

Brief Instruction On Using The JEOL J400 NMR Spectrometer

(2nd draft, 5/10/2018)

Sample Preparation

- Insert the NMR tube into the spinner and adjust the depth with the JEOL depth gauge. (Make sure the inner part of the spinner is fully extended.)
- Put the sample with the spinner into an empty slot of the carousel. Remember the slot number.

To change user, click on the Login tab in the Spectrometer Control window and enter your username and password.

Spectrometer Control - Walkup Mode - Harvard-ECZ400S

Compass Options Tools Config Queue Samples Columns

User: console Logout

Sample: sensitivity (2)
Job: Proton
Method: -
Action: Script
Collected: -
Time: -

Change Loading Sample
Change Loaded Sample
Loaded System Skims for Current Probe
Waiting to achieve Spin State 'SPIN OFF'
Achieved Spin State
Waiting Temp Delay 60[s]

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Force Tune	Upload Data	Scheduling	Submit Job
1										
2		sensitivity	0.1% ethylbenzene	Chloroform-D	Select a Method					
3		Sample Name Required		Select a Solvent	Select a Method					
4		Sample Name Required		Select a Solvent	Select a Method					
5		Sample Name Required		Select a Solvent	Select a Method					
6		Sample Name Required		Select a Solvent	Select a Method					
7		Sample Name Required		Select a Solvent	Select a Method					
8		Sample Name Required		Select a Solvent	Select a Method					
9		Sample Name Required		Select a Solvent	Select a Method					
10		Sample Name Required		Select a Solvent	Select a Method					
11		Sample Name Required		Select a Solvent	Select a Method					
12		Sample Name Required		Select a Solvent	Select a Method					
13		Sample Name Required		Select a Solvent	Select a Method					
14		Sample Name Required		Select a Solvent	Select a Method					
15		Sample Name Required		Select a Solvent	Select a Method					
16		Sample Name Required		Select a Solvent	Select a Method					
17		Sample Name Required		Select a Solvent	Select a Method					
18		Sample Name Required		Select a Solvent	Select a Method					
19		Sample Name Required		Select a Solvent	Select a Method					
20		Sample Name Required		Select a Solvent	Select a Method					
21		Sample Name Required		Select a Solvent	Select a Method					
22		Sample Name Required		Select a Solvent	Select a Method					
23		Sample Name Required		Select a Solvent	Select a Method					

Status	Slot	Sample	Submit Time	Method	Visualize	Scheduling	User	Est. End Time
	2	sensitivity	11-MAY-2018 10:53:30	Proton	Yes		console	11-MAY-2018 10:58
	2	sensitivity	11-MAY-2018 10:54:13	Carbon	Yes		console	11-MAY-2018 11:00

Receiver Gain: 56 Spin: 0[Hz] Lock: 0 Temp: 25.1[4C] Helium: 94[%] Nitrogen: 87[%] LOADED (2) Queued Jobs: 2

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10:51 AM 5/11/2018

Please note that there is a 24 slot automatic sample changer installed. The sample diagram shows the current sample in the probe in yellow, those samples queued in blue. If the slot has been occupied with an idling sample, you can take the sample tube out and use the slot for your sample.

The screenshot displays the 'Spectrometer Control - Walkup Mode - Harvard-ECZ4005' interface. The main window features a table with 24 slots for sample scheduling. The current sample in the probe is highlighted in yellow (Slot 9, Sample Name: test, Solvent: D2O). Other slots are in various states, some requiring sample names or solvents. A red box highlights a circular diagram of the 24-slot sample changer, showing the current sample in yellow and queued samples in blue. The diagram includes a legend for sample status: Current (yellow), Defined (blue), Pending (green), Unavailable (grey), Error (red), Verified (black), and Selected (orange).

