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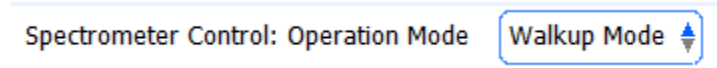
Walkup Mode

Overview

Over the years customers have requested a spreadsheet type interface for sample definition and submission. The design of this interface should contain all elements of Sample Creation, Method Selection, Data Destination, Queue Management and Queue Status.

Walkup Preferences

Walkup mode is activated by setting the “Operation Mode” preference to “Walkup Mode”.



The “Tools” menu in Spectrometer Control has parameters related to “Walkup Mode”

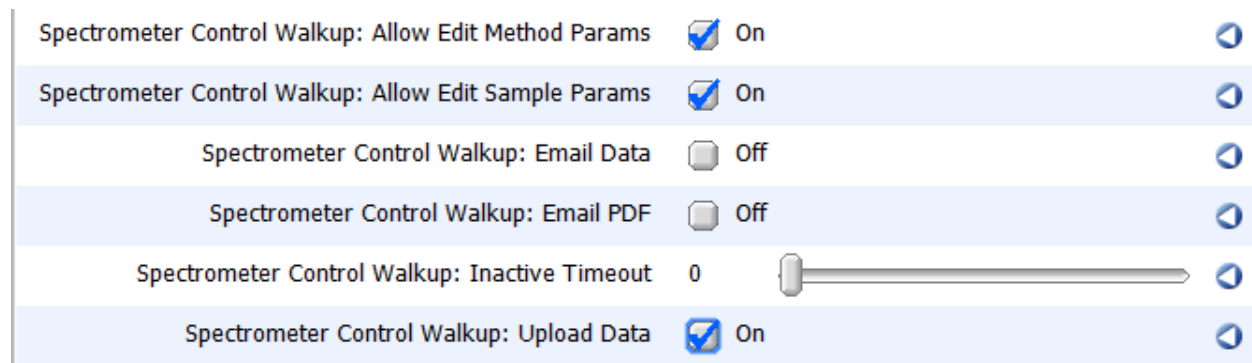


Figure 1

Spectrometer Control Walkup: Allow Edit Method Params – Enable/Disable ability to modify method parameters prior to method submission.

Spectrometer Control Walkup: Allow Edit Sample Params – Enable/Disable ability to modify sample attribute prior to method submission.

Spectrometer Control Walkup: Email Data – Hide or Display the e-mail Data column and disable the function. E-mail address is inherited from the User Profile definition using the “Manage User Accounts Tool”.

Spectrometer Control Walkup: Email PDF – Hide or Display the e-mail PDF column and disable the function. E-mail address is inherited from the User Profile definition using the “Manage User Accounts Tool”.

Spectrometer Control Walkup: Inactive Timeout – Amount of time before user is automatically logged out in minutes. Setting it to 0 will disable this function. Movement of the mouse will reset the timer.

