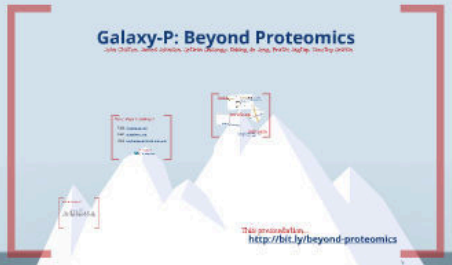

Toolbox Filters

Large Numbers of Files

Windows

LWR

Tool Macros

Cloud

Binary Data Types

Galaxy-P: Beyond Proteomics

Galaxy-P: Beyond Proteomics

John Chilton, James Johnson, Getiria Onsongo, Ebbing de Jong, Pratik Jagtap, Timothy Griffin

Three ways to Galaxy-P

Public usegalaxyp.org

Local getgalaxyp.org

Cloud biocloudcentral.msi.umn.edu

...or maybe 4

Twitter @usegalaxyp

Tools

Workflows

Outreach

What is Galaxy-P?

This presentation...

http://bit.ly/beyond-proteomics

What is Galaxy-P?

nearing end of year 1

Three year NSF funded grant to build mass spec & proteomics data analysis platform on top of Galaxy.

Three ways to Galaxy-P

Public **usegalaxyp.org**

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Tools

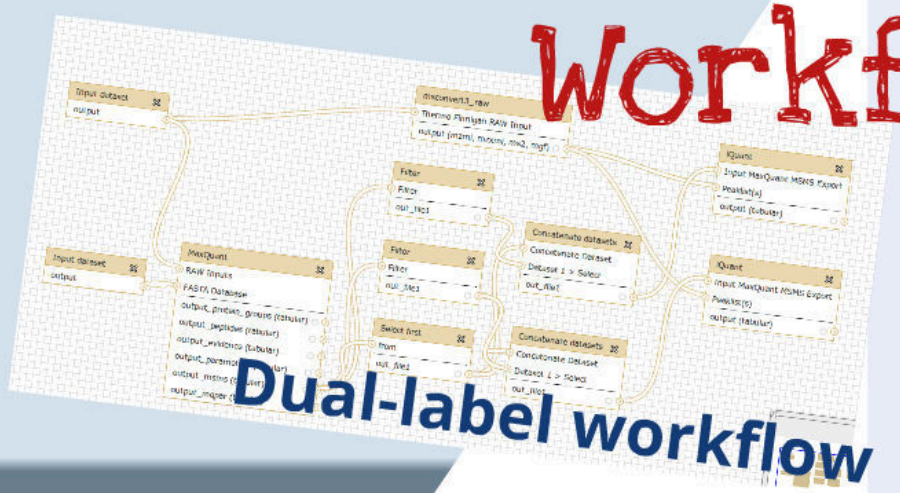
Category Proteomics

search repository name, description

Name ↓	Synopsis	Metadata Revisions	Tools Verified	Owner
appendfdr	Add false discovery rate to tabular data.	0:ef7cc296f063	no	galaxyp
bumbershoot	Tool wrappers for applications in the Tabb lab's Bumbershoot suite.	2:e07c19262374	no	galaxyp
dbbuilder	This tool allows users to download protein databases from common sources.	2:6c624803c5f9	no	galaxyp
	Galaxy tool wrapper for the			

Proteomics category has 3rd most repositories on tool shed.

Workflows



Dual-label workflow

Jagtap's Minnesota Two Step

Outreach

Huge presence at ASMS 2013, generated a lot of buzz.

