

Joseph B. Greer, Ryan T. Fellers, Bryan P. Early, Michael A. R. Hollas

User Guide for Performing High Throughput Searches on TDPortal

Part 1: Making Files Available in TDPortal..... 2

Part 2: Logging into OnDemand..... 3

Part 3: Launch TDPortal Session 3

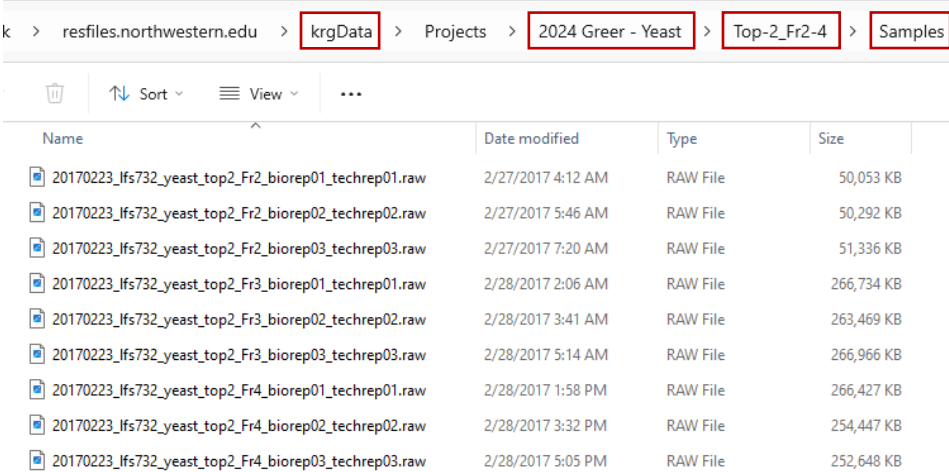
Part 4: Running searches on TDPortal..... 4

Part 5: Reviewing TDPortal Results..... 6

Part 6: Trouble Shooting..... 7

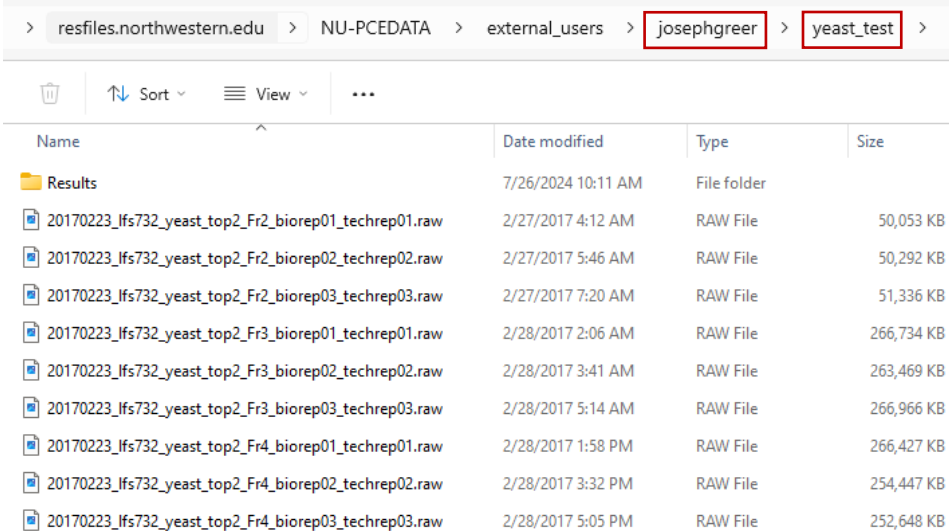
Part 1: Making Files Available in TDPortal

