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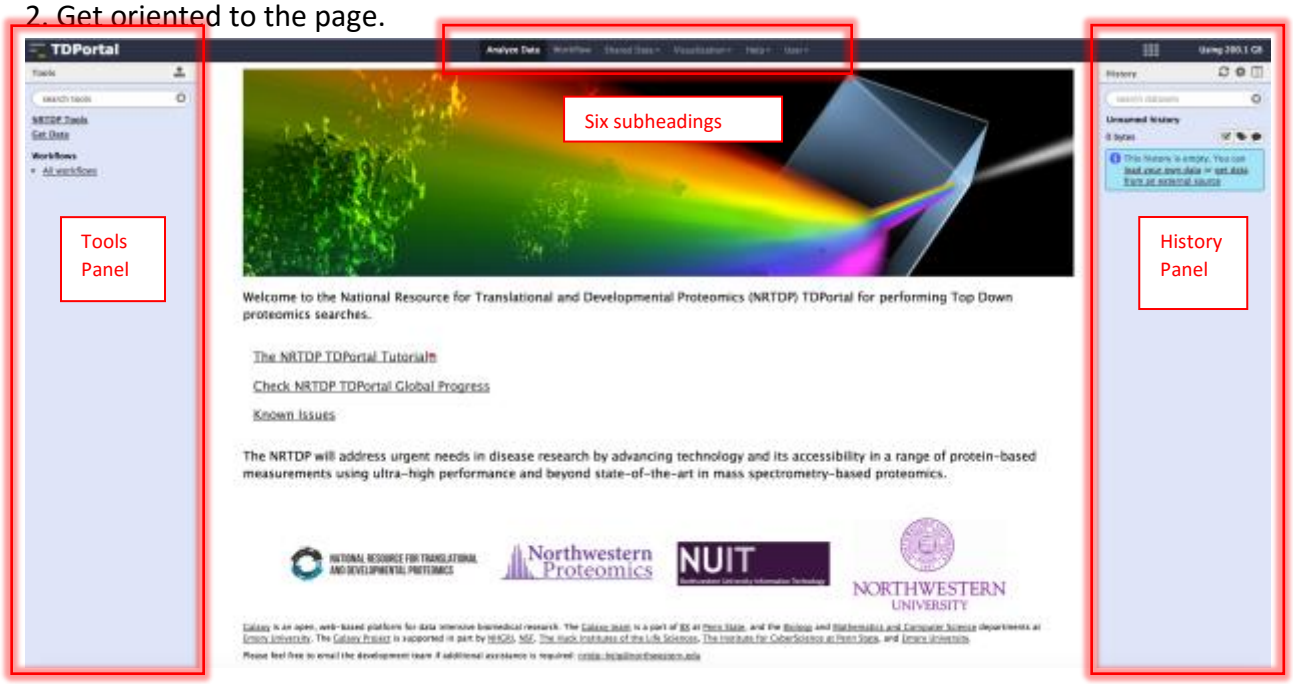
External User Guide for Performing High Throughput Searches on TDPortal

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

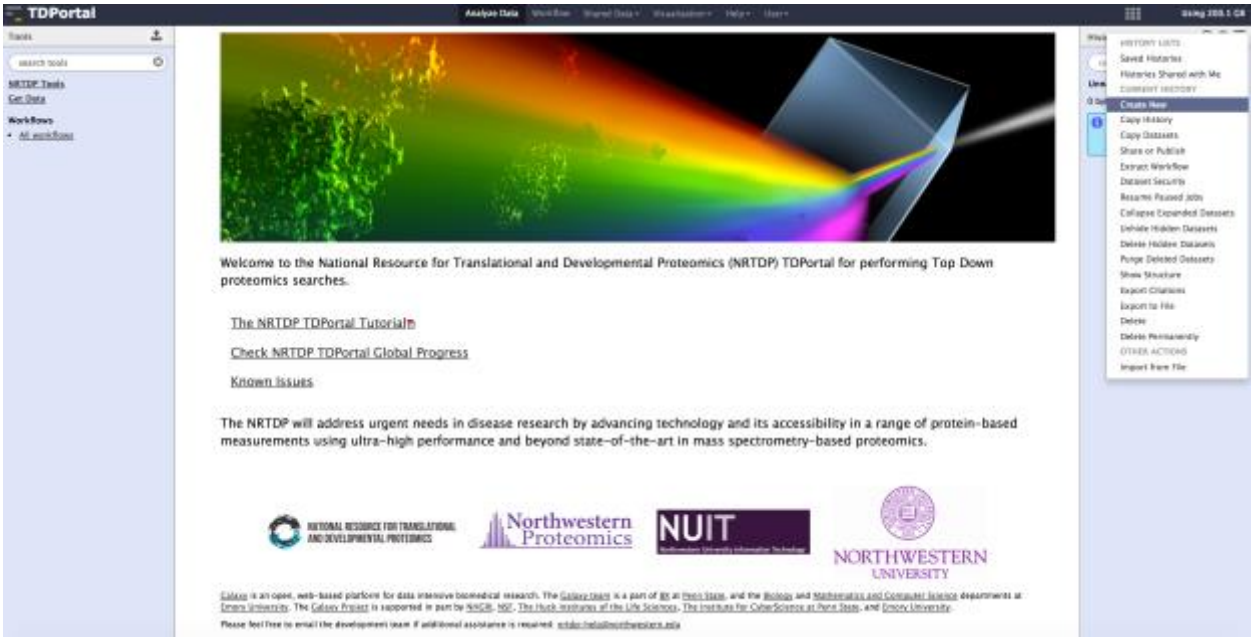
2. Get oriented to the page.



