NRTDP

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<u>User Guide for Performing High Throughput Searches on TDPortal</u>
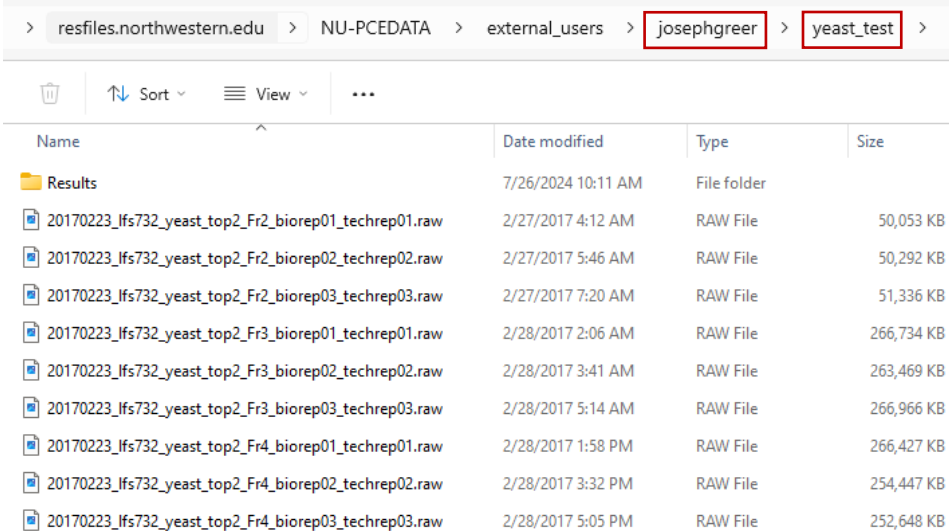
Part 1: Making Files Available in TDPortal

1. Copy files to correct location.
   a. Northwestern University Users:
      i. X Drive (krgData in the example below)
      ii. Project folder (2024 Greer – Yeast in the example below)
      iii. Dataset folder (Top-2_Fr2-4 in the example below)
      iv. Samples folder

Name	Date modified	Type	Size
20170223_lfs732_yeast_top2_Fr2_biorep01_techrep01.raw	2/27/2017 4:12 AM	RAW File	50,053 KB
20170223_lfs732_yeast_top2_Fr2_biorep02_techrep02.raw	2/27/2017 5:46 AM	RAW File	50,292 KB
20170223_lfs732_yeast_top2_Fr2_biorep03_techrep03.raw	2/27/2017 7:20 AM	RAW File	51,336 KB
20170223_lfs732_yeast_top2_Fr3_biorep01_techrep01.raw	2/28/2017 2:06 AM	RAW File	266,734 KB
20170223_lfs732_yeast_top2_Fr3_biorep02_techrep02.raw	2/28/2017 3:41 AM	RAW File	263,469 KB
20170223_lfs732_yeast_top2_Fr3_biorep03_techrep03.raw	2/28/2017 5:14 AM	RAW File	266,966 KB
20170223_lfs732_yeast_top2_Fr4_biorep01_techrep01.raw	2/28/2017 1:58 PM	RAW File	266,427 KB
20170223_lfs732_yeast_top2_Fr4_biorep02_techrep02.raw	2/28/2017 3:32 PM	RAW File	254,447 KB
20170223_lfs732_yeast_top2_Fr4_biorep03_techrep03.raw	2/28/2017 5:05 PM	RAW File	252,648 KB

Path: resfiles.northwestern.edu > krgData > Projects > 2024 Greer - Yeast > Top-2_Fr2-4 > Samples

   b. External Users:
      i. User folder (josephgreer in example below)
   ii. Dataset folder (yeast_test in example below)

Path: resfiles.northwestern.edu > NU-PCEDATA > external_users > josephgreer > yeast_test

