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

**Part 1: Transferring Project Files to TDPortal.....Step 1 - Step 7**

**Part 2: TDPortal Page Orientation.....Step 8**

**Part 3: Preparing Raw Files for the TDPortal Search.....Step 9 - Step 20**

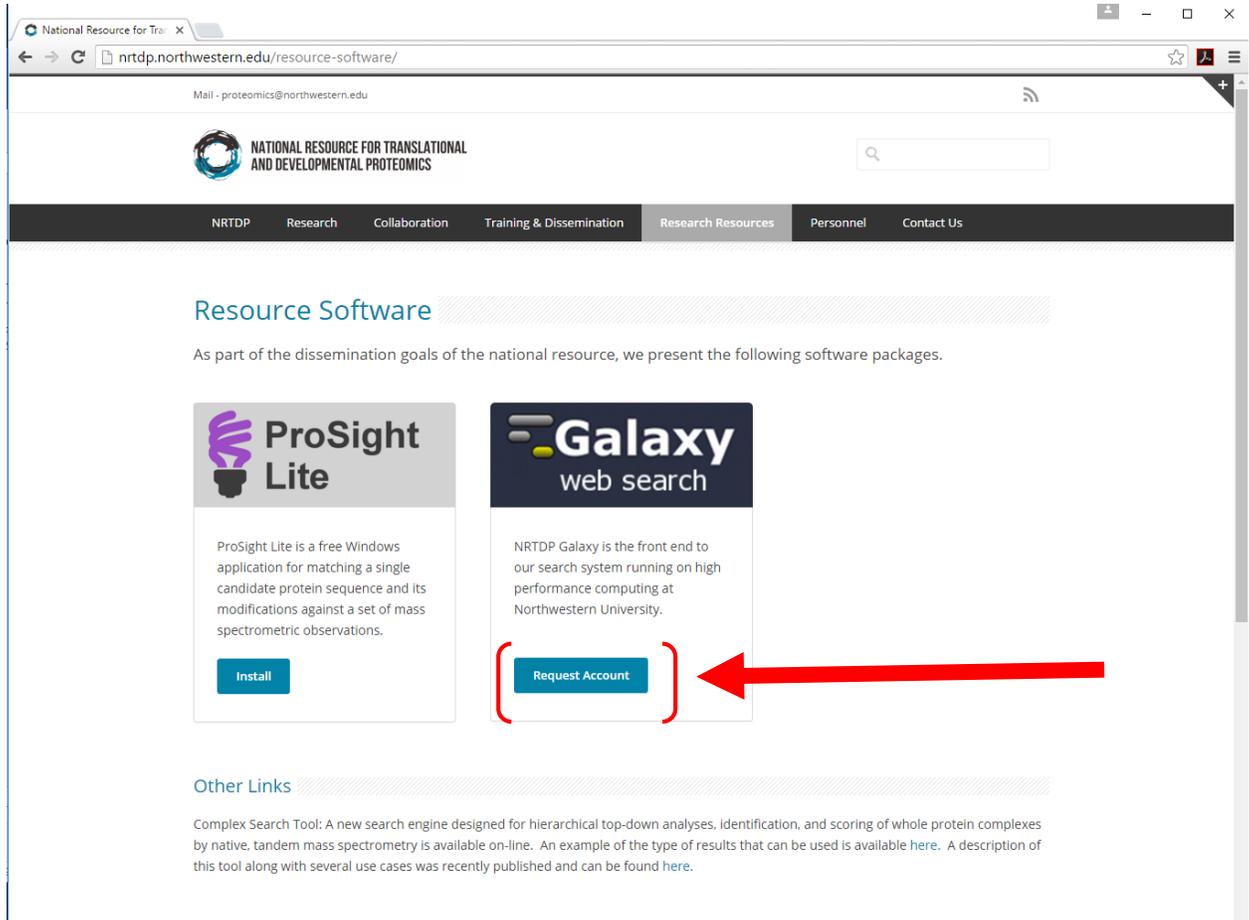
**Part 4: Running Searches on TDPortal.....Step 21 - Step 24**

**Part 5: Monitoring Progress of TDPortal Searches.....Step 25 - Step 34**

**Part 6: Generating and Viewing the Top Down Report.....Step 35 - Step 36**

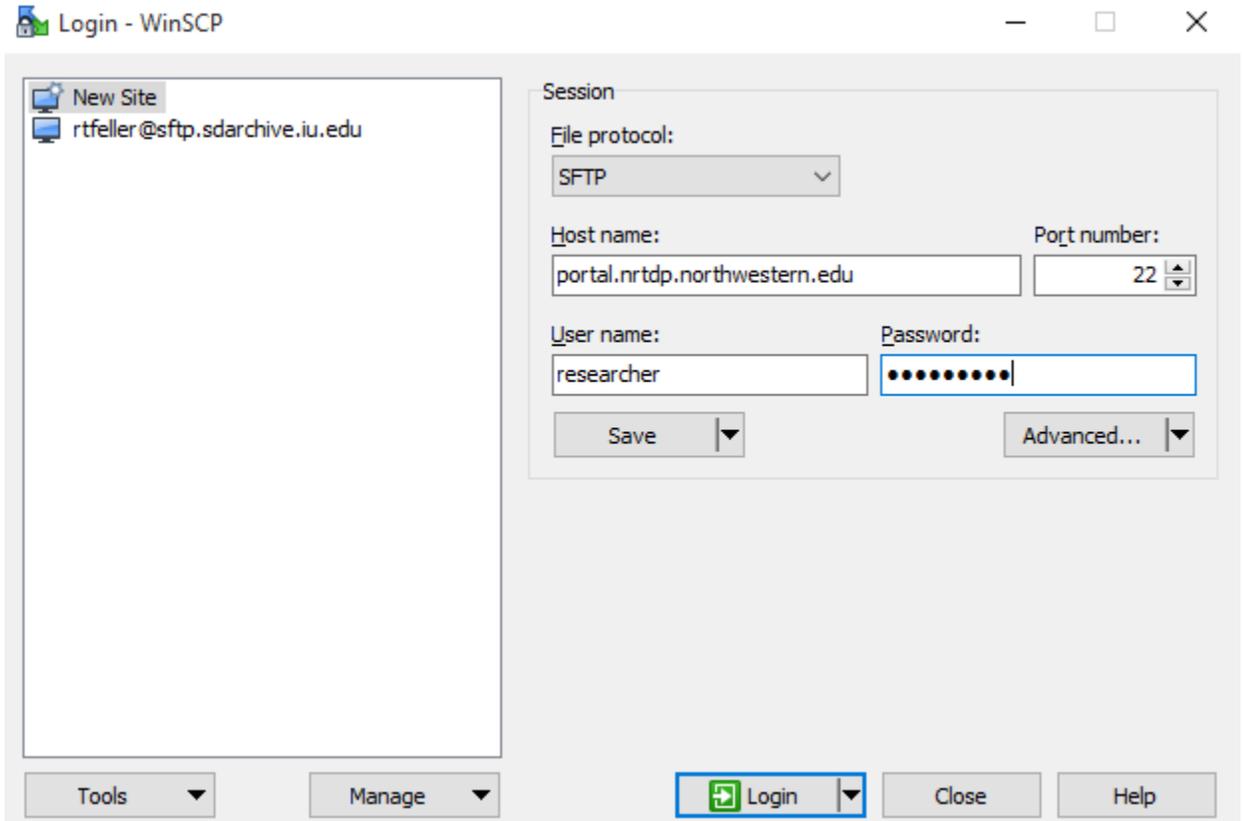
## Part 1: Transferring Project Files to TDPortal