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

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



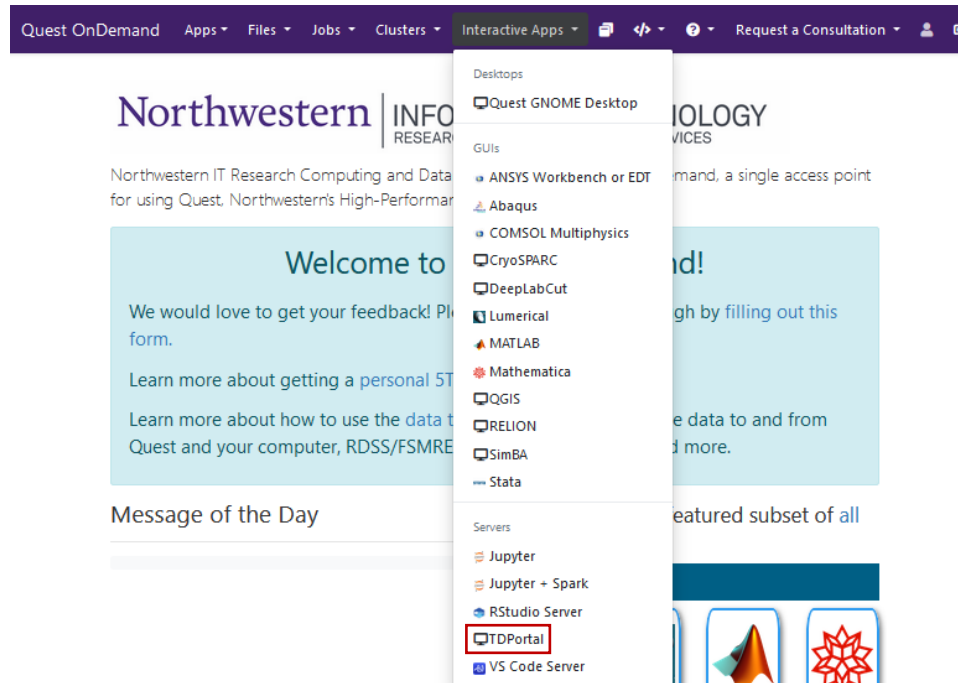
Name	Date modified	Type	Size
Results	7/26/2024 10:11 AM	File folder	
20170223_lfs732_yeast_top2_Fr2_biorep01_techrep01.raw	2/27/2017 4:12 AM	RAW File	50,053 KB
20170223_lfs732_yeast_top2_Fr2_biorep02_techrep02.raw	2/27/2017 5:46 AM	RAW File	50,292 KB
20170223_lfs732_yeast_top2_Fr2_biorep03_techrep03.raw	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

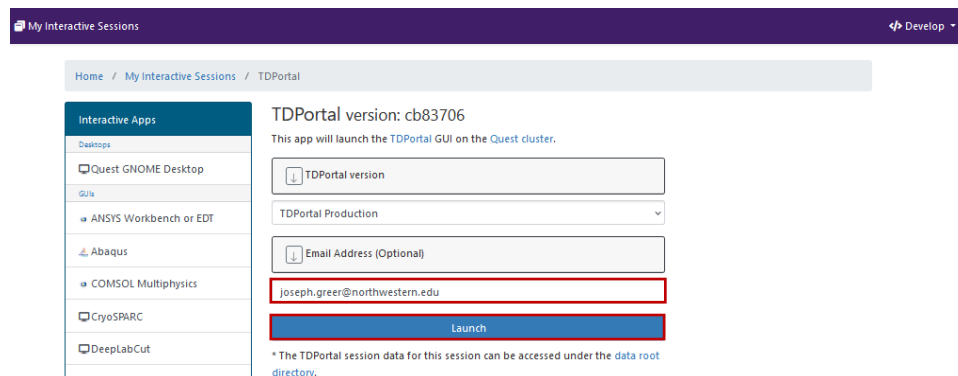
2. Log into OnDemand at <https://qondemand.ci.northwestern.edu> with your NetID and password.

