTS : PEAKLISTS and SEARCH db

6.2 Generating a sqlite Database

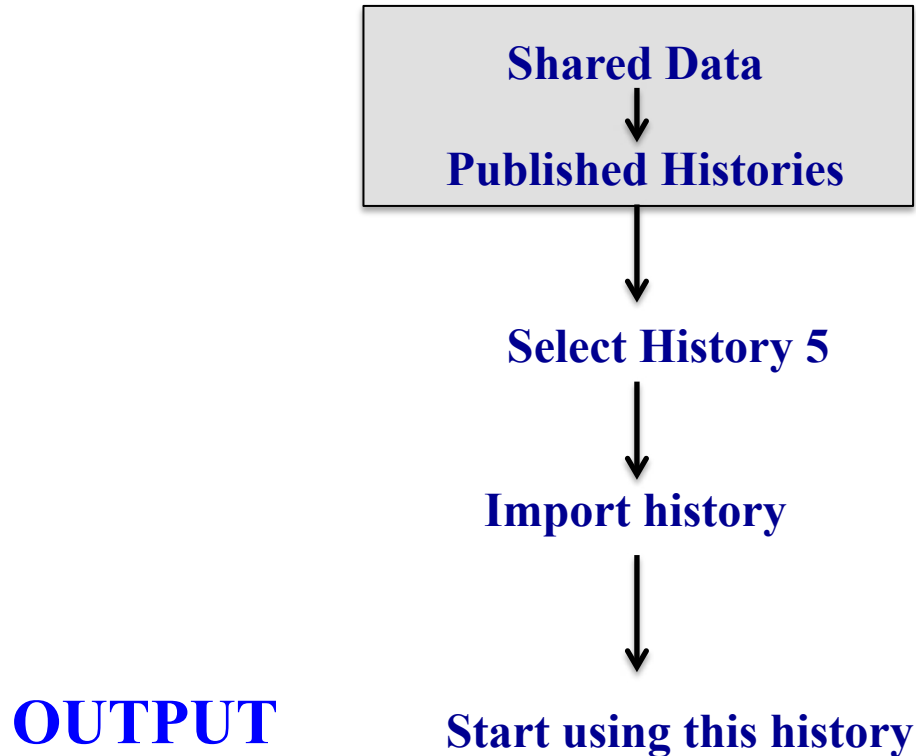
- a. From Shared Data at the top of the screen, import History 5 and Workflow 4: History 4 to History 5 .
- b. From the workflows menu , run Workflow 4: History 4 to History 5 on History 4.
- c. In the workflow run options, check that all inputs are correct and select the box Send results to a new history named: and enter History 5 into the field provided.
- d. Select Run and navigate to History 5 in the normal Galaxy view. For the purposes of this tutorial, a completed History 5 may be imported from Published Histories.



6.2 Generating a sqlite Database



6.3 PSM Evaluator in GalaxyP

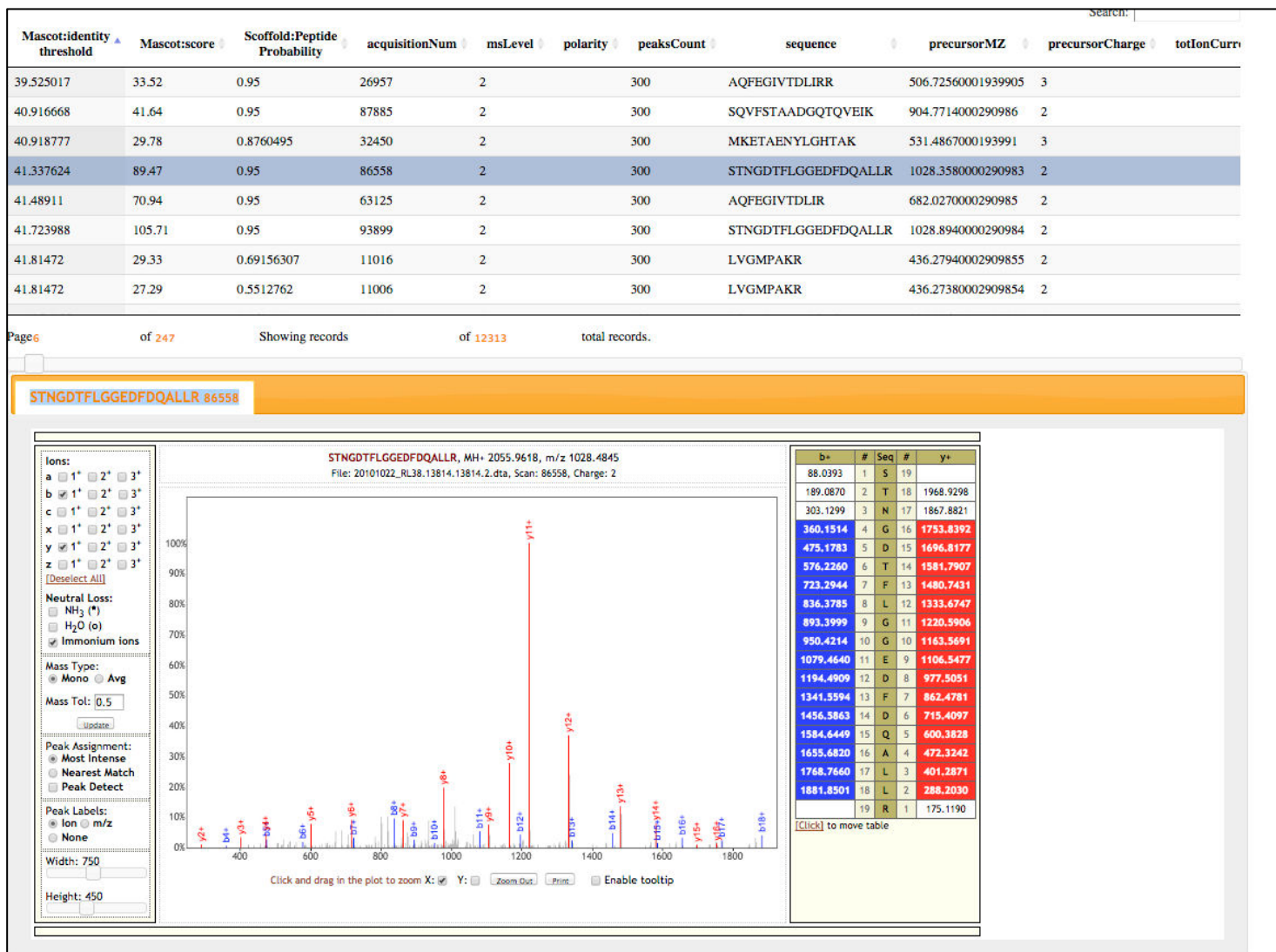


6.3 PSM Evaluator in GalaxyP

- a. From Shared Data at the top of the screen, import History 5
- b. Click on mz_to_sqlite dataset to expand, select Visualize in PSM Viewer .
- c. Select Peptide View from PSM Table at the top of the screen.
- d. To view the spectra of the novel peptides input the peptide sequences (LLSVGGLR, SPVLKPSR) into the filter peptides by sequence(s) field and select the sequence to generate the spectral data.
- e. Within the viewer users can utilize numerous organization tools to sort through data of each peptide.
 - i. Users may select which columns they prefer to see in their PSM Tables.
 - ii. Users may search the table for a specific piece of data.
 - iii. Users may sort data in each column and organize the order in which columns appear.
- f. To view the spectra of LLSVGGLR select anywhere with the peptide spectral data table.



PSM EVALUATION



July 7th 2015: Session II : 11:20 AM : *Proteomics Visualization in Galaxy*

James E. Johnson

PSM EVALUATION

- Go to 'Peptide' View.
- Type in 'LLSVGGLR, SPVLKPSR' in Filter box.

OR

Copy the peptide sequences from item #52 in history 5.