Name	Date modified	Type	Size
Results	7/26/2024 10:11 AM	File folder	
20170223_lfs732_yeast_top2_Fr2_biorep01_techrep01.raw	2/27/2017 4:12 AM	RAW File	50,053 KB
20170223_lfs732_yeast_top2_Fr2_biorep02_techrep02.raw	2/27/2017 5:46 AM	RAW File	50,292 KB
20170223_lfs732_yeast_top2_Fr2_biorep03_techrep03.raw	2/27/2017 7:20 AM	RAW File	51,336 KB
20170223_lfs732_yeast_top2_Fr3_biorep01_techrep01.raw	2/28/2017 2:06 AM	RAW File	266,734 KB
20170223_lfs732_yeast_top2_Fr3_biorep02_techrep02.raw	2/28/2017 3:41 AM	RAW File	263,469 KB
20170223_lfs732_yeast_top2_Fr3_biorep03_techrep03.raw	2/28/2017 5:14 AM	RAW File	266,966 KB
20170223_lfs732_yeast_top2_Fr4_biorep01_techrep01.raw	2/28/2017 1:58 PM	RAW File	266,427 KB
20170223_lfs732_yeast_top2_Fr4_biorep02_techrep02.raw	2/28/2017 3:32 PM	RAW File	254,447 KB
20170223_lfs732_yeast_top2_Fr4_biorep03_techrep03.raw	2/28/2017 5:05 PM	RAW File	252,648 KB

Part 2: Logging into OnDemand

2. Log into OnDemand at https://qondemand.ci.northwestern.edu with your NetID and password.
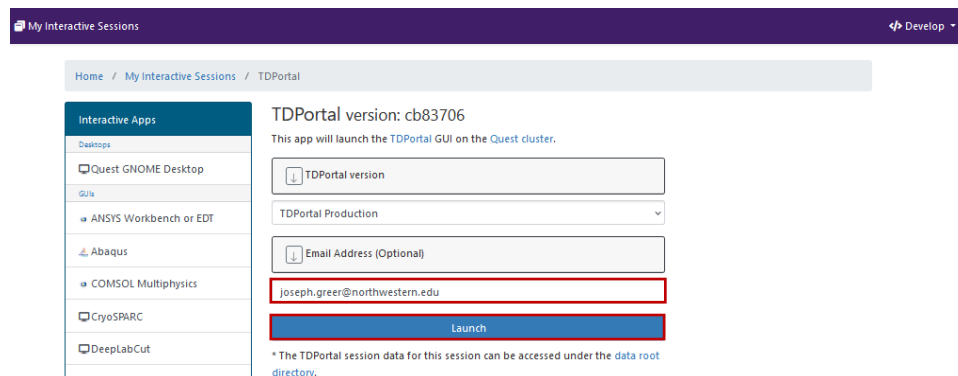
Part 3: Launch TDPortal Session

