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User Guide for Performing High Throughput Searches on TDPortal

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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

k > resfiles.northwestern.edu > krgData > Proje	cts > 2024 Greer -	Yeast > Top-2_	Fr2-4 > Samples
$\widehat{\mathbb{W}}$ \mathbb{N} Sort \sim \equiv View \sim \cdots			
Name	Date modified	Туре	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)

> resfiles.northwestern.edu > NU-PCEDATA >	external_users > jo	sephgreer >	yeast_test >			
$\hat{\mathbb{W}}$ \mathbb{N} Sort $\stackrel{\scriptstyle{\scriptstyle{\vee}}}{=}$ \mathbb{V} iew $\stackrel{\scriptstyle{\scriptstyle{\vee}}}{=}$ \cdots						
Name	Date modified	Туре	Size			
Caracteria 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 KE						
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.

active Sessions		
Home / My Interactive Sessions	/ TDPortal	
Interactive Apps	TDPortal version: cb83706	
Desktops	This app will launch the TDPortal GUI on the Quest cluster.	
Quest GNOME Desktop	TDPortal version	
GUIs		
ANSYS Workbench or EDT	TDPortal Production ~	
🚣 Abaqus	Email Address (Optional)	
 COMSOL Multiphysics 	joseph.greer@northwestern.edu	
CryoSPARC	Launch	
DeepLabCut	* The TDPortal session data for this session can be accessed under the data root	



Part 4: Running searches on TDPortal

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

active Apps 🝷 📄 My Interactive Sessions	;	🂠 Develop 👻 🚷
Session was successfully created.		×
Home / My Interactive Sessions		
Interactive Apps	TDPortal (7067389)	1 node 1 core Running
Desktops	Host: >_qgalaxy02	S Cancel
GUIs a ANSYS Workbench or EDT	Created at: 2024-11-18 09:10:30 CST Time Remaining: 29 minutes	
🛦 Abaqus	Session ID: dae643bf-463e-4665-9ab7-a9207cca8d5f	
COMSOL Multiphysics	🛠 Connect to TDPortal	
© CryoSPARC	TDPortal (6912081)	Completed 😰
Lumerical	Created at: 2024-11-15 10:33:27 CST	S Delete
MATLAB	Session ID: 0be25297-6c4f-4bdd-9925-c83448163bc2	
Mathematica	For debugging purposes, this card will be retained for 4 more days	
	TDPortal (6908627)	Completed 😰
C SimBA	Created at: 2024-11-15 09:44:13 CST	S Delete
Stata	Session ID: fd6e61ca-1544-441c-9eb1-770910eaddf3	
≓ Jupyter	For debugging purposes, this card will be retained for 4 more days	
Jupyter + Spark		



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

TDPortal				
Code Set O Top Down Search v 4.1				
Project* O 2024 Greer - Yeast *				
Dataset* O Top-2_Fr2-4 *				
Data Files Name	Туре	Size	Last Updated	Remove
20170223_lfs732_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				
Fragmentation Method O auto T				
Include ProSight Error Tolerant Search				
PPM Shift (4.1 only) O				
Include Spectra in tdReport (4.1 only)				
SUBMIT				



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)

> resfiles.northwestern.edu > NU-PCEDATA	> external_users	> josephgreer >	yeast_test	> Results > 2024-07-26-10-11-50
$\hat{\mathbb{W}}$ \mathbb{N} Sort $\tilde{\mathbb{V}}$ \mathbb{W} View $\tilde{\mathbb{V}}$				
Name	Date modified	Туре	Size	
\$ 2024-07-26-10-11-50_codeset_4_0_0.tdReport	7/26/2024 10:11 AM	TDReport	6,900 KB	

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

•	Setup	Study Design Use this verse's setup year experiment before data processing begins. This is a crucial step, in order to property we a study, it m	unt be dragment.
 × = ⊗ ∎ ■ 	Setup Proteins Proteoforms Compare Statistics Reports	Study Design Use this verifies the status place represented before data processing begins. This is a crucial status is series to property new a status, it is Project Factors Use these factors to anywhole your data files into logical groups. Add Terms Data Files and Categorization The status by factor before construct the discensations of your statuy. Add Data Files. Terms Terms	At the designed.
		goommode.	



Part 6: Trouble Shooting

10. Emails contain useful job information.

- a. Job ID
- b. Job Name
- c. Status

e.

d. Session beginning email

Slurm Job_id=6908627 Name=TDPortal Began, Queued time 00:00:59 slurm@quest.it.northwestern.edu To * Joseph Brent Greer	★ @ ← Reply ≪ Reply All → Forward for Fri 11/15/2024 945 AM
Error email	
Slurm Array Summary Job_id=6575540_* (6575540) Name=Se	arB_SB Failed, FAILED, ExitCode [134-134]
slurm@quest.it.northwestern.edu To • Joseph Brent Greer	



11. Download session output log file.

a. Click on Session ID in Interactive Sessions.