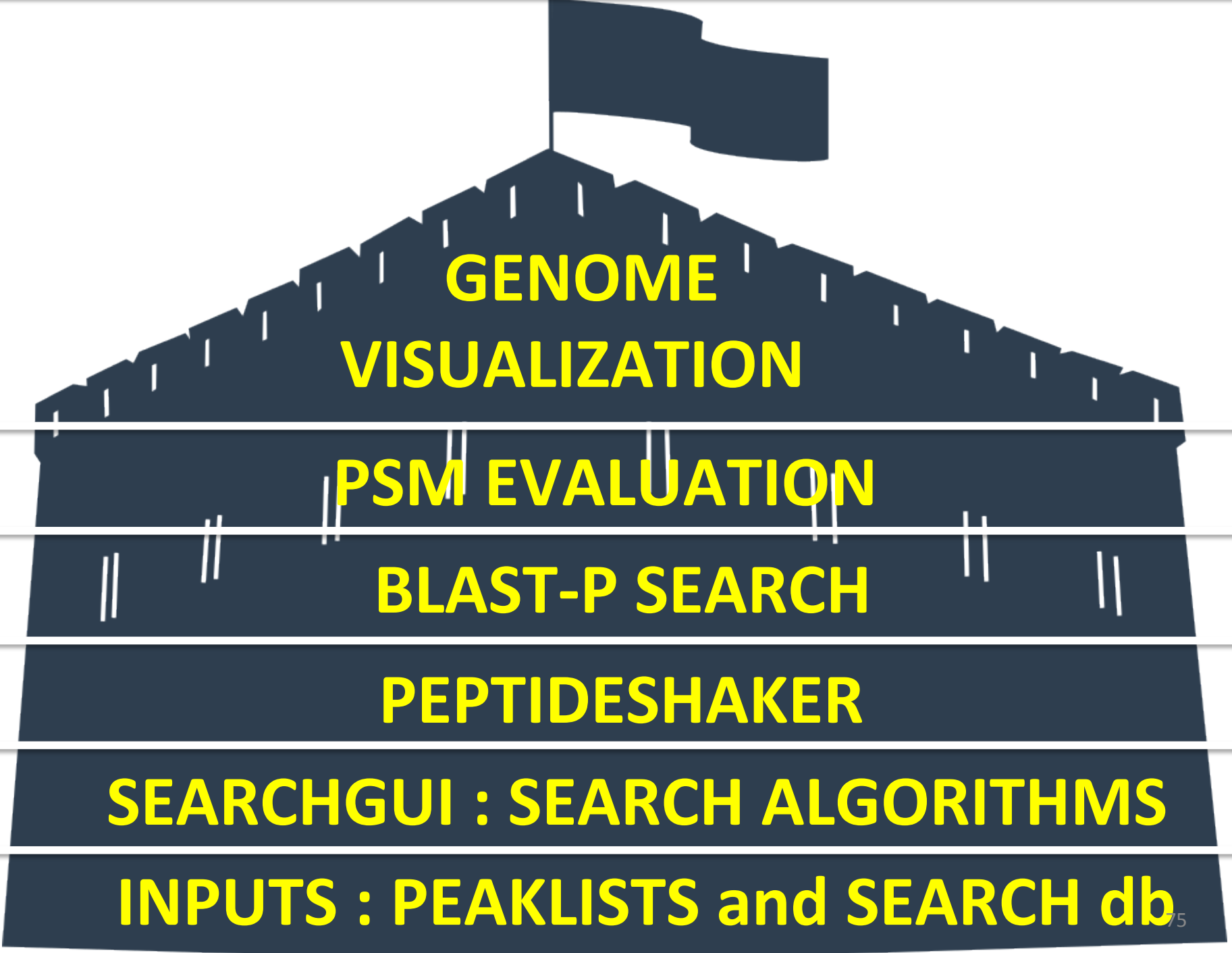
- Follow the instructor for demo.

- Go to 'Protein' View.
- Type in 'ABRF' in Filter box.
- Follow the instructor for demo.

July 7th 2015: Session II : 11:20 AM : [Proteomics Visualization in Galaxy](#)

James E. Johnson





**GENOME
VISUALIZATION**

PSM EVALUATION

BLAST-P SEARCH

PEPTIDESHAKER

SEARCHGUI : SEARCH ALGORITHMS

INPUTS : PEAKLISTS and SEARCH db

7. Mapping Peptides to a Genome

- Map the peptide to the SearchDB protein
- Find the mapping of the protein to the reference genome. An Ensembl GTF file shows how the exons of the protein sequence are mapped to the genome sequence
- Each SearchDB construction may need its own mapping to genome method.



7. Mapping Peptides to a Genome

7.2 Generating a GFF file

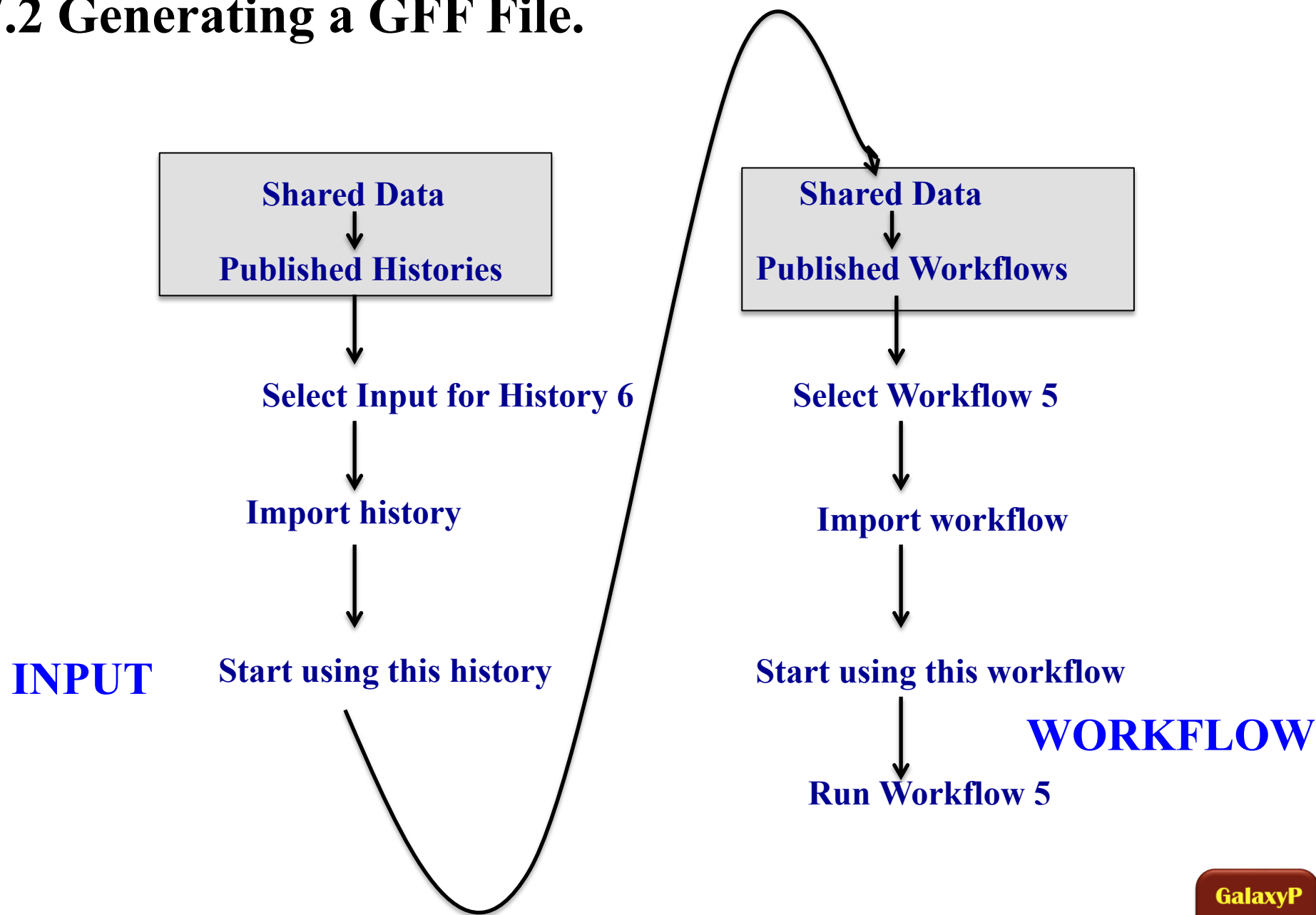
- From Shared Data at the top of the screen, import Input for History 6 and Workflow 5 : Workflow to History 6 from Published Histories and Workflows, respectively.
- From the workflow menu, Run Workflow 5 on Inputs for History 6.
- Select the appropriate inputs for Workflow 5 from Inputs to History 6.
- Check to send the results to a new history named History 6 and Run the workflow.

For the purposes of this tutorial, a completed History 6 may be imported from Published Histories.

