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**External User Guide for Performing High Throughput Searches on TDPortal**

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**Part 2: TDPortal Page Orientation.....Step 2**

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**Part 4: Running Searches on TDPortal.....Step 15 - Step 18**

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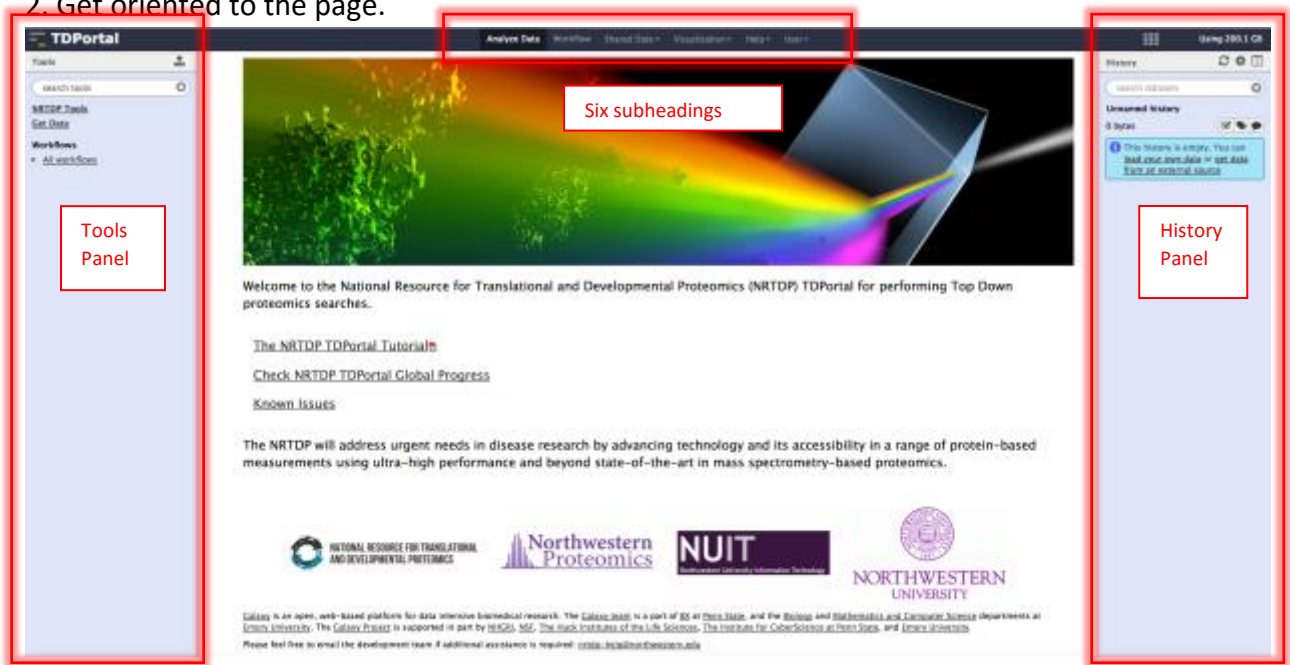
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## Part 1: Transferring Project Files to TDPortal

1. Log in to TDPortal at <https://portal.nrtdp.northwestern.edu> with your Northwestern email and password.

## Part 2: TDPortal Page Orientation

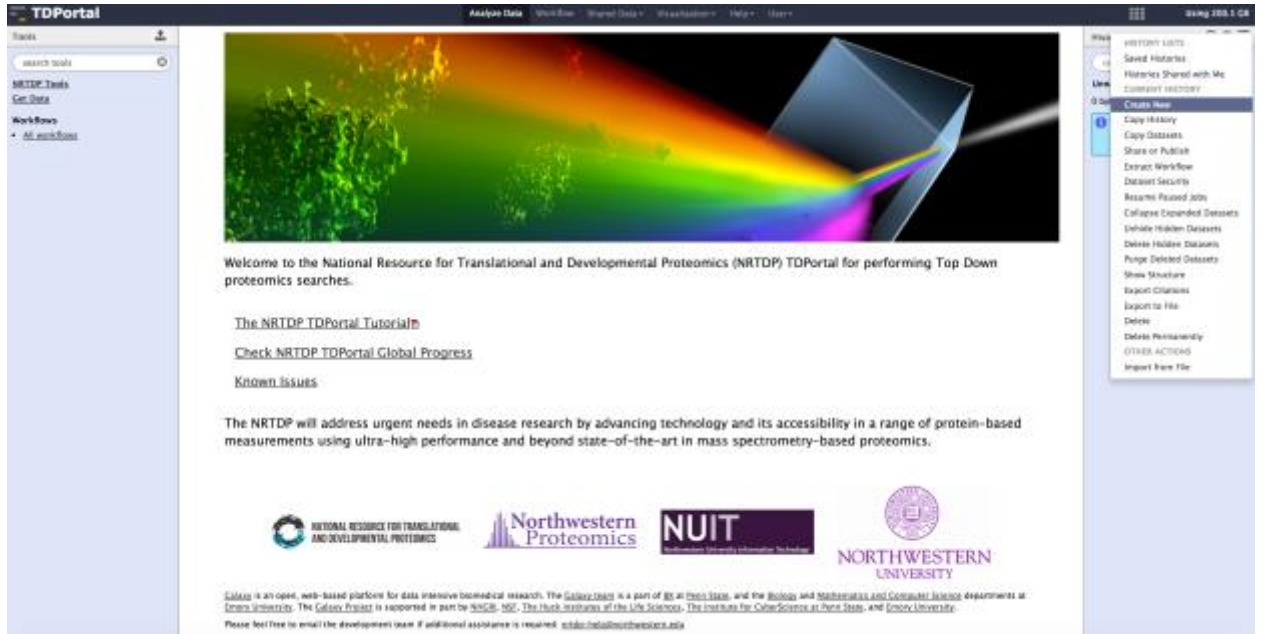
2. Get oriented to the page.