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Force Tune	Upload Data	Scheduling	Submit Job
3		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
4		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
5		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
6		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
7		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
8		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
9	✓	test		D2O	Select a Method			✓	↓	⏏
10		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
11		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
12		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
13		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
14		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
15		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
16		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
17		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
18		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
19		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
20		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
21		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
22		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
23		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏
24		Sample Name Required		Select a Solvent	Select a Method			✓	↓	⏏

Below the table, a summary row shows: Status: 9, Slot: 9, Sample: test, Submit Time: 10-MAY-2018 16:48:31, Method: HSQC, Visualize: Yes, User: delta, Est. End Time: 10-MAY-2018 17:13.

The bottom status bar displays: Receiver Gain: 52, Spin: 0[H2], Lock: 1150, Temp: 25[°C], Helium: 94[%], Nitrogen: 92[%], LOADED (V), Queued Jobs: 1.

Setting up jobs for the sample

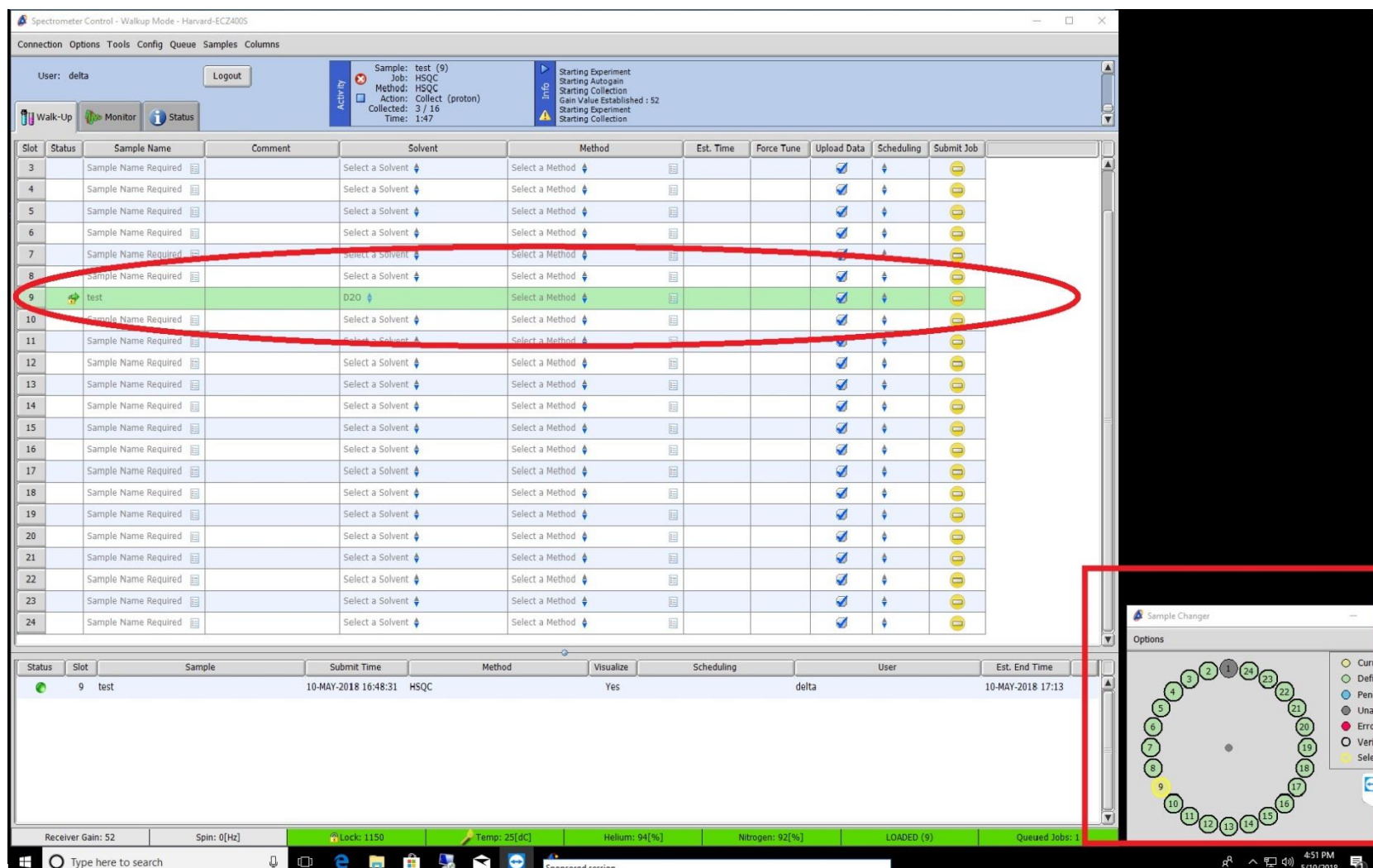
- Click on the line with the slot number of your sample or double-click on the circled number in the sample diagram to hi-light the line of the sample selected and enter all information needed.

