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External User Guide for Performing High Throughput Searches on TDPortal

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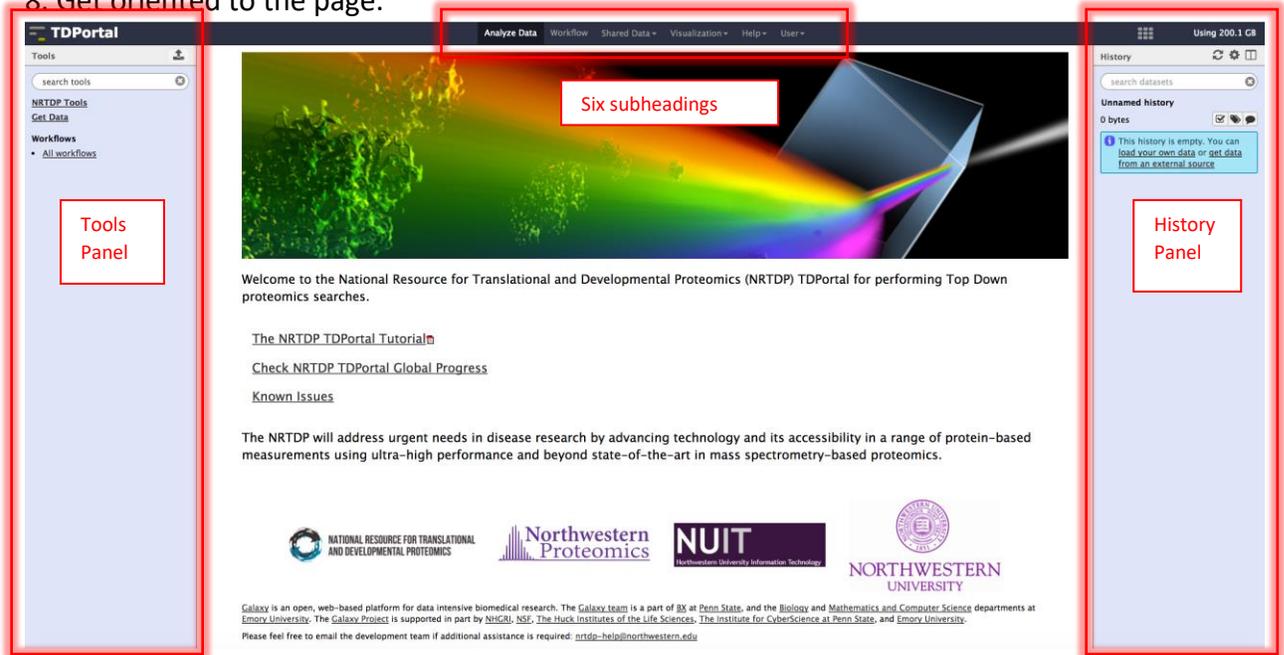
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Part 1: Transferring Project Files to TDPortal

1-7 Please email nrtdp-help@northwestern.edu

Part 2: TDPortal Page Orientation

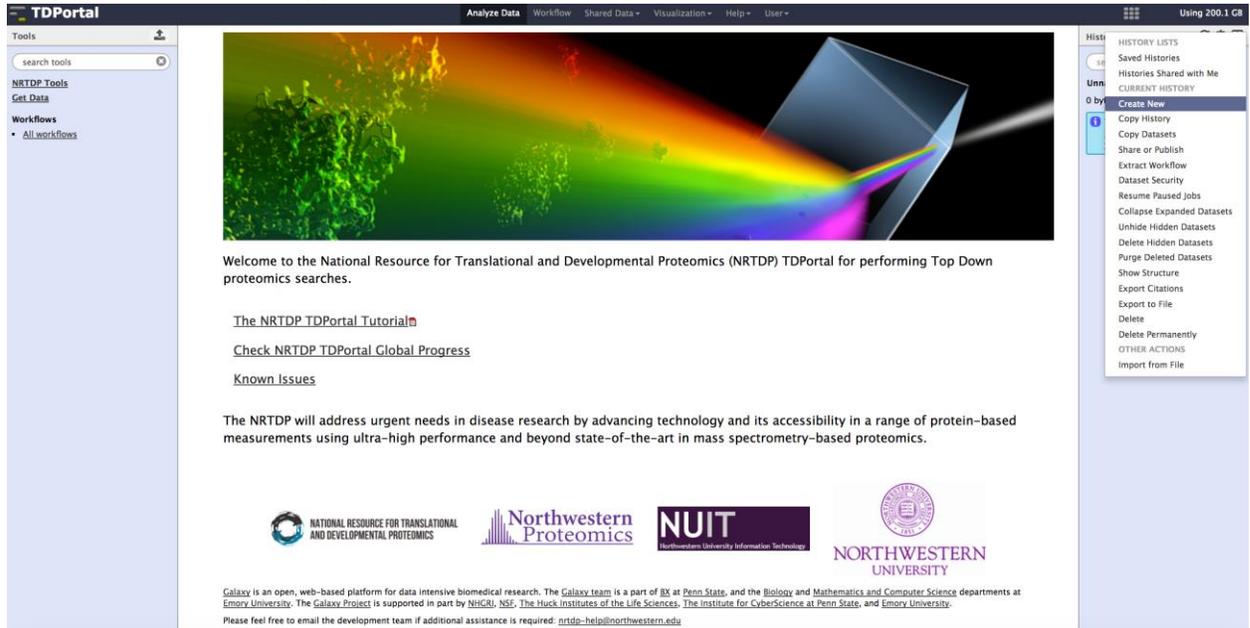
8. Get oriented to the page.



