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Internal User Guide for Performing High Throughput Searches on TDPortal

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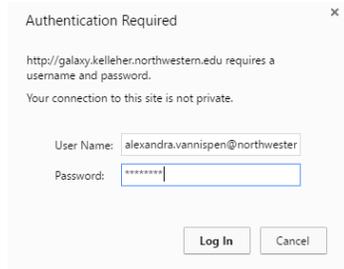
Part 3: Running Searches on TDPortal.....Step 15 - Step 18

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Part 1: TDPortal Orientation

1. Log into TDPortal at: <http://portal.nrtdp.northwestern.edu>. The username is your Northwestern email and password.



Authentication Required

<http://galaxy.kelleher.northwestern.edu> requires a username and password.

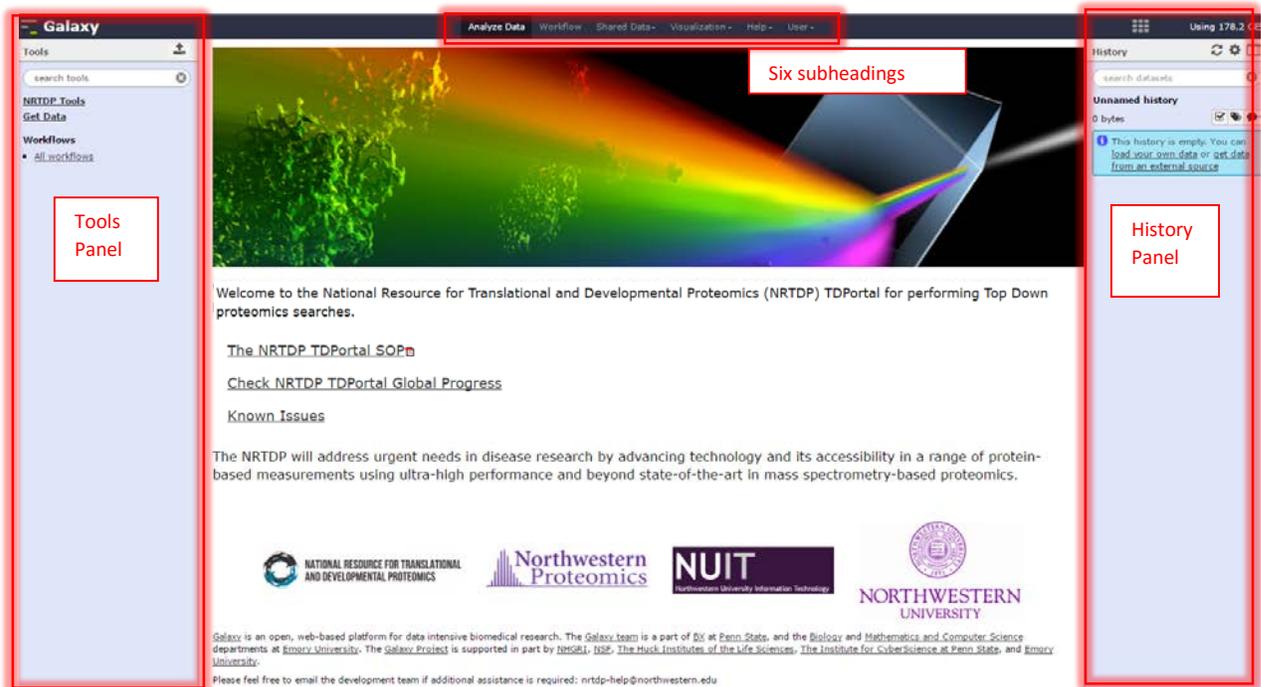
Your connection to this site is not private.

User Name: alexandra.vannispn@northwestern.edu

Password: [masked]