1. Request access to TDPortal on the Resource Software page of the NRTDP website:  
<http://nrtdp.northwestern.edu/resource-software/>

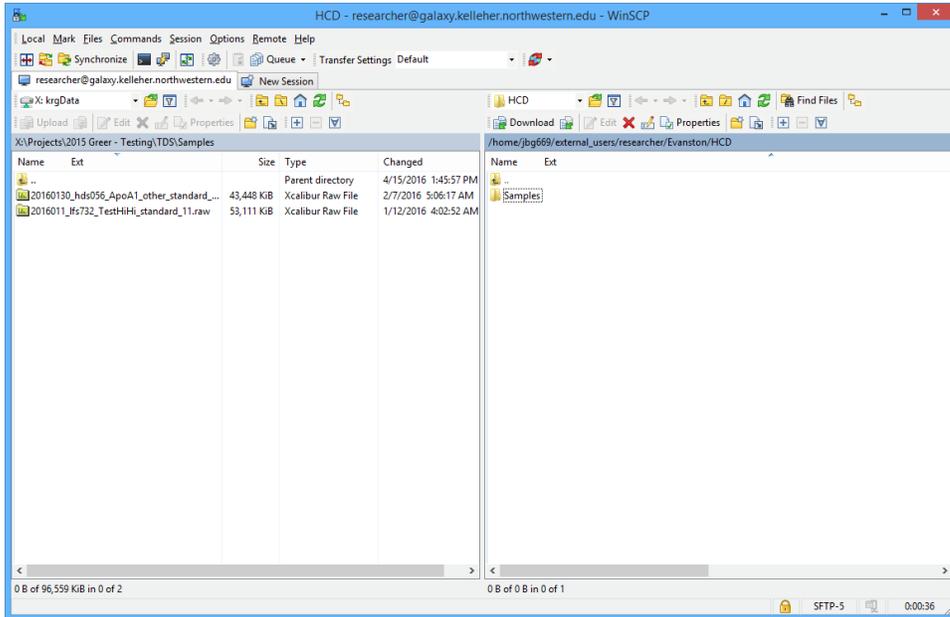


2. Complete the request form. The TDPortal administrator will email login information.
3. Use an SFTP application to transfer raw files to be searched. We recommend WinSCP.

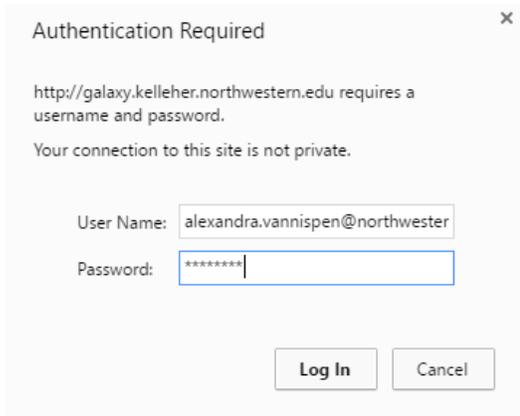
- 4. On WinSCP, create a New Site.
  - a. The File Protocol is SFTP, the Host name is portal.nrtdp.northwestern.edu, the port number is 22. The TDPortal administrator will provide username and password information. Click Save. Click login.



- Once logged in, ½ of the screen will show the local computer and ½ of the screen will show the SFTP folder.
- Create a folder that will contain all raw file(s) to be searched.

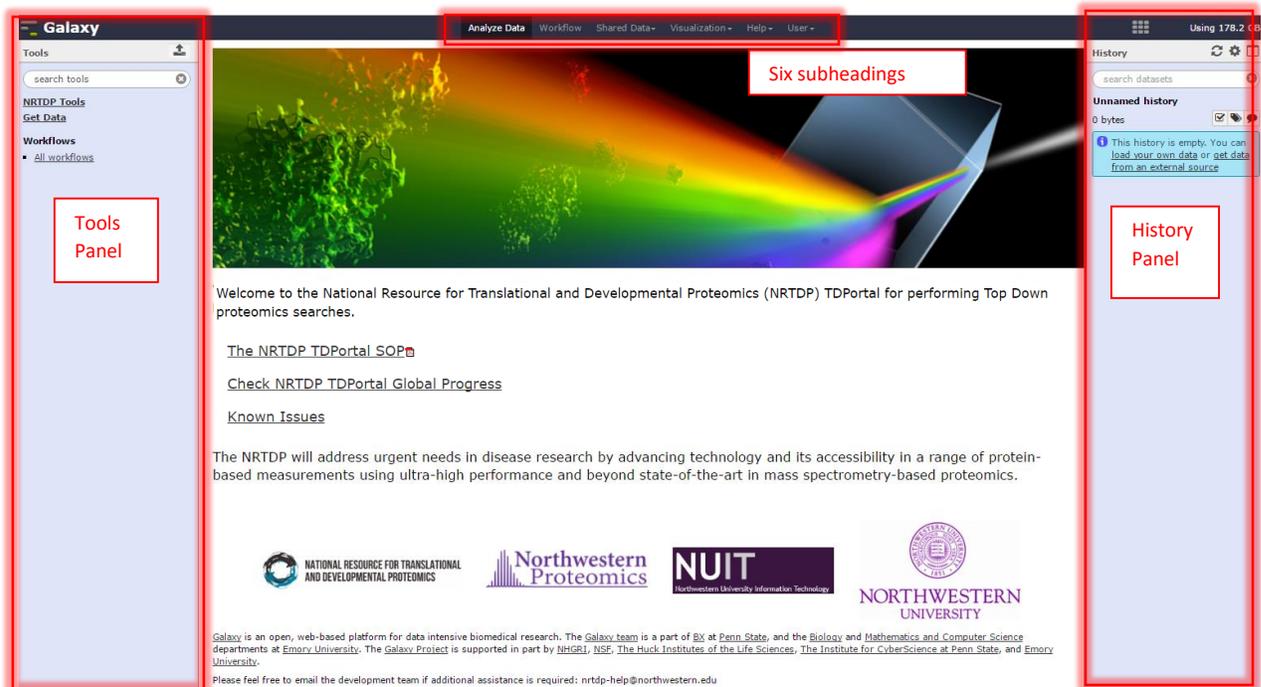


- Log into TDPortal at: <http://portal.nrtdp.northwestern.edu>. The TDPortal administrator will provide username and password information.