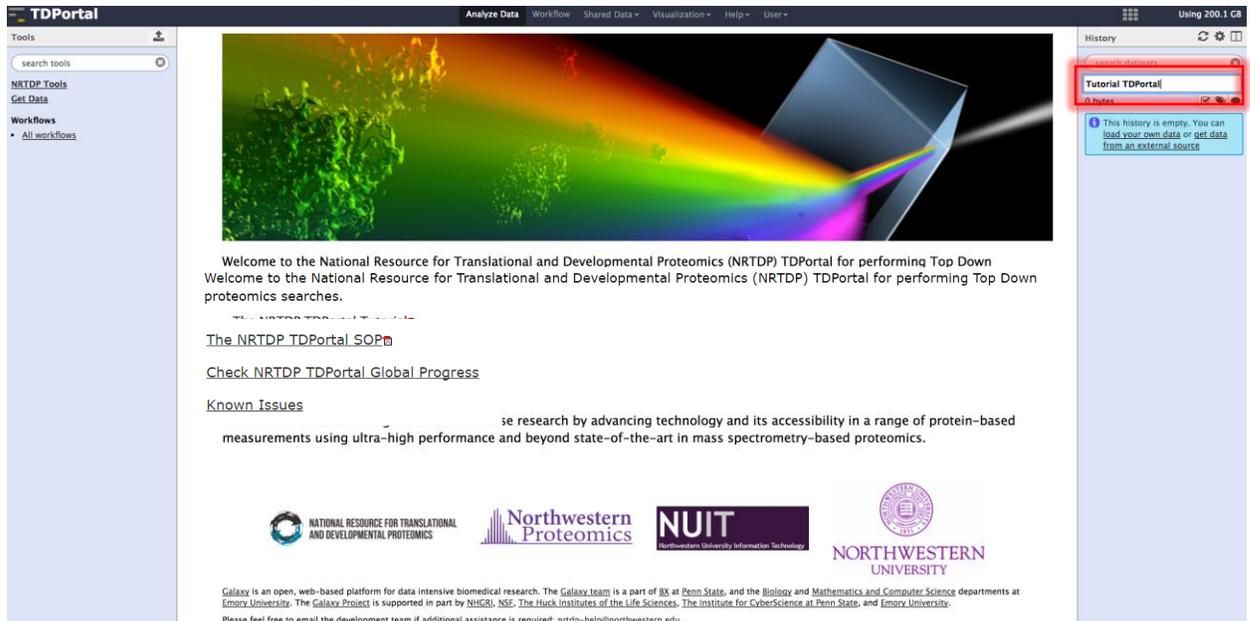
- a. There are six subheadings that link to different pages.
- b. The History Panel is on the right. When data is uploaded or an analysis is performed, each output generates a dataset. These datasets are stored by TDPortal in the History Panel.
- c. All of the available tools are located in the blue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

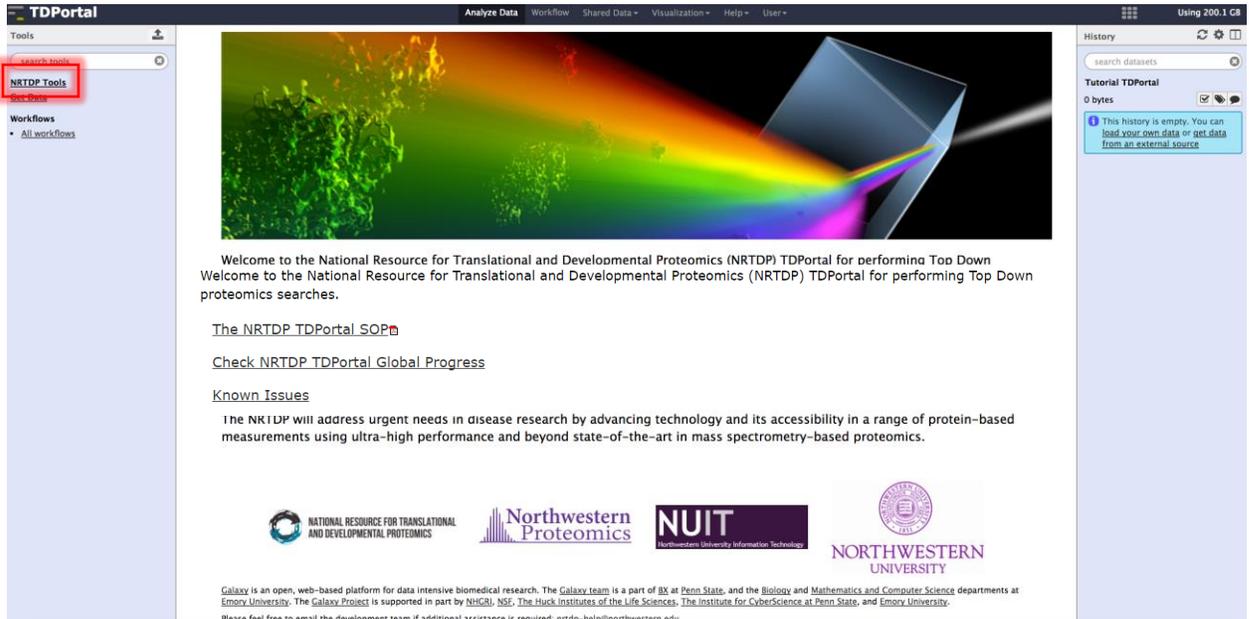
Create a new history. Go to the history column and click on the gear in the top right. A drop down menu will appear. Click on “Create New.”