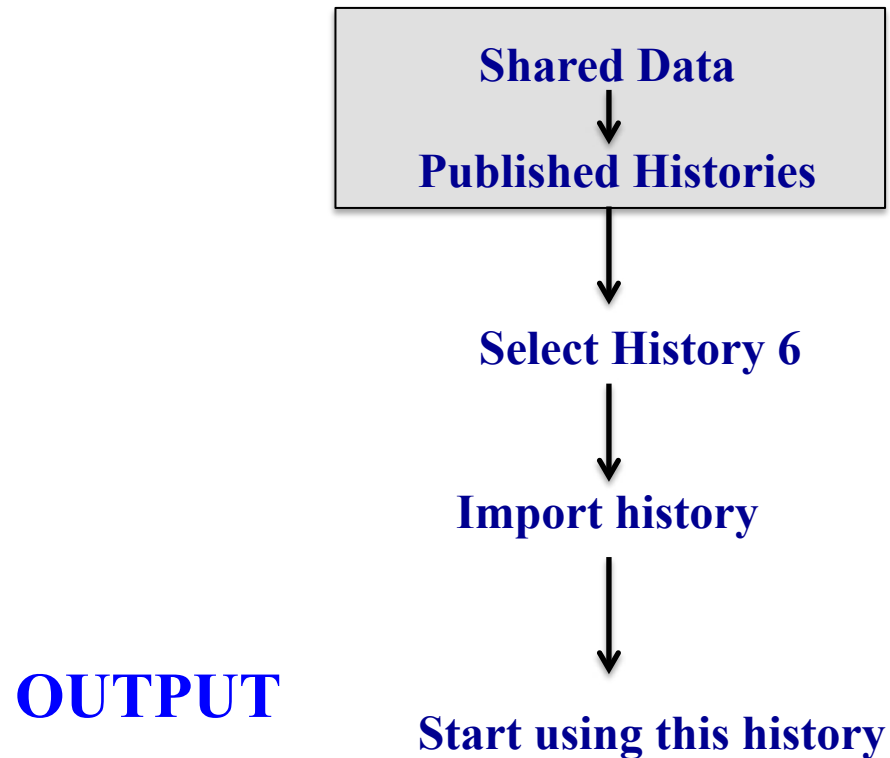
7.3 From GFF to IGV Browser



7.2 Generating a GFF File.



7.2 Generating a GFF File.



galaxyp.msi.umn.edu

Galaxy / GalaxyP

Analyze Data Workflow Shared Data Visualization Admin Help User

Tools

search tools

CORE TOOLS

Get Data

Send Data

Lift-Over

Text Manipulation

Filter and Sort

Join, Subtract and Group

Convert Formats

Extract Features

Statistics

Graph/Display Data

FASTA manipulation

PROTEOMICS

MS Data Conversion

Sequence Database Tools

NGS: QC and manipulation

Protein/Peptide Search Algorithms

Data Conversion Tools

Visualizers

Quantification

BLAST-P

Proteogenomics

GENOMICS

1	2	3	4	5	6	7	8	9	10	11	12	13	14
4398	ENST00000339452_9	LLSVGGLR	N12-LLSVGGLR-COOH	ER					1	1	96.82539682539682	0	Co
5511	ENST00000310343_104	SPVLKPSR	N12-SPVLKPSR-COOH	ET					1	1	100.0	0	Co

History

search datasets

novel proteoforms

3 shown

200 bytes

3: Homo_sapiens.GRCh37.canon.73.gtf

2: Homo_sapiens.GRCh37.73.cdna.all.fa

1: BLAST-P Filtered_Peptide_Report.tabular

2 lines

format: tabular, database: ?

uploaded tabular file

1	2	3	4
4398	ENST00000339452_9	LLSVGGLR	NH2
5511	ENST00000310343_104	SPVLKPSR	NH2

ENST00000339452_9

ENST00000310343_104

galaxy.msi.umn.edu/workflow/editor?id=0d57d5e9c8f1b11b

Galaxy / GalaxyP

Analyze Data Workflow Shared Data Visualization Admin Help User

Using 183.9 GB

Tools

search tools

CORE TOOLS

Get Data

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Lift-Over

Text Manipulation

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Data Conversion Tools

Visualizers

Quantification

BLAST-P

Proteogenomics

GENOMICS

Workflow Canvas | imported: GCC12: Workflow to generate Peptides to GTF for genome visualization

Input dataset x

output

Column Regex Find And Replace x

Select cells from

out_file1

Input dataset x

output

Peptide to GFF x

Source File

Sequence and Feature References for mapping the peptides 1 > CDNA Transcripts Fasta

Sequence and Feature References for mapping the peptides 1 > GTF feature file for the cdna transcripts

output_gff (gff3)

unmapped (tabular)

Details

Tool: Column Regex Find And Replace

Version: 0.1.0

Select cells from

Data input 'input' (tabular)

using column: ▾

2

Checks:

Check 1

Find Regex: ▾

^(.*(ENST\d+)_\d+.*)\$

Replacement: ▾

\\1\\t2

Remove Check 1

Add new Check

Edit Step Actions

Rename Dataset

out_file1 ▾ Create

Add actions to this step; actions are applied when this workflow step completes.

galaxy.msi.umn.edu/workflow/editor?id=0d57d5e9c8f1b11b

Galaxy / GalaxyP

Analyze Data Workflow Shared Data Visualization Admin Help User

Using 183.9 GB

Tools

search tools

CORE TOOLS

Get Data

Send Data

Lift-Over

Text Manipulation

Filter and Sort

Join, Subtract and Group

Convert Formats

Extract Features

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NGS: QC and manipulation

Protein/Peptide Search Algorithms

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Visualizers

Quantification

BLAST-P

Proteogenomics

GENOMICS

Workflow Canvas | imported: GCC12: Workflow to generate Peptides to GTF for genome visualization

Input dataset x

output

Column Regex Find And Replace x

Select cells from

out_file1

Input dataset x

output

Peptide to GFF x

Source File

Sequence and Feature References for mapping the peptides 1 > CDNA Transcripts Fasta

Sequence and Feature References for mapping the peptides 1 > GTF feature file for the cdna transcripts

output_gff (gff3)

unmapped (tabular)

Details

Tool: Peptide to GFF

Version: 1.0

Peptide Source Format:

Generic Tabular (with peptide)

Source File

Data input 'input_file' (tabular)

Peptide Column:

To be set at runtime

Accession Identifier Column:

To be set at runtime

Sequence and Feature References for mapping the peptides:

Sequence and Feature References for mapping the peptides 1

Select Peptide Mapping File Formats:

cdna sequence with G

CDNA Transcripts Fasta

Data input 'seqs' (fasta)

GTF feature file for the cdna transcripts

Data input 'feature_ref' (gff)

Remove Sequence and

galaxyp.msi.umn.edu/root?workflow_id=0d57d5e9c8f1b11b

Galaxy / GalaxyP

Peptides to GTF for genome visualization

Tools

search tools

CORE TOOLS

[Get Data](#)

[Send Data](#)

[Lift-Over](#)

[Text Manipulation](#)

[Filter and Sort](#)

[Join, Subtract and Group](#)

[Convert Formats](#)

[Extract Features](#)

[Statistics](#)

[Graph/Display Data](#)

[FASTA manipulation](#)

PROTEOMICS

[MS Data Conversion](#)

[Sequence Database Tools](#)

[NGS: QC and manipulation](#)

[Protein/Peptide Search Algorithms](#)

[Data Conversion Tools](#)

[Visualizers](#)

[Quantification](#)

[BLAST-P](#)

[Proteogenomics](#)

GENOMICS

Step 1: Input dataset

Peptide Report for Novel Proteoform Peptides (Potential)

1: BLAST-P_Filtered_Peptide_Report.tabular

type to filter

Step 2: Input dataset

CDNA FASTA File

2: Homo_sapiens.GRCh37.73.cdna.all.fa

type to filter

Step 3: Input dataset

EnSEMBL GTF File

3: Homo_sapiens.GRCh37_canon.73.gtf

type to filter

Step 4: Column Regex Find And Replace (version 0.1.0)

Peptide Source Format

Generic Tabular (with peptide and accession columns)

Source File

Output dataset 'out_file1' from step 4

Peptide Column

4

Accession Identifier Column

3

Step 5: Peptide to GFF (version 1.0)