Log In Cancel

2. Get oriented to the page.

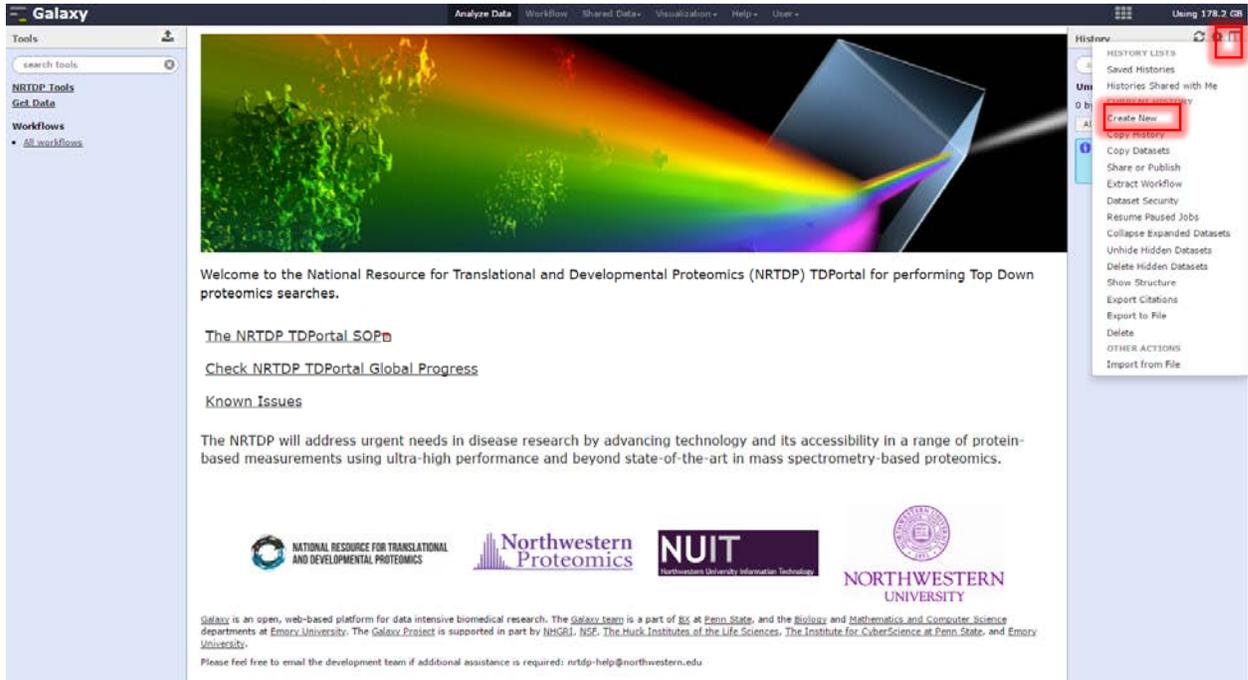


The screenshot shows the Galaxy web interface. On the left is a blue 'Tools Panel' containing a search bar and categories like 'NRTDP Tools', 'Get Data', and 'Workflows'. On the right is a 'History Panel' showing an 'Unnamed history' with 0 bytes. The main content area features a colorful 3D visualization of a protein structure. A red box labeled 'Six subheadings' points to a list of links: 'The NRTDP TDPortal SOP', 'Check NRTDP TDPortal Global Progress', and 'Known Issues'. Below this is a paragraph of text and logos for NRTDP, Northwestern Proteomics, NUIT, and Northwestern University.

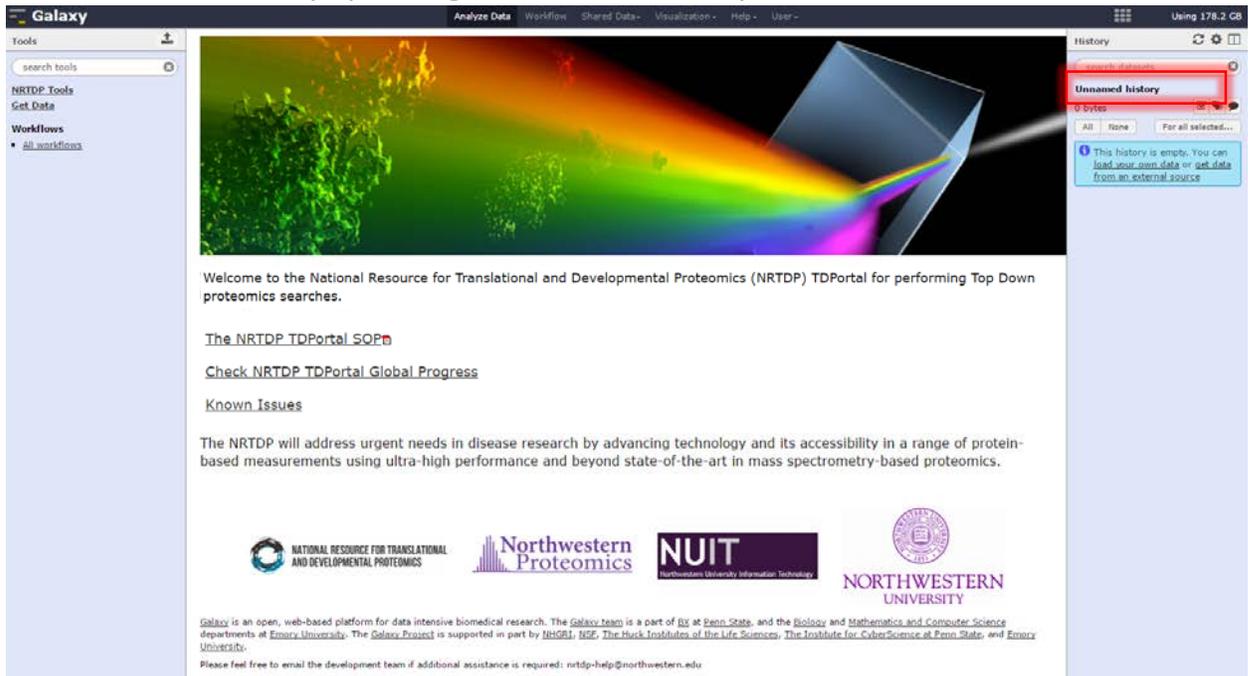
- a. There are six subheadings that link to different pages.
- b. The History Panel is on the right. When data is uploaded or an analysis is performed, each output generates a dataset. These datasets are stored by TDPortal in the History Panel.
- c. All of the available tools are located in the blue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

Part 2: Preparing Raw files for the TDPortal Search

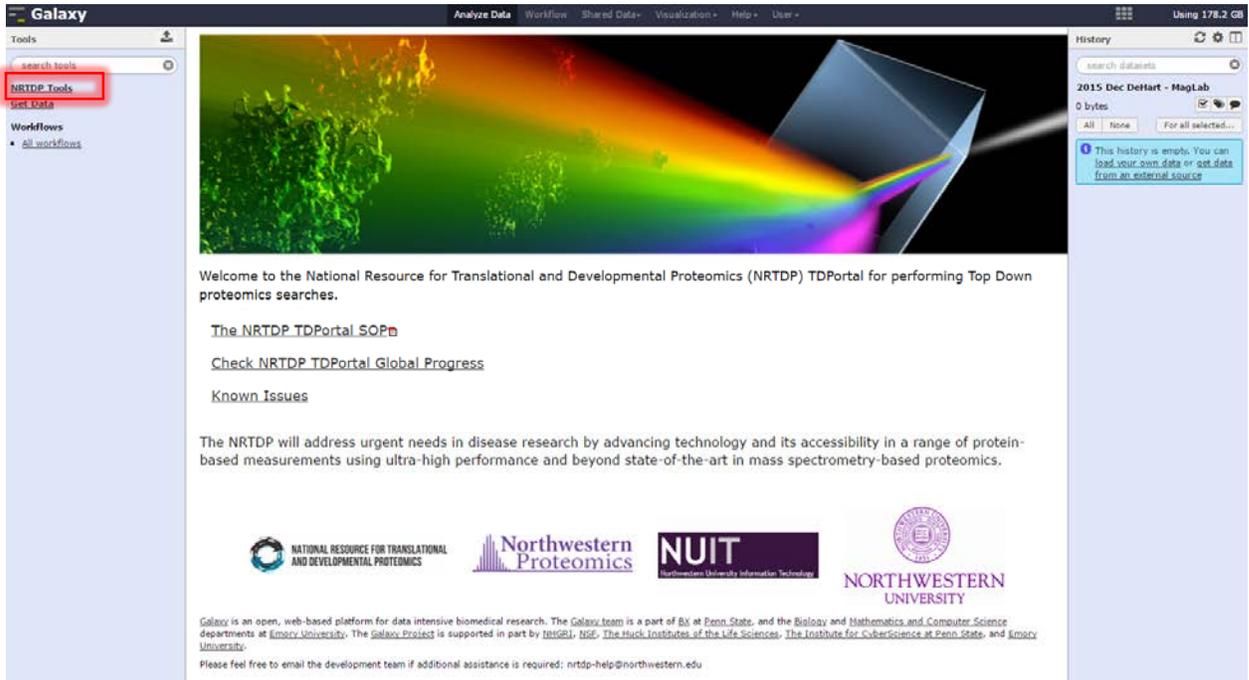
3. Create a new history. Go to the history column and click on the gear in the top right . A drop down menu will appear. Click on “Create New.”