## Part 2: TDPortal Page Orientation

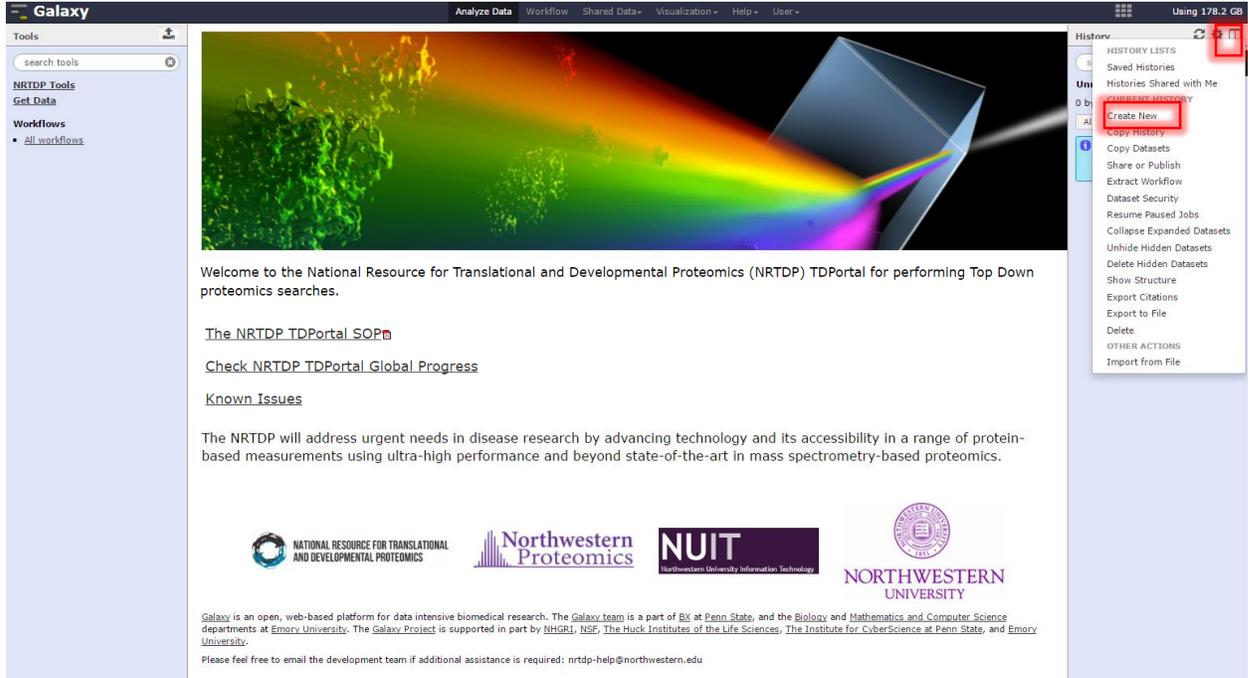
### 8. Get oriented to the page.



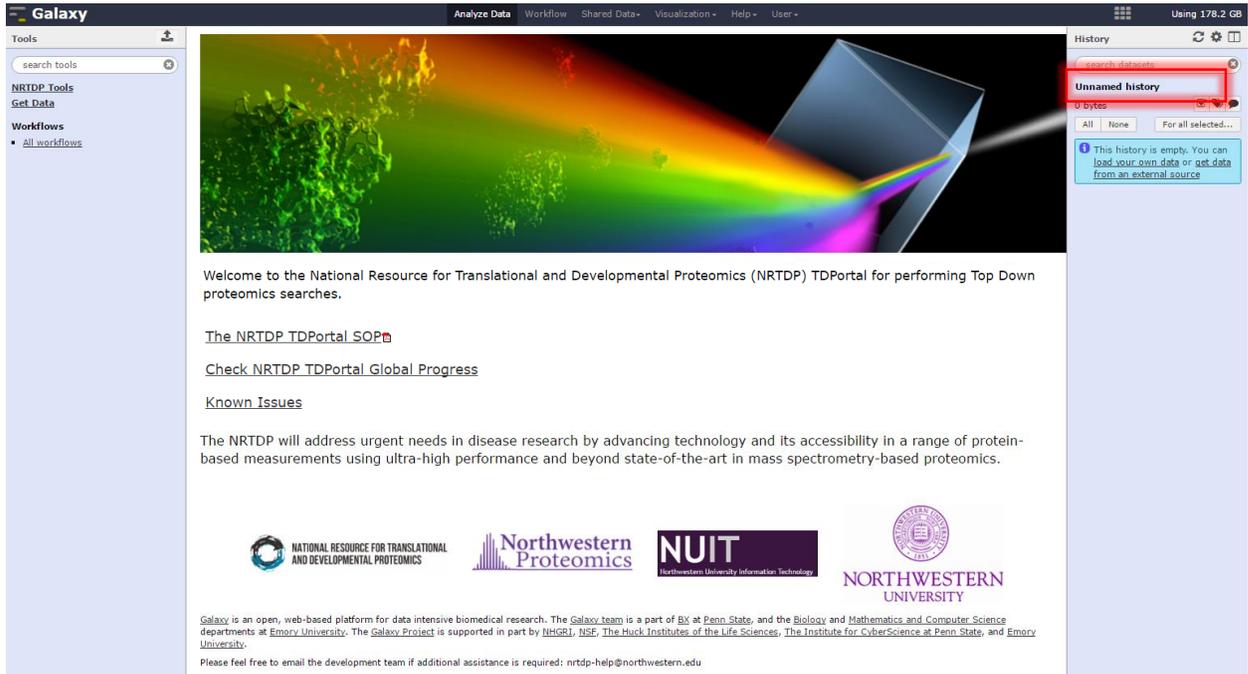
- a. There are six subheadings that link to different pages.
- b. The History Panel is on the right. When data is uploaded or an analysis is performed, each output generates a dataset. These datasets are stored by TDPortal in the History Panel.
- c. All of the available tools are located in the blue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

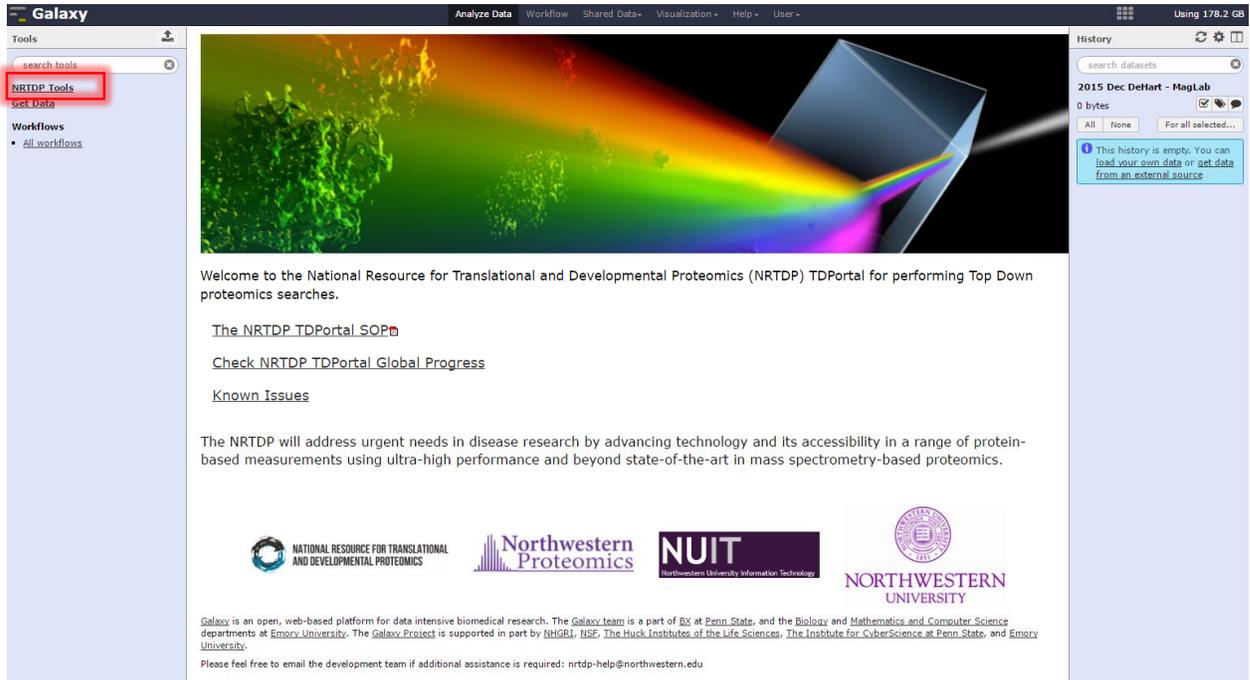
9. Create a new history. Go to the history column and click on the gear in the top right . A drop down menu will appear. Click on “Create New.”