Part 3: Launch TDPortal Session

3. Select TDPortal in Interactive Apps.

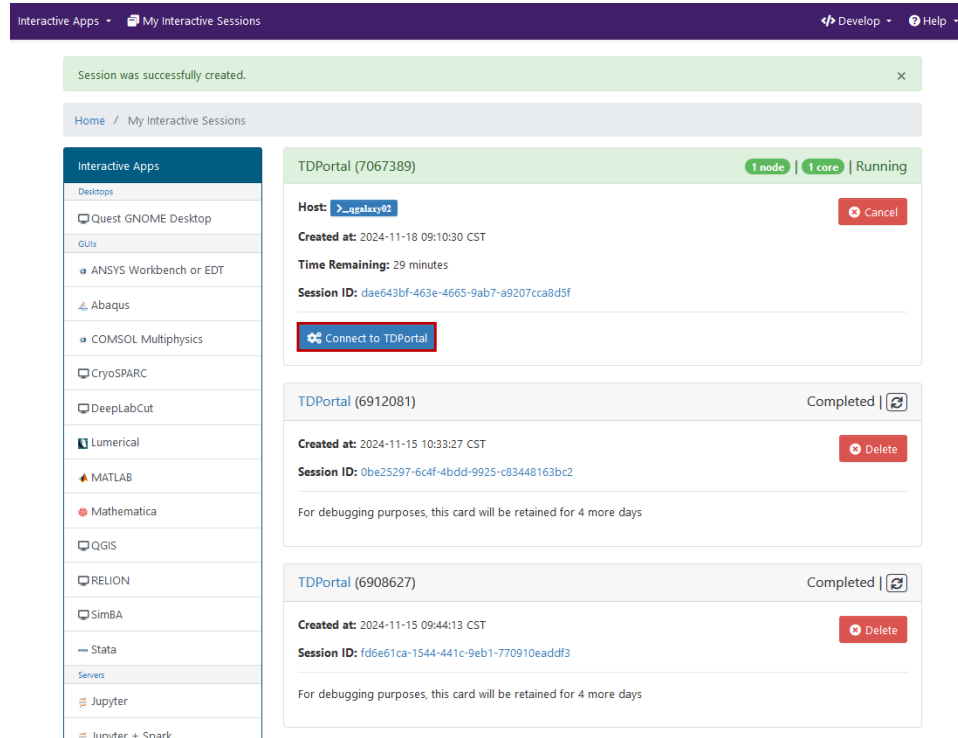


4. Add email address to receive notification.
5. Click Launch.



Part 4: Running searches on TDPortal

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



Interactive Apps | My Interactive Sessions | Develop | Help

Session was successfully created.

Home / My Interactive Sessions

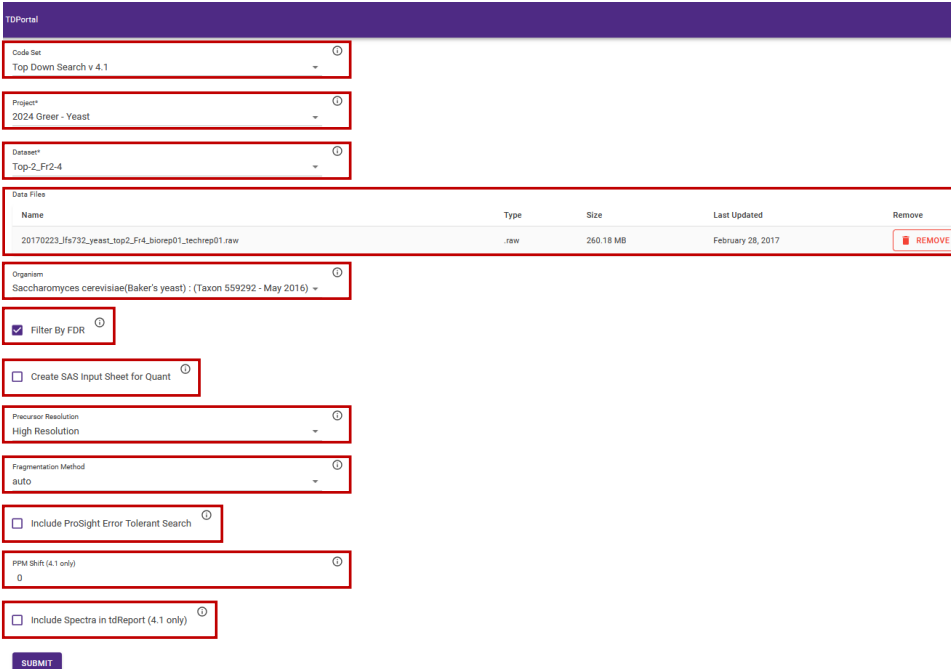
Interactive Apps	Session Details
Desktops	
Quest GNOME Desktop	
GUIS	
ANSYS Workbench or EDT	
Abaqus	
COMSOL Multiphysics	
CryoSPARC	
DeepLabCut	
Lumerical	
MATLAB	
Mathematica	
QGIS	
RELION	
SimBA	
Stata	
Servers	
Jupyter	
Jupyter + Soark	