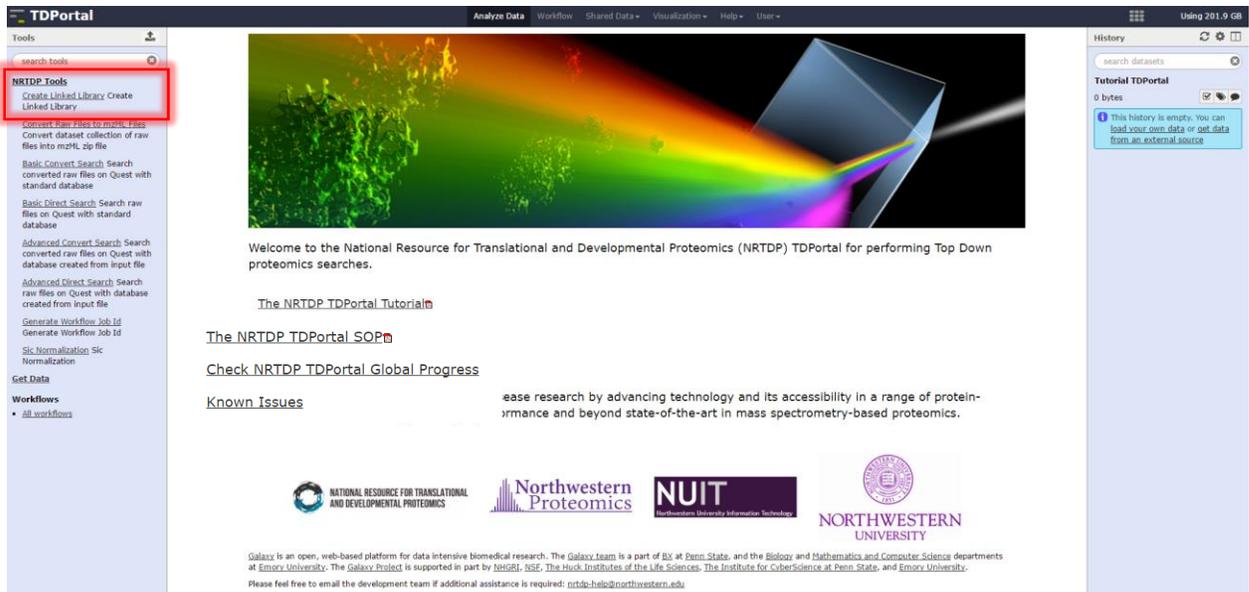
9. Rename the new history by clicking on “Unnamed History.”



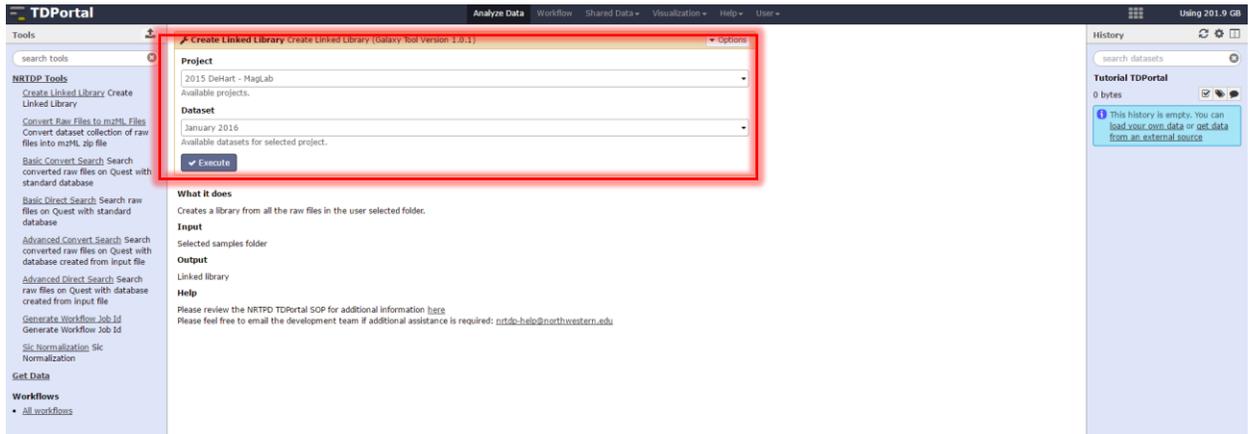
10. Go to Tools Panel and click on “NRTDP Tools.” A menu containing all the available NRTDP tools will appear.