Spectrometer Control: Open Delivered Data – ON/OFF for Visualize box

Example below shows all options turned on

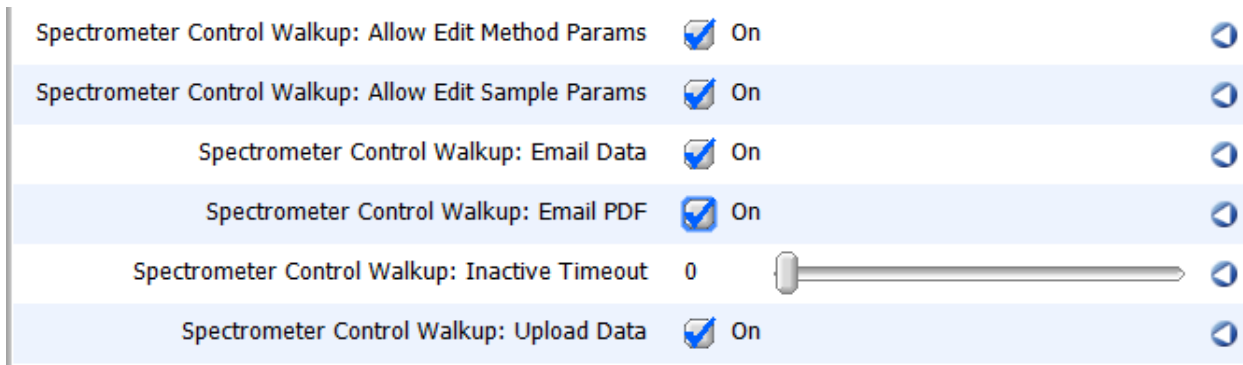


Figure 2

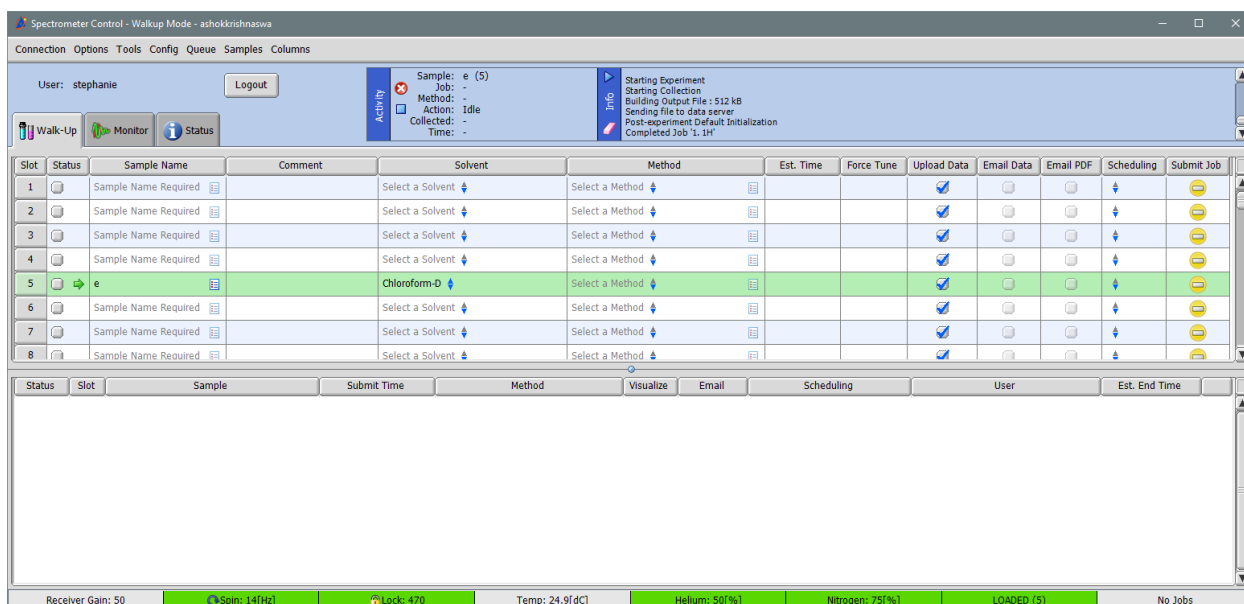


Figure 3

As one can see even though E-mail data and E-mail PDF was checked on the radio buttons are greyed out. This is because the logged in user does not have an e-mail associated with the account.

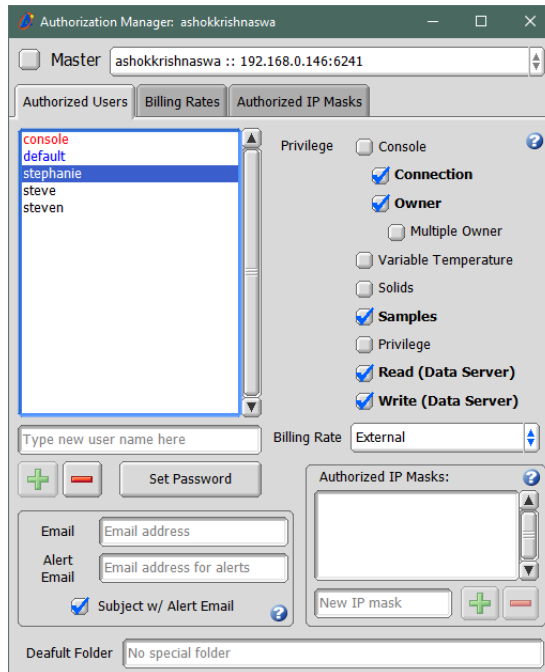


Figure 4

User Authorization settings

To be able to access “Walkup” mode, a USER account must be created on the spectrometer using the “Manage User Accounts” from the “Config” menu of Spectrometer Control.