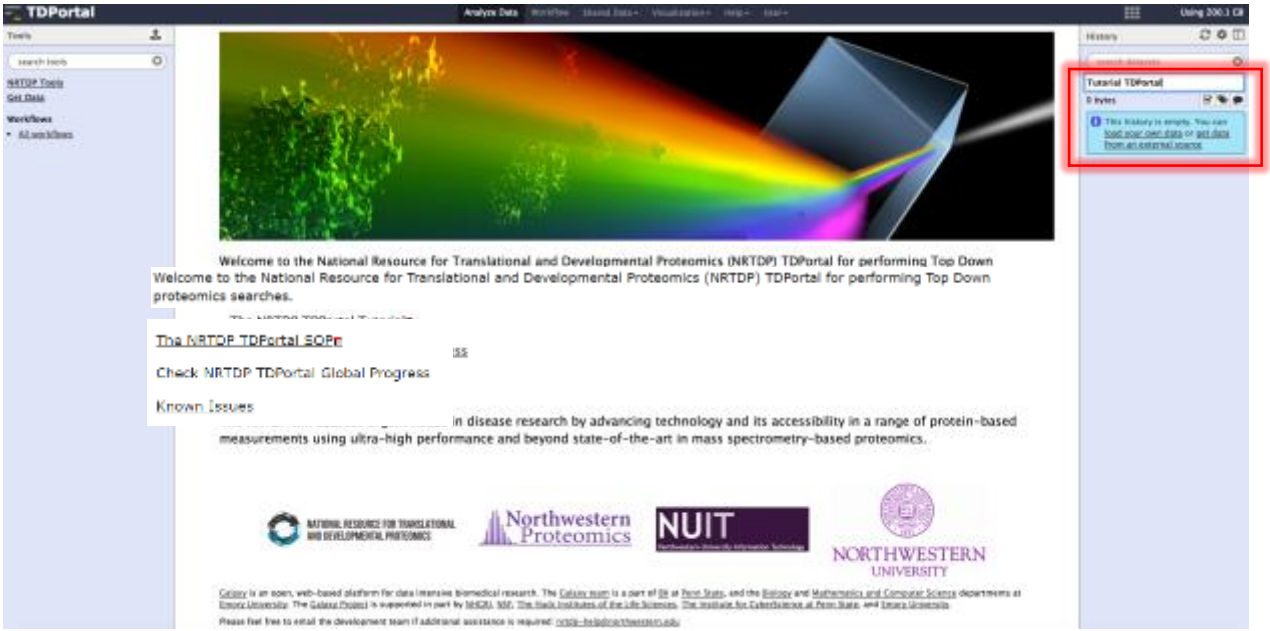
a. There are six subheadings that link to different pages.
b. The History Panel is on the right. When data is uploaded or an analysis is performed, each output generates a dataset. These datasets are stored by TDPortal in the History Panel.
c. All of the available tools are located in the blue Tools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