Galaxy-P: Beyond Proteomics

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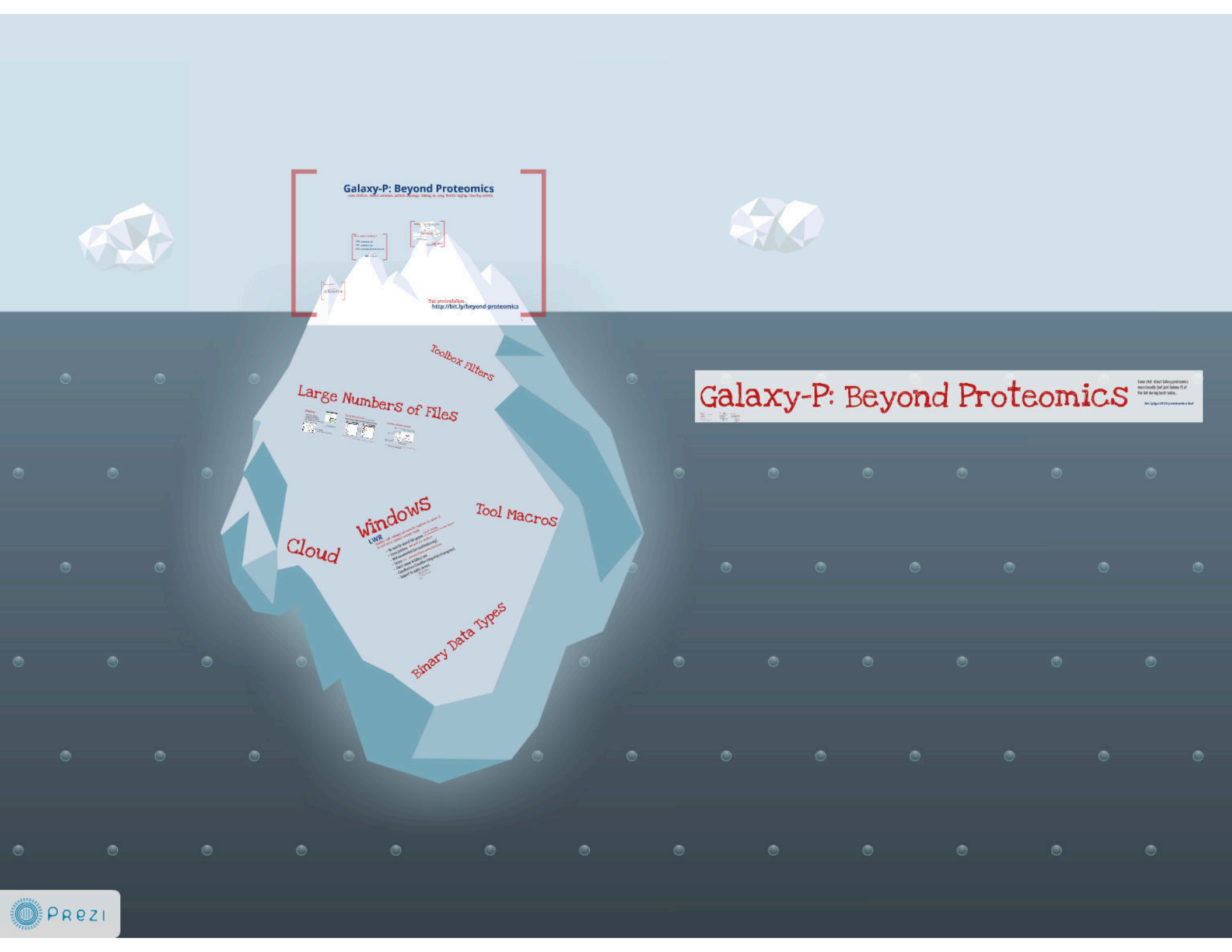
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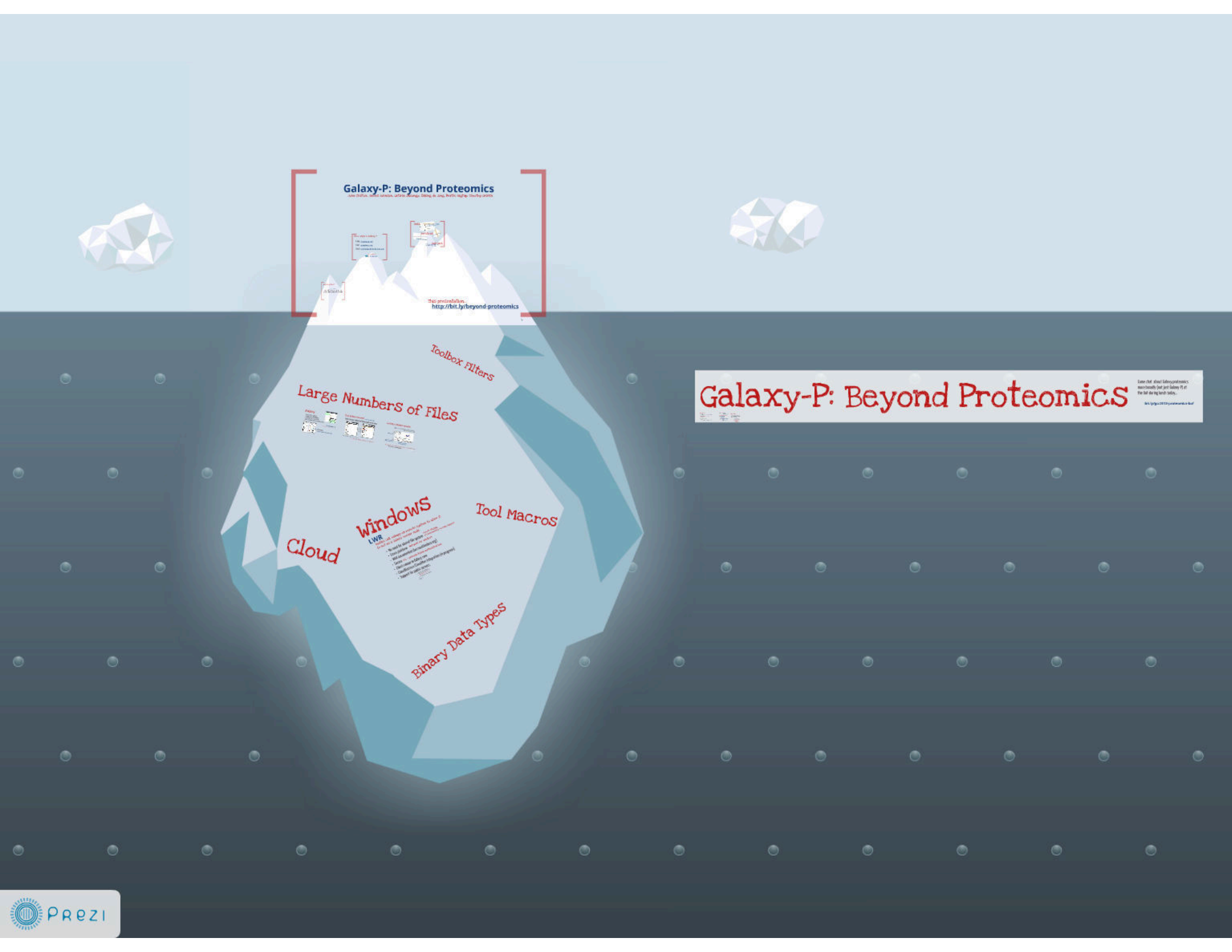
Come chat about Galaxy proteomics more broadly (not just Galaxy-P) at the BoF during lunch today...

bit.ly/gcc2013-proteomics-bof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windows

LWR

Install LWR webapp on remote system to allow it to act as a Galaxy worker node.