The screenshot displays the 'Spectrometer Control - Walkup Mode - Harvard-EC24005' software interface. The main window features a menu bar (Connection, Options, Tools, Config, Queue, Samples, Columns) and a toolbar with buttons for Walk-Up, Monitor, and Status. A status bar at the top shows the user as 'delta' and a 'Logout' button. Below this, a panel displays job details: Sample: test (9), Job: HSQC, Method: HSQC, Action: Collect (proton), Collected: 3 / 16, Time: 1:47. A 'Starting Experiment' button is also visible.

The central part of the interface is a table with columns: Slot, Status, Sample Name, Comment, Solvent, Method, Est. Time, Force Tune, Upload Data, Scheduling, and Submit Job. The table lists 24 slots. Slot 9 is highlighted in green and contains the sample 'test' with solvent 'D2O' and method 'HSQC'. The bottom status bar shows the current sample 'test' at slot 9, submitted at 10-MAY-2018 16:48:31, using the HSQC method, with a user of 'delta' and an estimated end time of 10-MAY-2018 17:13.

In the bottom right corner, a 'Sample Changer' window is open, showing a circular diagram of 24 sample positions. The positions are numbered 1 through 24. Position 9 is highlighted in yellow, corresponding to the selected sample 'test'.

Enter sample info (name, comment, solvent) and select the experiment in the Method area. You can click the little square on the right of the Method to open a window where you can change any acquisition parameter such as the number of scans, the spectral range, the relaxation delay, etc.



Spectrometer Control - Walkup Mode - Harvard-ECZ400S

Connection Options Tools Config Queue Samples Columns

User: delta Logout

Activity Sample: test (9)
Job: HSQC
Method: HSQC
Action: Collect (proton)
Collected: 3 / 16
Time: 1:47

Info Starting Experiment
Starting Autogain
Starting Collection
Gain Value Established: 52
Starting Experiment
Starting Collection

Walk-Up Monitor Status

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Force Tune	Upload Data	Scheduling	Submit Job
3		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
4		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
5		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
6		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
7		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
8		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
9		test		D2O	HSQC			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
10		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
11		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
12		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
13		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
14		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
15		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
16		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
17		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
18		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
19		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
20		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
21		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
22		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
23		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>
24		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Go"/>

Status Slot Sample SubMIT Time Method Visualize Scheduling User Est. End Time

9 test 10-MAY-2018 16:48:31 HSQC Yes delta 10-MAY-2018 17:13

Receiver Gain: 52 Spin: 0[H2] Lock: 1150 Temp: 25[°C] Helium: 94[%] Nitrogen: 92[%] LOADED (9) Queued Jobs: 1

Sample Changer

Options

Legend: Current (yellow), Defined (green), Pending (blue), Unavailable (grey), Error (red), Verified (black), Selected (yellow)

Starting the experiment

Click the blue triangle icon at the right end of the line to start the experiment.
(You can add more experiments to this sample by selecting the Method and click the blue triangle icon again.)