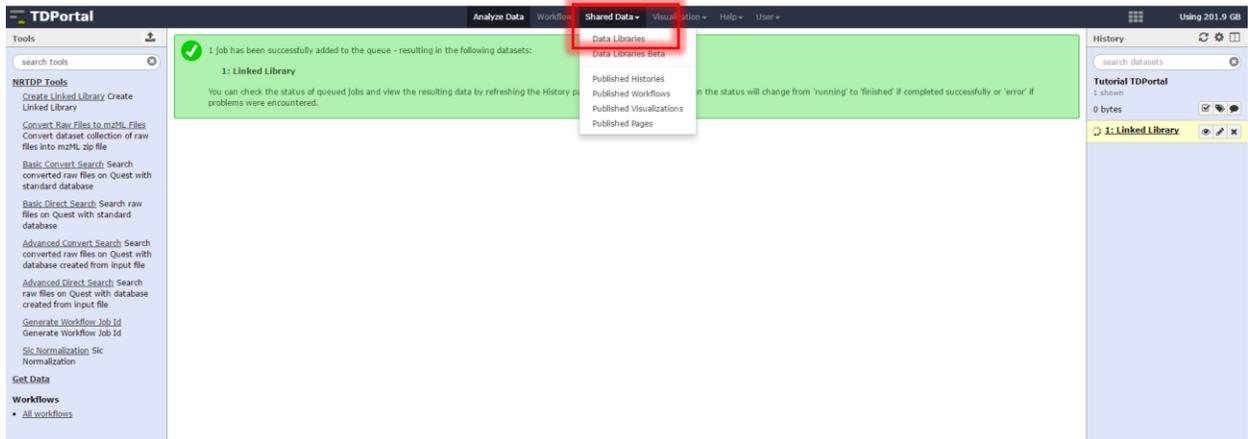
11. Click on “Create Linked Library” to create a linked library.



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



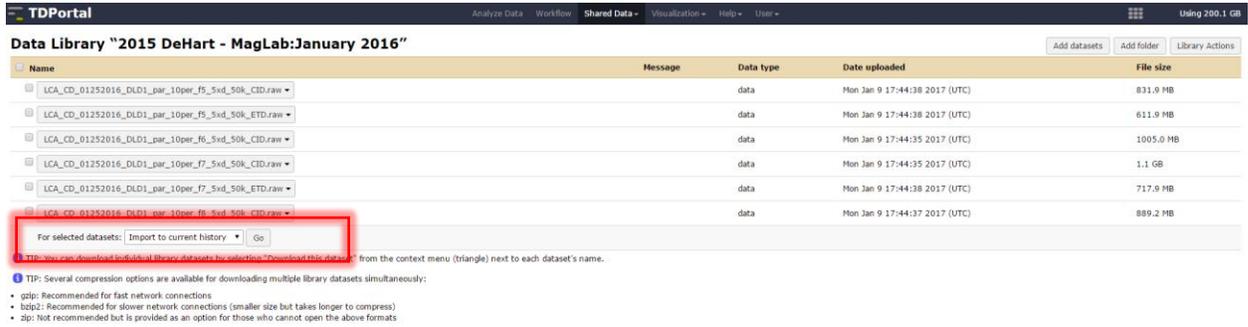
13. Click on the “Shared Data” subheading and “Data Libraries” view available linked library.



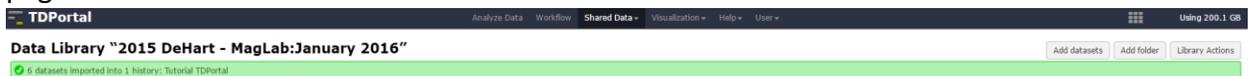
14. The Data Libraries screen displays available data libraries. Click on the desired data set library