- No need for shared file system — remote staging w/experimental caching support
- Cross-platform — Not just for windows
- Well documented (lwr.readthedocs.org)
- Secure — SSL + private token authentication
- Client runner in Galaxy now
- CloudBioLinux/CloudMan integration (in progress)
- Support for public servers.

public servers

- Point LWR at a toolbox to describe what it can run.
- Markup your standard Galaxy tool XML to lock down how it runs. then any Galaxy instance can run these tools on your resource
- Easily share access to specialized hardware, large datasets, etc...
- One click access...

http://bit.ly/galaxy-extras

```
<tool>
  ...
  <default_destination runner="lwr">
    <param id="url">https://example.com:8913/</param>
  </default_destination>
  ...
```

Publish tools with default public server instances to the tool shed

ne click access

http://bit.ly/galaxy-extras

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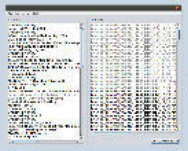
  </default_destination>
  ...
```

Publish tools with default public server instances to the tool shed and provide one-click access to your compute and data.

Large Numbers of Files

JGalaxy

- Java Web Start Application
- Batch Download and Upload Files
- Get around browser upload limits
- Many API enhancements contributed upstream



bit.ly/galaxy-extras

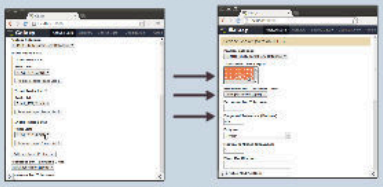
Optional Galaxy extensions for direct access

Built on blend4j

github.com/jmchilton/blend4j

Tool Enhancements (in your Galaxy now)

Tools can now take in multiple inputs at all once.

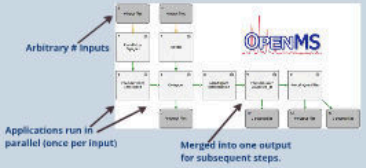


Convenient for a specifying a few inputs, necessary for dozens or hundreds.

Replace dataset <repeat> elements with <input type="data" multiple="true">

Workflow Enhancements

"An Automated Pipeline for High-Throughput Label-Free Quantitative Proteomics (J. Proteome Res., 2013, PMID: 23391308)."



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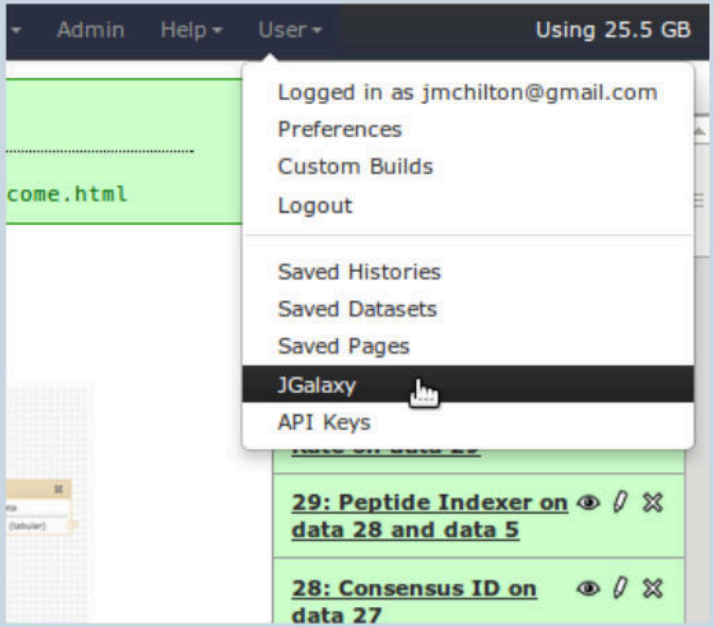
http://toolshed.g2.bx.psu.edu/view/jpaprotsys/openms

JGalaxy



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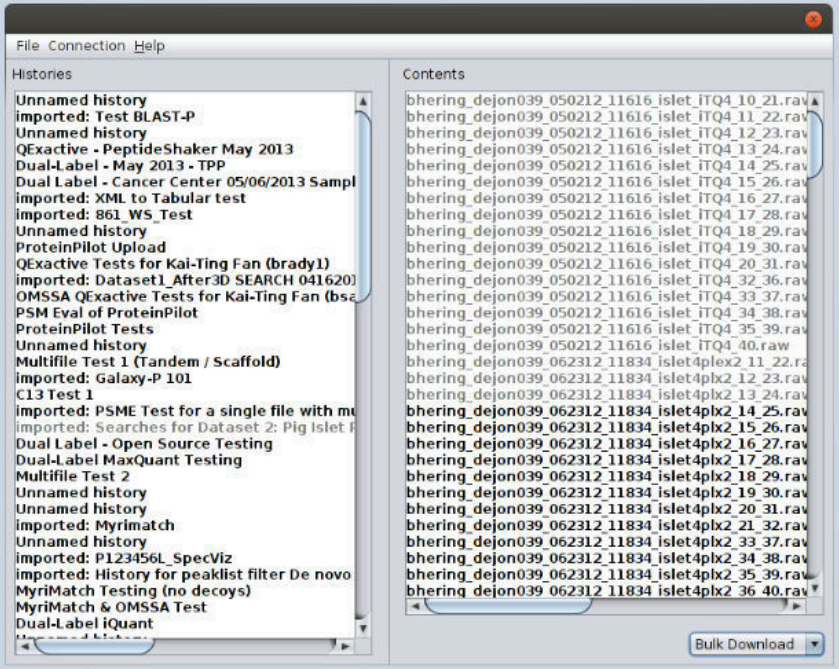

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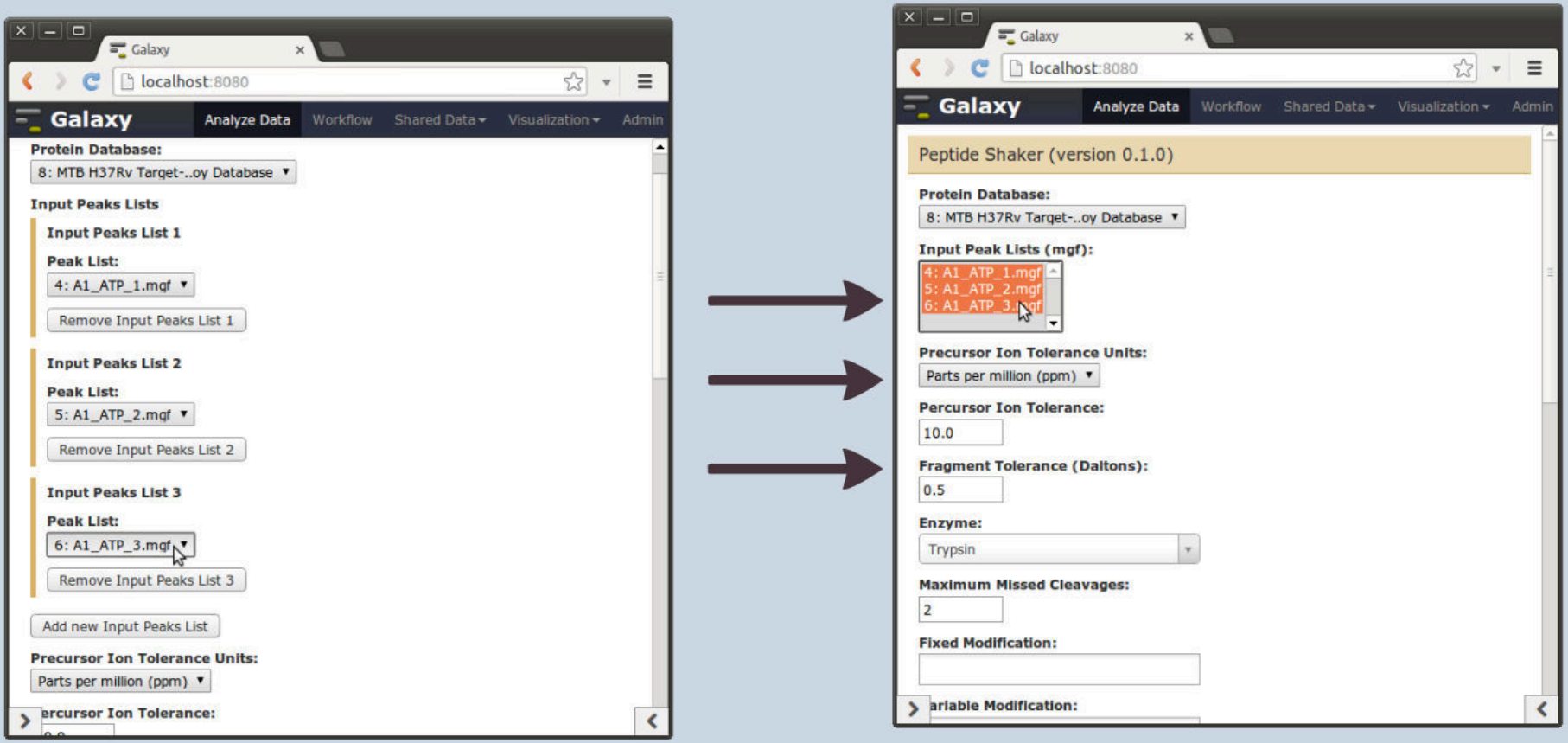

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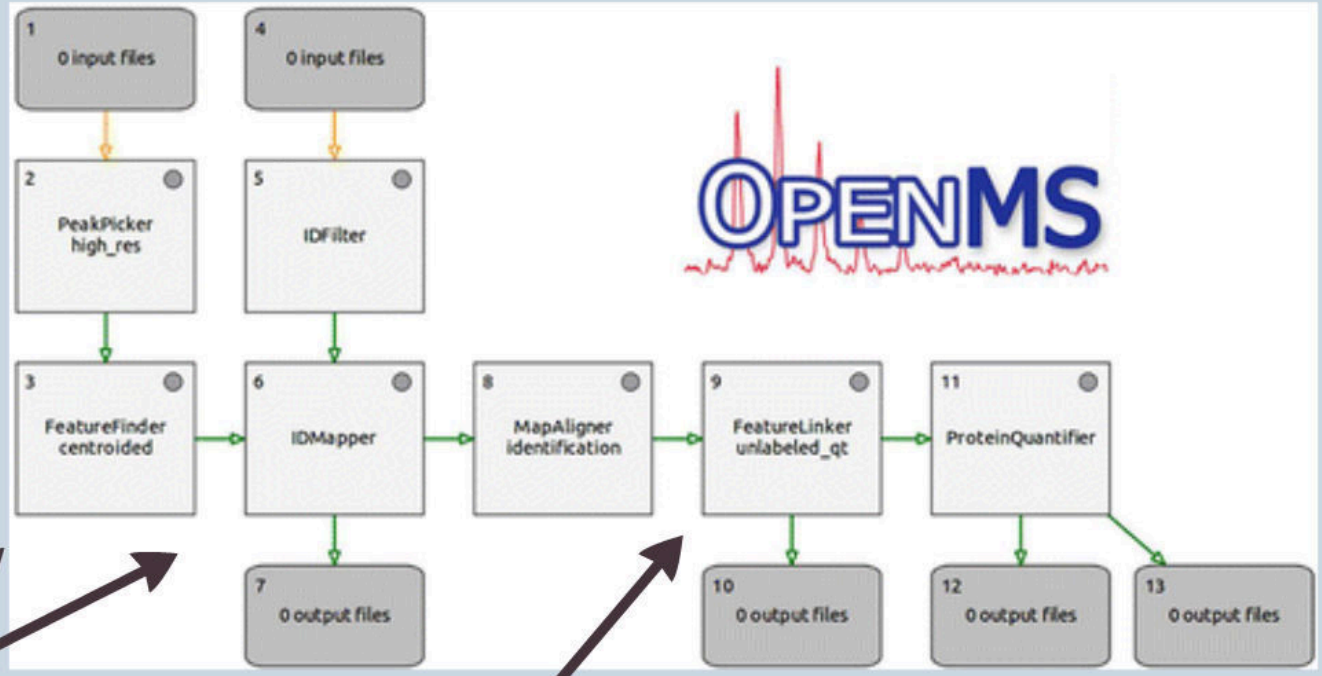

Arbitrary # Inputs

Applications run in parallel (once per input)

Merged into one output for subsequent steps.

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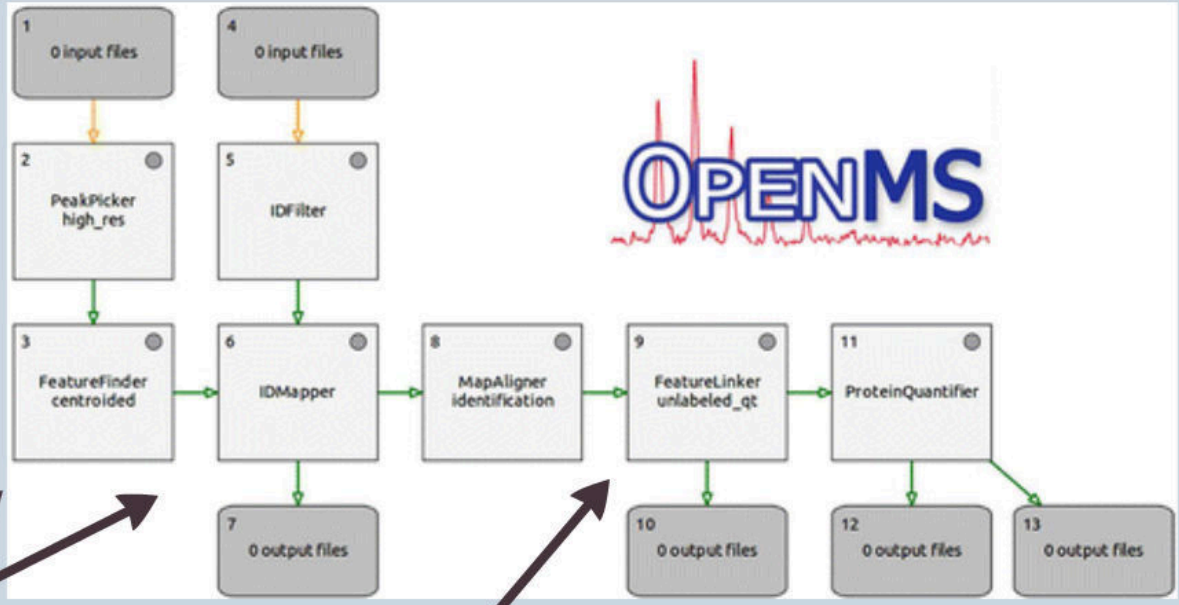

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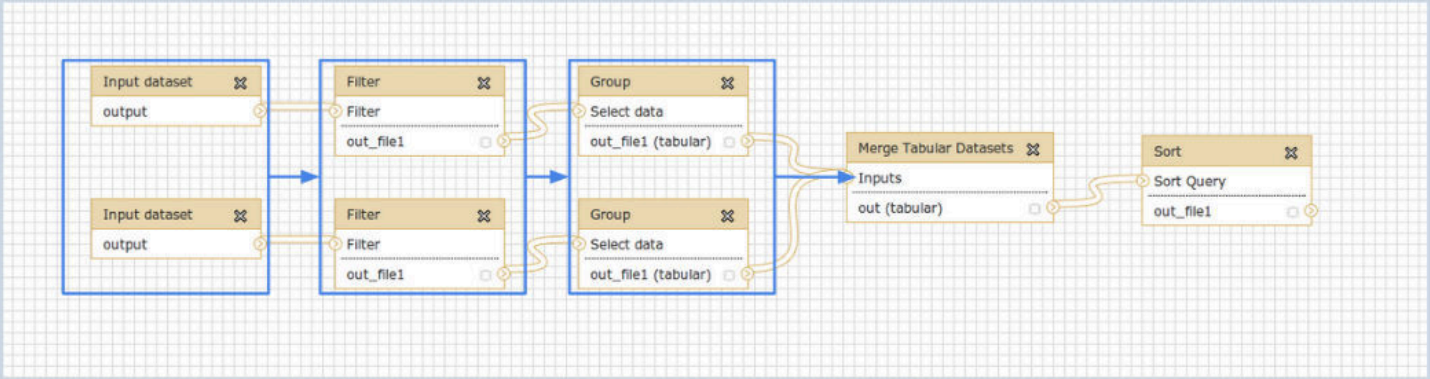