As an example “Steve” has an e-mail address.

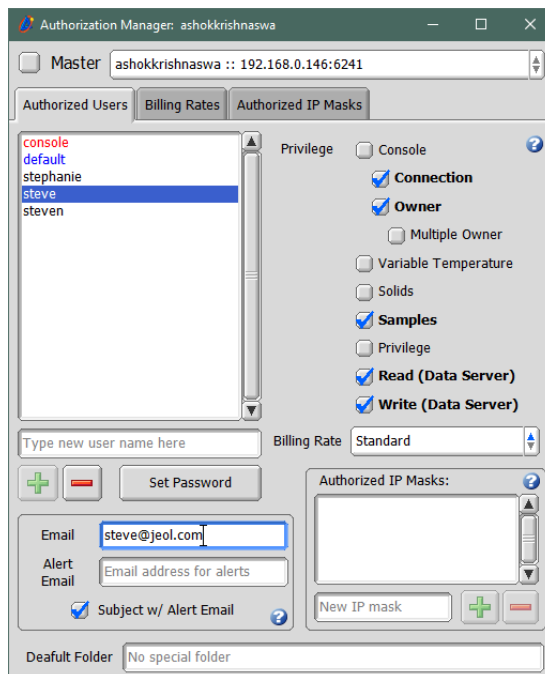


Figure 5

When “Steve” logs in to the spectrometer, the e-mail radio buttons are active.

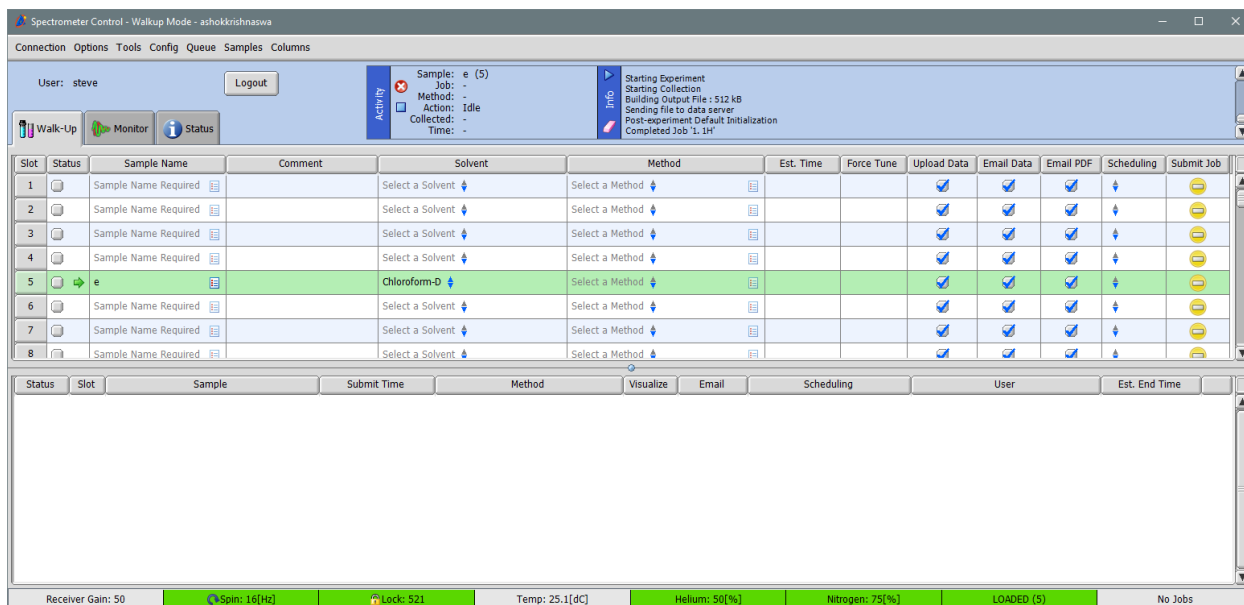


Figure 6

Note: If a SMTP server is not specified in “Instrument Preferences”, Email Data and Email PDF columns will not be visible.

Column Display

Columns that don't need to be displayed can be hidden. The list of Columns that can be displayed/hidden are available under the “Column” menu.