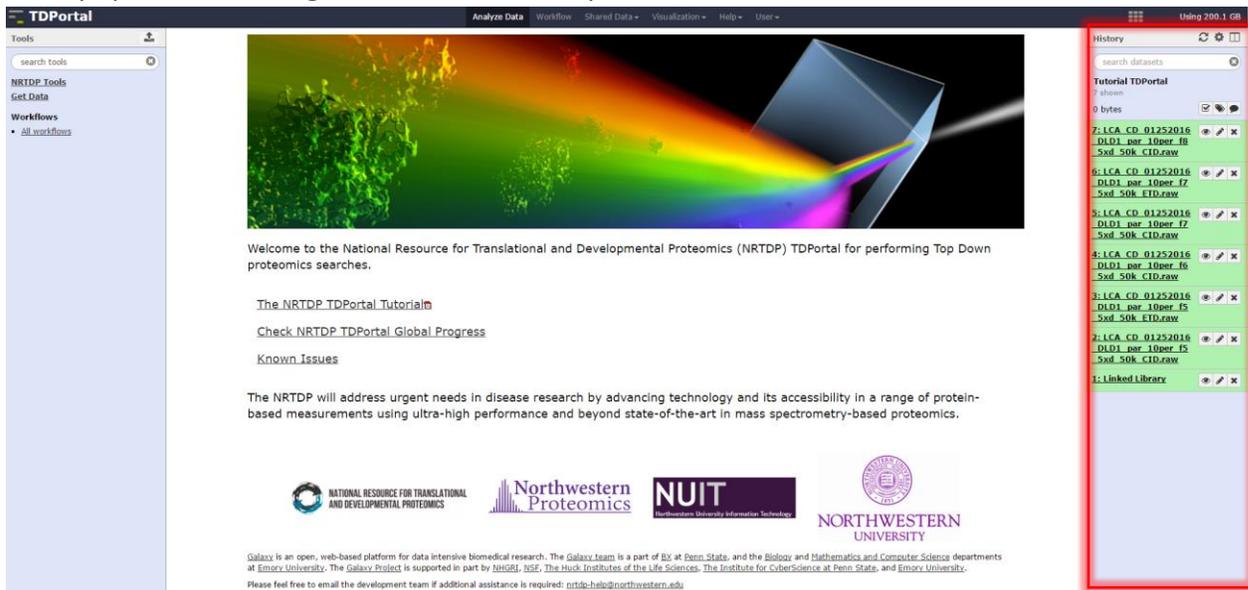
15. The next screen displays the dataset raw files. Select files to import to history by checking their checkboxes. At the bottom of the page there is a “For selected datasets” dropdown menu. Set the dropdown next to “Import to current history” and click “Go.”



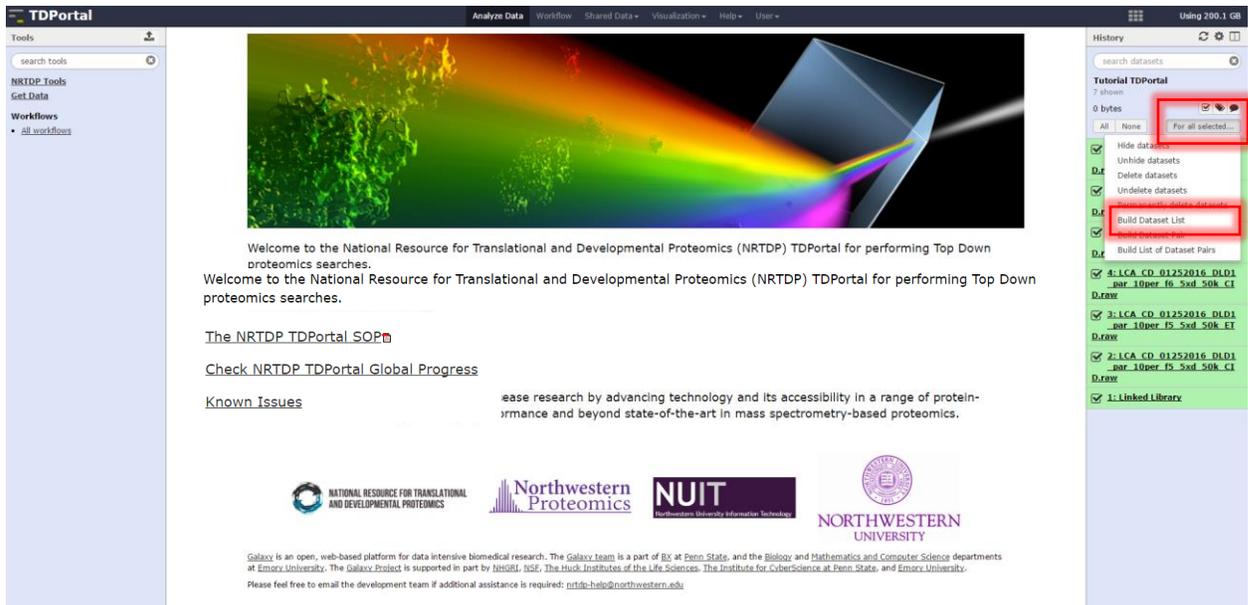
16. Once the files are successfully imported this confirmation will be displayed at the top of the page.