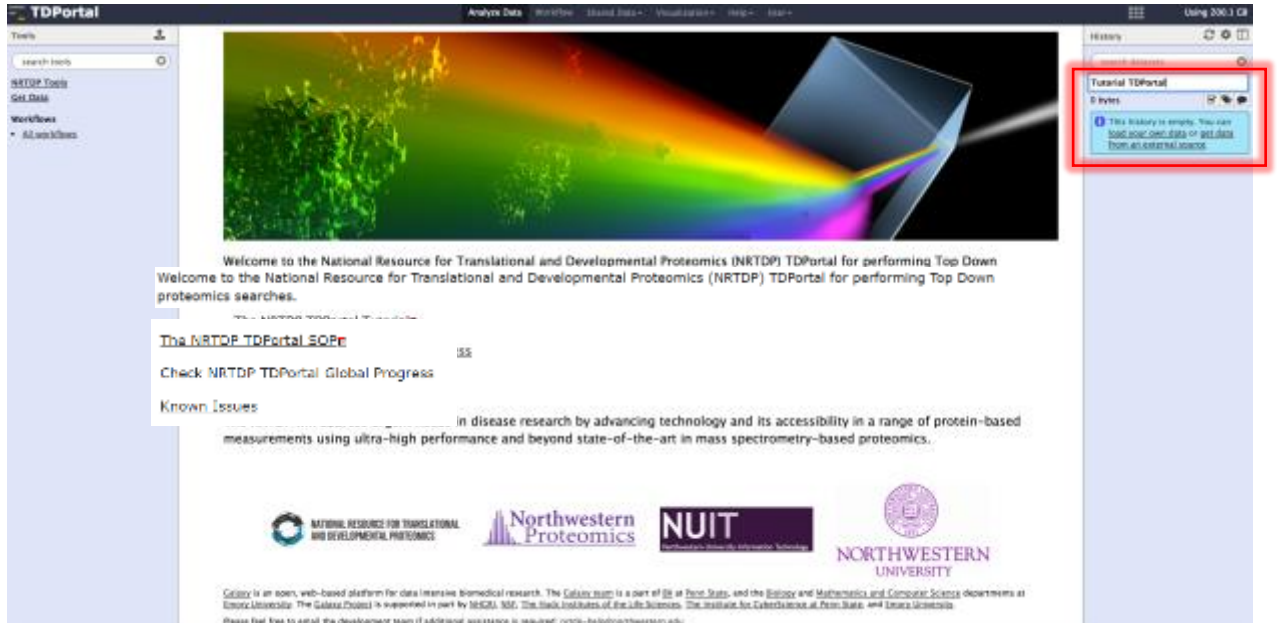
- a. There are six subheadings that link to different pages.
- b. The History Panel is on the right. When data is uploaded or an analysis is performed, each output generates a dataset. These datasets are stored by TDPortal in the History Panel.
- c. All of the available tools are located in the blue Tools Panel on the left.
- d. The NRTDP designed tools are located in the NRTDP Tools menu in the Tools Panel.

### Part 3: Preparing Raw files for the TDPortal Search

- 3. Create a new history. Go to the history column and click on the gear in the top right. A drop down menu will appear. Click on "Create New."



- 4. Rename the new history by clicking on "Unnamed History."



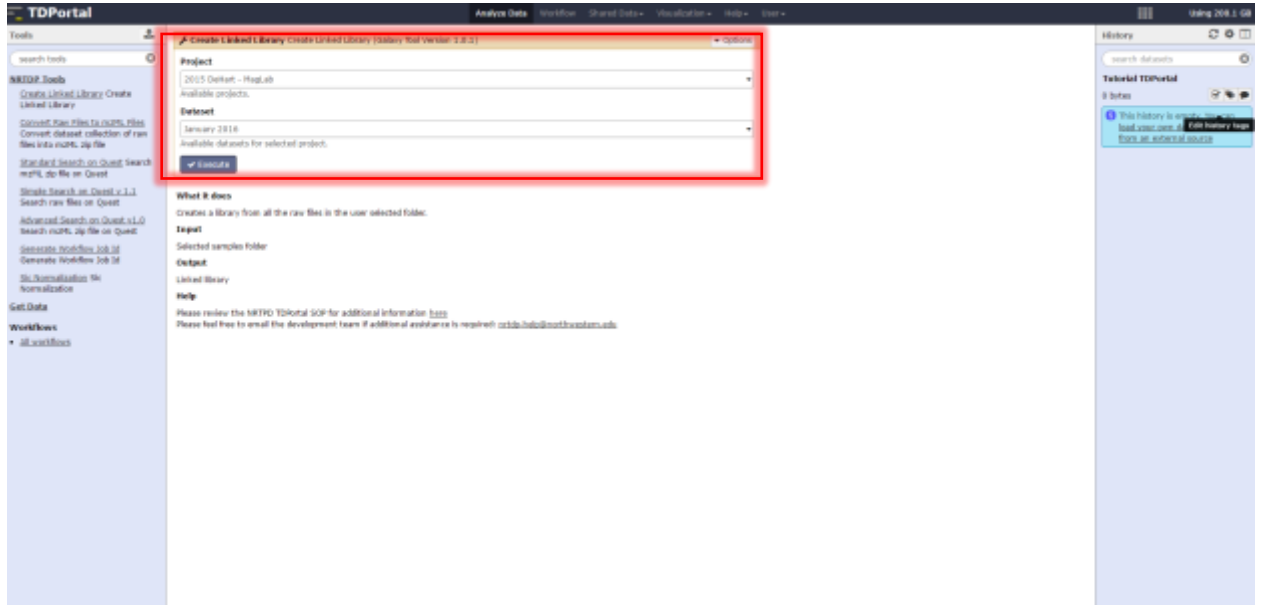
- 5. Go to Tools Panel and click on “NRTDP Tools.” A menu containing all the available NRTDP tools will appear.