History

search datasets

novel proteoforms

3 shown

200 bytes

3: Homo_sapiens.GRCh37_canon.73.gtf

~2,000,000 lines

format: gtf, database: hg19

uploaded gtf file

display in IGB [View](#)

display with IGV [web](#) [current](#) [local](#)

display at Ensembl [Current](#)

display at UCSC [main](#)

1. Seqname	2. Source
1	processed_transcript
1	processed_transcript
1	processed_transcript
1	unprocessed_pseudogene
1	unprocessed_pseudogene
1	unprocessed_pseudogene

2: Homo_sapiens.GRCh37.cdna.all.fa

1: BLAST-P_Filtered_Peptide_Report.tabular

galaxy.msi.umn.edu/root?workflow_id=0d57d5e9c8f1b11b

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[Visualizers](#)

[Quantification](#)

[BLAST-P](#)

[Proteogenomics](#)

GENOMICS

Successfully ran workflow "Imported: GCC12: Workflow to generate Peptides to GTF for genome visualization". The following datasets have been added to the queue:

- 1: BLAST-P_Filtered_Peptide_Report.tabular
- 2: Homo_sapiens.GRCh37.73.cdna.all.fa
- 3: Homo_sapiens.GRCh37_canon.73.gtf
- 4: Column Regex Find And Replace on data 1
- 6: Peptide to GFF peptides.unmapped
- 5: peptides.gff3

History

search datasets

novel proteoforms

6 shown

200 bytes

6: Peptide to GFF peptides.unmapped

5: peptides.gff3

4: Column Regex Find And Replace on data 1

3: Homo_sapiens.GRCh37_canon.73.gtf

~2,000,000 lines

format: gtf, database: hg19

uploaded gtf file

display in IGB View

display with IGV web current local

display at Ensembl Current

display at UCSC main

1. Seqname	2. Source
1	processed_transcript
1	processed_transcript
1	processed_transcript
1	unprocessed_pseudogene

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[Protein/Peptide Search Algorithms](#)

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[Quantification](#)

[BLAST-P](#)

[Proteogenomics](#)

GENOMICS

Successfully ran workflow "imported: GCC12: Workflow to generate Peptides to GTF for genome visualization". The following datasets have been added to the queue:

- 1: BLAST-P_Filtered_Peptide_Report.tabular
- 2: Homo_sapiens.GRCh37.73.cdna.all.fa
- 3: Homo_sapiens.GRCh37_canon.73.gtf
- 4: Column Regex Find And Replace on data 1
- 6: Peptide to GFF peptides.unmapped
- 5: peptides.gff3

History

search datasets

novel proteoforms

5 shown, 1 hidden

200 bytes

6: Peptide to GFF peptides.unmapped

5: peptides.gff3

3: Homo_sapiens.GRCh37_canon.73.gtf

~2,000,000 lines

format: gtf, database: hg19

uploaded gtf file

display in IGB View

display with IGV web current local

display at Ensembl Current

display at UCSC main

1.Seqname	2.Source
1	processed_transcript
1	processed_transcript
1	processed_transcript
1	unprocessed_pseudogene
1	unprocessed_pseudogene
1	unprocessed_pseudogene