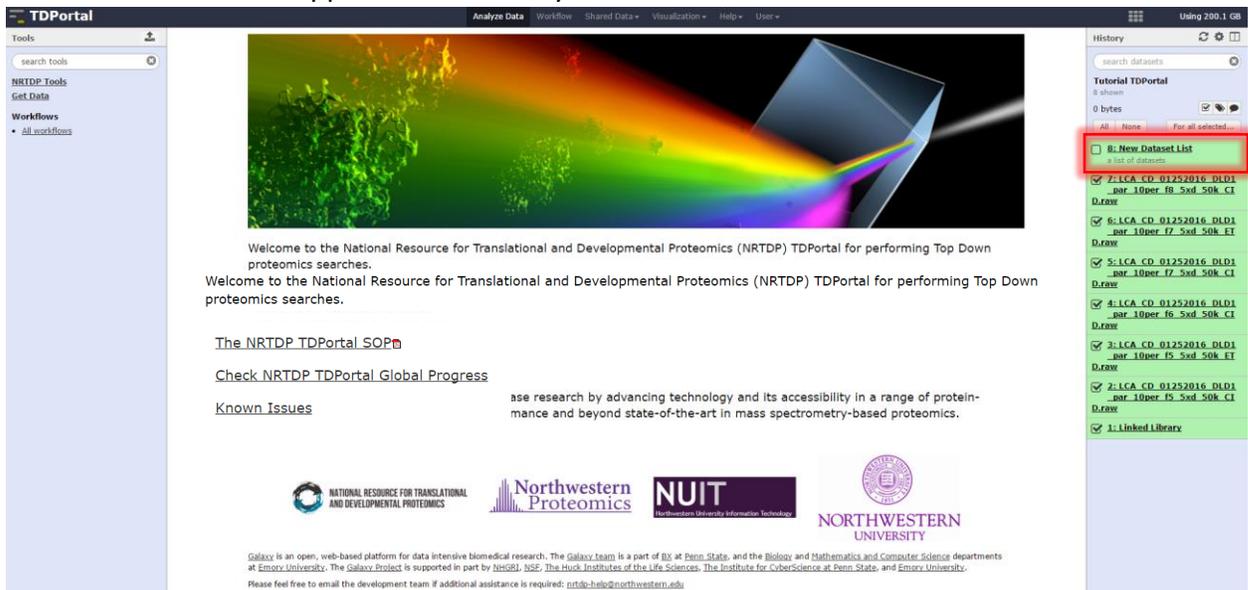
17. Click the TDPortal icon at the top of the page to return to the home page. The history has been populated with a green box for each imported raw file.



18. 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



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

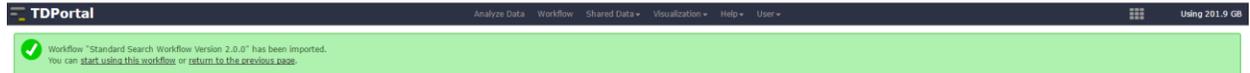


Step 4: Running searches on TDPortal

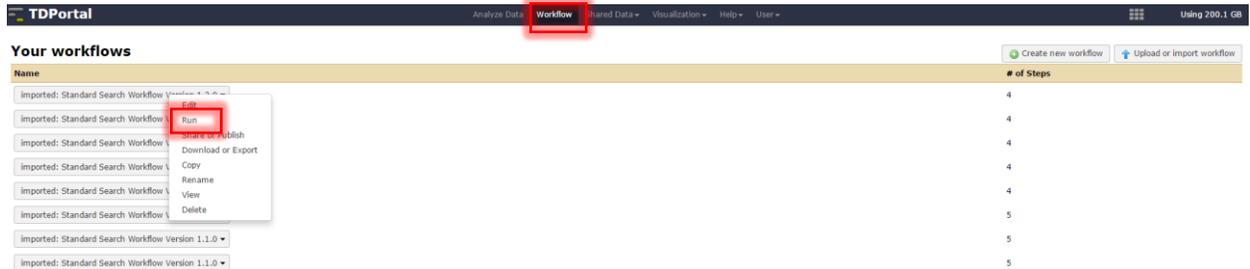
20. Navigate to Shared Data. Click on “Published Workflows” in the drop down menu. Import the latest Standard Search Workflow. In this Tutorial we use Published Standard Search Workflow 2.0 by clicking on the down arrow of the “Standard Search Workflow Version 12.0” tab.