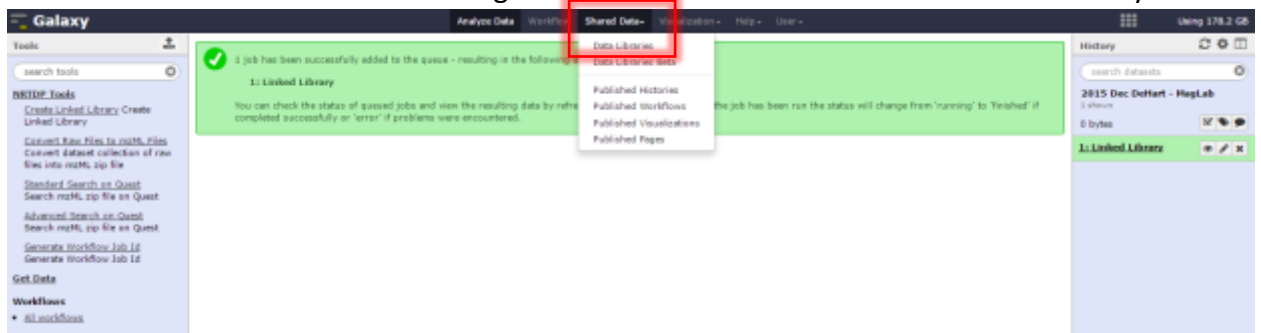
- 6. Click on “Create Linked Library” to create a linked library.



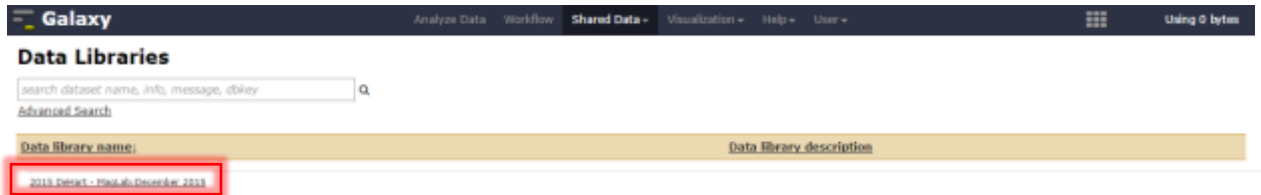
7. Select the dataset that will be searched. Click “Execute.”



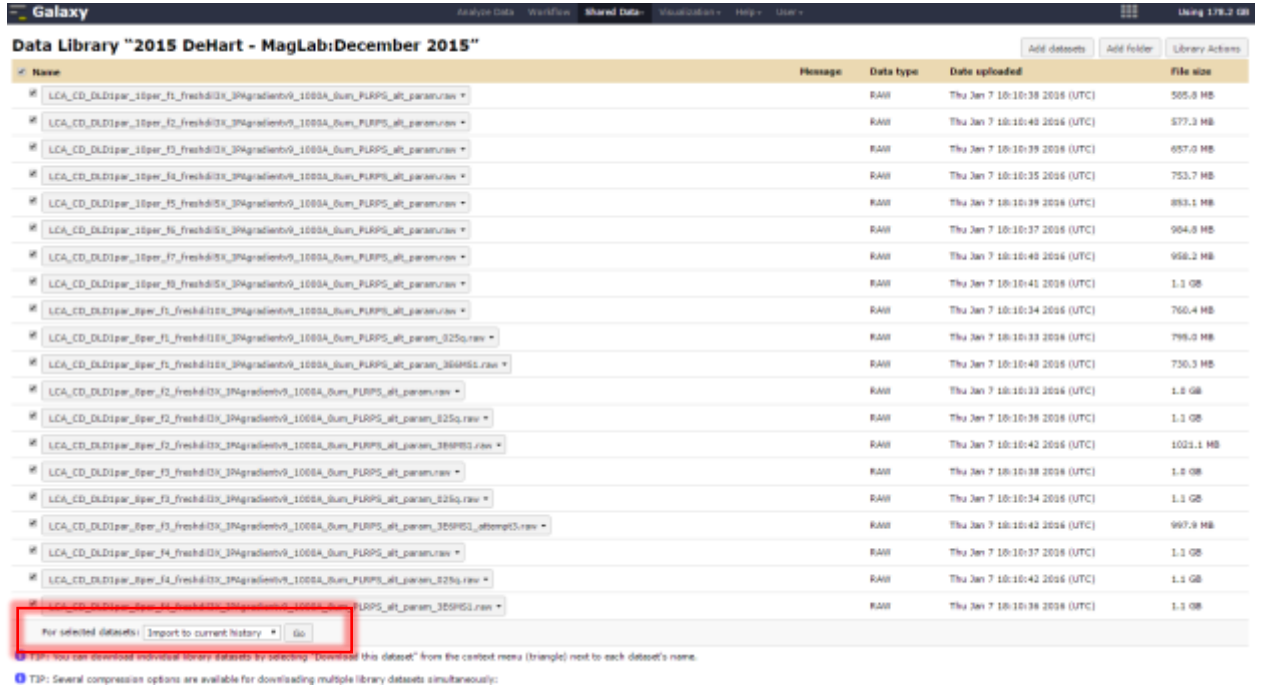
8. Click on the “Shared Data” subheading and “Data Libraries” view available linked library.