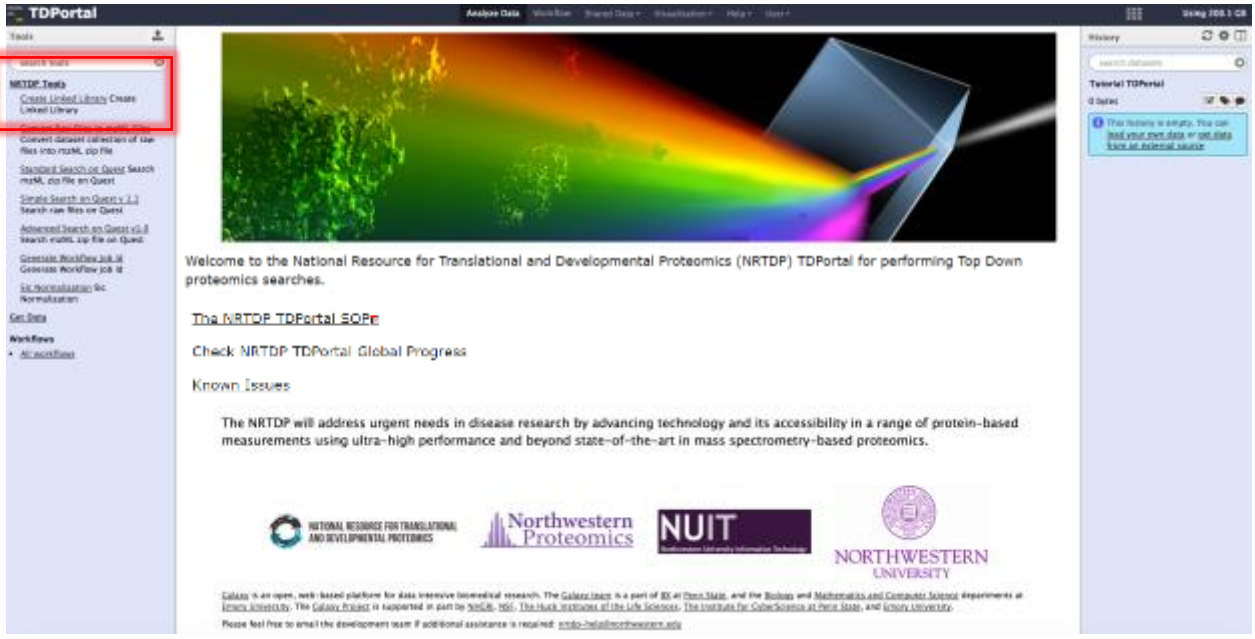


4. Rename the new history by clicking on “Unnamed History.”

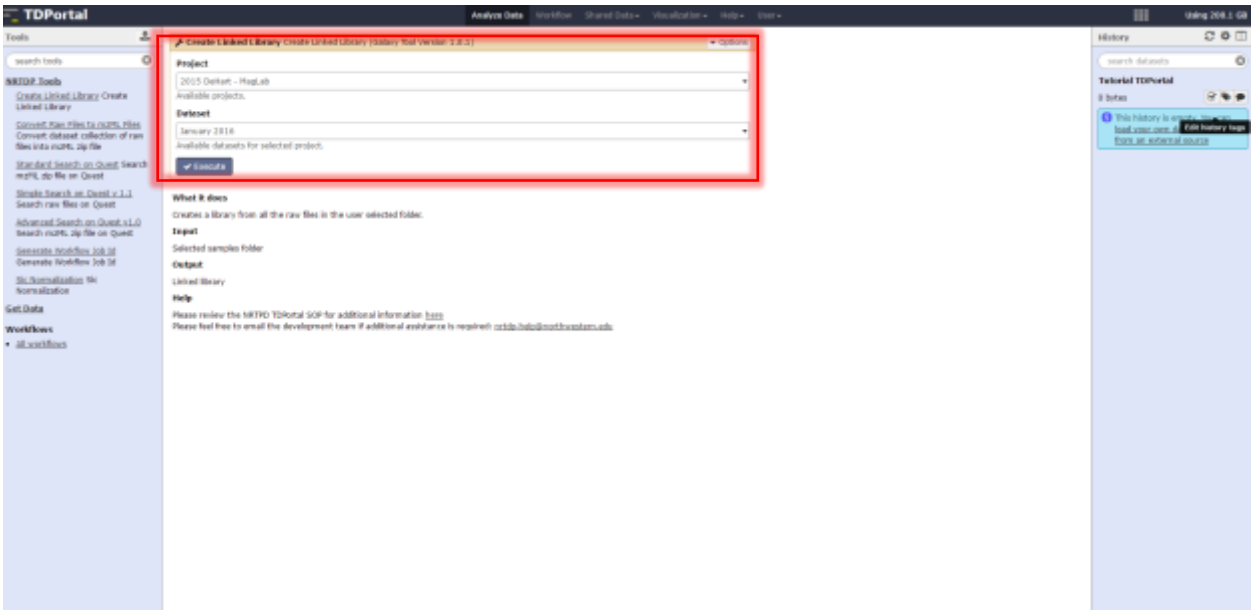


5. Go to Tools Panel and click on “NRTDP Tools.” A menu containing all the available NRTDP tools will appear.

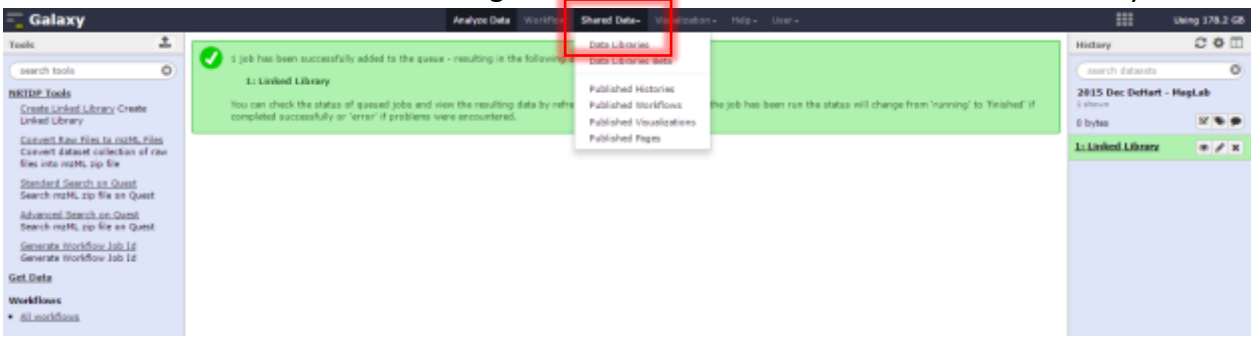
6. Click on “Create Linked Library” to create a linked library.