Galaxy-P can!

Multiple File Datasets



...group multiple files into a single dataset to "flatten" workflow.

Not just for toy workflows...

Jagtap's "Shamelessly Seamless" Proteogenomics workflow

- 150+ steps - Multiple identifications, BLAST, custom tools for spectral validation and genome mapping
- Takes 3 days to run on a Fractionated 52 RAW file sample
- Multiple LWR steps.
- Tools and datatypes are NOT adapted for multiple file datasets

Not just for proteomics...

nothing proteomics related

bit.ly/galaxy-extras

Track or merge multiple file datasets into your Galaxy.

Other Applications:

Imaging:

"...it is needed for the community. I don't think we have other options for our requirements. [The] multiple file datasets implementation was a real saver for us."

Alex Khassapov, CSIRO

Genomics:

I am using it with success for chip-seq and rna-seq analysis.

Hagai Cohen, Hebrew University

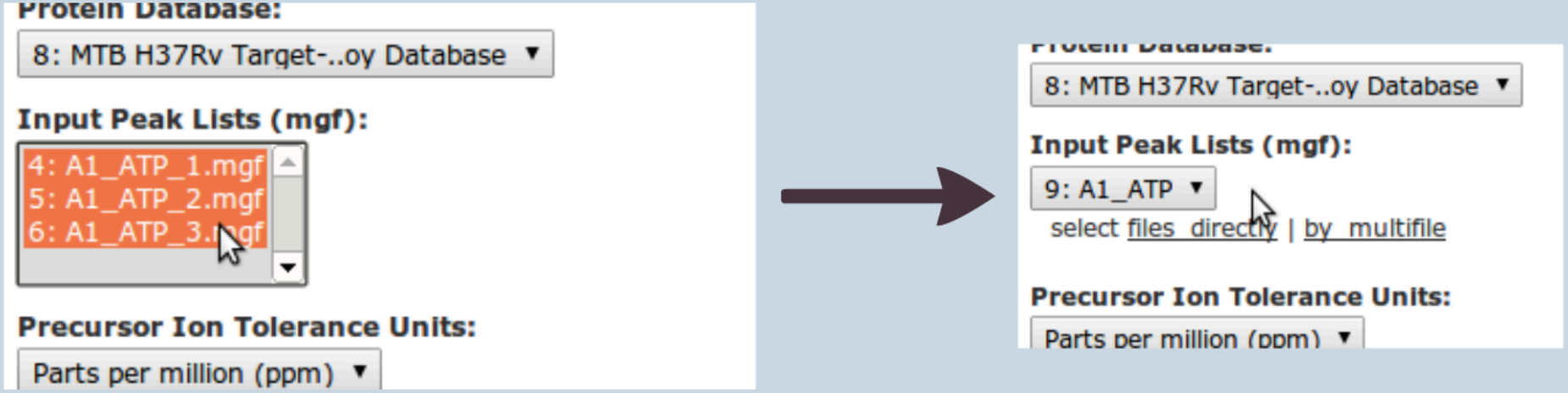
Not just improved grouping...

Addresses additional limitations of Galaxy.

Sample tracking throughout complex workflows...

Tools with many-to-many outputs...

Merging or many-to-one tools...



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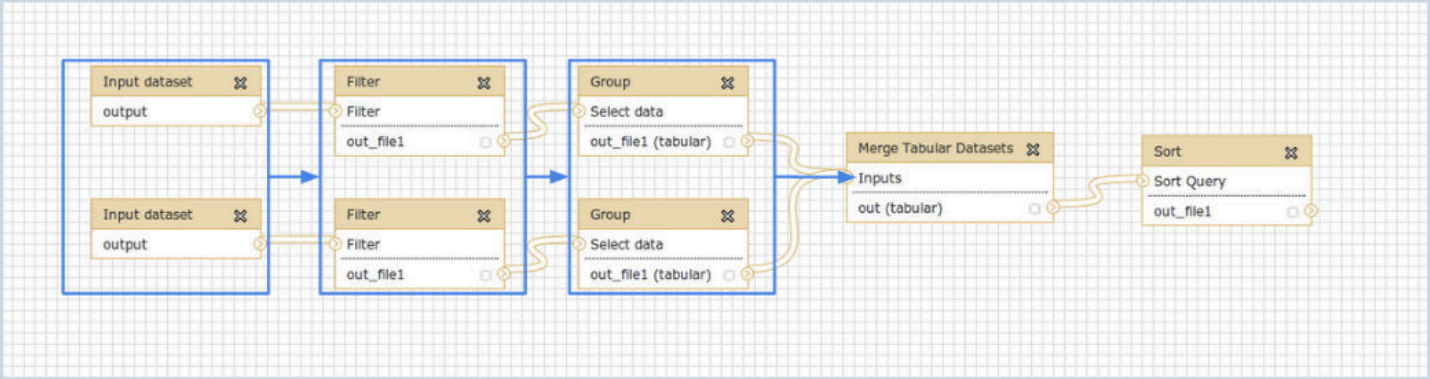

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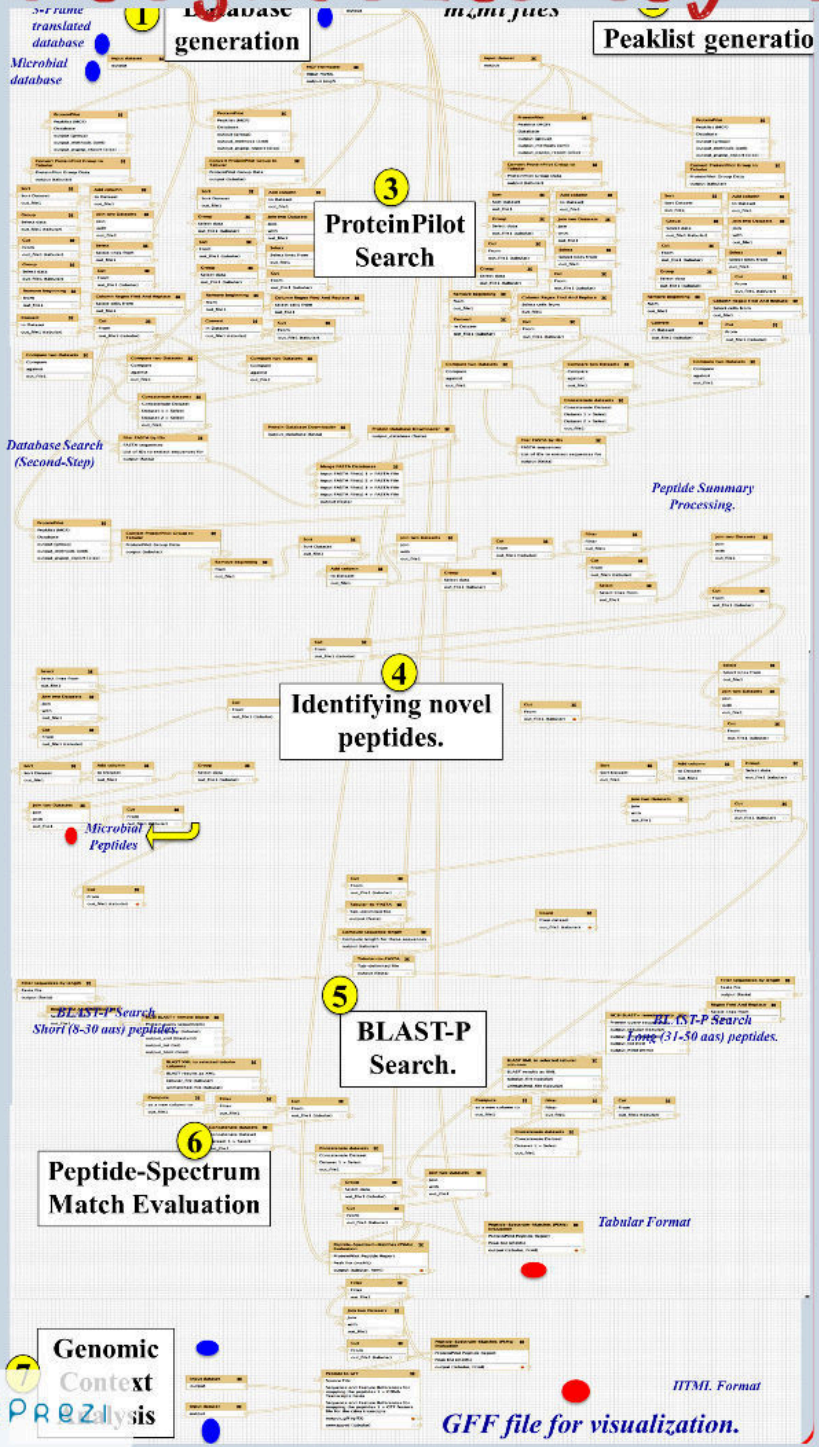