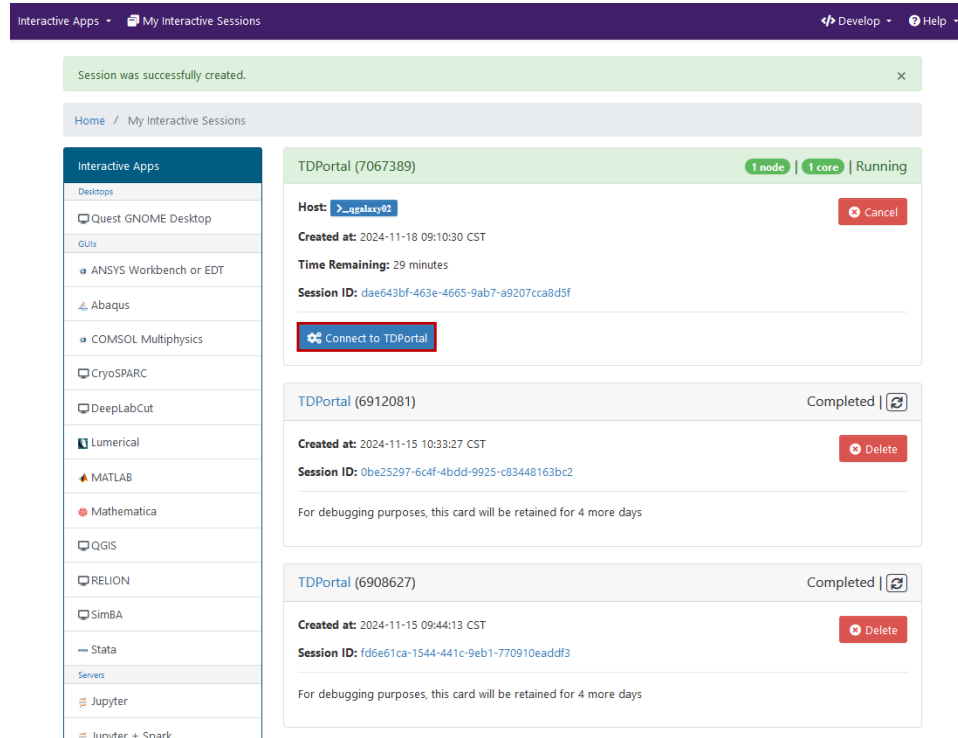3. Select TDPortal in Interactive Apps.
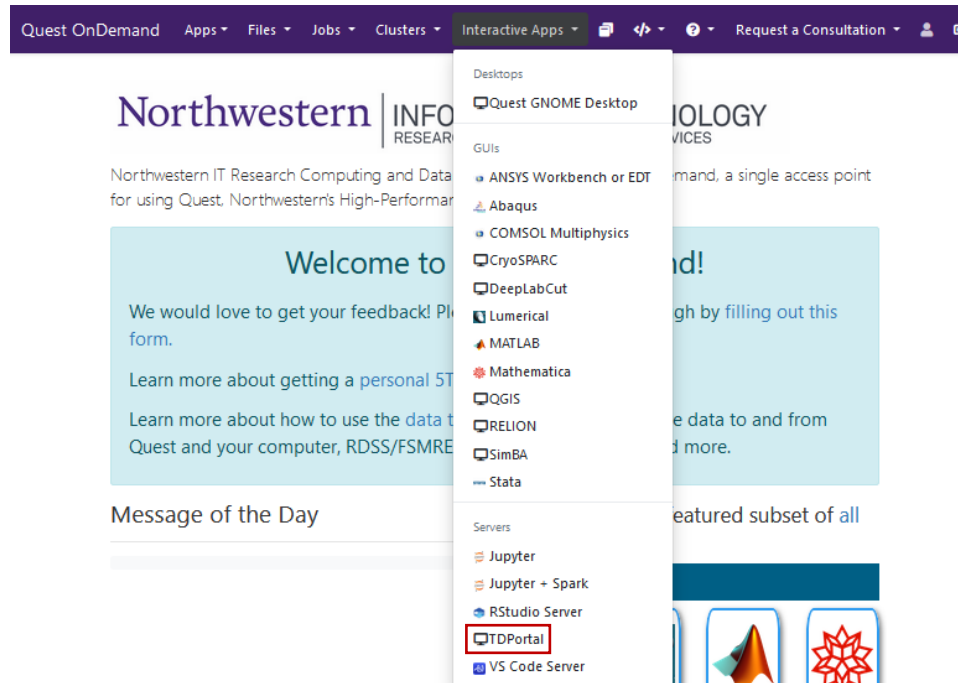
4. Add email address to receive notification.
5. Click Launch.

Part 4: Running searches on TDPortal

6. Click Connect to TDPortal from list of interactive sessions. The connect button might not be immediately available.

7. Select search parameters and click SUBMIT.

   a. Select Code Set. The newest code is selected by default. Older versions are available in the drop down.

   b. Select Project.

   c. Select Dataset.

   d. Select Data Files.

   e. Select Organism.

   f. If filtering by FDR, check Filter by FDR.

   g. If performing quant, check Create SAS Input sheet.

   h. Select Precursor Resolution.

   i. Select Fragmentation Method.

   j. If including the ProSight Error Tolerant Search, check Include ProSight Error Tolerant Search.

   k. If using Code Set 4.1 and applying a ppm shift, enter PPM Shift value.

   l. If using Code Set 4.1 and including spectra in output, check Include Spectra in tdReport.