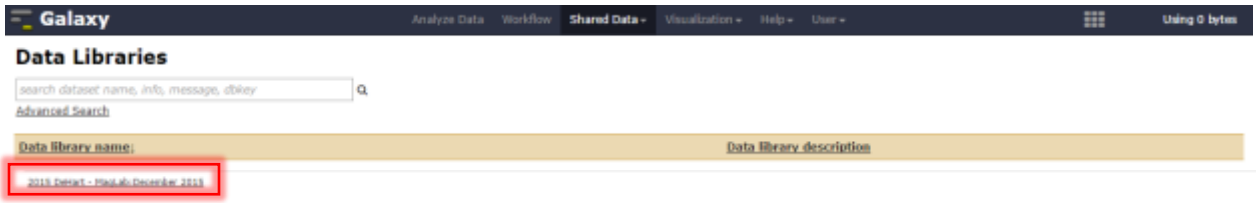
7. Select the dataset that will be searched. Click “Execute.”



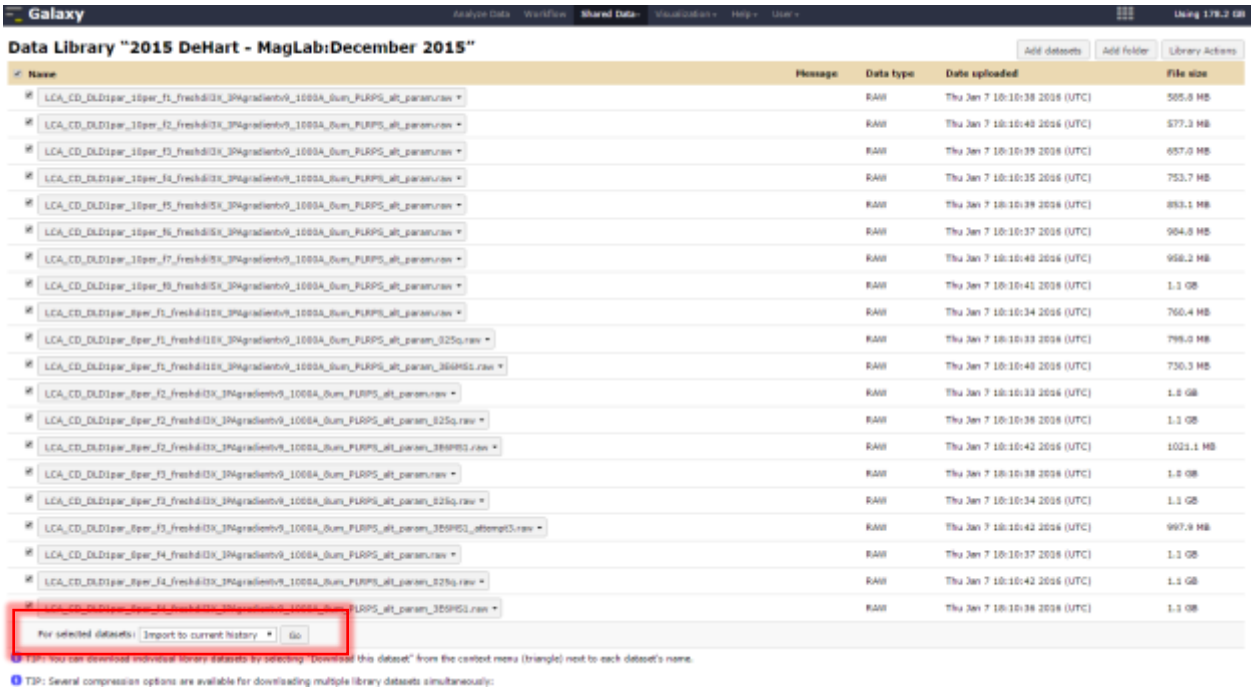
8. Click on the “Shared Data” subheading and “Data Libraries” view available linked library.



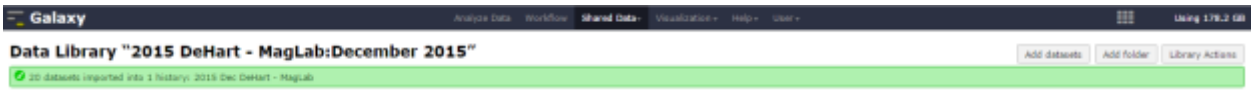
9. The Data Libraries screen displays available data libraries. Click on the desired data set library