9. The Data Libraries screen displays available data libraries. Click on the desired data set library



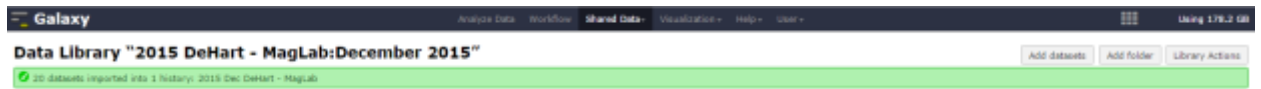
10. The next screen displays the dataset raw files. Select files to import to history by checking their checkboxes. At the bottom of the page there is a “For selected datasets” dropdown menu. Set the dropdown next to “Import to current history” and click “Go.”



The screenshot shows the Galaxy Data Library interface for "2015 DeHart - MagLab:December 2015". It displays a table of datasets with columns for Name, Message, Data type, Date uploaded, and File size. A red box highlights the "For selected datasets" dropdown menu at the bottom, which is currently set to "Import to current history" and has a "Go" button next to it.

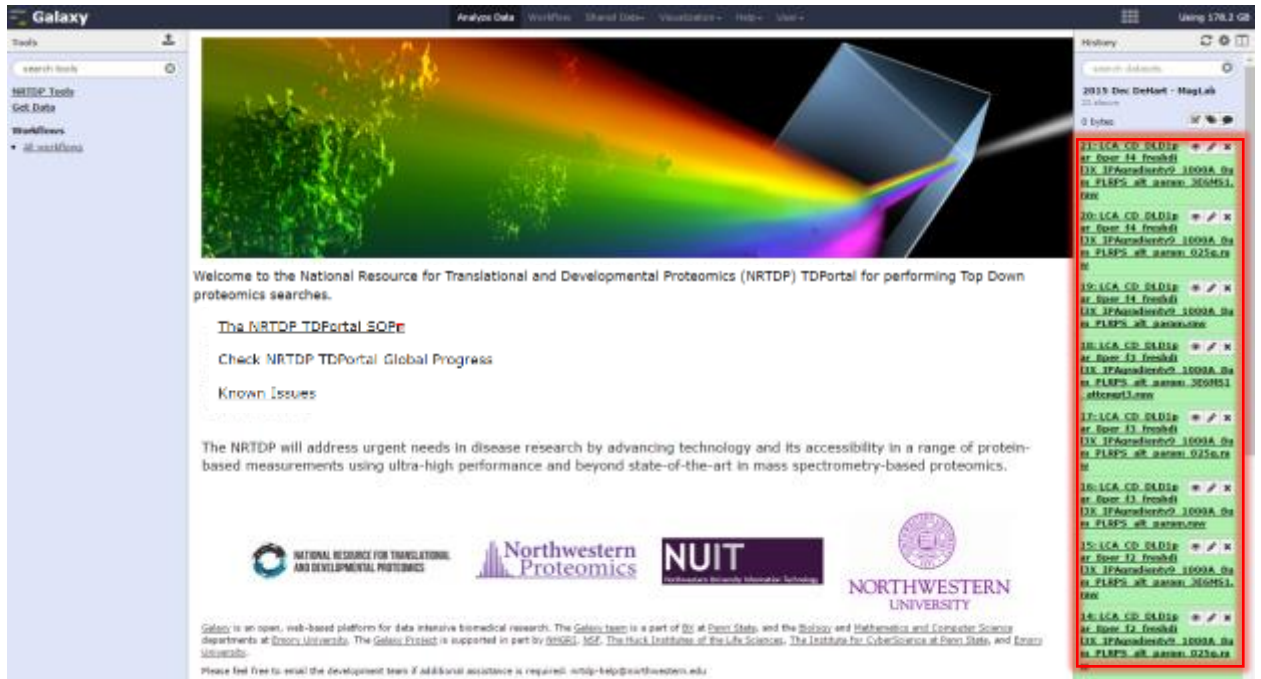
Name	Message	Data type	Date uploaded	File size
LCA_CD_DD1pw_10pw_f1_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:38 2016 (UTC)	505.8 MB
LCA_CD_DD1pw_10pw_f2_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:40 2016 (UTC)	577.3 MB
LCA_CD_DD1pw_10pw_f3_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:39 2016 (UTC)	657.0 MB
LCA_CD_DD1pw_10pw_f4_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:35 2016 (UTC)	753.7 MB
LCA_CD_DD1pw_10pw_f5_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:39 2016 (UTC)	853.1 MB
LCA_CD_DD1pw_10pw_f6_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:37 2016 (UTC)	904.8 MB
LCA_CD_DD1pw_10pw_f7_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:40 2016 (UTC)	956.2 MB
LCA_CD_DD1pw_10pw_f8_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:41 2016 (UTC)	1.3 GB
LCA_CD_DD1pw_10pw_f9_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:34 2016 (UTC)	760.4 MB
LCA_CD_DD1pw_10pw_f10_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_825q.raw		RAW	Thu Jan 7 10:10:33 2016 (UTC)	799.0 MB
LCA_CD_DD1pw_10pw_f1_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_364MS.raw		RAW	Thu Jan 7 10:10:40 2016 (UTC)	730.3 MB
LCA_CD_DD1pw_10pw_f2_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:33 2016 (UTC)	1.0 GB
LCA_CD_DD1pw_10pw_f3_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_825q.raw		RAW	Thu Jan 7 10:10:38 2016 (UTC)	1.3 GB
LCA_CD_DD1pw_10pw_f4_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_384MS.raw		RAW	Thu Jan 7 10:10:42 2016 (UTC)	1023.1 MB
LCA_CD_DD1pw_10pw_f5_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:38 2016 (UTC)	1.0 GB
LCA_CD_DD1pw_10pw_f6_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_825q.raw		RAW	Thu Jan 7 10:10:34 2016 (UTC)	1.3 GB
LCA_CD_DD1pw_10pw_f7_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_359MS_attempt3.raw		RAW	Thu Jan 7 10:10:42 2016 (UTC)	997.9 MB
LCA_CD_DD1pw_10pw_f8_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param.raw		RAW	Thu Jan 7 10:10:37 2016 (UTC)	1.3 GB
LCA_CD_DD1pw_10pw_f9_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_825q.raw		RAW	Thu Jan 7 10:10:42 2016 (UTC)	1.3 GB
LCA_CD_DD1pw_10pw_f10_freshd1X_3Mgradient9_1000A_sum_FURPS_at_param_359MS.raw		RAW	Thu Jan 7 10:10:38 2016 (UTC)	1.3 GB