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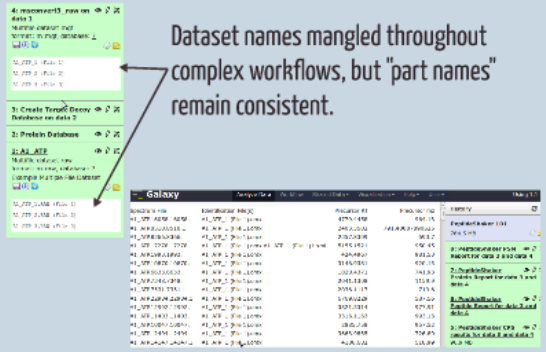

Dataset names mangled throughout complex workflows, but "part names" remain consistent.

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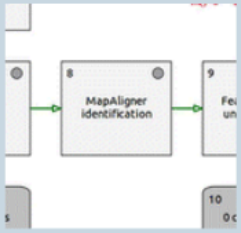


Aligns feature space of each input against all others...

With current implementation, the tool does "need to know" it produces multiple file dataset.

Sample tracking th

4: msconvert3_raw on data 1
Multifile dataset mgf
format: m:mgf, database: ?

A1_ATP_1 (File 1)
A1_ATP_2 (File 2)
A1_ATP_3 (File 3)

3: Create Target-Decoy Database on data 2

2: Protein Database

1: A1_ATP
Multifile dataset raw
format: m:raw, database: ?
Example Multiple File Dataset

A1_ATP_1.RAW (File 1)
A1_ATP_2.RAW (File 2)
A1_ATP_3.RAW (File 3)

Dataset names mangled throughout complex workflows, but "part names" remain consistent.

Galaxy | Analyze Data | Workflow | Shared Data | Visualization | Help | User | Using 1.1

Spectrum File	Identification File(s)	Precursor RT	Precursor mz
A1_ATP.16058.16058.	A1_ATP_1 (File 1).omx	4779.4458	964.13
A1_ATP.8510.8510.1	A1_ATP_1 (File 1).omx	2403.5502	791.40087890625
A1_ATP.8366.8366.	A1_ATP_1 (File 1).omx	2357.8309	693.7
A1_ATP.17278.17278.	A1_ATP_1 (File 1).omx A1_ATP_1 (File 1).t.xml	5155.1521	950.45