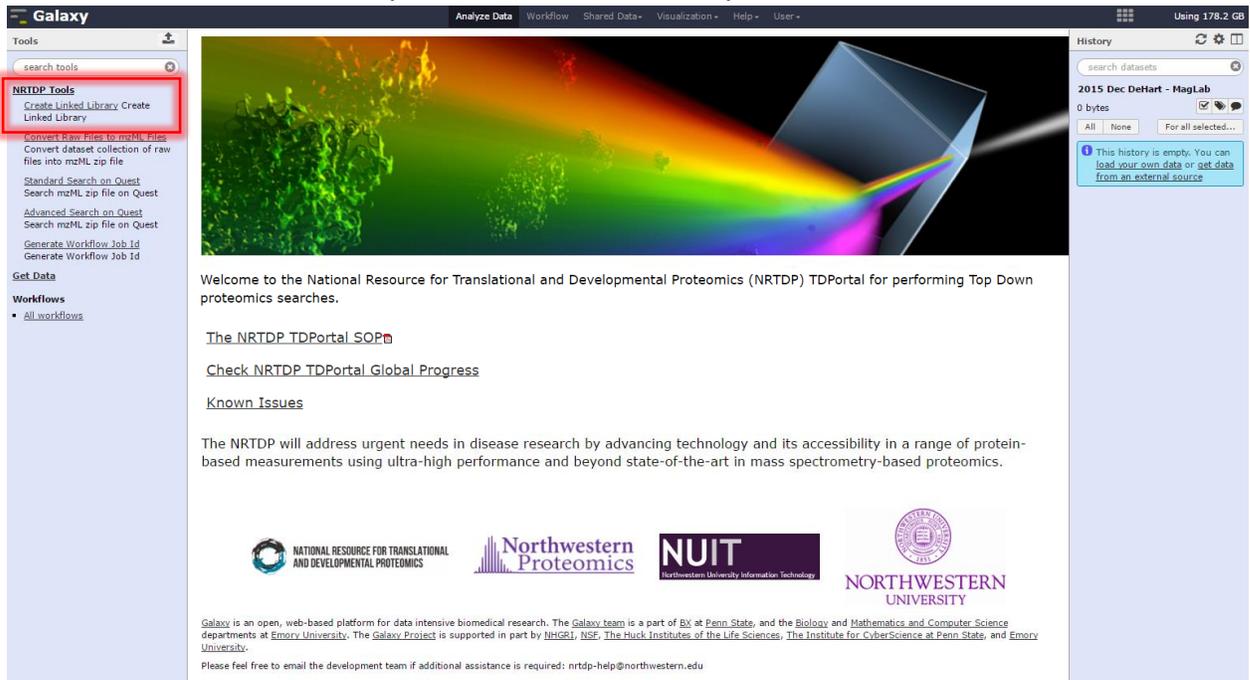
10. Rename the new history by clicking on “Unnamed History.”



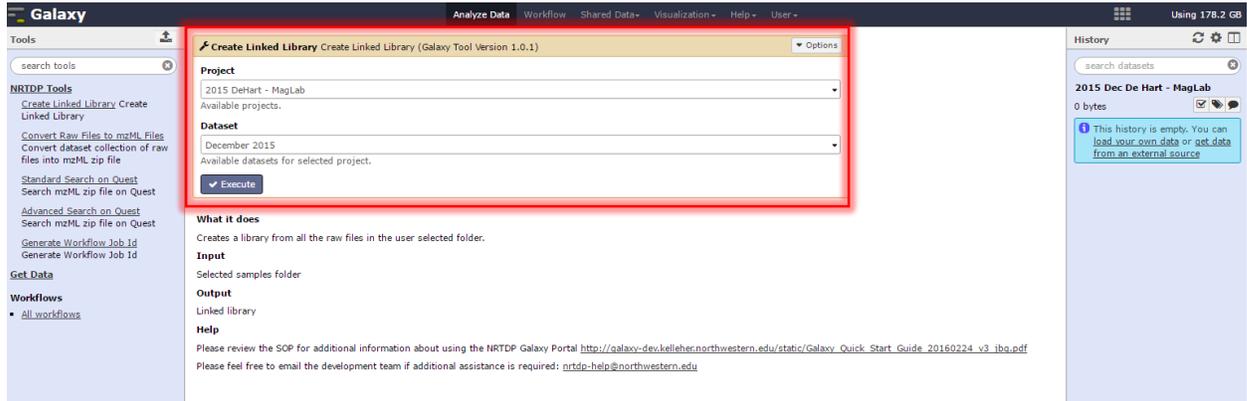
11. Go to Tools Panel and click on “NRTDP Tools.” A menu containing all the available NRTDP tools will appear.



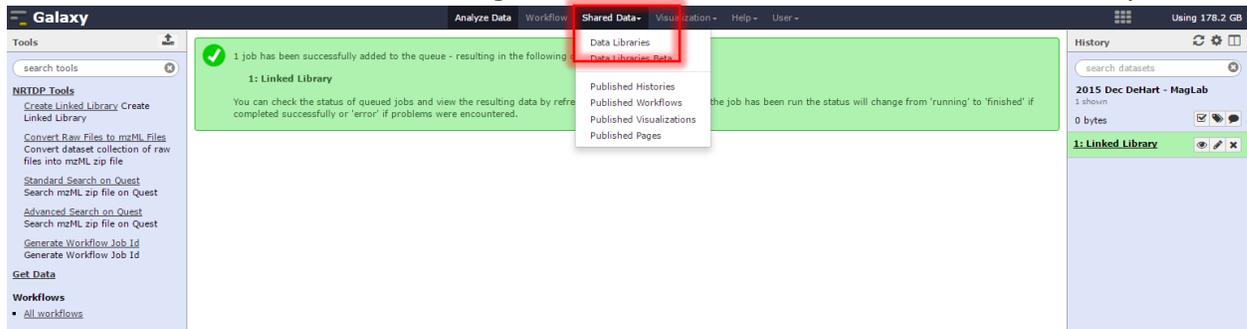
12. Click on “Create Linked Library” to create a linked library.



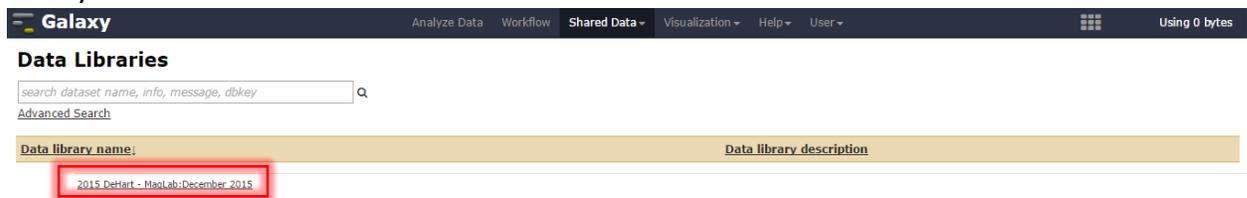
13. Select the dataset that will be searched. Click “Execute.”