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BLAST-P

Proteogenomics

GENOMICS

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

display with IGV web current local

display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Start

##gff-version 3

##sequence-region 4 1 155412208

4 MassSpec peptide 1554121

4 MassSpec CDS 1554121

##sequence-region 11 1 128838569

11 MassSpec peptide 1288385

3: Homo_sapiens.GRC

h37_canon.73.gtf

~2,000,000 lines

format: gtf, database: hg19

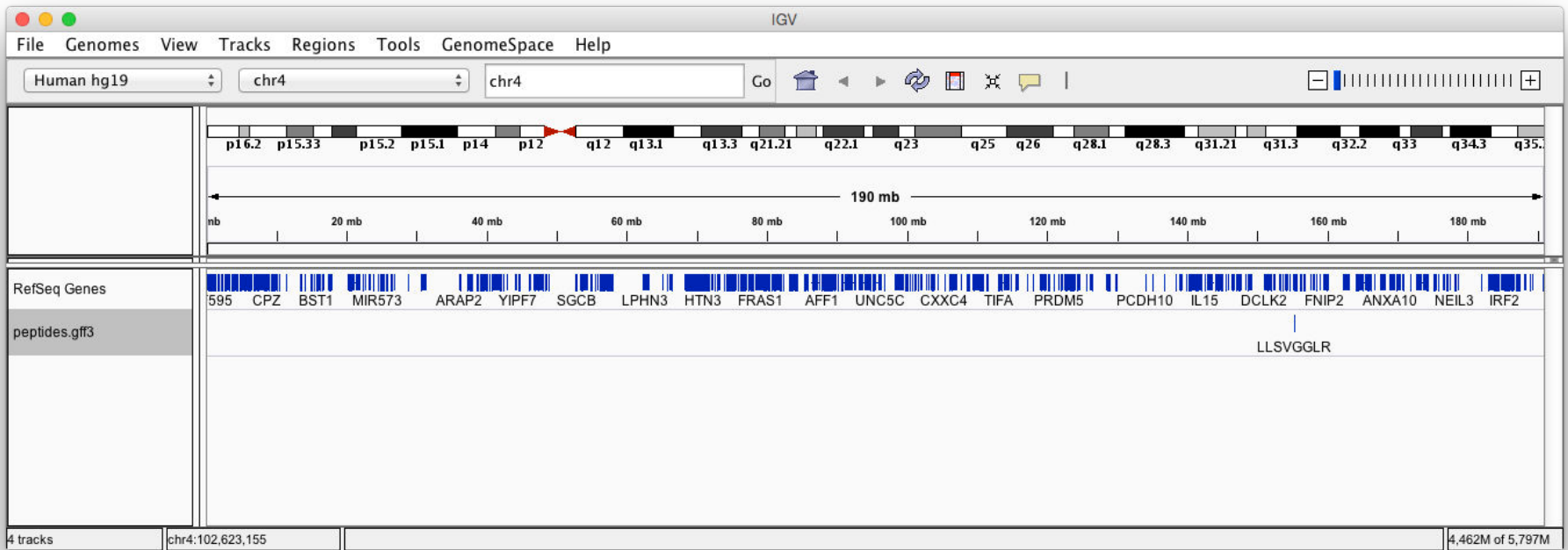
uploaded gtf file

display in IGV View

display with IGV web current local

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Extract Features

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

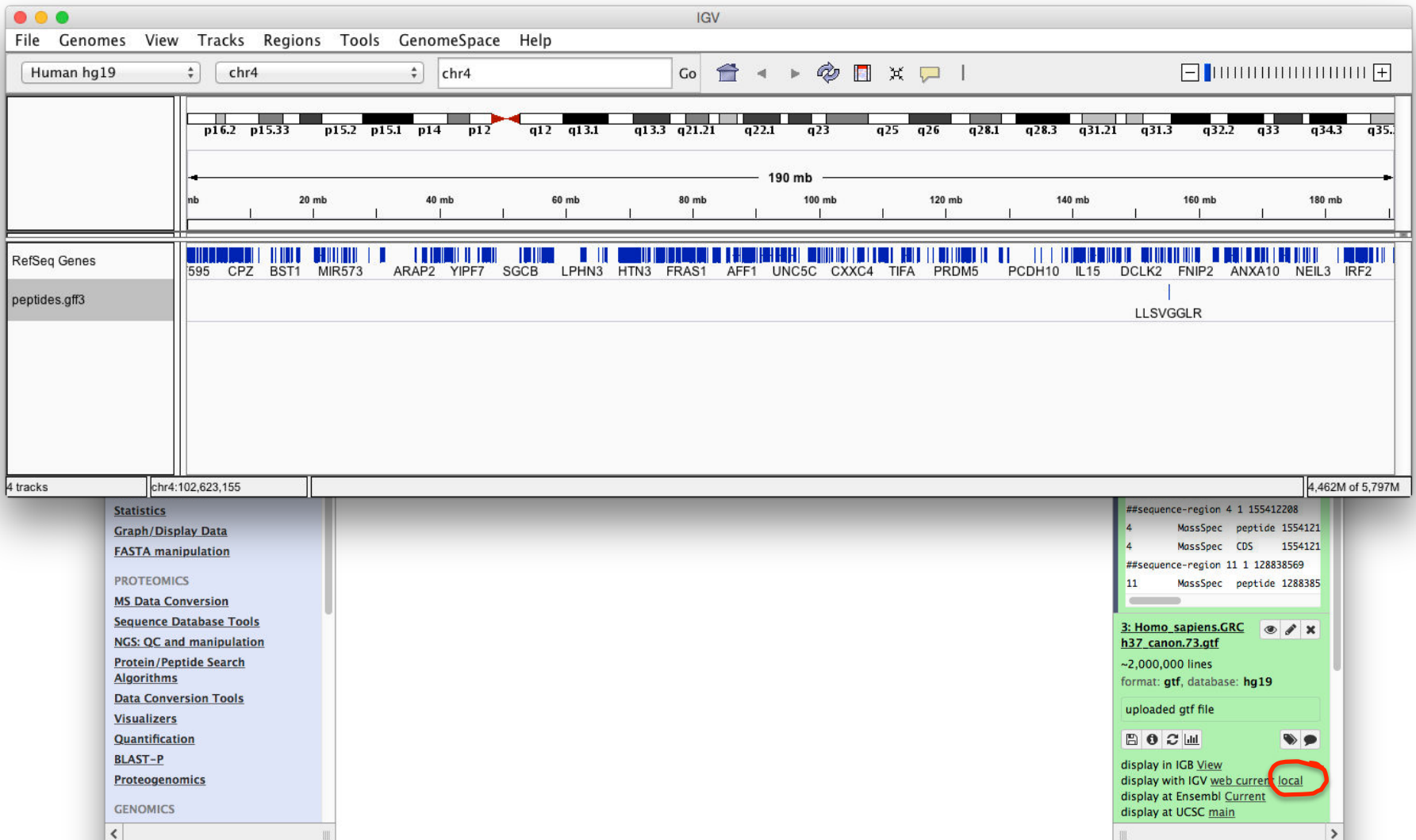
display with IGV web current local

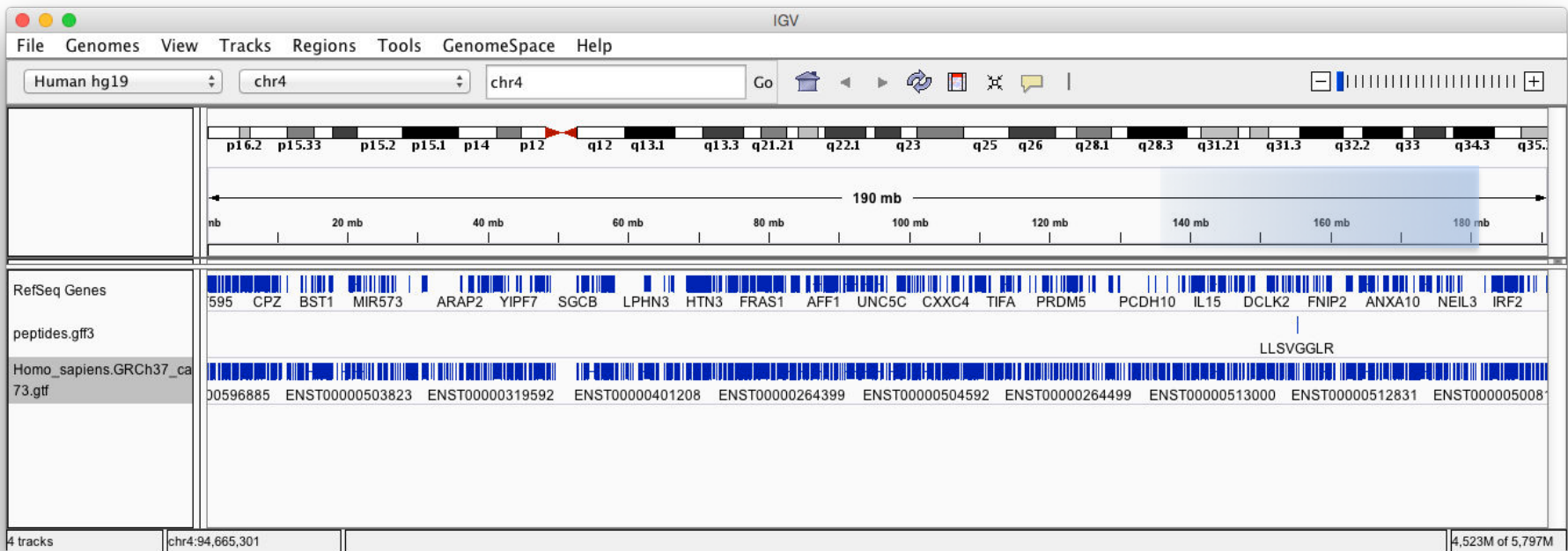
display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Strand