11. Once the files are successfully imported this confirmation will be displayed at the top of the page.

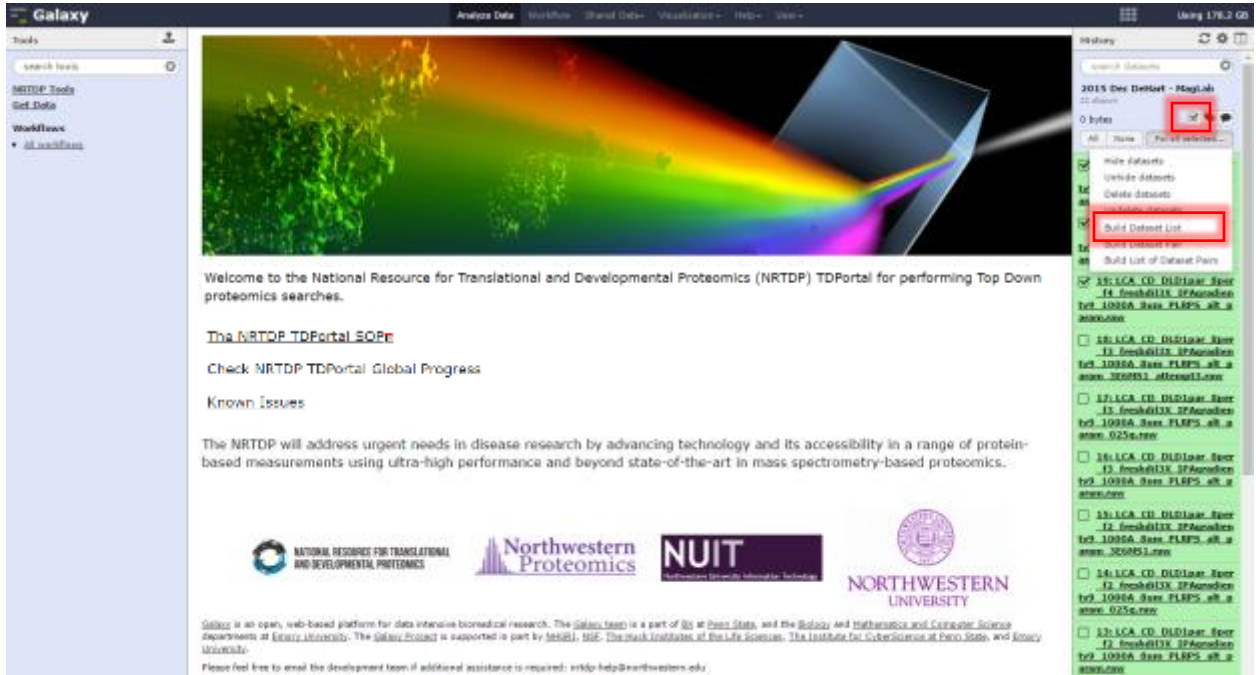


The screenshot shows the Galaxy Data Library interface with a green confirmation message at the top: "20 datasets imported into 1 history: 2015 DeHart - MagLab".