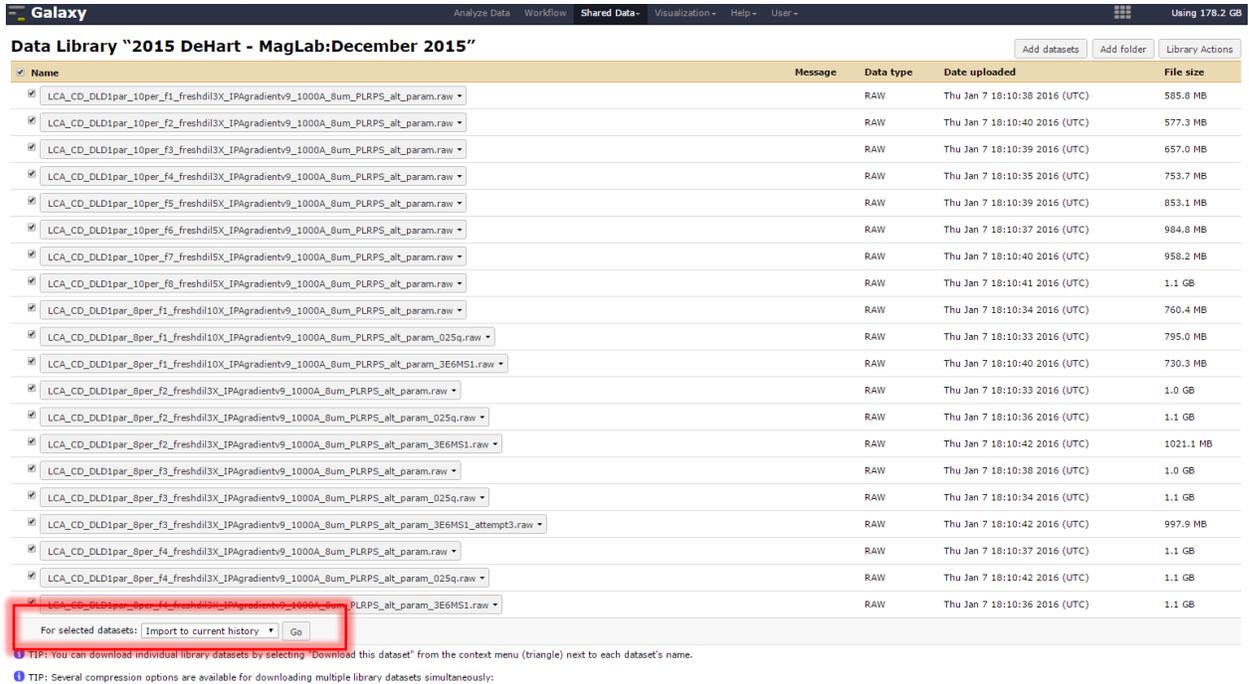
14. Click on the “Shared Data” subheading and “Data Libraries” view available linked library.



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



16. 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 raw files 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. Below the table, there are two tips: one about downloading individual datasets and another about simultaneous downloads.

Name	Message	Data type	Date uploaded	File size
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f1_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:38 2016 (UTC)	585.8 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f2_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:40 2016 (UTC)	577.3 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f3_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:39 2016 (UTC)	657.0 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f4_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:35 2016 (UTC)	753.7 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f5_freshdil5X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:39 2016 (UTC)	853.1 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f6_freshdil5X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:37 2016 (UTC)	984.8 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f7_freshdil5X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:40 2016 (UTC)	958.2 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f8_freshdil5X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:41 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f1_freshdil10X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:34 2016 (UTC)	760.4 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f1_freshdil10X_IPAgradientv9_1000A_sum_PLRPS_alt_param_025q.raw		RAW	Thu Jan 7 18:10:33 2016 (UTC)	795.0 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f1_freshdil10X_IPAgradientv9_1000A_sum_PLRPS_alt_param_3E6MS1.raw		RAW	Thu Jan 7 18:10:40 2016 (UTC)	730.3 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f2_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:33 2016 (UTC)	1.0 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f2_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param_025q.raw		RAW	Thu Jan 7 18:10:36 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f2_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param_3E6MS1.raw		RAW	Thu Jan 7 18:10:42 2016 (UTC)	1021.1 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f3_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:38 2016 (UTC)	1.0 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f3_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param_025q.raw		RAW	Thu Jan 7 18:10:34 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f3_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param_3E6MS1_attempt3.raw		RAW	Thu Jan 7 18:10:42 2016 (UTC)	997.9 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f4_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:37 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f4_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param_025q.raw		RAW	Thu Jan 7 18:10:42 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f4_freshdil3X_IPAgradientv9_1000A_sum_PLRPS_alt_param_3E6MS1.raw		RAW	Thu Jan 7 18:10:36 2016 (UTC)	1.1 GB

For selected datasets:

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

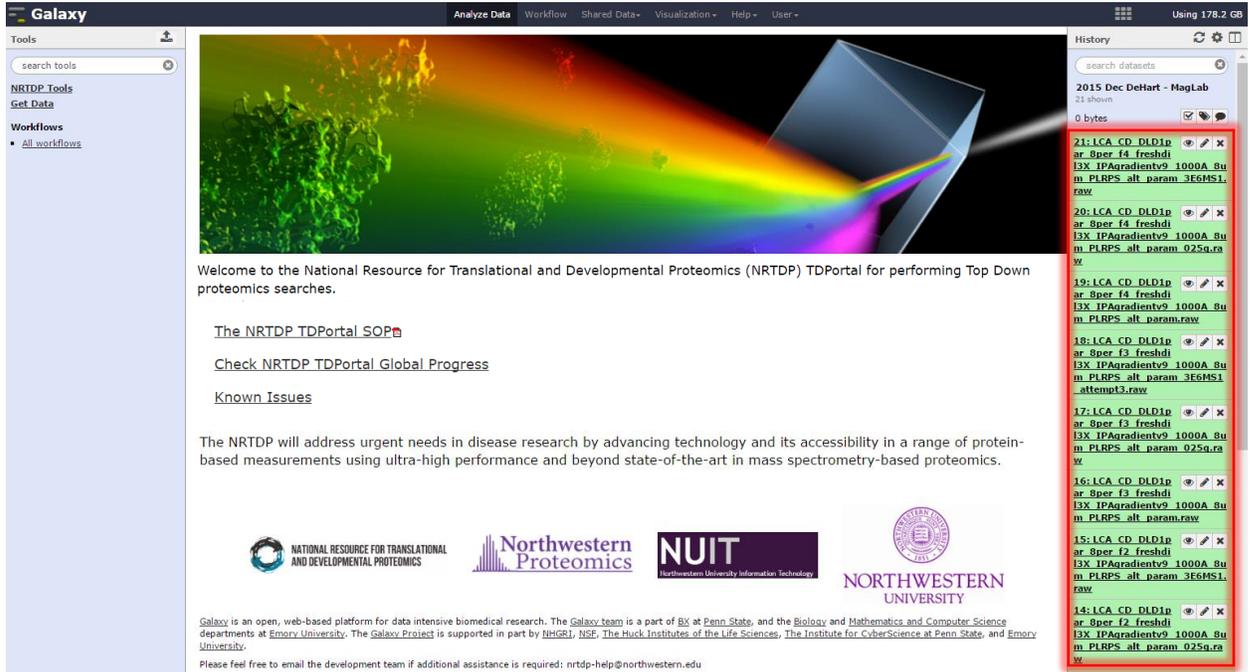
TIP: Several compression options are available for downloading multiple library datasets simultaneously:

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



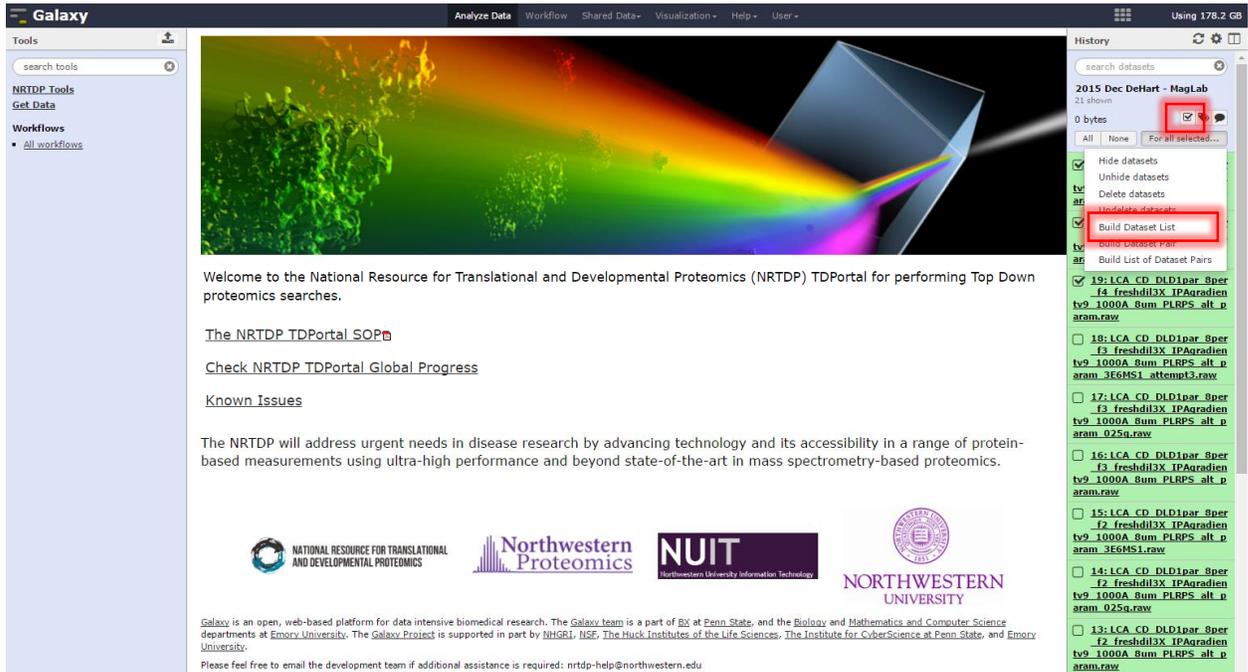
The screenshot shows the Galaxy Data Library interface with a green confirmation banner at the top: "20 datasets imported into 1 history: 2015 Dec DeHart - MagLab". The rest of the interface is the same as in the previous screenshot.

18. 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.



The screenshot shows the Galaxy web interface. The main content area displays a welcome message for the NRTDP TDPortal, a navigation menu on the left, and a central visualization of a protein structure. On the right, the 'History' panel is open, showing a list of datasets. A red box highlights a list of raw files, including entries like '21: LCA\_CD\_DLD1p\_ar\_8per\_14\_freshdi', '20: LCA\_CD\_DLD1p\_ar\_8per\_14\_freshdi', '19: LCA\_CD\_DLD1p\_ar\_8per\_14\_freshdi', '18: LCA\_CD\_DLD1p\_ar\_8per\_13\_freshdi', '17: LCA\_CD\_DLD1p\_ar\_8per\_13\_freshdi', '16: LCA\_CD\_DLD1p\_ar\_8per\_13\_freshdi', '15: LCA\_CD\_DLD1p\_ar\_8per\_12\_freshdi', and '14: LCA\_CD\_DLD1p\_ar\_8per\_12\_freshdi'. Each entry includes a search icon, a refresh icon, and a delete icon.

19. 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

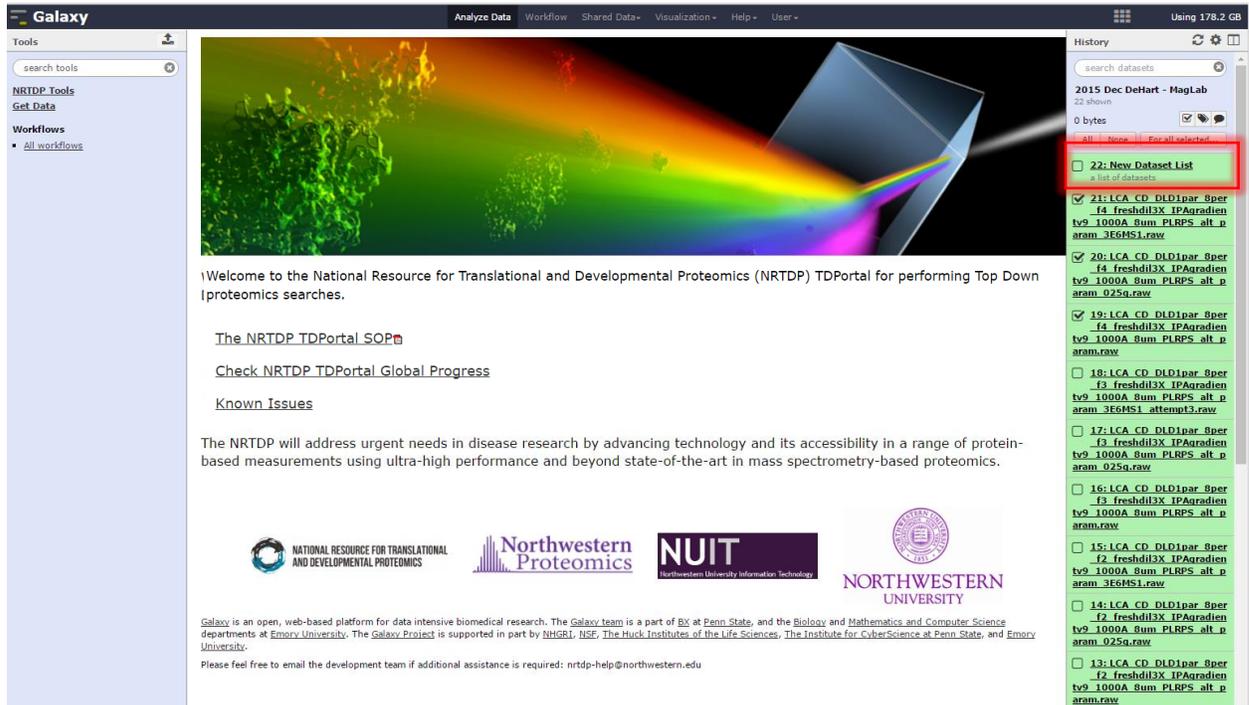


The screenshot shows the Galaxy web interface. The main content area displays a welcome message for the NRTDP TDPortal, including links for SOPs, global progress, and known issues. The History panel on the right shows a list of datasets with checkboxes. A red box highlights the 'Build Dataset List' button in the History panel.