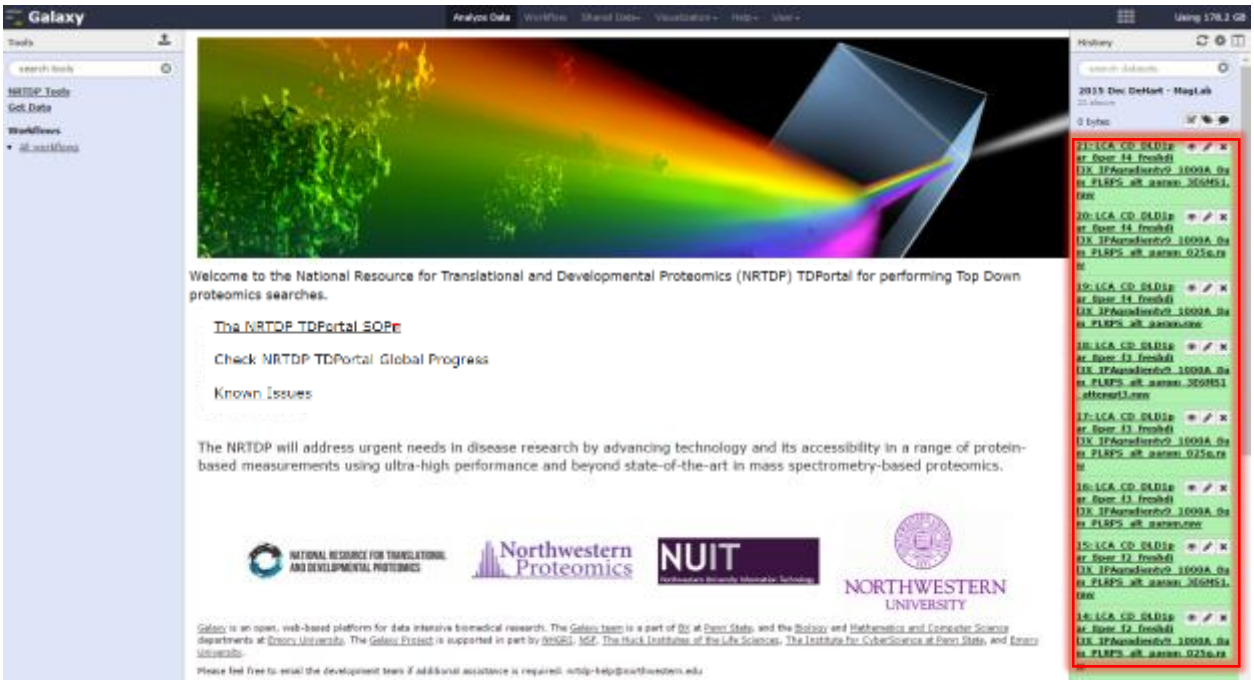
10. The next screen displays the dataset raw files. Select files to import to history by checking their checkboxes. At the bottom of the page there is a “For selected datasets” dropdown menu. Set the dropdown next to “Import to current history” and click “Go.”



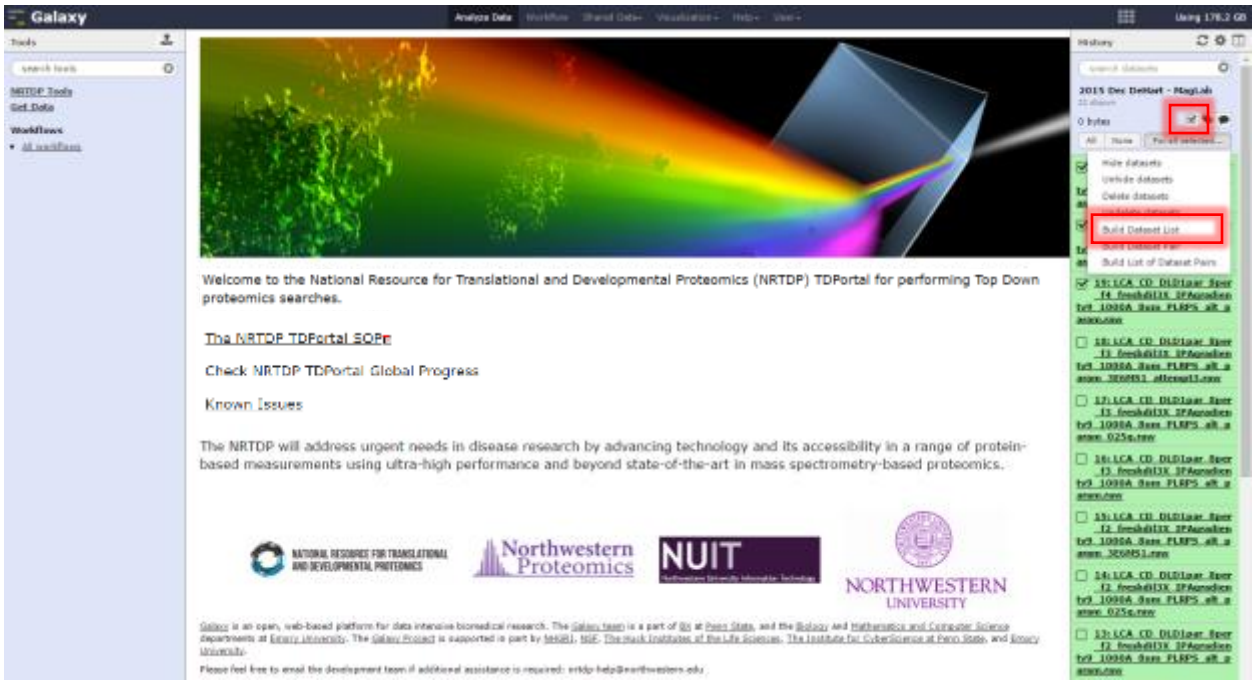
11. Once the files are successfully imported this confirmation will be displayed at the top of the page.