##gff-version 3





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Extract Features

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

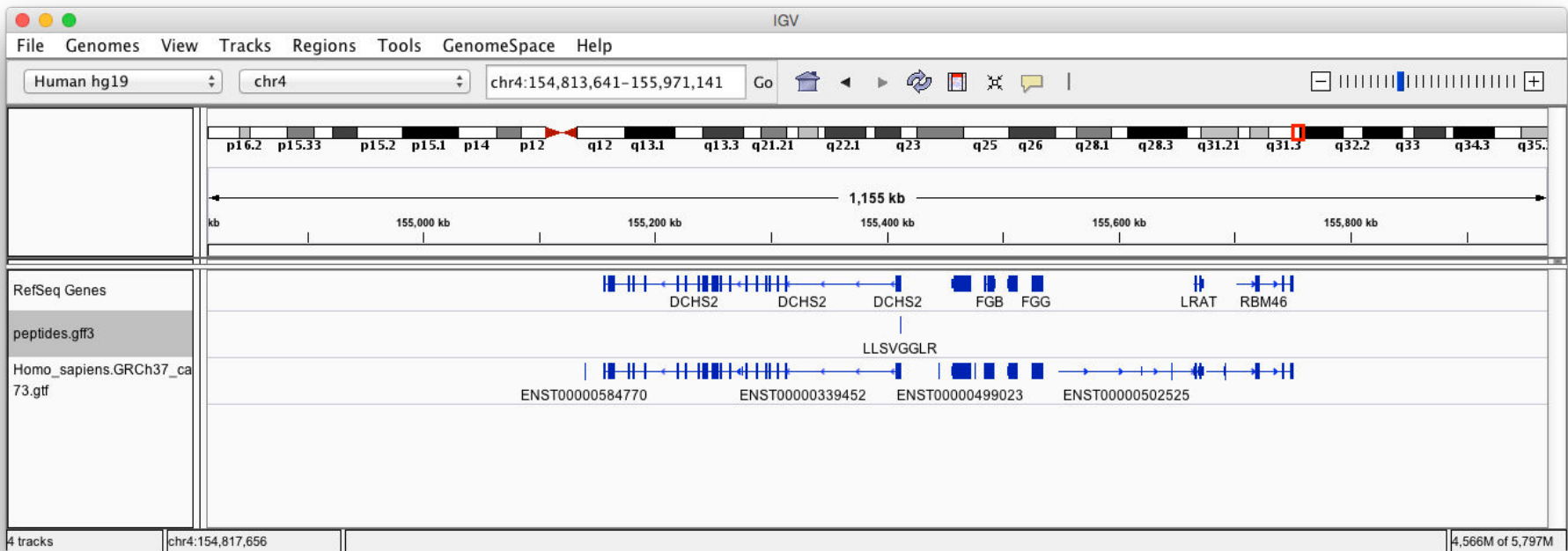
display with IGV web current local

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display at UCSC main

1.Seqid 2.Source 3.Type 4.Start

##gff-version 3



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Extract Features

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

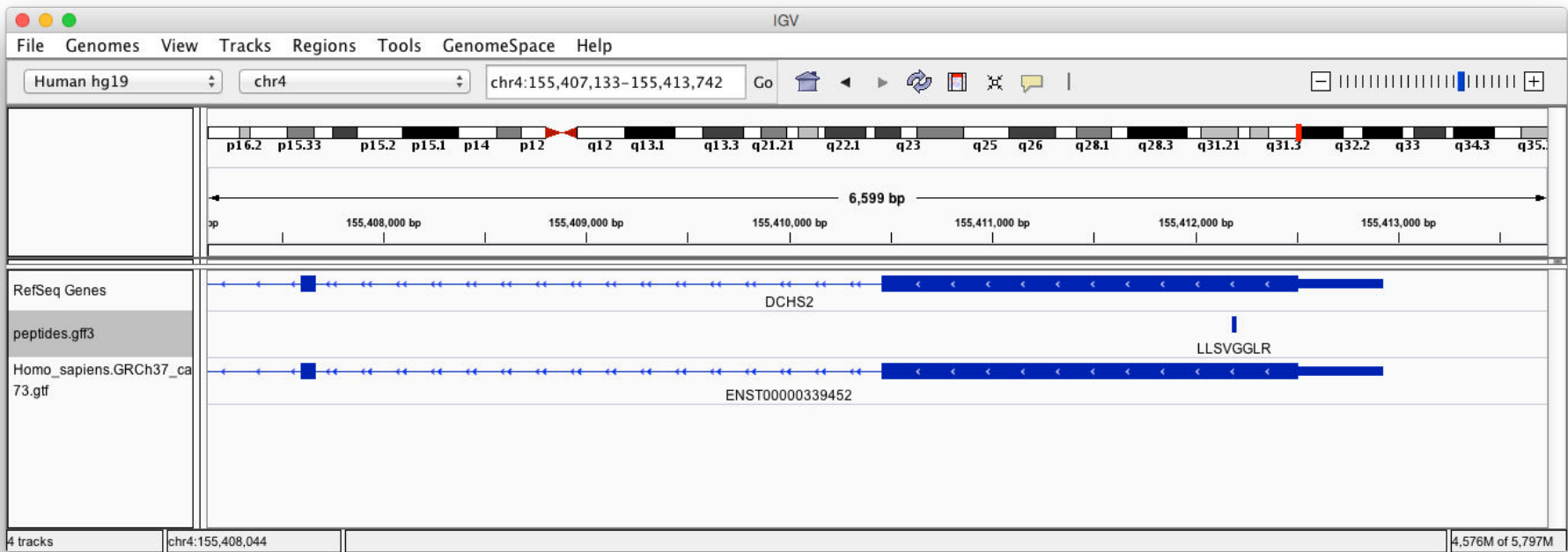
display with IGV web current local

display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Star

##gff-version 3



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Extract Features

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

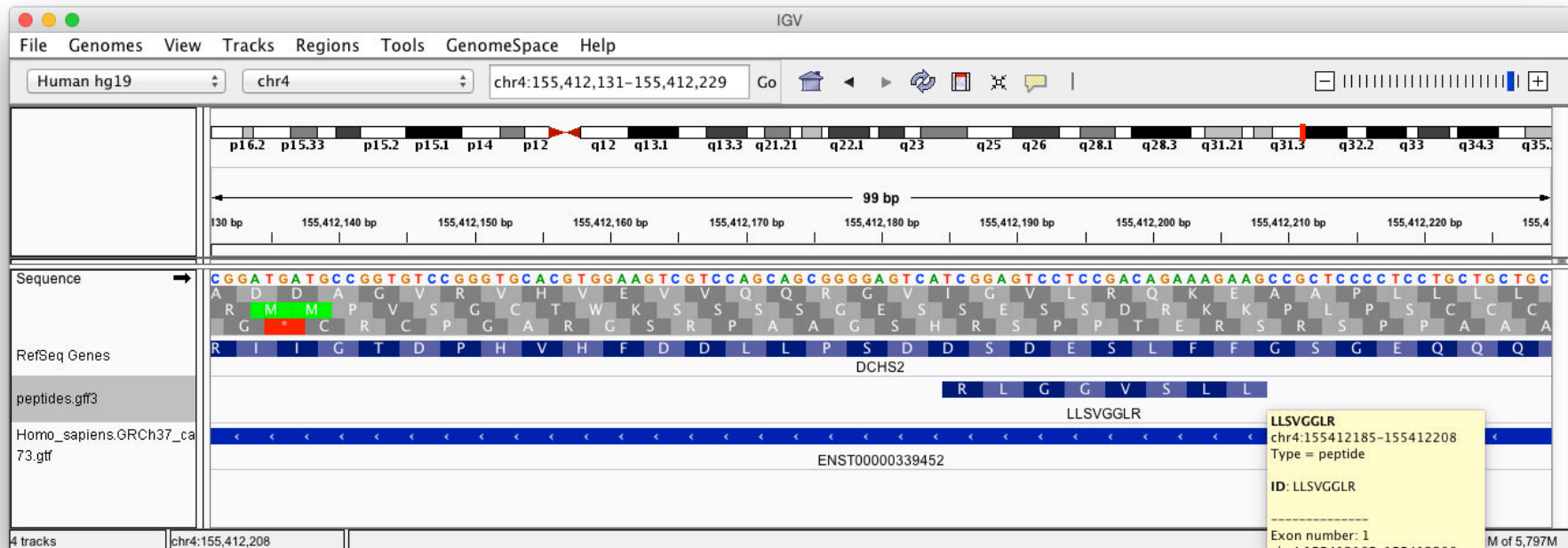
display with IGV web current local

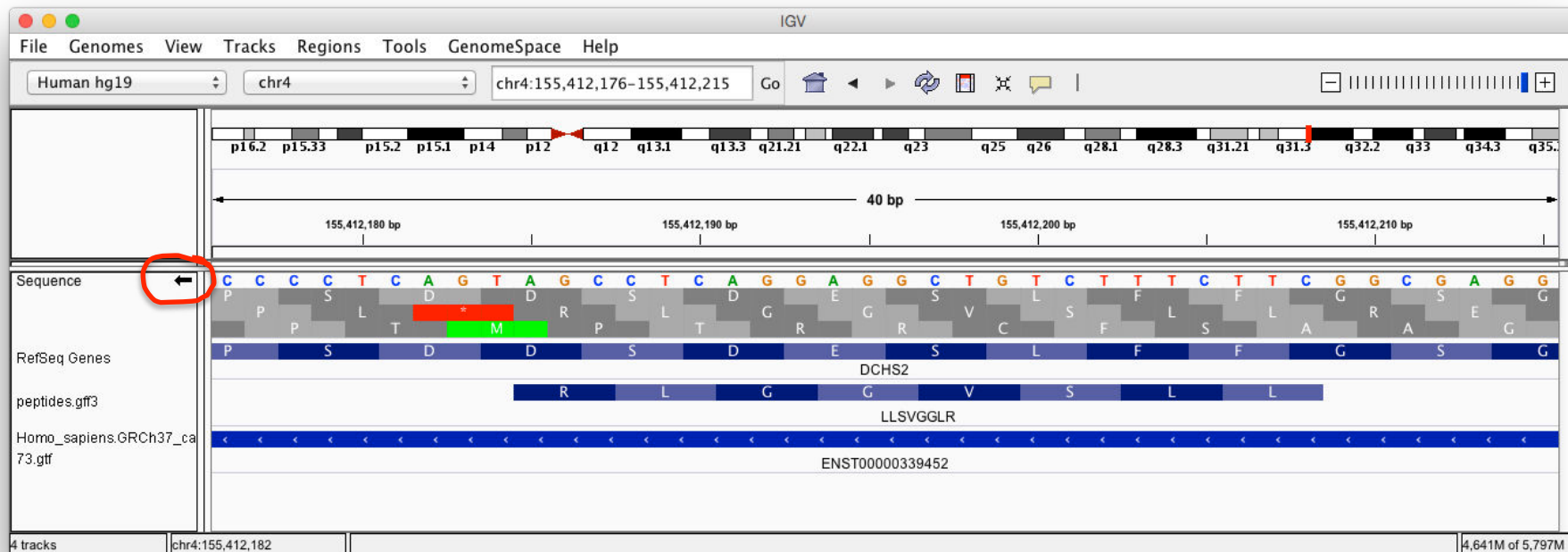
display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Star