Part 5: Reviewing TDPortal Results

8. Search result files are automatically saved to the Results folder.
    a. Northwestern University Users:
        i. X Drive (krgData in example the below)
        ii. Project folder (2024 Greer – Yeast in the example below)
        iii. Dataset folder (Top-2_Fr2-4 in the example below)
        iv. Results folder
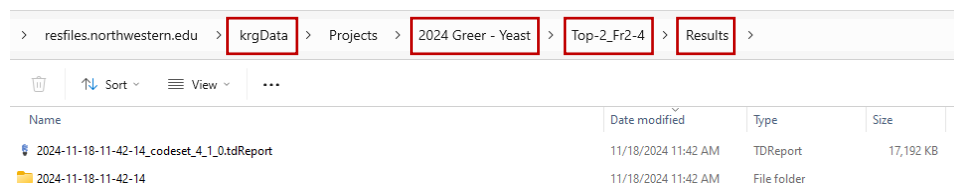
    b. External Users:
        i. User folder (josephgreer in the example below)
        ii. Dataset folder (yeast_test in the example below)
        iii. Results folder
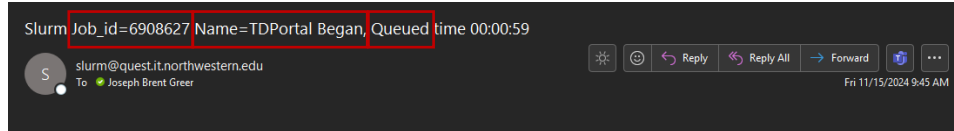   iv. Specific search result folder (2024-07-26-10-11-50 in the example below)
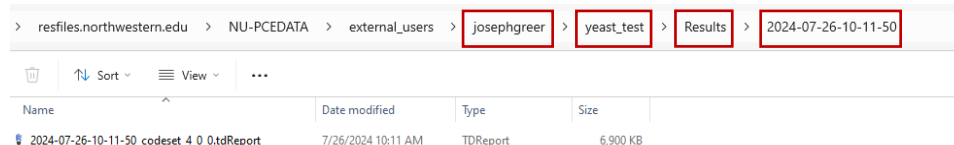
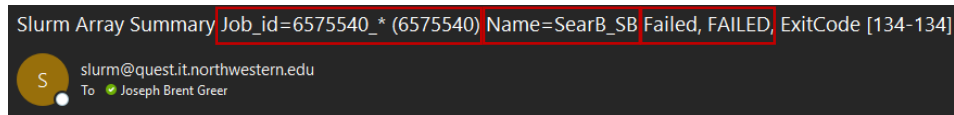9. tdReport files can be reviewed in TDViewer (http://psptm.kelleher.northwestern.edu/).
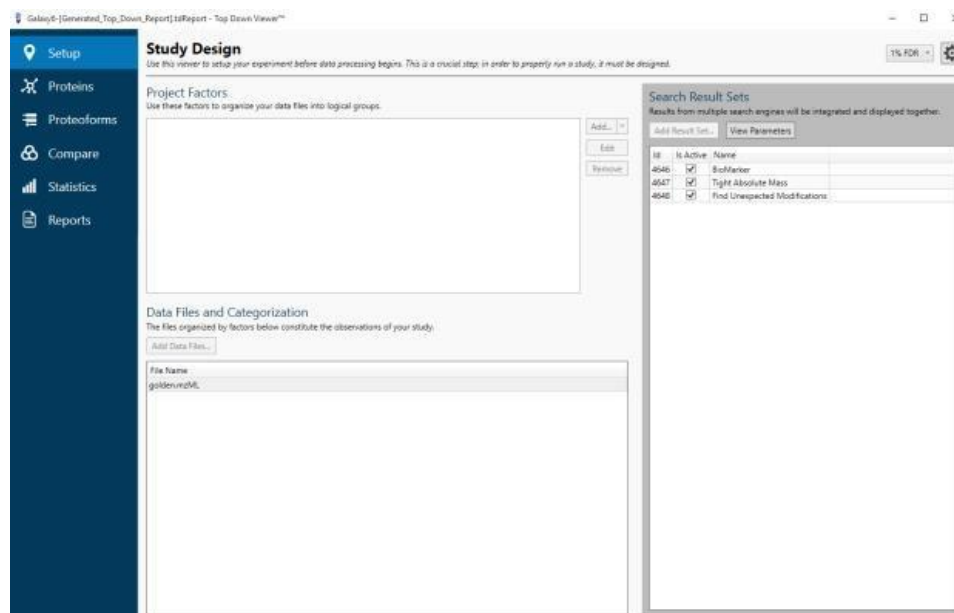
Part 6: Trouble Shooting