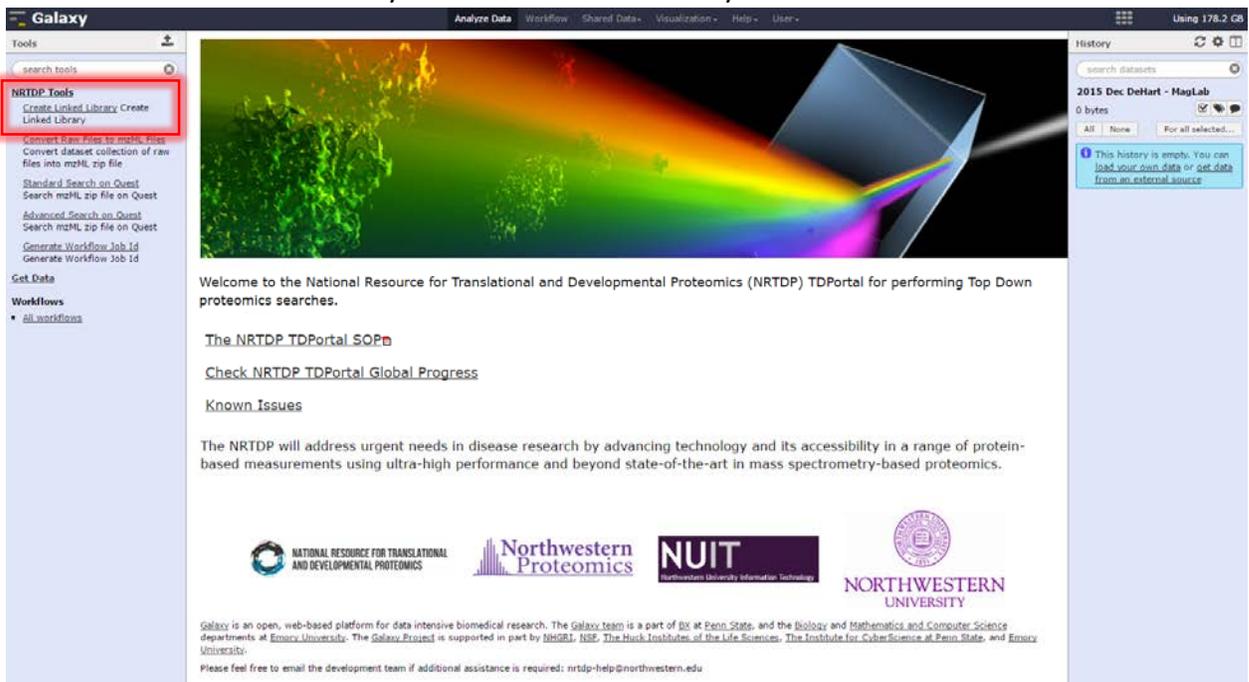
4. Rename the new history by clicking on “Unnamed History.”



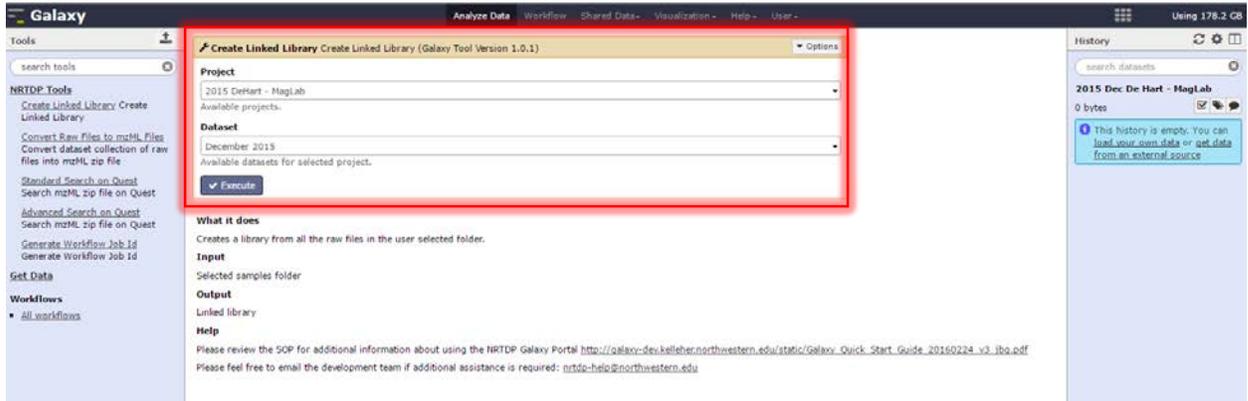
- Go to Tools Panel and click on “NRTDP Tools.” A menu containing all the available NRTDP tools will appear.



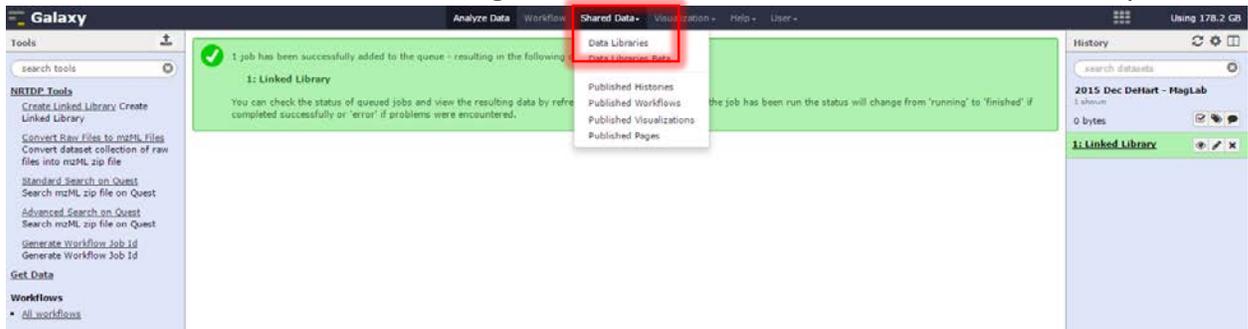
- Click on “Create Linked Library” to create a linked library.