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

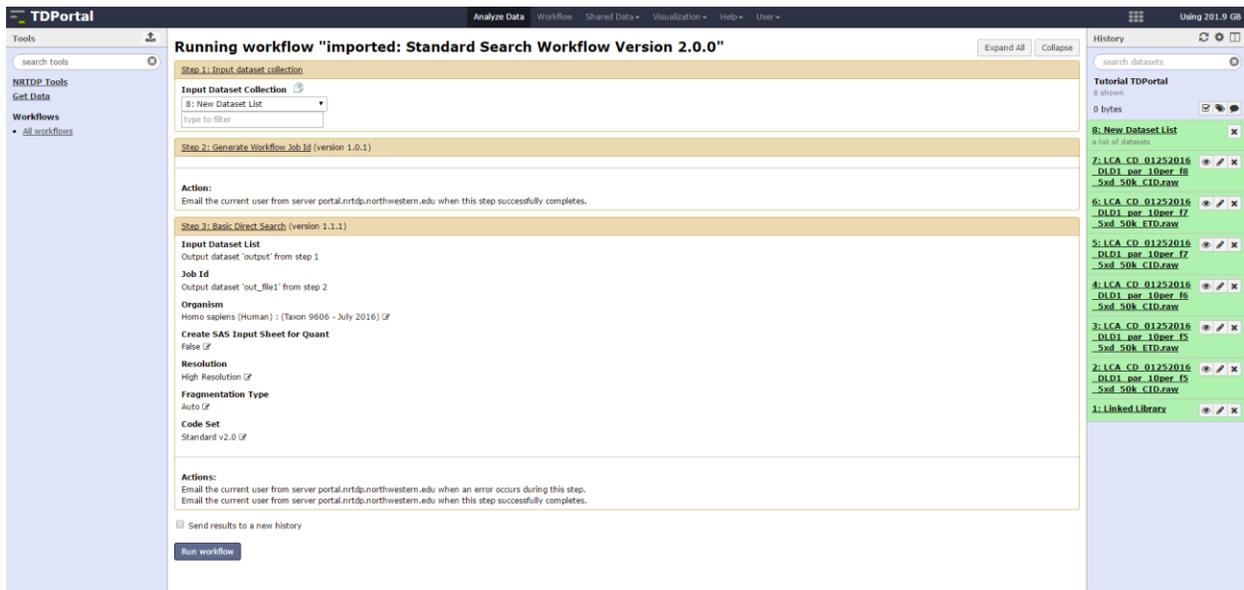


22. Click the “Workflow” Subheading. Click “Run” in Standard Search Workflow Version 2.0 dropdown.



23. You will run a Basic Direct Search unless otherwise instructed by the NRTDP bioinformatics team. 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 Set Standard 2.0 (unless otherwise updated).
- h. Click Run Workflow



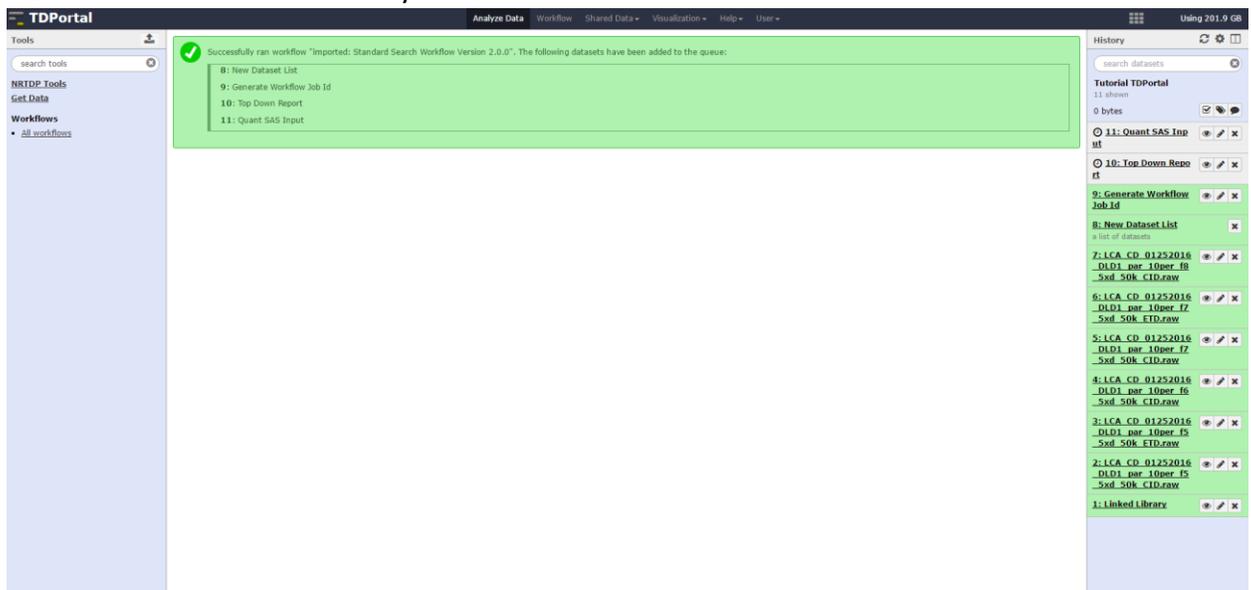
Step 5: Monitoring Progress of TDPortal Searches

24. 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 TDPortal.