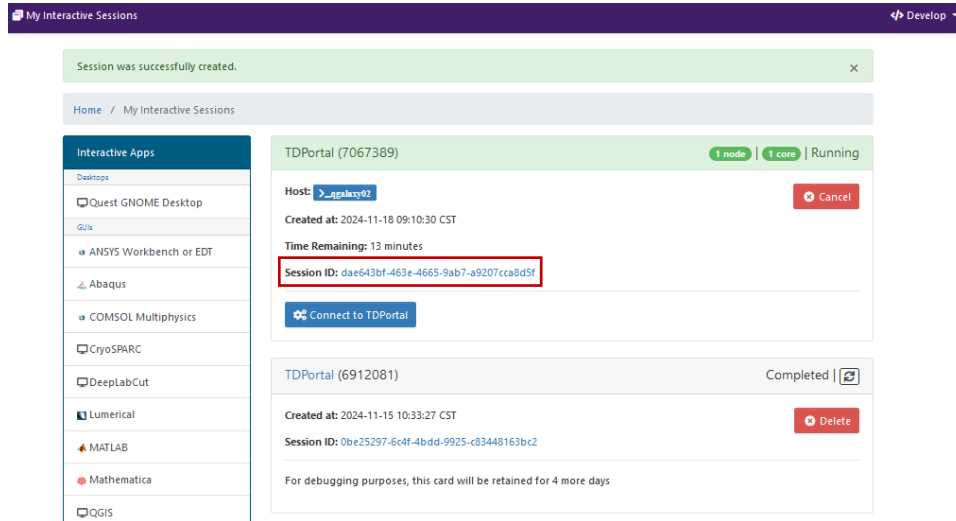10. Emails contain useful job information.
    a. Job ID
    b. Job Name
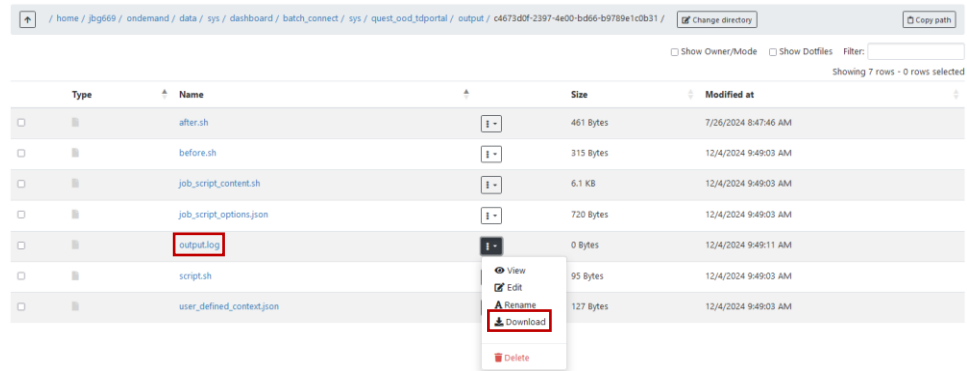   c. Status
    d. Session beginning email