##gff-version 3





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Using 183.9 GB

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

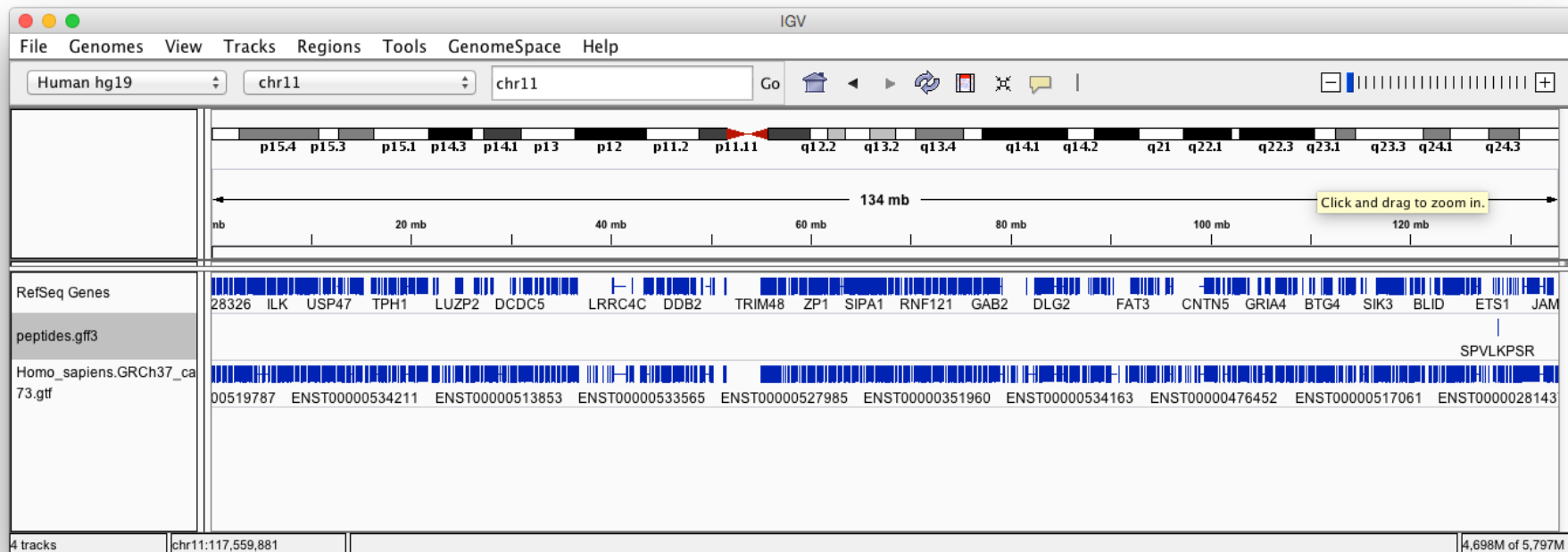
display with IGV web current local

display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Strand

##gff-version 3



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vim java py ruby GWT Galaxy MSI docker News DB bio prot html Mothur RickRack reg Norsk Apple HealthCare UniSci 2008 FMS CFS

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https://galaxy.msi.umn.edu/datasets/20e4f86aacb54c7f/show_params

Untitled

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Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

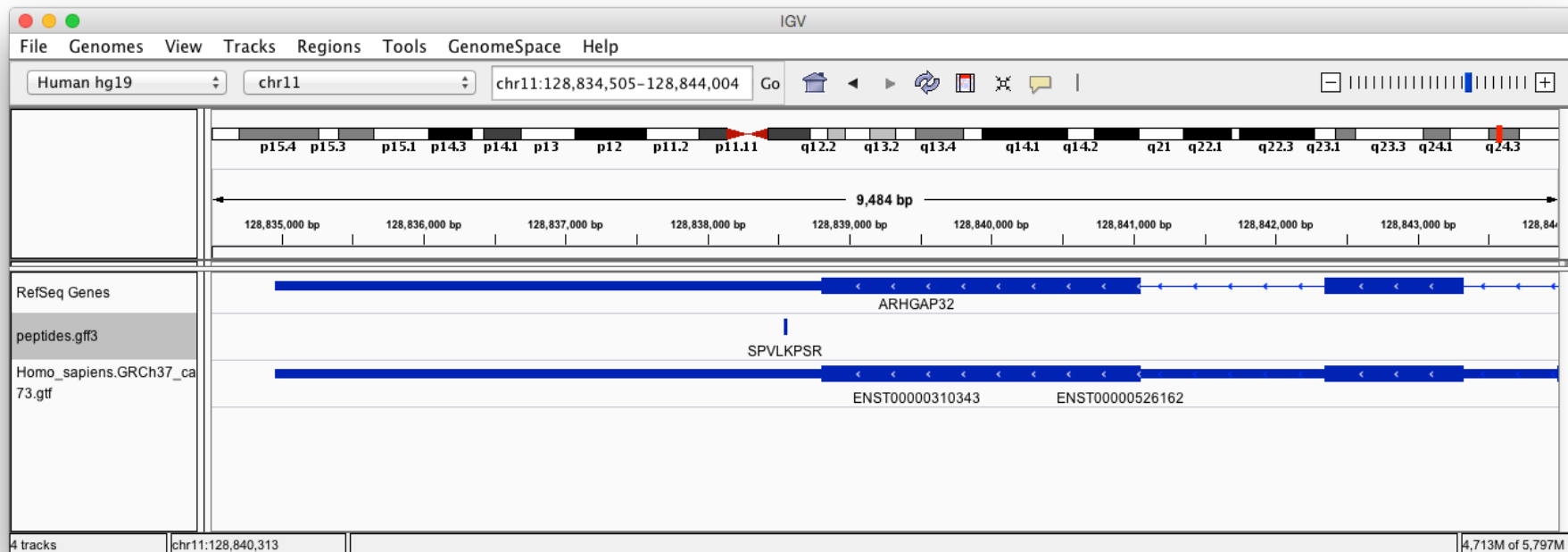
display with IGV web current local

display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Strand

##gff-version 3



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Extract Features

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

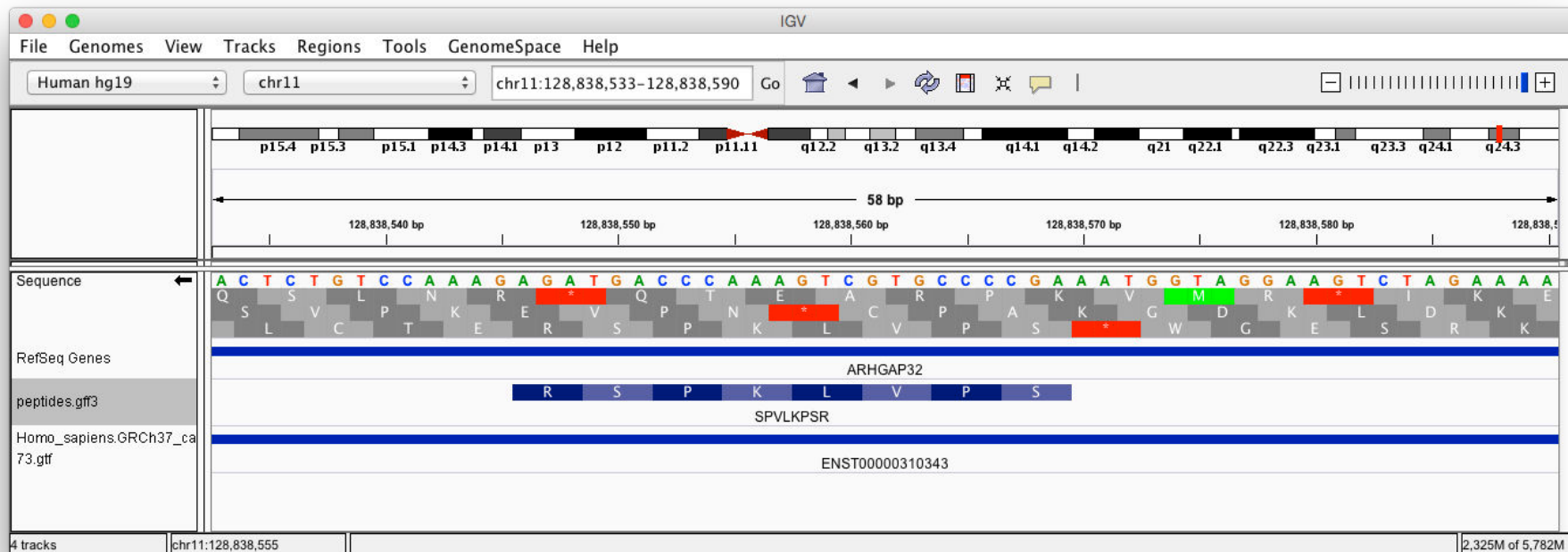
display with IGV web current local

display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Star

##gff-version 3



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Extract Features

Seqid	Source	Type	Start	End	Score	Strand	Phase	Attributes
##gff-version 3								
##sequence-region 4 1 155412208								
4	MassSpec	peptide	155412185	155412208	10.0	-	0	ID=LLSVGGLR
4	MassSpec	CDS	155412185	155412208	.	-	0	Parent=LLSVGGLR;transcript_id=ENST00000339452
##sequence-region 11 1 128838569								
11	MassSpec	peptide	128838546	128838569	10.0	-	0	ID=SPVLKPSR
11	MassSpec	CDS	128838546	128838569	.	-	0	Parent=SPVLKPSR;transcript_id=ENST00000310343