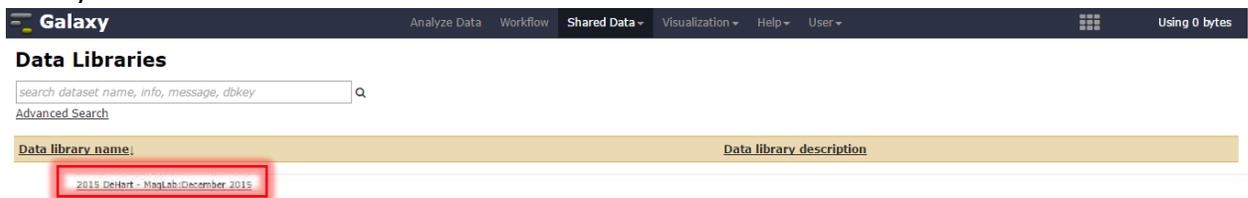
7. Select the dataset that will be searched. Click “Execute.”



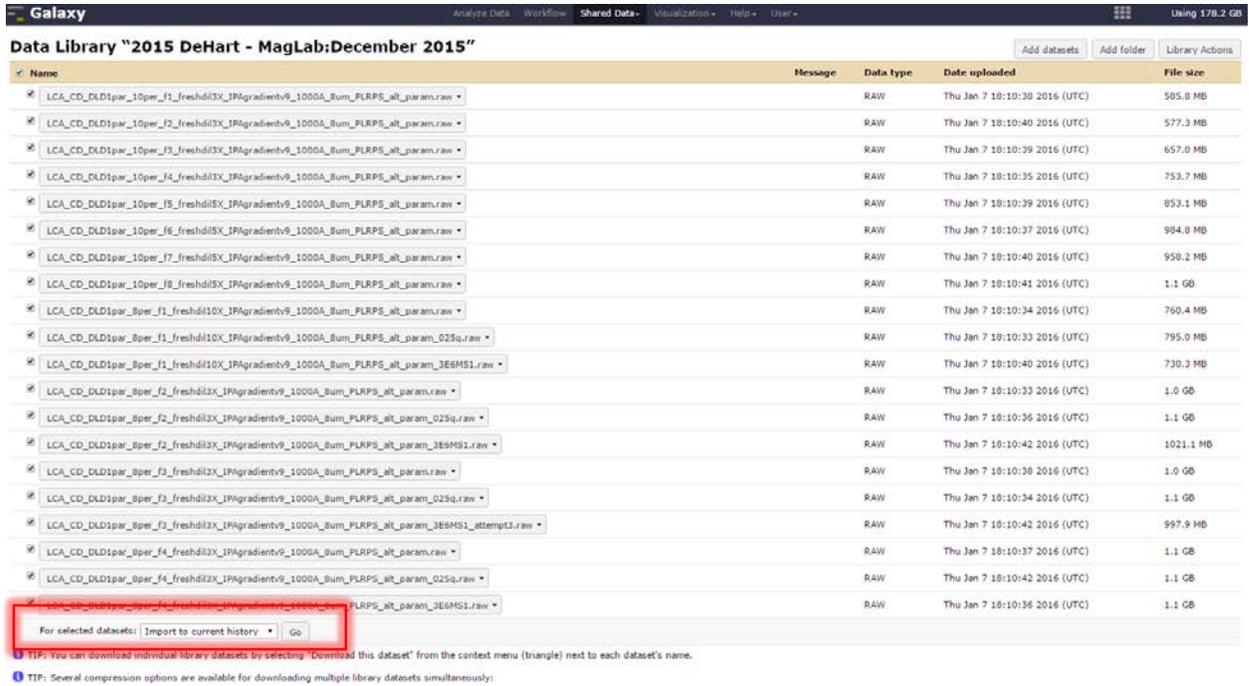
8. Click on the “Shared Data” subheading and “Data Libraries” view available linked library.



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 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 set to "Import to current history" and a "Go" button next to it.

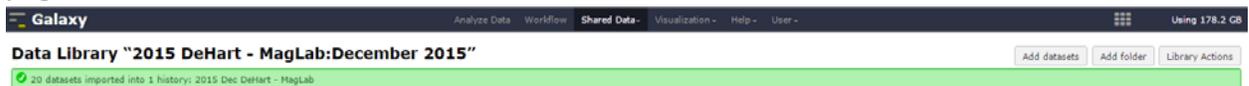
Name	Message	Data type	Date uploaded	File size
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f1_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:38 2016 (UTC)	505.8 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f2_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:40 2016 (UTC)	577.3 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f3_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param.raw		RAW	Thu Jan 7 18:10:37 2016 (UTC)	994.8 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_10per_f7_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param_Q25q.raw		RAW	Thu Jan 7 18:10:33 2016 (UTC)	795.0 MB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f1_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param_Q25q.raw		RAW	Thu Jan 7 18:10:36 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f2_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param_Q25q.raw		RAW	Thu Jan 7 18:10:34 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f3_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_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_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param_Q25q.raw		RAW	Thu Jan 7 18:10:42 2016 (UTC)	1.1 GB
<input checked="" type="checkbox"/> LCA_CD_DLD1par_8per_f4_freshd13X_IPAgradientv9_1000A_Bum_PLRPS_alt_param_3E6MS1.raw		RAW	Thu Jan 7 18:10:36 2016 (UTC)	1.1 GB