Session Name	Status	Host	Created at	Time Remaining	Session ID	Actions
TDPortal (7067389)	Running	galaxy02	2024-11-18 09:10:30 CST	29 minutes	dae643bf-463e-4665-9ab7-a9207cca8d5f	Cancel
TDPortal (6912081)	Completed		2024-11-15 10:33:27 CST		0be25297-6c4f-4bdd-9925-c83448163bc2	Delete
TDPortal (6908627)	Completed		2024-11-15 09:44:13 CST		fd6e61ca-1544-441c-9eb1-770910eaddf3	Delete

For debugging purposes, this card will be retained for 4 more days

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.



The screenshot shows the TDPortal search interface with the following fields highlighted by red boxes:

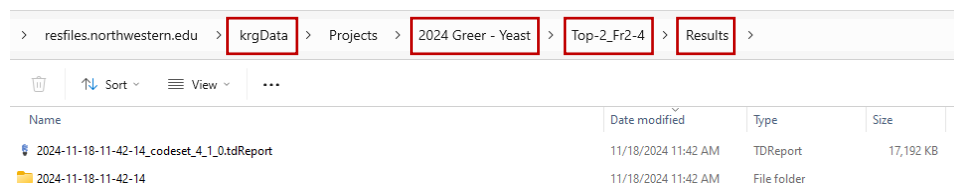
- Code Set: Top Down Search v 4.1
- Project: 2024 Greer - Yeast
- Dataset: Top-2_Fr2-4
- Data Files table:

Name	Type	Size	Last Updated	Remove
20170223_Jf5732_yeast_top2_Fr4_biorep01_techrep01.raw	.raw	260.18 MB	February 28, 2017	REMOVE
- Organism: Saccharomyces cerevisiae(Baker's yeast) : (Taxon 559292 - May 2016)
- Filter By FDR
- Create SAS Input Sheet for Quant
- Precursor Resolution: High Resolution
- Fragmentation Method: AUTO
- Include ProSight Error Tolerant Search
- PPM Shift (4.1 only): 0
- Include Spectra in tdReport (4.1 only)

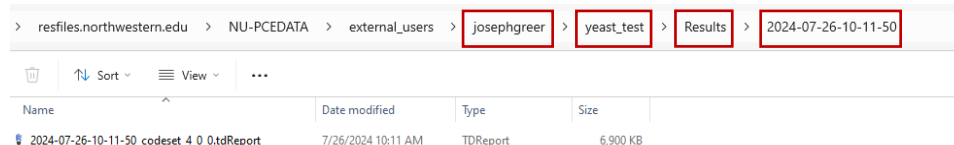
A SUBMIT button is located at the bottom of the form.