12. Click the Galaxy icon at the top of the page to return to the home page. The history has been populated with a green box for each imported raw file.



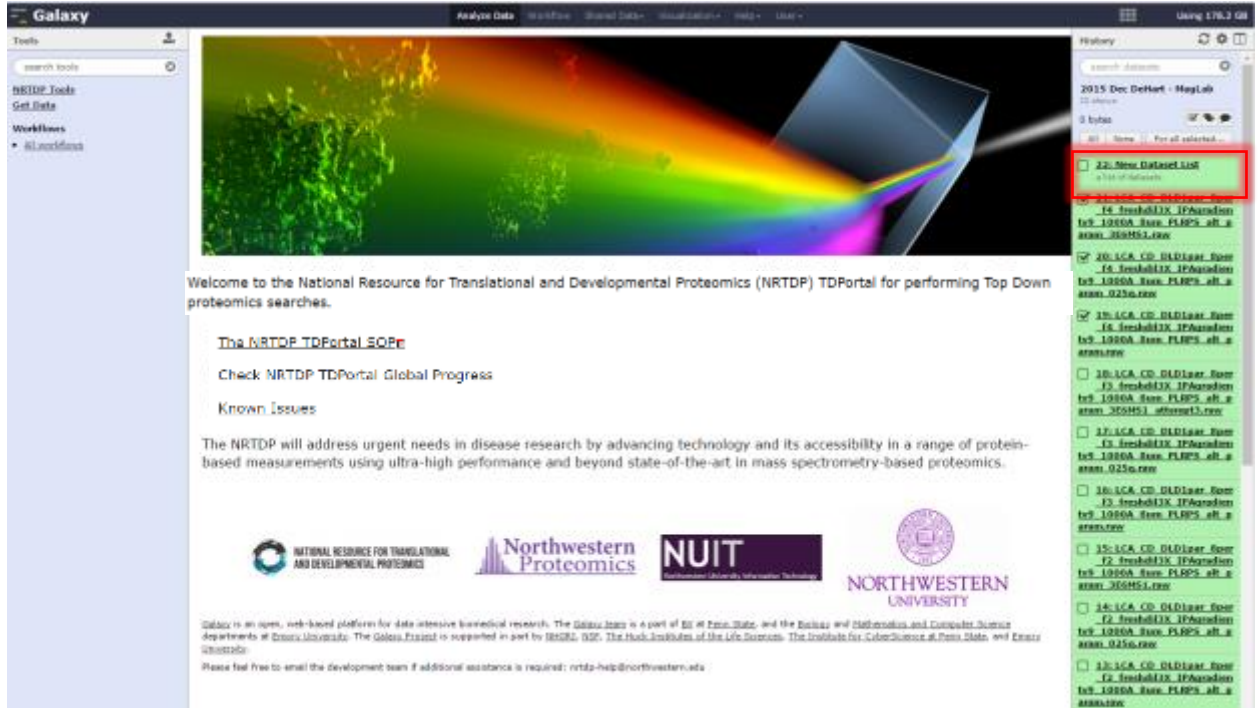
- 13. Next create the dataset list. To do this, navigate to the History Panel.
  - a. Click on the checkbox.
  - b. Select the raw files that will be searched.
  - c. Click For all selected
  - d. Select Build Dataset List



The screenshot shows the Galaxy web interface. The main content area displays a welcome message for the NRTDP TDPortal, including links for 'The NRTDP TDPortal SOPs', 'Check NRTDP TDPortal Global Progress', and 'Known Issues'. It also features logos for the National Resource for Translational and Developmental Proteomics, Northwestern Proteomics, NUIT, and Northwestern University. The History panel on the right shows a list of datasets with checkboxes for selection. A red box highlights the 'Build Dataset List' button in the History panel.