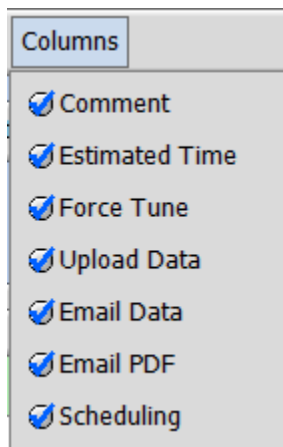


Figure 7

Sample Changer Map Display

The Map of the Sample Changer tray is available under the “Samples” menu.

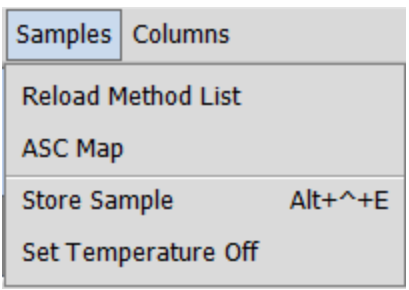


Figure 8

Selecting the “ASC Map” entry spawns a separate window that displays the tray pattern of the sample changer.

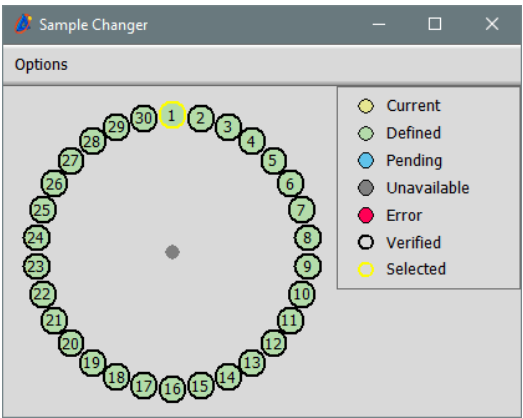


Figure 9

Double clicking on an available slot will select that line in the main Walkup window. Additionally the legend associated with the map provides feedback on the current state of the queue.

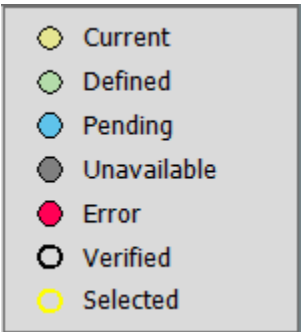



Figure 10

Note: In Walkup mode all samples will appear as “Defined” and “Verified” as all slot positions are created (Defined) and Verified.

Sample Attributes

If the preference “Spectrometer Control Walkup: Allow Edit Sample Params” is set to “ON”, the parameter icon  appears next to the Sample name.

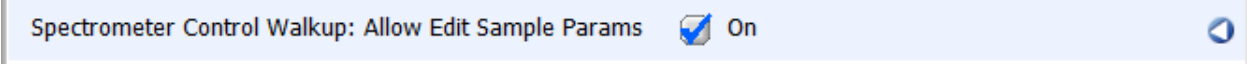


Figure 11

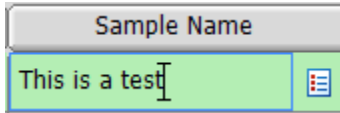


Figure 12

If the preference “Spectrometer Control Walkup: Allow Edit Sample Params” is set to “OFF” then Sample Attributes cannot be changed prior to method submission.

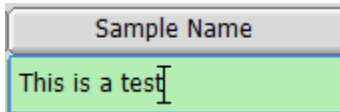



Figure 13

Clicking on  displays the Sample Attributes for the sample prior to Method submission.

Parameter	Value
gradient shim	<input checked="" type="checkbox"/>
lock_state	AUTOLOCK
preparation	<input checked="" type="checkbox"/>
spin_set	15[Hz]
spin_state	SPIN ON
temp_set	25[dC]
temp_state	TEMP OFF

Figure 14

Estimated Time column

Time calculation is performed by evaluation the expression defined in the “Duration” statement in a method. If a “Duration” Statement is not present in a given method, the estimated time is simply an additive result of all experiments within the defined method.

Shown below are examples of duration statements

DURATION Proton + (force_tune ? 60[s] : 0[s]) + (calculate_proton_90 ? 120[s] : 0[s]) + 120[s];

DURATION Proton + (acquire_13C_data ? carbon : 0[s]) + hmbc + (force_tune ? 60[s] : 0[s]) + (calculate_90s ? 240[s] : 0[s]) + 120[s];

Note: The “Duration” statement re-evaluates the method if any changes are made.