For selected datasets: Import to current history Go

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

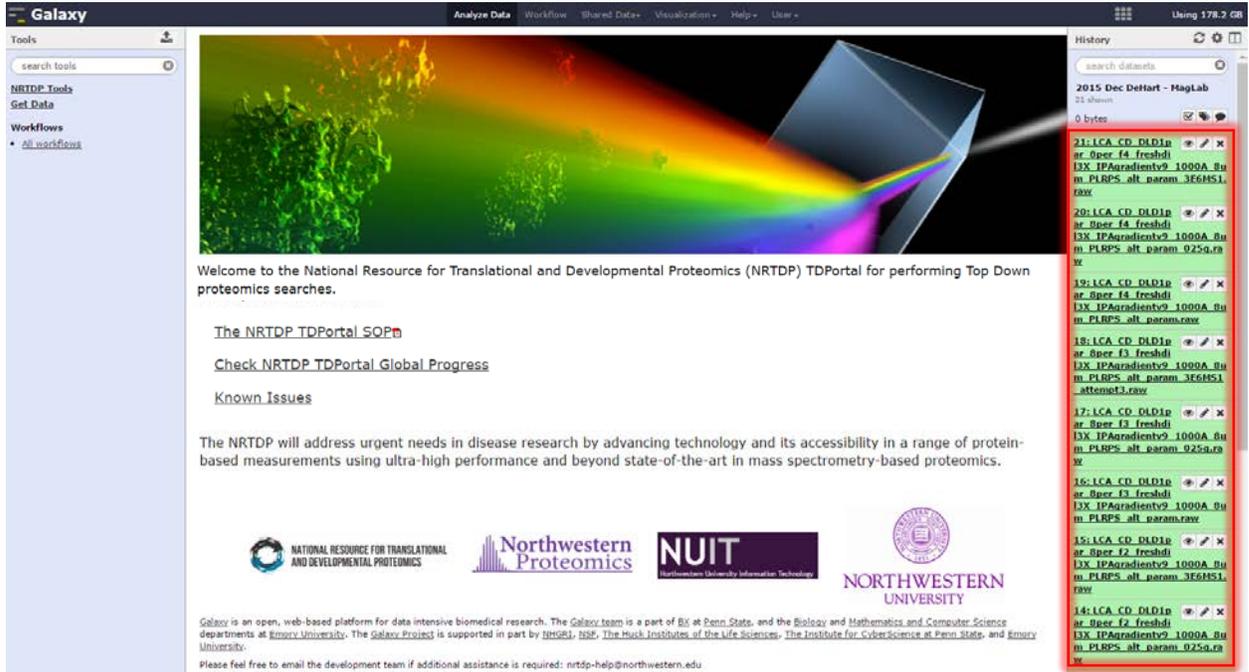
TIP: Several compression options are available for downloading multiple library datasets simultaneously:

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 Dec DeHart - MagLab".

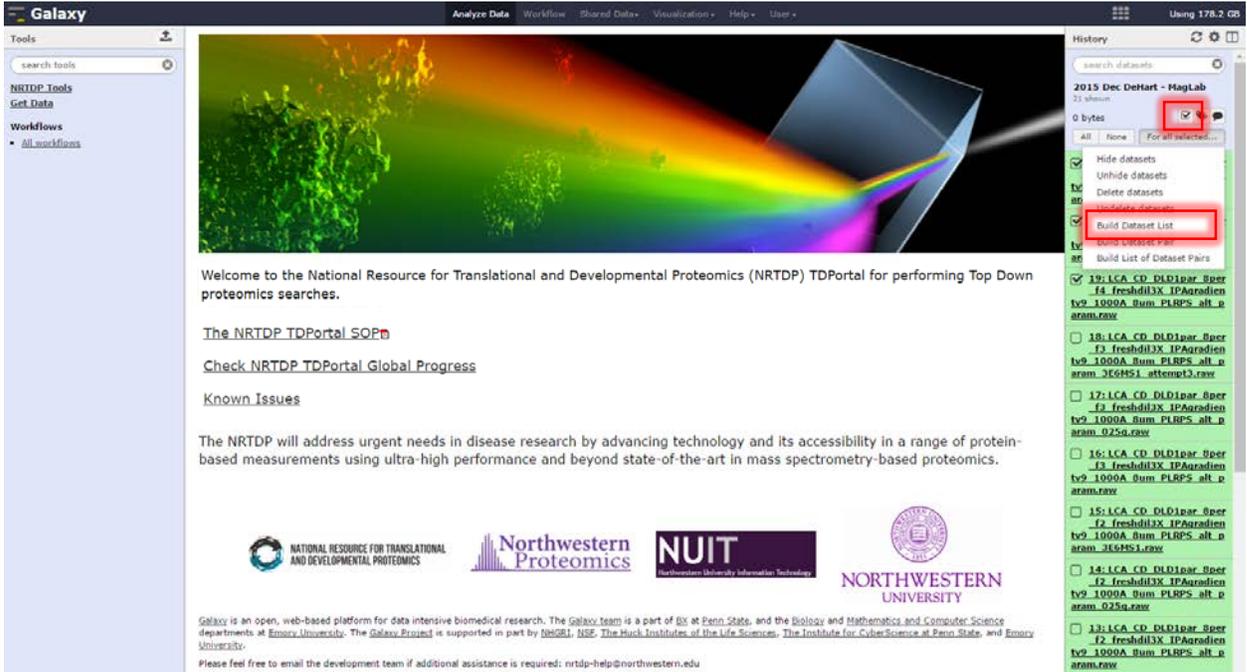
12. Click the Galaxy icon at the top of the page to return to the home page. The history has been populated with a green box for each imported raw file.