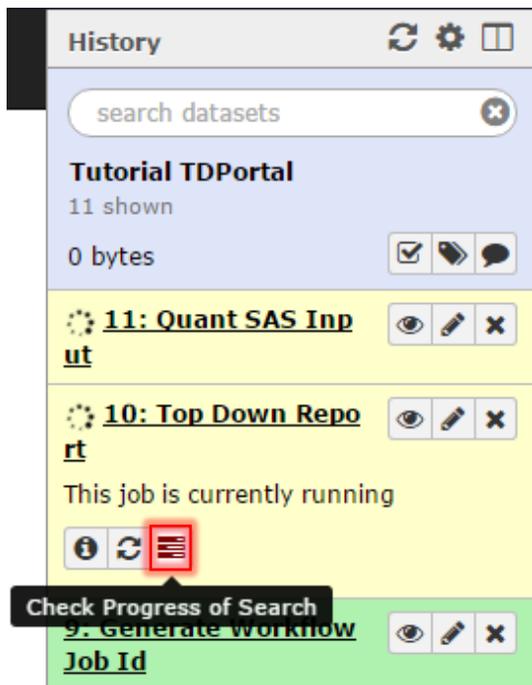
Action:

Email the current user from server portal.nrtdp.northwestern.edu when this step successfully completes.

25. The search will be added to History Panel.



26. Monitor Search progress by clicking on Check Progress button under the Top Down Report file in the History Panel. Two percentages are displayed in search progress. The page refreshes every 30 seconds.



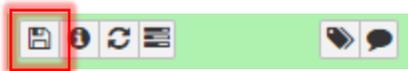
27. In progress, the date of the search, and user email will be visible.

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

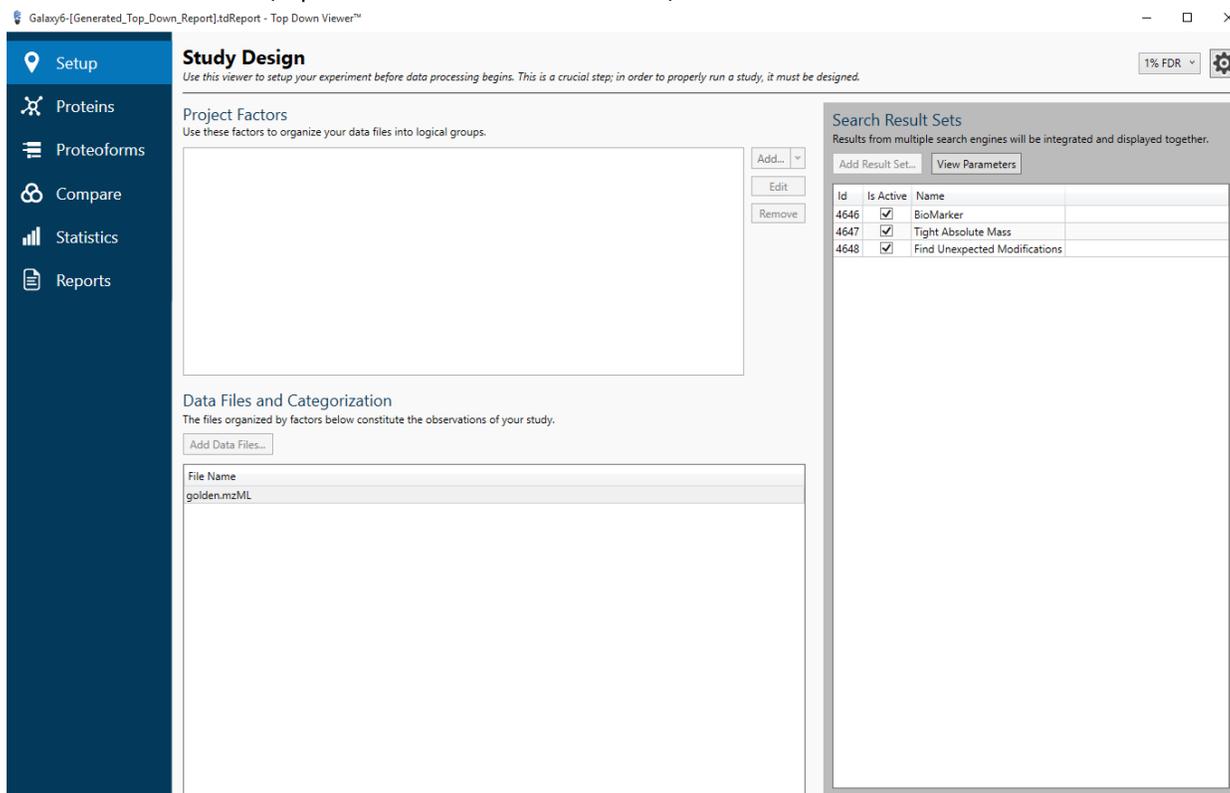
28. TDPortal will send an email immediately if a step in the workflow fails. The email will contain history and job id information. An email will also be sent when the search completes. The History Panel items will also turn green when the search fully completes.

Step 6: Generating and Viewing the Top Down Report

29. Download search results by clicking the floppy disk “download” button under the Top Down Report subsection in the History Panel.



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



Id	Is Active	Name
4646	<input checked="" type="checkbox"/>	BioMarker
4647	<input checked="" type="checkbox"/>	Tight Absolute Mass
4648	<input checked="" type="checkbox"/>	Find Unexpected Modifications