14. A new dataset list will appear in the History Panel.

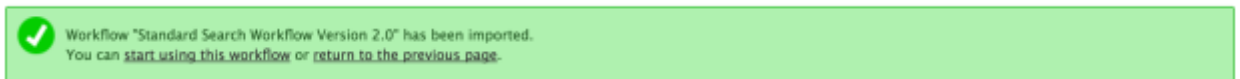


### Step 4: Running searches on TDPortal

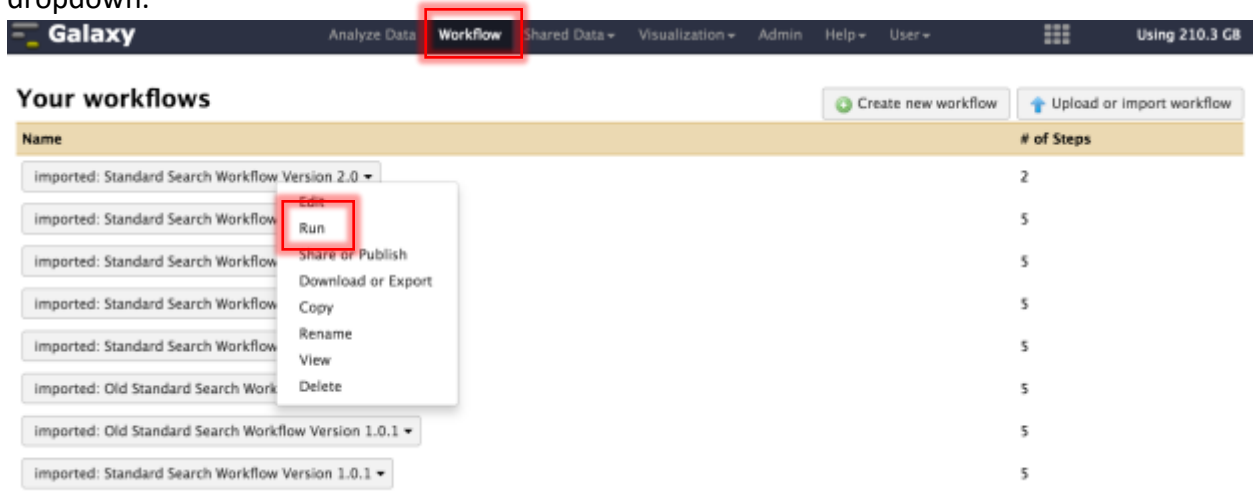
15. Navigate to Shared Data. Click on “Published Workflows” in the drop down menu. Import Published Standard Search Workflow 2.0 by clicking on the down arrow of the “Standard Search Workflow Version 2.0” tab.



16. When the workflow has successfully imported, this screen will appear.



17. Click the “Workflow” Subheading. Click “Run” in Standard Search Workflow Version 2.0 dropdown.



The screenshot shows the Galaxy web interface. The top navigation bar includes 'Galaxy', 'Analyze Data', 'Workflow' (highlighted with a red box), 'Shared Data', 'Visualization', 'Admin', 'Help', and 'User'. Below the navigation bar, the 'Your workflows' section is displayed. It features a table with columns for 'Name' and '# of Steps'. The table lists several workflows, including 'imported: Standard Search Workflow Version 2.0'. A dropdown menu is open for this workflow, showing options: 'Edit', 'Run' (highlighted with a red box), 'Share or Publish', 'Download or Export', 'Copy', 'Rename', 'View', and 'Delete'. Buttons for 'Create new workflow' and 'Upload or import workflow' are also visible.

Name	# of Steps
imported: Standard Search Workflow Version 2.0	2
imported: Standard Search Workflow	5
imported: Standard Search Workflow	5
imported: Standard Search Workflow	5
imported: Standard Search Workflow	5
imported: Old Standard Search Work	5
imported: Old Standard Search Workflow Version 1.0.1	5
imported: Standard Search Workflow Version 1.0.1	5

18. Input search parameters and click “Run Workflow.”
- Select Dataset list.
  - Input Parameters File (optional).
  - Select Organism to be searched.
  - If performing quant, select True to create SAS Input sheet.
  - Select Data file Resolution
  - Select Fragmentation Type.
  - Select Code Search v2.0.
  - Run Workflow.

## Running workflow "imported: Standard Search Workflow Version 2.0"

Expand All

Collapse

Step 1: Generate Workflow Job Id (version 1.1.1)

Step 2: Simple Search on Quest (version 1.1.1)

### Input Dataset List

4: New Dataset List ↕

### Job Id

Output dataset 'out\_file1' from step 1

### Search Parameters File

7: Quant SAS Input  
8: parameterss.json  
10: Quant SAS Input  
Selection is Optional