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. Logos for NRTDP, Northwestern Proteomics, NUIT, and Northwestern University are visible. A history panel on the right side of the interface is highlighted with a red border, showing a list of imported raw files with green boxes around each entry. The history list includes:

- 21: ICA_CD_D1D1p ar_Sper_14_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param_3E6H51].raw
- 20: ICA_CD_D1D1p ar_Sper_14_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param_0259.c9.w
- 19: ICA_CD_D1D1p ar_Sper_14_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param.raw
- 18: ICA_CD_D1D1p ar_Sper_13_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param_3E6H51_attenu3.raw
- 17: ICA_CD_D1D1p ar_Sper_13_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param_0259.c9.w
- 16: ICA_CD_D1D1p ar_Sper_13_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param.raw
- 15: ICA_CD_D1D1p ar_Sper_12_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param_3E6H51.raw
- 14: ICA_CD_D1D1p ar_Sper_12_freshhd [3X_IPAgradientv2_1000A_Bu m_PLRPS_all_param_0259.c9.w

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

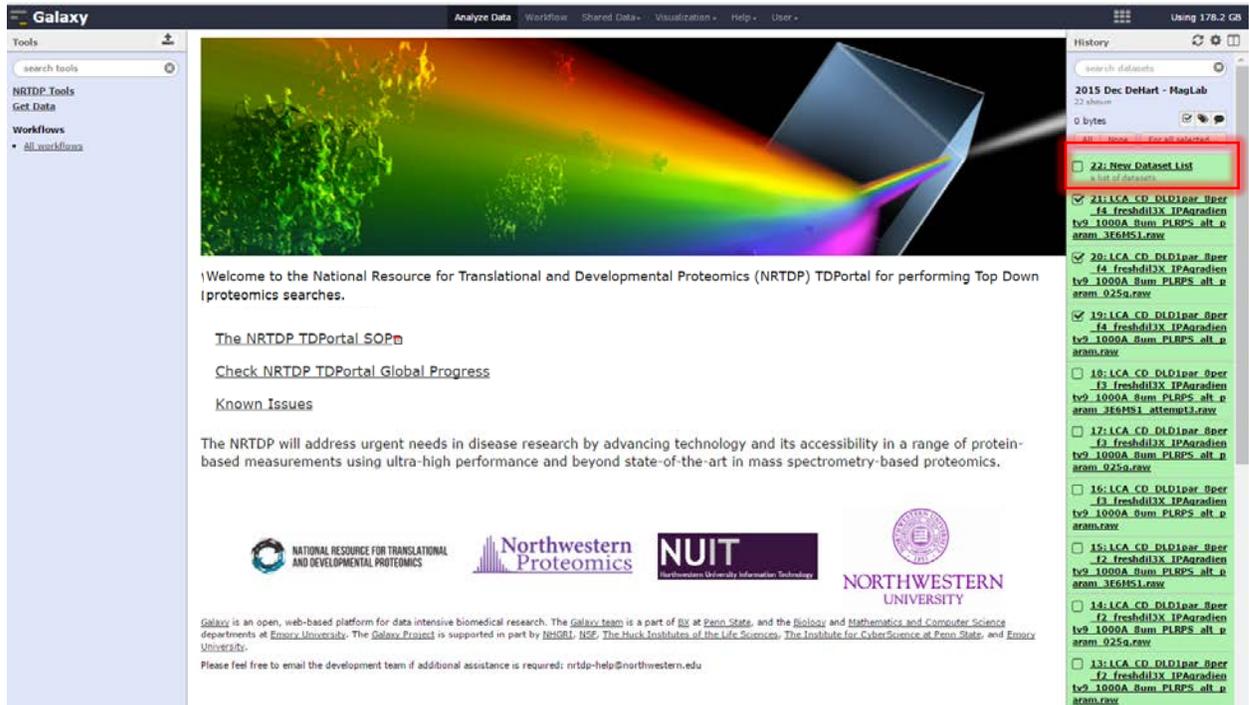


The screenshot shows the Galaxy web interface. The main content area displays a welcome message for the NRTDP TDPortal, including links to SOPs, global progress, and known issues. Logos for the National Resource for Translational and Developmental Proteomics, Northwestern Proteomics, NUIT, and Northwestern University are visible. The History panel on the right shows a list of datasets with checkboxes. The 'Build Dataset List' button is highlighted with a red box.

Galaxy is an open, web-based platform for data intensive biomedical research. The Galaxy team is a part of IIS at Penn State, and the Biology and Mathematics and Computer Science departments at Emory University. The Galaxy Project is supported in part by NHGRI, NSF, The Huck Institutes of the Life Sciences, The Institute for CyberScience at Penn State, and Emory University.

Please feel free to email the development team if additional assistance is required: nrtdp-help@northwestern.edu

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

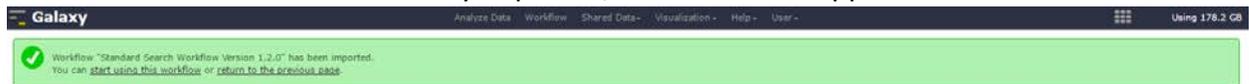


Step 3: Running searches on TDPortal

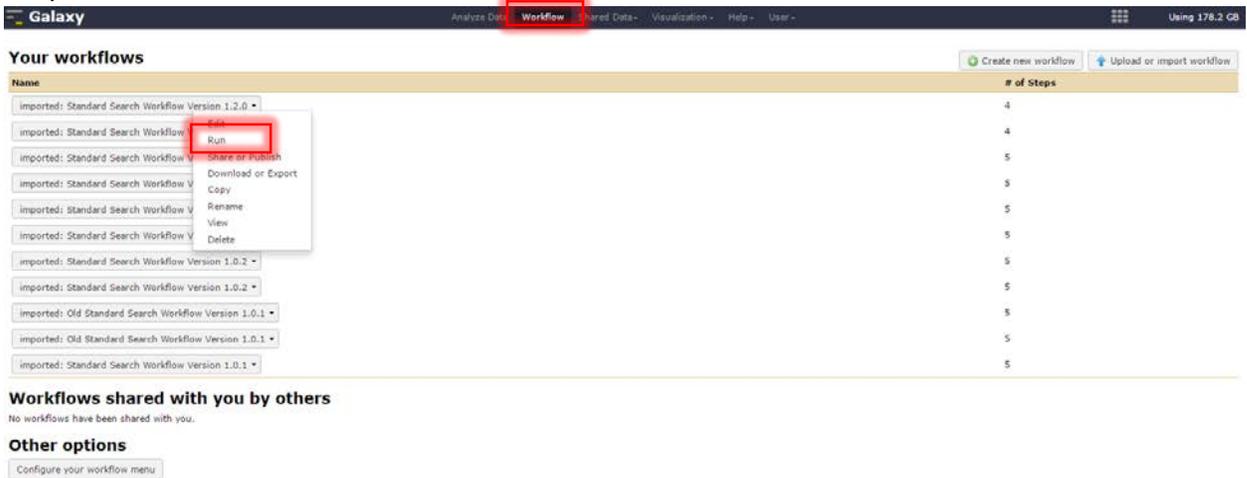
15. Navigate to Shared Data. Click on “Published Workflows” in the drop down menu. Import Published Standard Search Workflow 1.2.0 by clicking on the down arrow of the “Standard Search Workflow Version 1.2.0” tab.