History

5: peptides.gff3

4 lines, 3 comments

format: gff3, database: hg19

Mapped 2 entries

display with IGV web current local

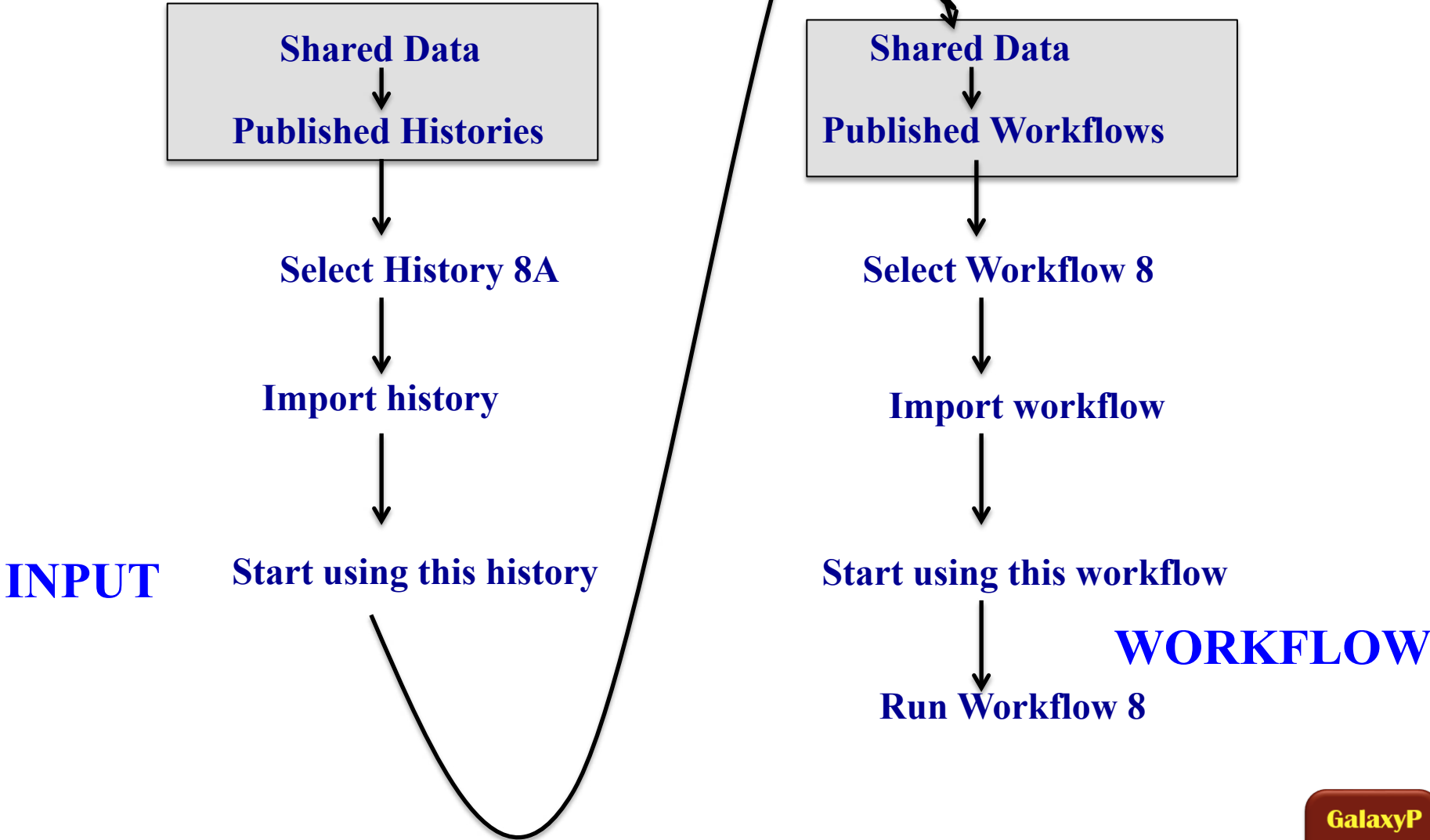
display at Ensembl Current

display at UCSC main

1.Seqid 2.Source 3.Type 4.Strand

##gff-version 3

8 Running the Entire Workflow



ENTIRE PROTEOGENOMICS WORKFLOW

INPUT

History 8A: Input for Entire Workflow
151.1 MB

search datasets

Dataset

- 1: ABRF-Spike4.fasta.fasta
- 2: FASTA File from EnSEMBL Searches.fasta
- 3: Mascot formatted MGF of data 7.mgf
- 4: Mascot formatted MGF of data 6.mgf
- 5: MGF Data Set List
- 6: Homo_sapiens.GRCh37.73.cdna.chr_4_17.fa
- 7: Homo_sapiens.GRCh37.canon.73.chr_4_17.gtf

WORKFLOW

Published Workflows

search name, annotation, owner, and tag

Advanced Search

Name

Workflow 8: Entire Proteogenomics Workflow.

Published Histories

search name, annotation, owner, and tag

Advanced Search

Name

Entire History

Running workflow "Workflow 8: Entire Proteogenomics Workflow."

Expand All Collapse

Step 1: Input dataset

Subset of 3-frame translated database

2: FASTA File from EnSEMBL Searches.fasta

type to filter

Step 2: Protein Database Downloader (version 0.2.0)

Step 3: Input dataset

Spiked in proteins

1: ABRF-Spike4.fasta.fasta

type to filter

Step 4: Protein Database Downloader (version 0.2.0)

Step 5: Input dataset collection

MGF Files (dataset collection)

5: MGF Data Set List

type to filter

Step 6: Input dataset

cDNA database

55: Homo_sapiens.GRCh37.73.cdna.chr_4_17.fa

type to filter

Step 7: Input dataset

GTF File

56: Homo_sapiens.GRCh37.canon.73.chr_4_17.gtf

type to filter

Step 8: Regex Find And Replace (version 0.1.0)

Step 9: FASTA Merge Files and Filter Unique Sequences (version 1.0)

History

search datasets

imported: Entire History

57 shown

907.4 MB

60: Peptide to GFF peptide.gff3

59: Peptide to GFF peptide.unmapped

57: Column Regex Find And Replace on data 56

56: Homo_sapiens.GRCh37.canon.73.chr_4_17.gtf

55: Homo_sapiens.GRCh37.73.cdna.chr_4_17.fa

54: mz to sqLite on data 14, data 3, and others

53: BLAST-P Filtered Peptide Report

52: BLAST-P Filtered Peptides

51: Concatenate datasets on data 49 and data 50

50: Concatenate datasets on data 48 and data 42

49: Concatenate datasets on data 40 and data 47

48: Cut on data 46

47: Cut on data 45

OUTPUT

INPUTS SEARCHGUI PEPTIDESHAKER BLAST-P PSM Viz Genome Visualization



UNIVERSITY OF MINNESOTA
Driven to DiscoverSM

Biochemistry, Molecular Biology &
Biophysics

Kevin Murray

Ray Sajulga

Candace Guerrero

Center for Mass Spectrometry
and Proteomics

Ebbing de Jong

LeeAnn Higgins

Todd Markowski

UNIVERSITY OF MINNESOTA
**SUPERCOMPUTING
INSTITUTE**

Tom McGowan

Trevor Wennblom

Getiria Onsongo

Bill Gallip

Ben Lynch



**COMMUNITY BASED
SOFTWARE DEVELOPMENT**

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University of Bergen, Bergen,

Norway

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*University of Freiburg, Freiburg,
Germany*

Lennart Martens

*VIB Department of Medical Protein
Research, Ugent, Belgium*

Ira Cooke

*La Trobe University, Melbourne ,
Australia*

John Chilton

Galaxy Team

Penn State University

July 7th 2015: Session II : 11:20 AM [Proteomics Visualization in Galaxy](#)

James E. Johnson

July 8th 2015: Session 7 : 2:05 PM: Extending Galaxy's reach: recent progress towards complete multi-omic data analysis workflows.

Timothy J Griffin

Funding
NSF, NIH