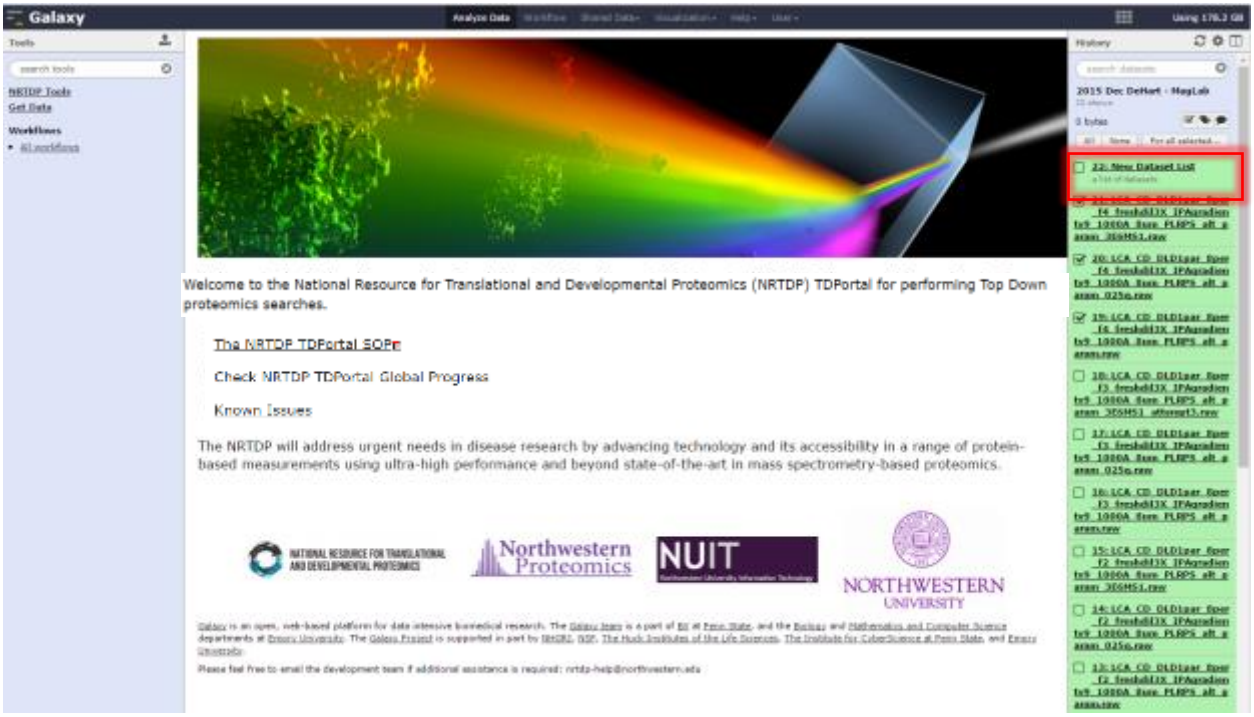
12. Click the Galaxy icon at the top of the page to return to the home page. The history has been populated with a green box for each imported raw file.



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



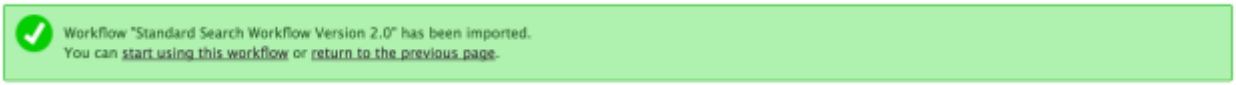
14. A new dataset list will appear in the History Panel.