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

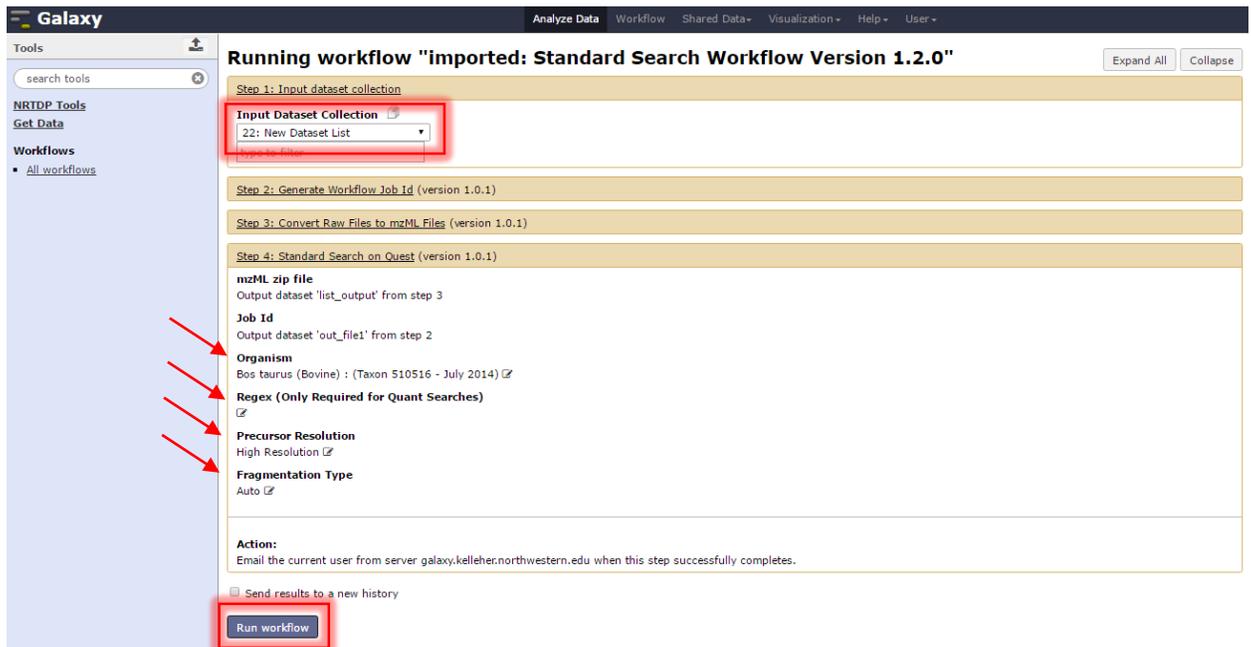


17. Click the “Workflow” Subheading. Click “Run” in Standard Search Workflow Version 1.2.0 dropdown.



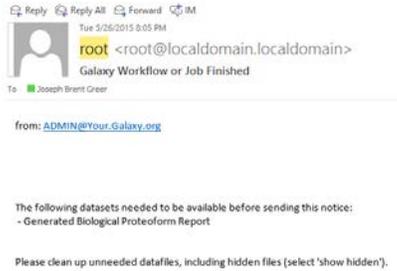
18. Input search parameters and click “Run Workflow.”

- 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.

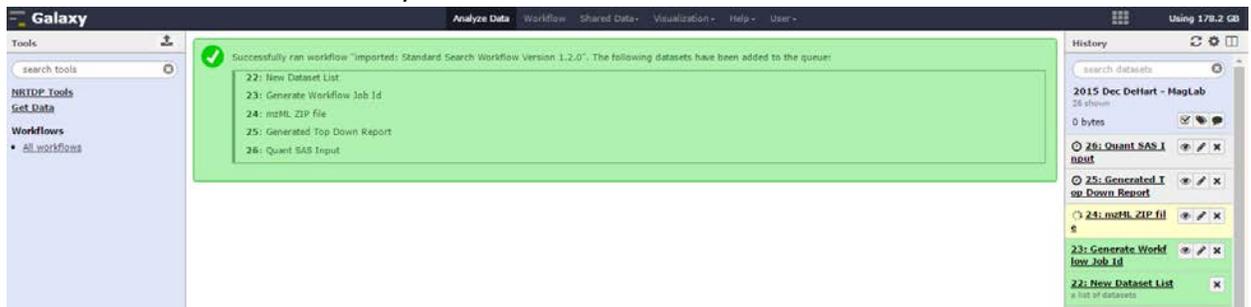


Step 4: Monitoring Progress of TDPortal Searches

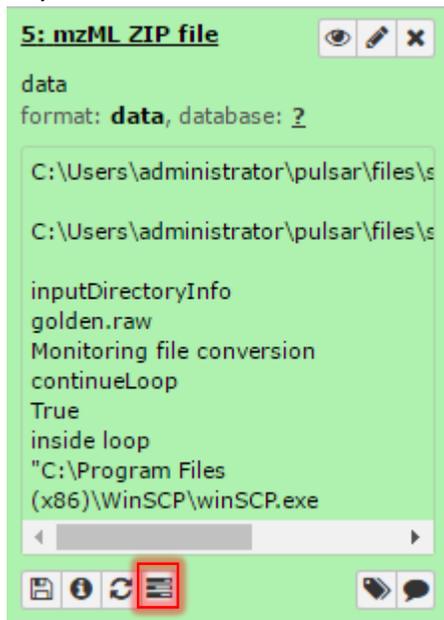
19. An email will be sent once the workflow has started containing history and job id information as well as a link to check progress outside of Galaxy.