🗐 My Inter	ractive Sessions			� Develop ▼
	Session was successfully created.		×	
	Home / My Interactive Sessions			
	Interactive Apps	TDPortal (7067389)	1 node 1 core Running	
	Desktops Quest GNOME Desktop	Host: >_qgalaxy02	Cancel	
	GUIs	Created at: 2024-11-18 09:10:30 CST		
	ANSYS Workbench or EDT	Time Remaining: 13 minutes		
	🚵 Abaqus	Session ID: dae643bf-463e-4665-9ab7-a9207cca8d5f		
	 COMSOL Multiphysics 	✿\$ Connect to TDPortal		
	CryoSPARC C			
	□DeepLabCut	TDPortal (6912081)	Completed 😰	
	Lumerical	Created at: 2024-11-15 10:33:27 CST	S Delete	
	📣 MATLAB	Session ID: 0be25297-6c4f-4bdd-9925-c83448163bc2		
	🐢 Mathematica	For debugging purposes, this card will be retained for 4 more days		
	QGIS			

b. Download output.log.

^ /	home / jbg669 /	ondemand ,	/ data / sys / dashboard / batch_connect / sys / que	st_ood_tdportal / output / c4673d0f-	2397-4e00-bd66-b9789e1c0b3	1/ 😰 ci	hange directory	Copy path
						🗆 Shov	v Owner/Mode 🗌 Show Dotfil	les Filter: Showing 7 rows - 0 rows selected
	Туре	÷	Name	÷	Size		Modified at	÷
			after.sh	1-	461 Bytes		7/26/2024 8:47:46 AM	
			before.sh	1 -	315 Bytes		12/4/2024 9:49:03 AM	
			job_script_content.sh	1 -	6.1 KB		12/4/2024 9:49:03 AM	
	8		job_script_options.json	1 -	720 Bytes		12/4/2024 9:49:03 AM	
			output.log	1.	0 Bytes		12/4/2024 9:49:11 AM	
			script.sh	 View Edit 	95 Bytes		12/4/2024 9:49:03 AM	
			user_defined_context.json	A Rename	e 127 Bytes		12/4/2024 9:49:03 AM	
				2,0000				
				🗑 Delete				



12. Active jobs contain other useful information.

a. Click on Active Jobs.

Quest OnDemand Apps - F	iles + Jobs + Clusters +	Interactive Apps 🝷 🗐		Request a Consultation		
Home / My Interactive Se	Active Jobs X Job Composer					
Interactive Apps	TDPortal (8801190)		1 node 1 co	re Running		
Desktops						
Quest GNOME Desktop	Host: >_qgalaxy02 Created at: 2024-12-04 09	9:49:02 CST		🙁 Cancel		
GUIs	Time Remaining: 24 minutes					
 ANSYS Workbench or EDT 	Session ID: c4673d0f-239	7-4e00-bd66-b9789e1c0b	31			
🔌 Abaqus	😂 Connect to TDPortal					
COMSOL						

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

Quest	OnDeman	ıd Apps▼ Files	- Jobs	Clusters	 Interact 	tive Apps 🝷	a 4>	- 0-	Request a Con:	
Your Jobs * All Clusters * Active Jobs Show 50 ÷ entries Filter:										
	ID ÷	\$	User 🔶	Account	Time Used [♦]	Queue 🔶	Status 🗘	Cluster	Actions 🗘	
>	7069439	TDP_Error_Report	jbg669	b1035	00:00:00	b1035	Queued	Quest S	â	
>	7069436	TDP_Error_Report	jbg669	b1035	00:00:00	b1035	Queued	Quest S	Ô	
>	7069435	TDP_Error_Report	jbg669	b1035	00:00:00	b1035	Queued	Quest S	Î	
>	9607462	TDP_S_R_P	jbg669	b1035	00:00:00	b1035	Queued	Quest S	â	
>	7077864	TDPortal	jbg669	b1035	00:08:04	b1035	Running	Quest S	ā	
Showing 1 to 5 of 5 entries									1 Next	



- 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	Ē		
•	7077864	TDPortal	jbg669	b1035	00:08:04	b1035	Running	Quest S	Ē		
	Running	TDPortal 7077	864								
	Cluster			Quest S							
	Job Id		7077864	7077864							
	Job Nan	ne	TDPortal	TDPortal							
	User			jbg669	jbg669						
	Account	Account			b1035						
	Partition	ı		b1035							
	State			RUNNING							
	Reason			None							
	Total No	odes		1							
	Node Lis	st		qgalaxy02							
	Total CPUs			1	1						
	Time Lin	Time Limit			30:00						
	Time Us	Time Used			12:25						
	Start Tir	Start Time			2024-11-18 15:43:38						
	End Tim	End Time			2024-11-18 16:13:38						
	Memory	/		4096M							
	Output Lo	ocation:									
	/home/jbg669/ondemand/data/sys/dashboard/batch_connect/sys/quest_ood_tdportal/ output/1e7f43bd-759b-4b90-a484-72359c95fae5										