The screenshot displays the 'Spectrometer Control - Walkup Mode - Harvard-ECZ400S' software interface. The main window features a menu bar (Connection, Options, Tools, Config, Queue, Samples, Columns) and a toolbar with 'Walk-Up', 'Monitor', and 'Status' buttons. A status bar at the top shows 'User: delta' and a 'Logout' button. Below this, a panel displays sample information: 'Sample: test (9)', 'Job: HSQC', 'Method: HSQC', 'Action: Collect (proton)', 'Collected: 3 / 16', and 'Time: 1:47'. A 'Starting Experiment' button is also visible. The main area is a table with columns: Slot, Status, Sample Name, Comment, Solvent, Method, Est. Time, Force Tune, Upload Data, Scheduling, and Submit Job. A red oval highlights row 9, which is selected and shows 'test' as the sample name. The bottom status bar displays various parameters: Receiver Gain: 52, Spin: 0[HHz], Lock: 1150, Temp: 25[°C], Helium: 94[%], Nitrogen: 92[%], LOADED (9), and Queued Jobs: 1. A red box in the bottom right corner highlights a 'Sample Changer' window, which shows a circular diagram of 24 sample positions. The legend indicates: Current (yellow), Defined (green), Pending (blue), Unavailable (grey), Error (red), Verified (black), and Selected (yellow). Position 9 is highlighted in yellow.

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Force Tune	Upload Data	Scheduling	Submit Job
3		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
4		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
5		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
6		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
7		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
8		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
9		test		D2O	HSQC			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
10		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
11		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
12		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
13		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
14		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
15		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
16		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
17		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
18		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
19		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
20		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
21		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
22		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
23		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>
24		Sample Name Required		Select a Solvent	Select a Method			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="button" value="Start"/>

Summary of Sample Changer Status:

Position	Status
1	Current
2	Defined
3	Defined
4	Defined
5	Defined
6	Defined
7	Defined
8	Defined
9	Current
10	Defined
11	Defined
12	Defined
13	Defined
14	Defined
15	Defined
16	Defined
17	Defined
18	Defined
19	Defined
20	Defined
21	Defined
22	Defined
23	Defined
24	Defined

Stopping current experiment

To stop the current experiment, simply click the blue square icon, the data collected will be saved. Clicking on the red X icon will abort the current experiment without saving the data.

The screenshot shows the 'Spectrometer Control - Walkup Mode - Harvard-ECZ400S' interface. The 'Activity' panel is highlighted with a red circle, showing the 'Stop' (blue square) and 'Abort' (red X) icons. The 'Sample' panel shows 'sensitivity (2)' with 'Job: Proton', 'Method: -', 'Action: Script', 'Collected: -', and 'Time: -'. The 'Change Loading Sample' panel shows 'Change Loading Sample', 'Loaded System Shims for Current Probe', 'Waiting to achieve Spin State 'SPIN OFF'', 'Achieved Spin State', and 'Waiting Temp Delay 60[s]'. The 'Queue' table lists 22 slots, with slot 2 selected. The 'Status' table shows the current experiment status.

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Force Tune	Upload Data	Scheduling	Submit Job
1										
2		sensitivity	0.1% ethylbenzene	Chloroform-D	Select a Method					
3		Sample Name Required		Select a Solvent	Select a Method					
4		Sample Name Required		Select a Solvent	Select a Method					
5		Sample Name Required		Select a Solvent	Select a Method					
6		Sample Name Required		Select a Solvent	Select a Method					
7		Sample Name Required		Select a Solvent	Select a Method					
8		Sample Name Required		Select a Solvent	Select a Method					
9		Sample Name Required		Select a Solvent	Select a Method					
10		Sample Name Required		Select a Solvent	Select a Method					
11		Sample Name Required		Select a Solvent	Select a Method					
12		Sample Name Required		Select a Solvent	Select a Method					
13		Sample Name Required		Select a Solvent	Select a Method					
14		Sample Name Required		Select a Solvent	Select a Method					
15		Sample Name Required		Select a Solvent	Select a Method					
16		Sample Name Required		Select a Solvent	Select a Method					
17		Sample Name Required		Select a Solvent	Select a Method					
18		Sample Name Required		Select a Solvent	Select a Method					
19		Sample Name Required		Select a Solvent	Select a Method					
20		Sample Name Required		Select a Solvent	Select a Method					
21		Sample Name Required		Select a Solvent	Select a Method					
22		Sample Name Required		Select a Solvent	Select a Method					
23		Sample Name Required		Select a Solvent	Select a Method					