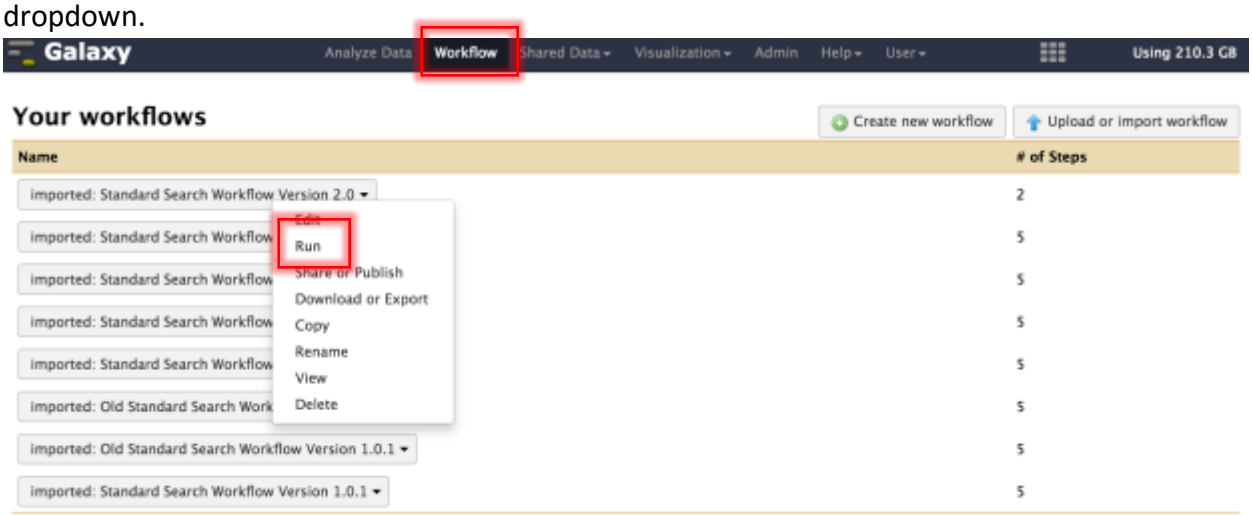
Step 4: Running searches on TDPortal

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.



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

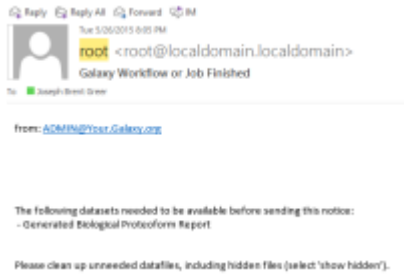
Auto

Code Set

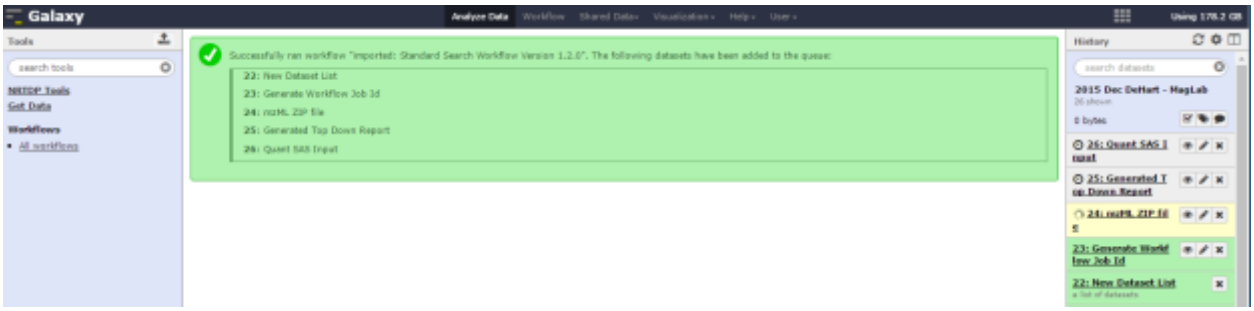
Search v2.0

Step 5: Monitoring Progress of TDPortal Searches

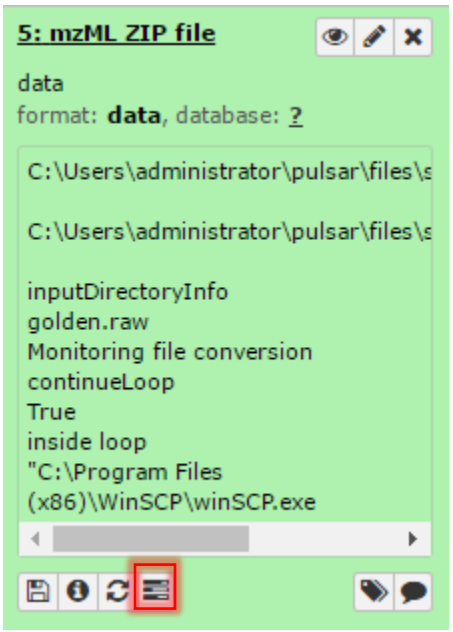
19. An email will be sent once the workflow has started containing history and job id information as well as a link to check progress outside of Galaxy.