A1_ATP.1993.1993.	A1_ATP_1 (File 1).omx	424.4967	981.53
A1_ATP.10870.10870.	A1_ATP_1 (File 1).omx	3146.9381	920.13
A1_ATP.6633.6633.	A1_ATP_1 (File 1).omx	1820.4371	741.93
A1_ATP.7348.7348.	A1_ATP_1 (File 1).omx	2041.1308	1159.9
A1_ATP.7331.7331.1	A1_ATP_1 (File 1).omx	2036.1117	719.6
A1_ATP.22984.22984.1	A1_ATP_1 (File 1).omx	6769.8229	587.56
A1_ATP.12992.12992.	A1_ATP_1 (File 1).omx	3821.3314	977.91
A1_ATP.11403.11403.	A1_ATP_1 (File 1).omx	3316.1163	993.13
A1_ATP.10047.10047.	A1_ATP_1 (File 1).omx	2885.758	957.52
A1_ATP.12494.12494.	A1_ATP_1 (File 1).omx	3663.9835	726.89
A1_ATP.14147.14147.1	A1_ATP_1 (File 1).omx	4186.682	518.99

History

PeptideShaker 101
764.5 MB

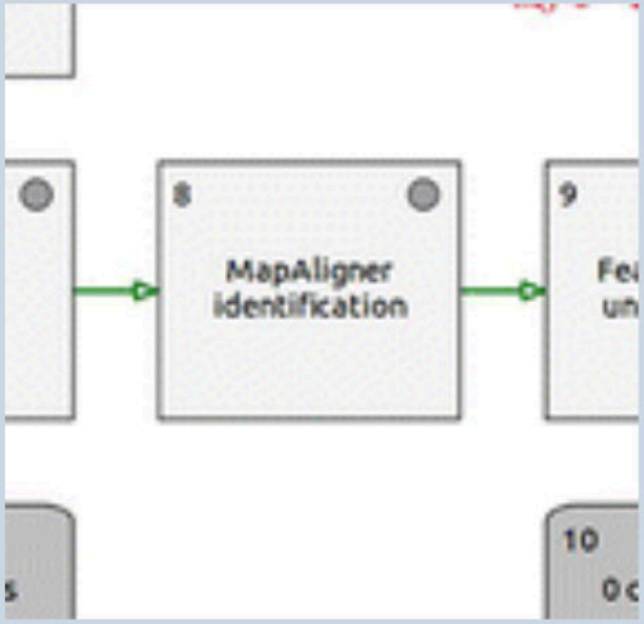
8: PeptideShaker PSM Report for data 3 and data 4

7: PeptideShaker Protein Report for data 3 and data 4

6: PeptideShaker Peptide Report for data 3 and data 4

5: PeptideShaker CPS results for data 3 and data 4
96.9 MB

many-to-many outputs...



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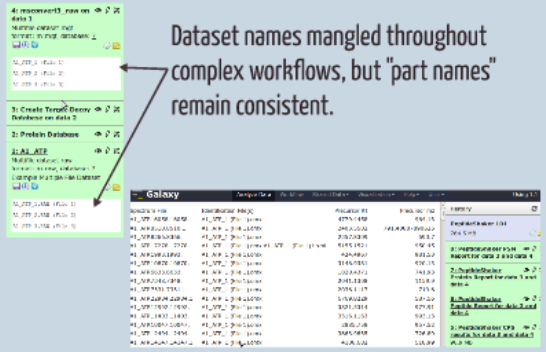

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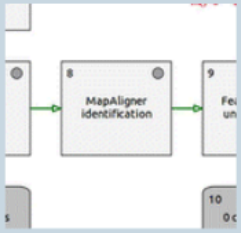

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Special Thanks...

Jorrit Boekel

Implemented an early version of multiple file datasets at tool and datatype level.