**History Panel Dataset List:**

Dataset ID	Dataset Name	Selected
19	LCA_CD_DLD1par_Sper_f4_freshd13X_IPAgradien_tv9_1000A_Sum_PLRPS_alt_p_aram.raw	<input checked="" type="checkbox"/>
18	LCA_CD_DLD1par_Sper_f3_freshd13X_IPAgradien_tv9_1000A_Sum_PLRPS_alt_p_aram_3EGMS1_attempt3.raw	<input type="checkbox"/>
17	LCA_CD_DLD1par_Sper_f3_freshd13X_IPAgradien_tv9_1000A_Sum_PLRPS_alt_p_aram_0259a.raw	<input type="checkbox"/>
16	LCA_CD_DLD1par_Sper_f3_freshd13X_IPAgradien_tv9_1000A_Sum_PLRPS_alt_p_aram.raw	<input type="checkbox"/>
15	LCA_CD_DLD1par_Sper_f2_freshd13X_IPAgradien_tv9_1000A_Sum_PLRPS_alt_p_aram_3EGMS1.raw	<input type="checkbox"/>
14	LCA_CD_DLD1par_Sper_f2_freshd13X_IPAgradien_tv9_1000A_Sum_PLRPS_alt_p_aram_0259a.raw	<input type="checkbox"/>
13	LCA_CD_DLD1par_Sper_f2_freshd13X_IPAgradien_tv9_1000A_Sum_PLRPS_alt_p_aram.raw	<input type="checkbox"/>

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

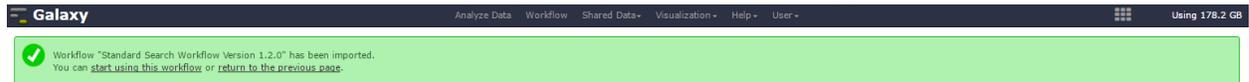


### Step 4: Running searches on TDPortal

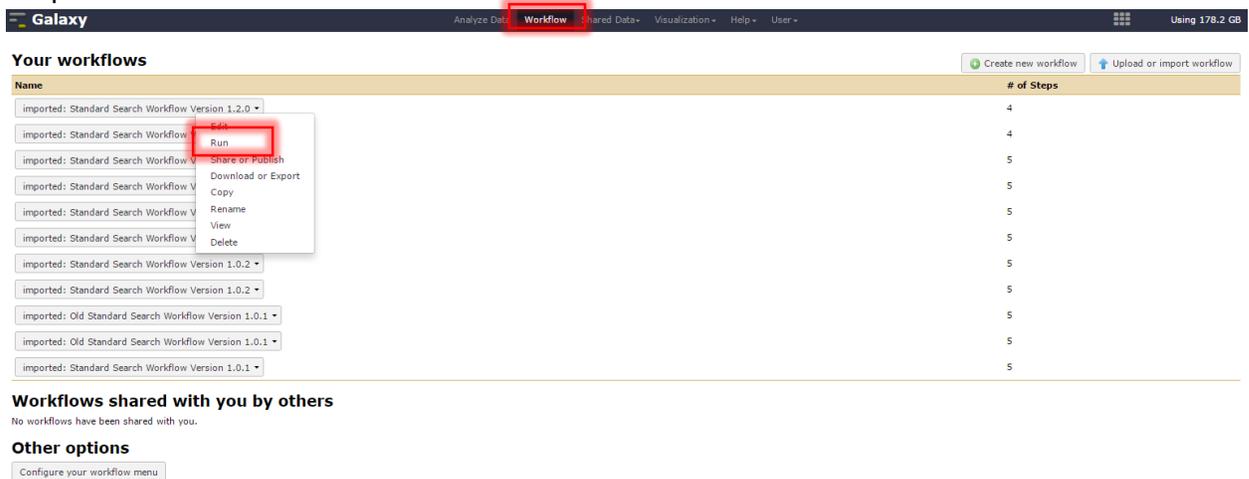
21. Navigate to Shared Data. Click on “Published Workflows” in the drop down menu. Import Published Standard Search Workflow 1.2.0 by clicking on the down arrow of the “Standard Search Workflow Version 1.2.0” tab.



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



23. Click the “Workflow” Subheading. Click “Run” in Standard Search Workflow Version 1.2.0 dropdown.



**Your workflows**

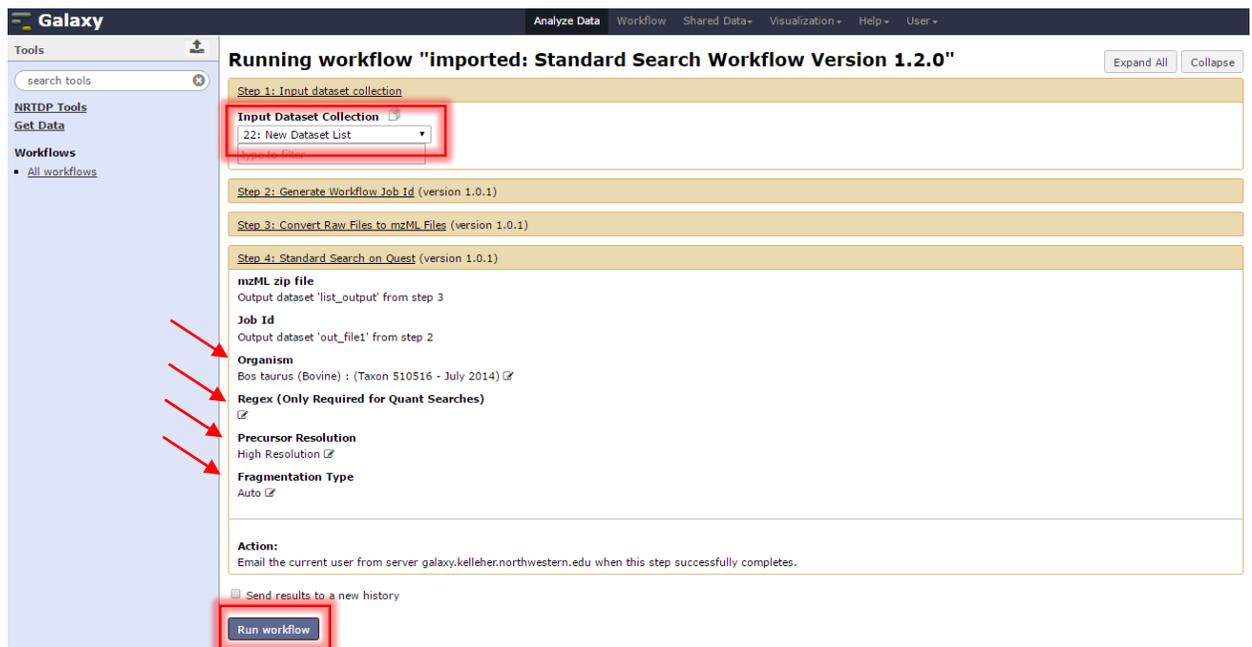
Name	# of Steps
imported: Standard Search Workflow Version 1.2.0	4
imported: Standard Search Workflow	4
imported: Standard Search Workflow	5
imported: Standard Search Workflow Version 1.0.2	5
imported: Standard Search Workflow Version 1.0.2	5
imported: Old Standard Search Workflow Version 1.0.1	5
imported: Old Standard Search Workflow Version 1.0.1	5
imported: Standard Search Workflow Version 1.0.1	5

**Workflows shared with you by others**  
No workflows have been shared with you.

**Other options**  
Configure your workflow menu

24. Input search parameters and click “Run Workflow.”

- a. Select Dataset list.
- b. Select Organism to be searched.
- c. If performing quant, insert regex provided by an administrator.
- d. Select Data file Resolution
- e. Select Fragmentation Type.
- f. Run Workflow.