Part 5: Reviewing TDPortal Results

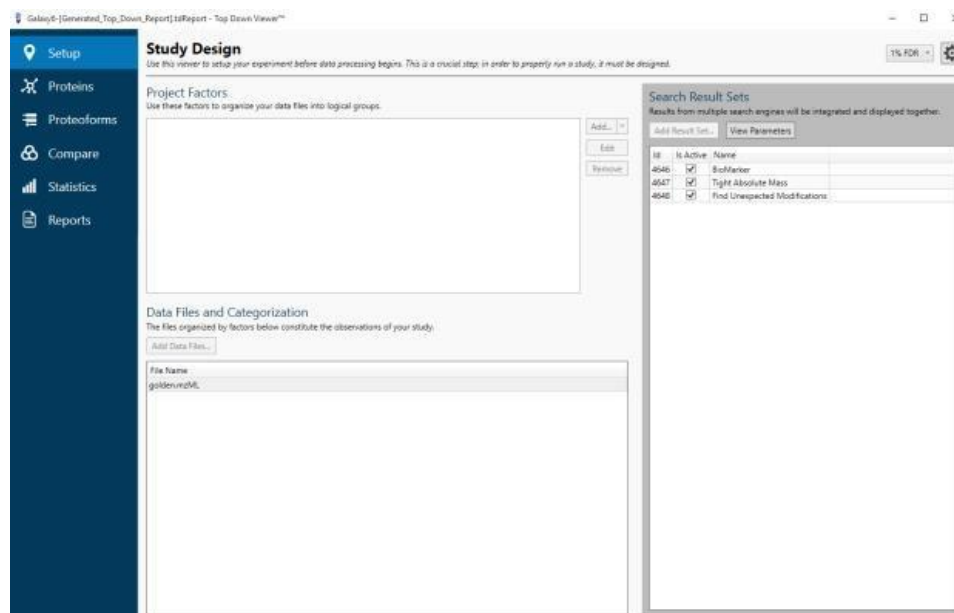
8. Search result files are automatically saved to the Results folder.
 - a. Northwestern University Users:
 - i. X Drive (krgData in example the below)
 - ii. Project folder (2024 Greer – Yeast in the example below)
 - iii. Dataset folder (Top-2_Fr2-4 in the example below)
 - iv. Results folder



- 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)



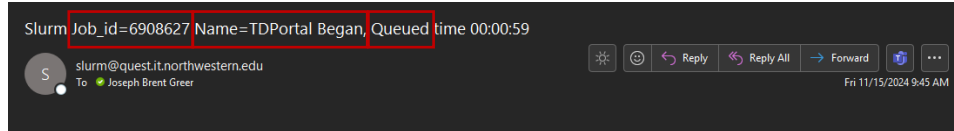
9. tdReport files can be reviewed in TDViewer (<http://psptm.kelleher.northwestern.edu/>).