    e. Error email

11. Download session output log file.
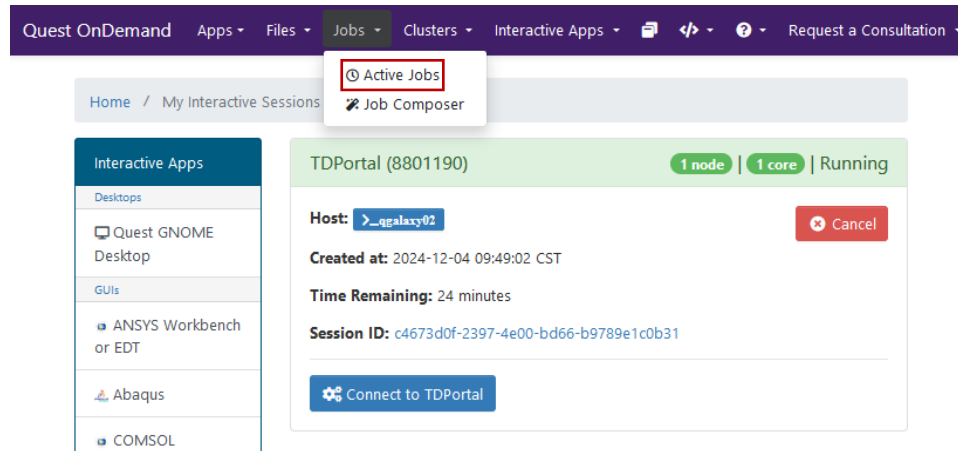   a. Click on Session ID in Interactive Sessions.

    b. Download output.log.

12. Active jobs contain other useful information.
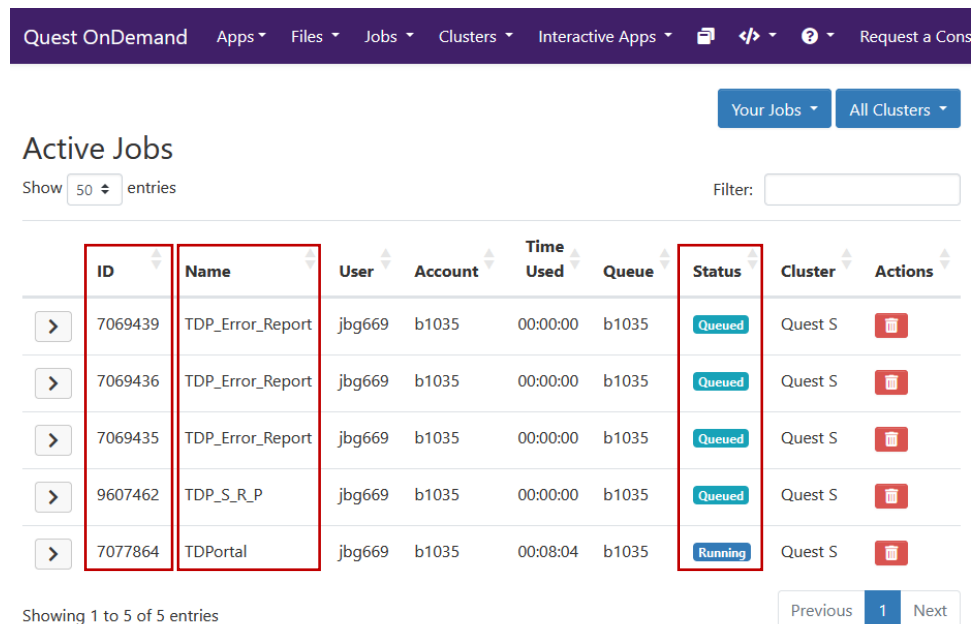
    a. Click on Active Jobs.

    b. Useful information:

      i. Job ID

      ii. Job Name

      iii. Status:

        1. Completed

        2. Queued

        3. Running

c. Click dropdown for additional information.
  i. Job Id
  ii. Job Name
  iii. State
  iv. Node list: where job is running
  v. Start time
  vi. End time
  vii. Output location: folder contains session log

>	9607462	TDP_S_R_P	jbg669	b1035	00:00:00	b1035	Queued	Quest S	🗑
⌄	7077864	TDPortal	jbg669	b1035	00:08:04	b1035	Running	Quest S	🗑

Running TDPortal 7077864

Cluster	Quest S
Job Id	7077864
Job Name	TDPortal
User	jbg669
Account	b1035
Partition	b1035
State	RUNNING
Reason	None
Total Nodes	1
Node List	qgalaxy02
Total CPUs	1
Time Limit	30:00
Time Used	12:25
Start Time	2024-11-18 15:43:38
End Time	2024-11-18 16:13:38
Memory	4096M

Output Location:

/home/jbg669/ondemand/data/sys/dashboard/batch_connect/sys/quest_ood_tdportal/
output/1e7f43bd-759b-4b90-a484-72359c95fae5