Status	Slot	Sample	Submit Time	Method	Visualize	Scheduling	User	Est. End Time
	2	sensitivity	11-MAY-2018 10:53:30	Proton	Yes		console	11-MAY-2018 10:58
	2	sensitivity	11-MAY-2018 10:54:13	Carbon	Yes		console	11-MAY-2018 11:00

Receiver Gain: 56 Spin: 0[Hz] Lock: 0 Temp: 25.1[°C] Helium: 94[%] Nitrogen: 87[%] LOADED (2) Queued Jobs: 2

Aborting the queued job

You can delete the queued experiment by clicking on the X icon on the left side of the line (only the user who submitted this job can do this deletion).

Spectrometer Control - Walkup Mode - Harvard-ECZ400S

Connection Options Tools Config Queue Samples Columns

User: console Logout

Activity

Sample: sensitivity (2)
Job: Proton
Method: -
Action: Script
Collected: -
Time: -

Changer Loading Sample
Changer Loaded Sample
Loaded System Skims for Current Probe
Waiting to achieve Spin State 'SPIN OFF'
Achieved Spin State
Waiting Temp Delay 60[s]

Walk-Up Monitor Status

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Force Tune	Upload Data	Scheduling	Submit Job
1										
2		sensitivity	0.1% ethylbenzene	Chloroform-D	Select a Method					
3		Sample Name Required		Select a Solvent	Select a Method					
4		Sample Name Required		Select a Solvent	Select a Method					
5		Sample Name Required		Select a Solvent	Select a Method					
6		Sample Name Required		Select a Solvent	Select a Method					
7		Sample Name Required		Select a Solvent	Select a Method					
8		Sample Name Required		Select a Solvent	Select a Method					
9		Sample Name Required		Select a Solvent	Select a Method					
10		Sample Name Required		Select a Solvent	Select a Method					
11		Sample Name Required		Select a Solvent	Select a Method					
12		Sample Name Required		Select a Solvent	Select a Method					
13		Sample Name Required		Select a Solvent	Select a Method					
14		Sample Name Required		Select a Solvent	Select a Method					
15		Sample Name Required		Select a Solvent	Select a Method					
16		Sample Name Required		Select a Solvent	Select a Method					
17		Sample Name Required		Select a Solvent	Select a Method					
18		Sample Name Required		Select a Solvent	Select a Method					
19		Sample Name Required		Select a Solvent	Select a Method					
20		Sample Name Required		Select a Solvent	Select a Method					
21		Sample Name Required		Select a Solvent	Select a Method					
22		Sample Name Required		Select a Solvent	Select a Method					
23		Sample Name Required		Select a Solvent	Select a Method					

Status	Slot	Sample	Submit Time	Method	Visualize	Scheduling	User	Est. End Time
	2	sensitivity	11-MAY-2018 10:53:30	Proton	Yes		console	11-MAY-2018 10:58
X	2	sensitivity	11-MAY-2018 10:54:13	Carbon	Yes		console	11-MAY-2018 11:00

Receiver Gain: 56 Spin: 0[Hz] Lock: 0 Temp: 25.1[4C] Helium: 94[%] Nitrogen: 87[%] LOADED (2) Queued Jobs: 2

Type here to search

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Finishing up

You can log out after submitting all your samples and experiments. Other users can then log in to submit their samples. If there is no more job submission, the dummy spinner in slot #1 will be automatically loaded 60 seconds after the end of all experiments. The last user will also be automatically logged out.