20. The search will be added to History Panel.



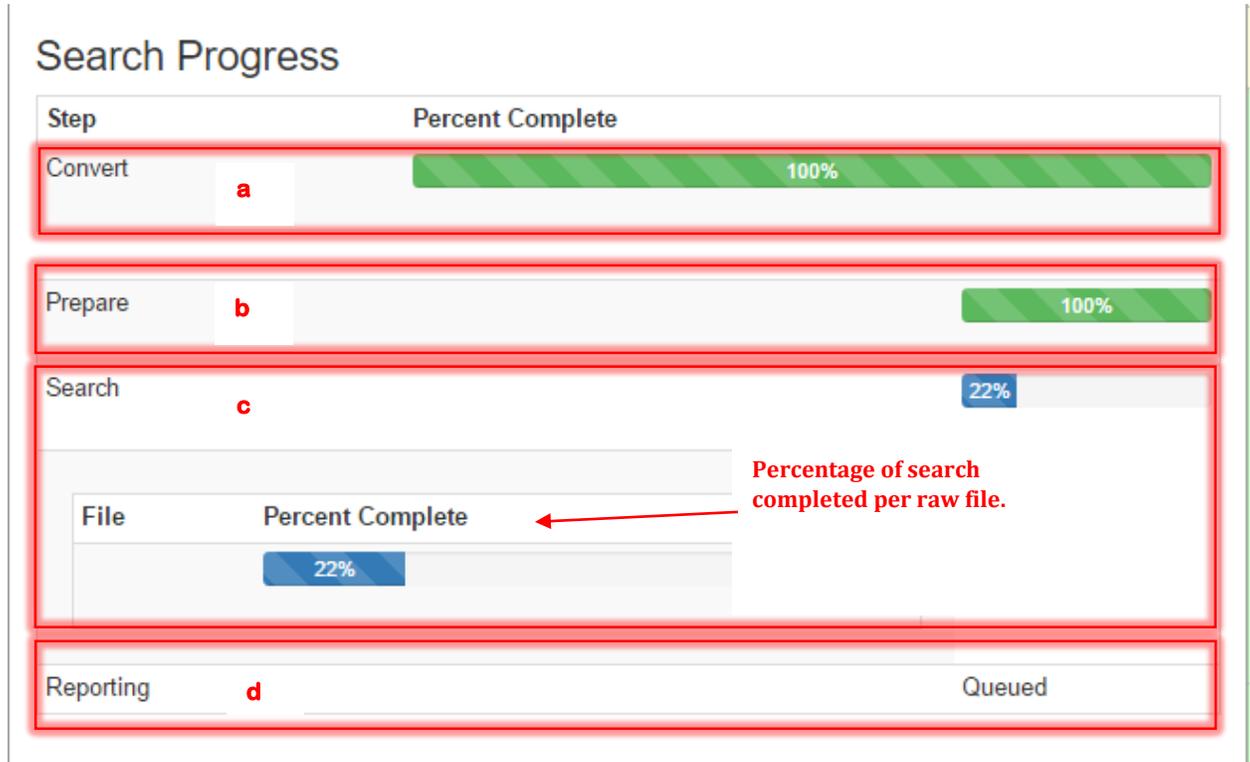
21. Monitor Search progress by clicking on Check Progress button under mzML Zip file in the History Panel.



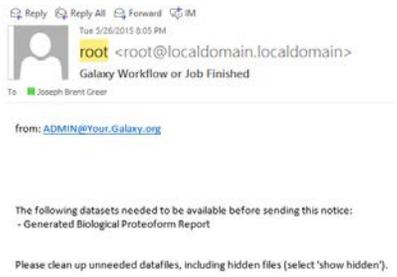
22. In progress, the date of the search, and user email will be visible.

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

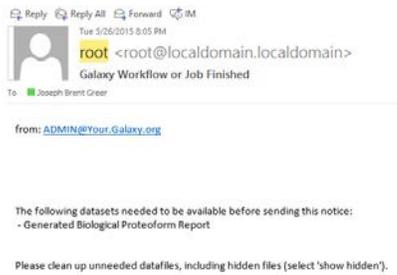
23. Four percentages are displayed in search progress. The page refreshes every 30 seconds.



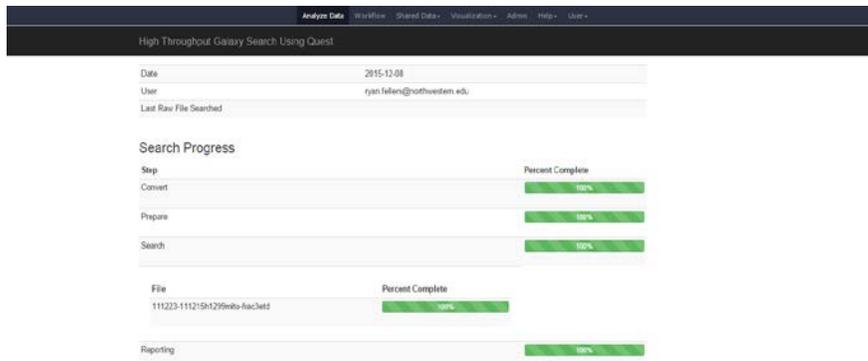
- The Convert percent is the percentage of raw files that have been converted to mzML.
 - The Prepare percent is the percent of mzML files that have been prepared for search.
 - The Search percent is the percent of searching all the mzML that has completed.
 - The search percent for each mzML file is 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.

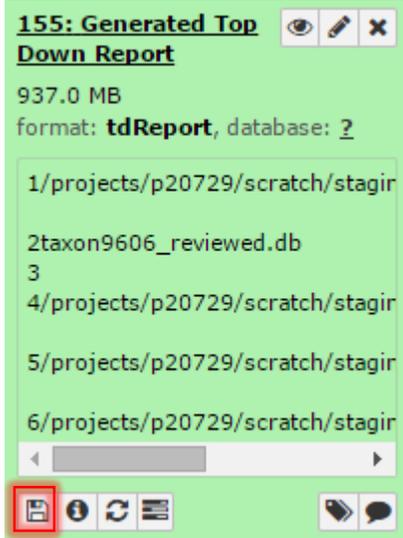


26. The History Panel items will turn green when the search fully completes.



Step 5: 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)