20. The search will be added to History Panel.

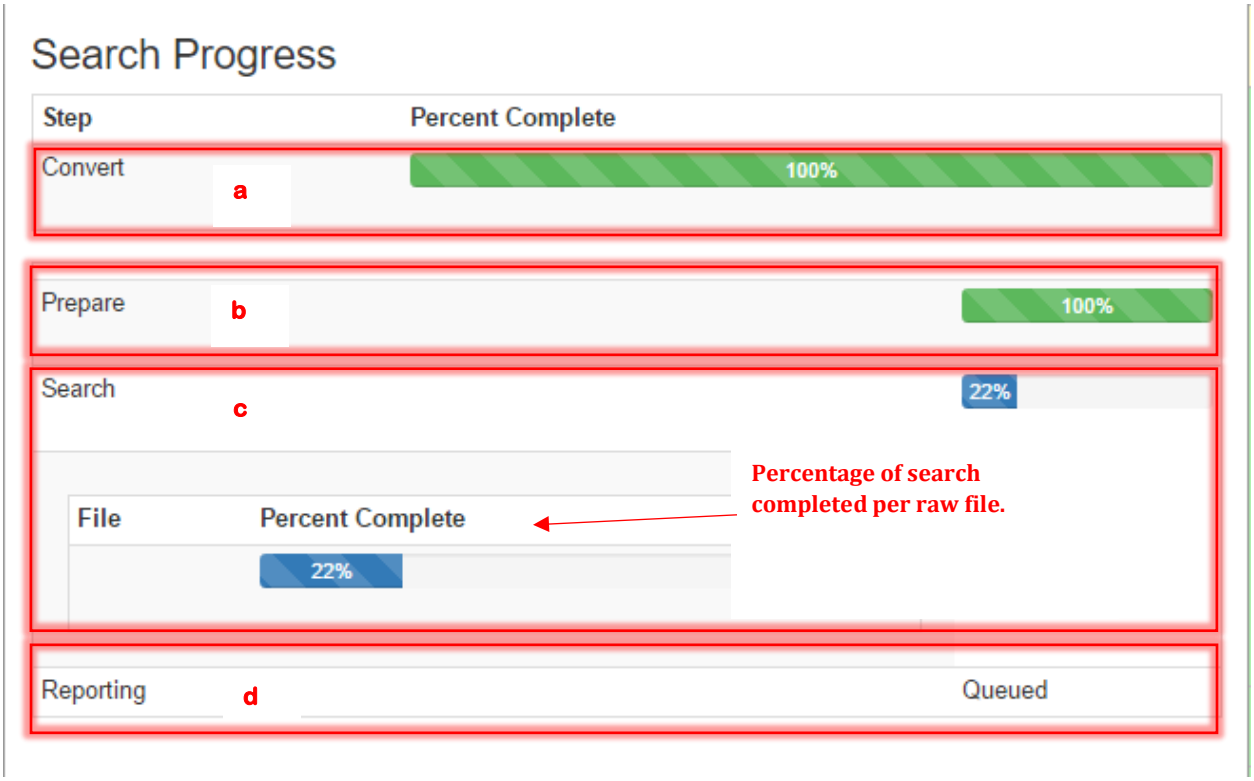


21. Monitor Search progress by clicking on Check Progress button under mzML Zip file in the History Panel.



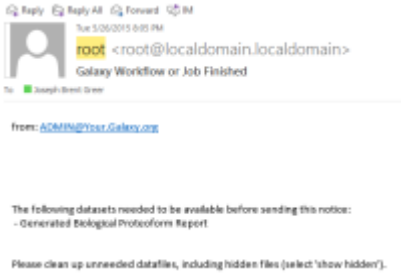
22. In progress, the date of the search, and user email will be visible.

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

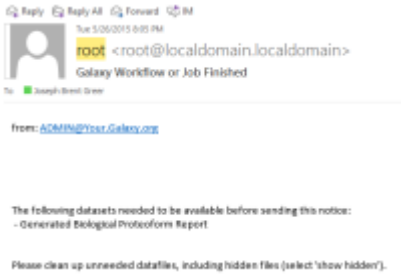


a. The Convert percent is the percentage of raw files that have been converted to mzML.
b. The Prepare percent is the percent of mzML files that have been prepared for search.
c. The Search percent is the percent of searching all the mzML that has completed.
d. The search percent for each mzML file is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

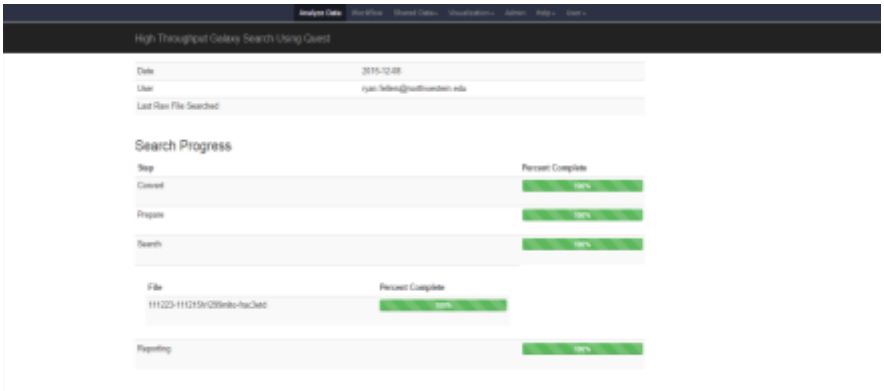
24. TDPortal will send an email immediately if a step in the workflow fails. The email will contain history and job id information.



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

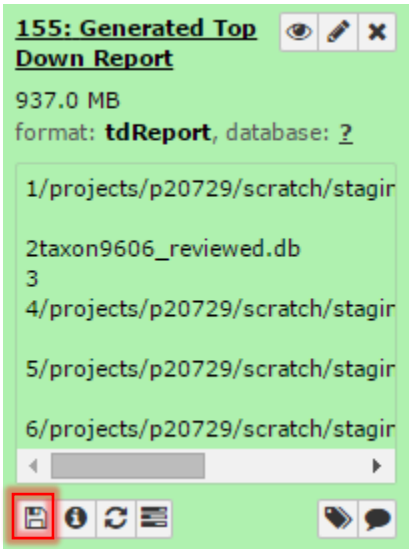


26. The History Panel items will turn green when the search fully completes.



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)