Galaxy-P and Galaxy Teams @ MSI

w/Special, Special thanks to Anne-Francoise Lamblin & Benjamin Lynch

Dannon, Nate, Enis, Brad, Jeremy, Ira & Dave Clements

Hardest working man in Galaxy

People in Galaxy community who helped with various parts of this

Have mass spec data?

Galaxy-P!

Three ways to Galaxy-P...

Public **usegalaxyp.org**

Local **getgalaxyp.org**

Cloud **biocloudcentral.msi.umn.edu**

or maybe 4...

Twitter **@usegalaxyp**

Why fork?

Because the Galaxy team would like a more flexible, deeply integrated concept of dataset grouping.

I do too!

Galaxy team doesn't want to support this.

Make me a committer on Bitbucket, problem solved!

Encumber the code base with special cases. (Technical debt.)

Pull Requests:

#86: Datatype Tracking Enhancements

#169: Support config files with task parallelism.

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Pull Requests:

#86: Datatype Tracking Enhancements

#169: Support config files with task parallelism.

#87: Framework for per job task parallelism.

#:83 More flexible task merging.

#122: Eliminate hard coding of upload1 tool hacks.

#133: Fix file_ext in image datatypes.

#123: Refactor huge functions in library_common.

#:142 Simplify task splitting input specification.

#156: Fix 'from_work_dir' with task splitting.