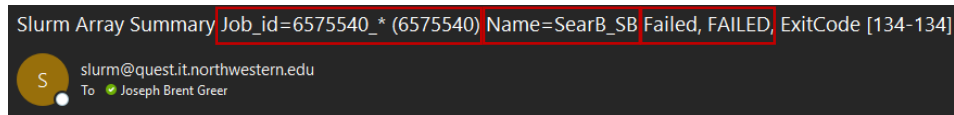
Part 6: Trouble Shooting

10. Emails contain useful job information.

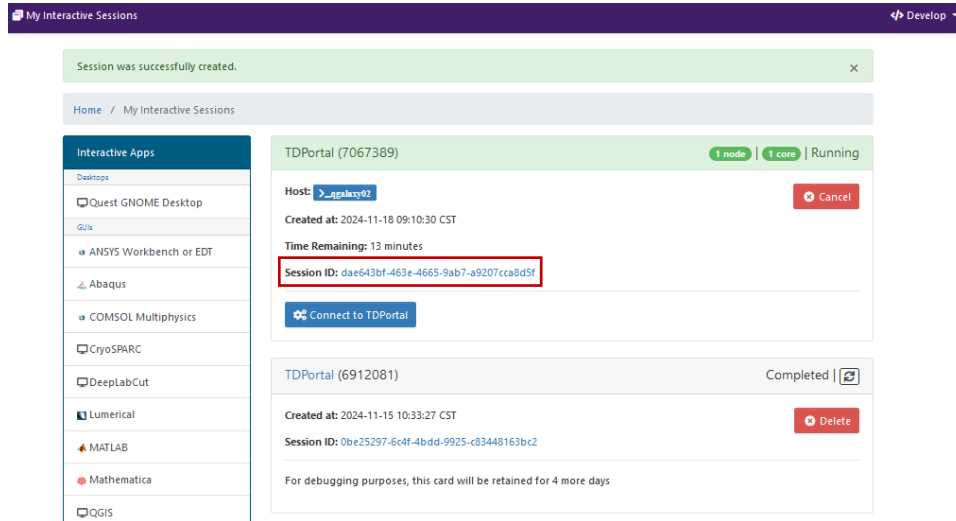
- a. Job ID
- b. Job Name
- c. Status
- d. Session beginning email



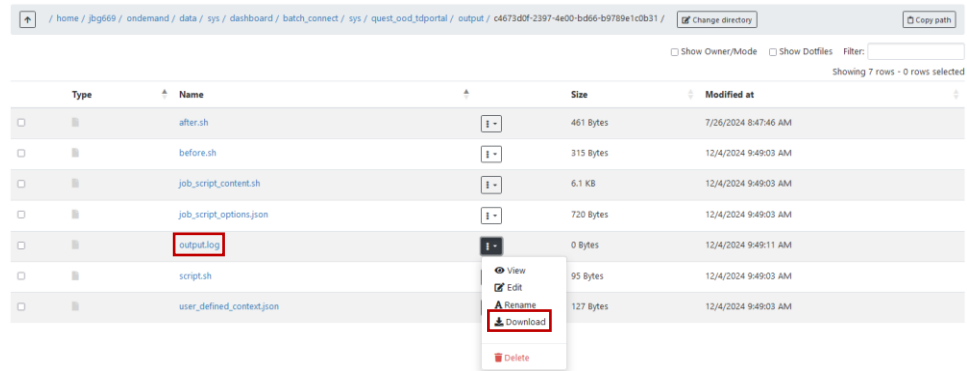
- e. Error email



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



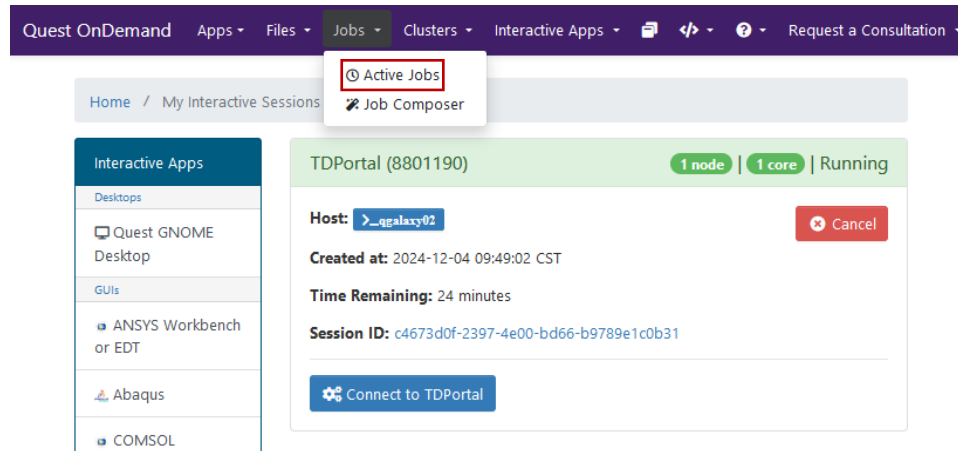
- b. Download output.log.