### Organism

Homo sapiens (Human) : (Taxon 9606 - July 2016) ✎

### Create SAS Input Sheet for Quant

False ✎

### Resolution

High Resolution ✎

### Fragmentation Type

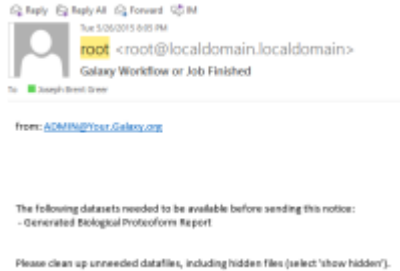
Auto ✎

### Code Set

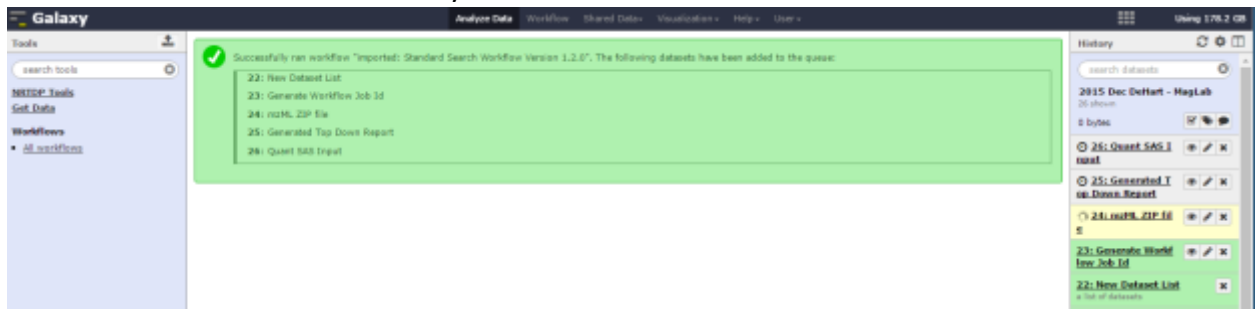
Search v2.0

### Step 5: Monitoring Progress of TDPortal Searches

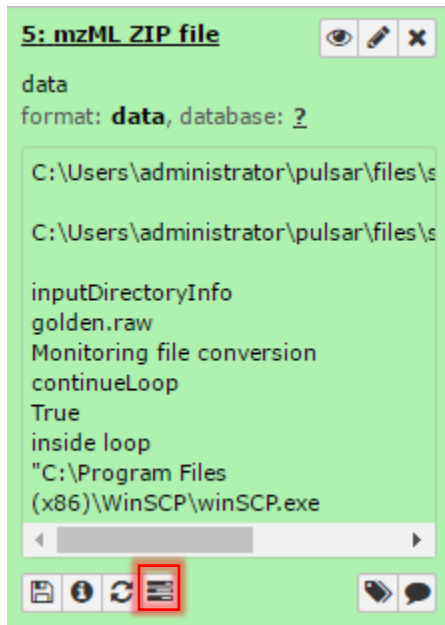
19. An email will be sent once the workflow has started containing history and job id information as well as a link to check progress outside of Galaxy.



20. The search will be added to History Panel.



21. Monitor Search progress by clicking on Check Progress button under mzML Zip file in the History Panel.



22. In progress, the date of the search, and user email will be visible.

Date	2016-04-25
User	alexandra.vannispn@northwestern.edu
Last Raw File Searched	

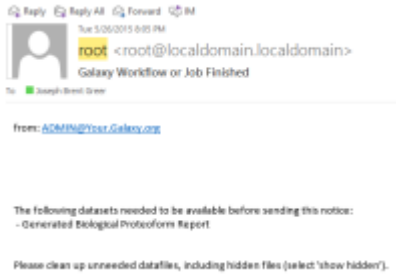
23. Four percentages are displayed in search progress. The page refreshes every 30 seconds.

### Search Progress

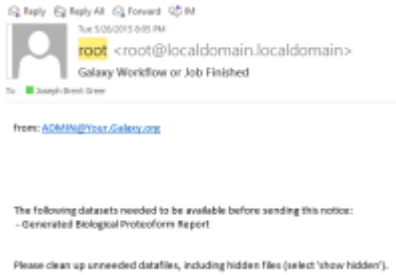
Step	Percent Complete				
Convert <b>a</b>	100%				
Prepare <b>b</b>	100%				
Search <b>c</b>	22%				
<table border="1"> <thead> <tr> <th>File</th> <th>Percent Complete</th> </tr> </thead> <tbody> <tr> <td></td> <td>22%</td> </tr> </tbody> </table> <p><b>Percentage of search completed per raw file.</b></p>		File	Percent Complete		22%
File	Percent Complete				
	22%				
Reporting <b>d</b>	Queued				

- The Convert percent is the percentage of raw files that have been converted to mzML.
- The Prepare percent is the percent of mzML files that have been prepared for search.
- The Search percent is the percent of searching all the mzML that has completed.
- The search percent for each mzML file is also displayed.
- The Reporting percent is the percentage of the creation of the tdReport that has completed.
- The Search Progress also displays errors during search with a descriptive message.

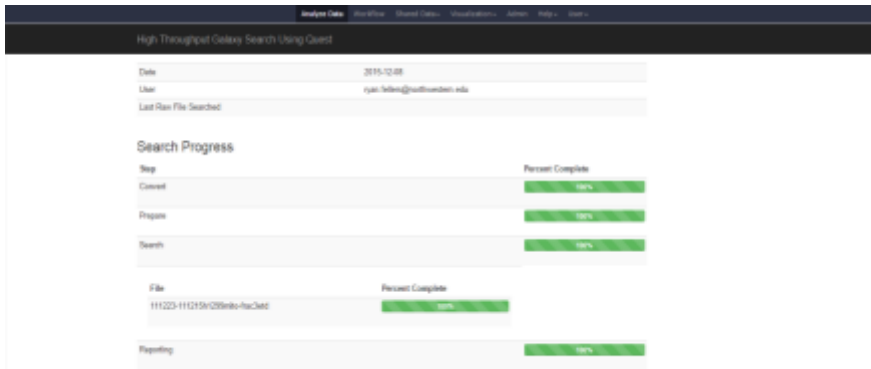
24. TDPortal will send an email immediately if a step in the workflow fails. The email will contain history and job id information.



25. An email will be sent when the search completes.

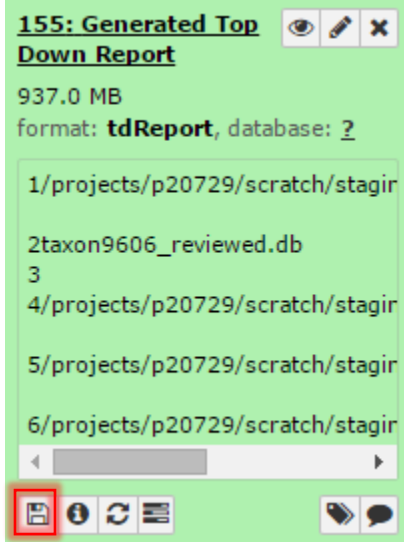


26. The History Panel items will turn green when the search fully completes.



### Step 6: Generating and Viewing the Top Down Report

27. Download search results by clicking “download” button under the Generated Top Down Report subsection in the History Panel.



28. Open results in TDViewer (topdownviewer.northwestern.edu)