**Running workflow "imported: Standard Search Workflow Version 1.2.0"**

Step 1: Input dataset collection

**Input Dataset Collection**  
22: New Dataset List

Step 2: Generate Workflow Job Id (version 1.0.1)

Step 3: Convert Raw Files to mzML Files (version 1.0.1)

Step 4: Standard Search on Quest (version 1.0.1)

**mzML zip file**  
Output dataset 'list\_output' from step 3

**Job Id**  
Output dataset 'out\_file1' from step 2

**Organism**  
Bos taurus (Bovine) : (Taxon 510516 - July 2014)

**Regex (Only Required for Quant Searches)**

**Precursor Resolution**  
High Resolution

**Fragmentation Type**  
Auto

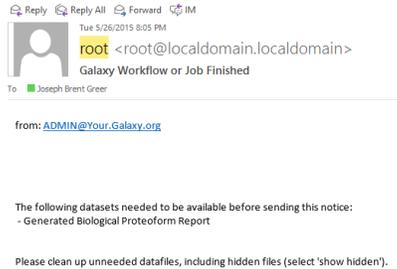
**Action:**  
Email the current user from server galaxy.kelleher.northwestern.edu when this step successfully completes.

Send results to a new history

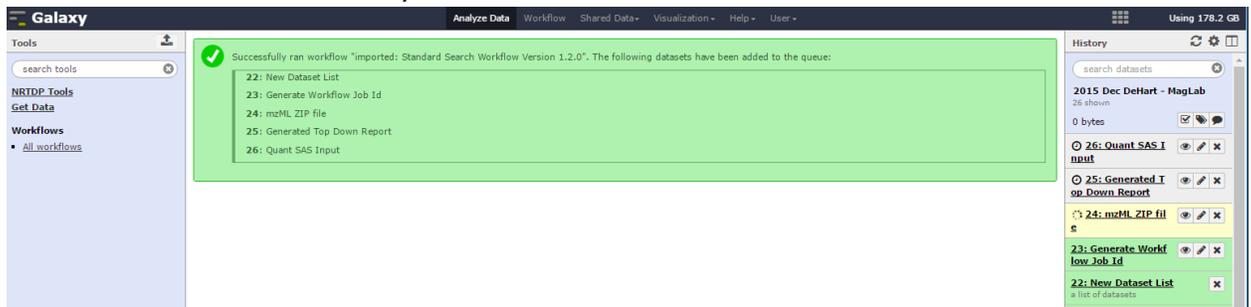
**Run workflow**

### Step 5: Monitoring Progress of TDPortal Searches

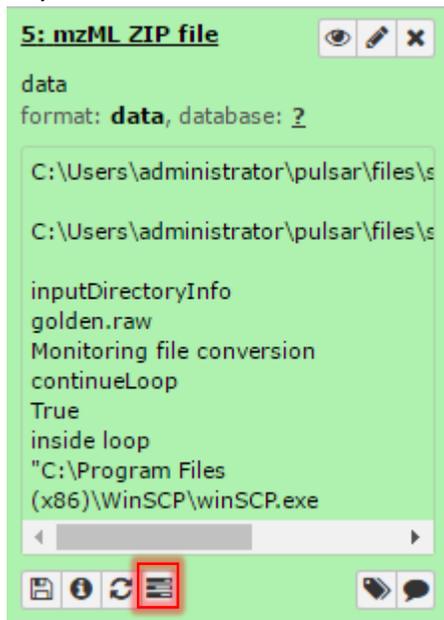
25. An email will be sent once the workflow has started containing history and job id information as well as a link to check progress outside of Galaxy.



26. The search will be added to History Panel.



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



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

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

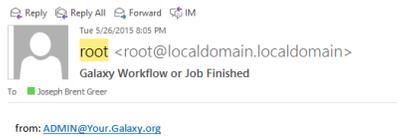
29. Four percentages are displayed in search progress. The page refreshes every 30 seconds.

### 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>Percentage of search completed per raw file.</p>		File	Percent Complete		22%
File	Percent Complete				
	22%				
Reporting <b>d</b>	Queued				

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

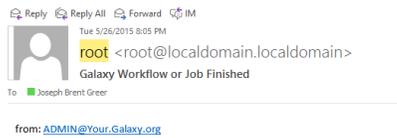
30. TDPortal will send an email immediately if a step in the workflow fails. The email will contain history and job id information.



The following datasets needed to be available before sending this notice:  
- Generated Biological Proteoform Report

Please clean up unneeded datafiles, including hidden files (select 'show hidden').

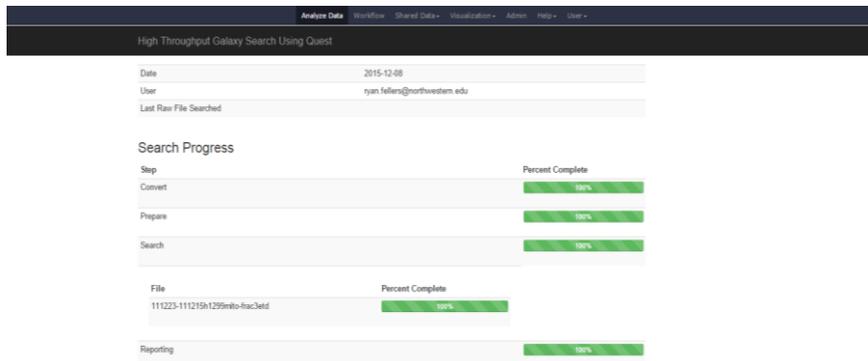
### 31. An email will be sent when the search completes.



The following datasets needed to be available before sending this notice:  
- Generated Biological Proteoform Report

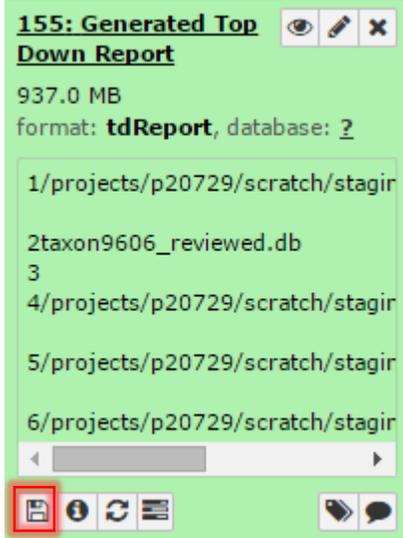
Please clean up unneeded datafiles, including hidden files (select 'show hidden').

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



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

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



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