Type	Name	Size	Modified at
File	after.sh	461 Bytes	7/26/2024 8:47:46 AM
File	before.sh	315 Bytes	12/4/2024 9:49:03 AM
File	job_script_content.sh	6.1 KB	12/4/2024 9:49:03 AM
File	job_script_options.json	720 Bytes	12/4/2024 9:49:03 AM
File	output.log	0 Bytes	12/4/2024 9:49:11 AM
File	script.sh	95 Bytes	12/4/2024 9:49:03 AM
File	user_defined_context.json	127 Bytes	12/4/2024 9:49:03 AM

12. Active jobs contain other useful information.

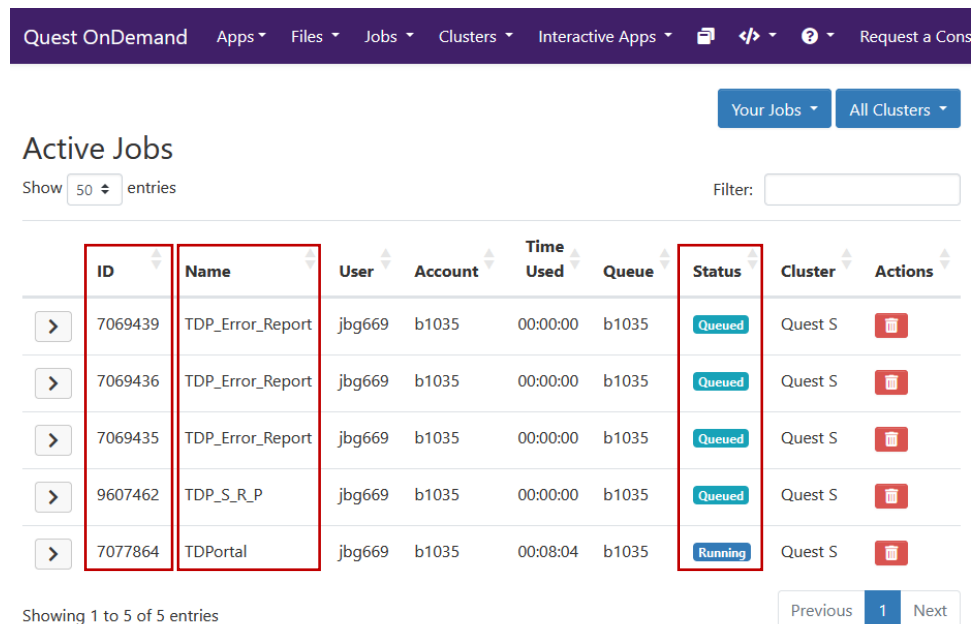
- a. Click on Active Jobs.



The screenshot shows the TDPortal navigation bar with 'Jobs' selected. A dropdown menu highlights 'Active Jobs'. Below, the 'My Interactive Sessions' page shows a job named 'TDPortal (8801190)' with 1 node and 1 core, currently 'Running'. The job details include: Host: >_qgalaxy02, Created at: 2024-12-04 09:49:02 CST, Time Remaining: 24 minutes, and Session ID: c4673d0f-2397-4e00-bd66-b9789e1c0b31. A 'Connect to TDPortal' button is visible at the bottom.

- b. Useful information:

- i. Job ID
- ii. Job Name
- iii. Status:
 1. Completed
 2. Queued
 3. Running



The screenshot shows the 'Active Jobs' page with a table of job entries. The table has columns for ID, Name, User, Account, Time Used, Queue, Status, Cluster, and Actions. The 'Status' column is highlighted with a red box, showing 'Queued' for most jobs and 'Running' for the last one. The 'ID' and 'Name' columns are also highlighted with a red box.

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
7069439	TDP_Error_Report	jbg669	b1035	00:00:00	b1035	Queued	Quest S	
7069436	TDP_Error_Report	jbg669	b1035	00:00:00	b1035	Queued	Quest S	
7069435	TDP_Error_Report	jbg669	b1035	00:00:00	b1035	Queued	Quest S	
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	

Showing 1 to 5 of 5 entries

- 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_tdpportal/output/1e7f43bd-759b-4b90-a484-72359c95fae5
```