Estimated time for method “1H” with “force_tune” set to False.

Method	Est. Time	Force Tune
1. 1H	4:25	<input type="radio"/>

Figure 15

As the “Duration” statement adds 60[s] for the tune process, the Estimated time for method “1H” with “force_tune” set to TRUE is shown below.

Method	Est. Time	Force Tune
1. 1H	5:25	<input checked="" type="checkbox"/>

Figure 16

If the Delta Preference “Spectrometer Control Walkup: Allow Edit Method Params” is TRUE then the “Duration” statement is also evaluated. See section “**Modifying Parameters Prior to Submission**” below.

Force Tune column

The “Force Tune” column is linked to the “force_tune” variable in the method. This is a **reserved variable** and should **ONLY** be used for triggering the check box in the GUI.

The method “1H” has the “force_tune” variable defined in the method. As can be seen below, when the method “1H” is used the “force_tune” radio button appears in the GUI.

Method	Est. Time	Force Tune
1. 1H	4:25	<input type="radio"/>

Figure 17

The method “Fluorine” does not have the “force_tune” variable defined in the method. As can be seen below, when the method “Fluorine” is used the “force_tune” radio button does not appear in the GUI.

Method	Est. Time	Force Tune
Fluorine	1:16	

Figure 18

Blocked/Un-available Samples

It is expected that "Walkup" mode will be the exclusive mode of operation for the spectrometer. When Walkup mode is active and the spectrometer is connected to, a set of pre-defined "blank" samples are created which represent the number of available slots in the Sample Changer.

The "Owner" of these samples is "Walkup".

If prior to "Walkup" mode if samples were created in "Advanced" mode **and are verified**, they will not be available for use in "Walkup" mode.

Note: If there is a need to reserve sample changer positions for Service support, it is recommended to create and "block" out these changer positions using "Advanced" mode prior to entering "Walkup Mode".




Slot	Status	Sample
1		Another Sample is verified on slot 2. Jobs submitted with this Sample will not run until the Sample is verified.
2		
3		

Figure 19

In addition to samples that have been reserved by "Advanced Mode", the slot that is reserved for Sample Parking is also blocked out from use in Walkup Mode.




29	<input type="checkbox"/>	This slot is set as the Automatic Parking Slot. Slot 30 cannot be used.
30		

Figure 20

Submission of Jobs

Submission of Jobs to the spectrometer queue is straightforward. Start from the left, fill in the cells and hit the  button.



There are required fields that MUST be filled out before the  button is available. These required fields are

Sample

Solvent


Method

Comment, Force Tune, Upload Data, Email Data, Email PDF, Scheduling are optional.

If the required fields are blank the  button will not be available. Instead the  icon will indicate that some fields need to be filled in.

Note: While the Estimated Time is being calculated the Submit button will not be available.

Modifying Parameters Prior to Method Submission

If the preference “Spectrometer Control Walkup: Allow Edit Method Params” is set to “ON”, the parameter icon  appears next to the Method name.

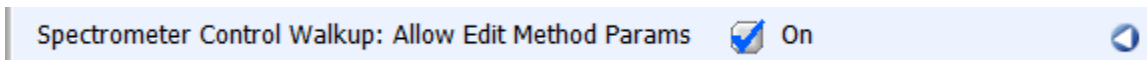


Figure 21

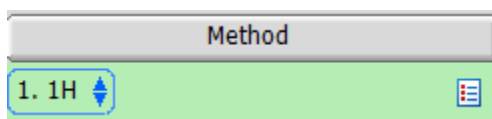


Figure 21

If the preference “Spectrometer Control Walkup: Allow Edit Method Params” is set to “OFF” then parameters cannot be changed prior to method submission.

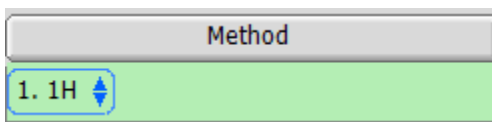




Figure 22

Note: If Preferences related to “Walkup” mode are changed while “Walkup” mode is active, it is necessary to close the “Spectrometer Control” tool and re-connect.

When  is pushed a popup window with “Exposed” variables for the method appears. Make the appropriate changes and hit the  button to close the parameter dialog box.

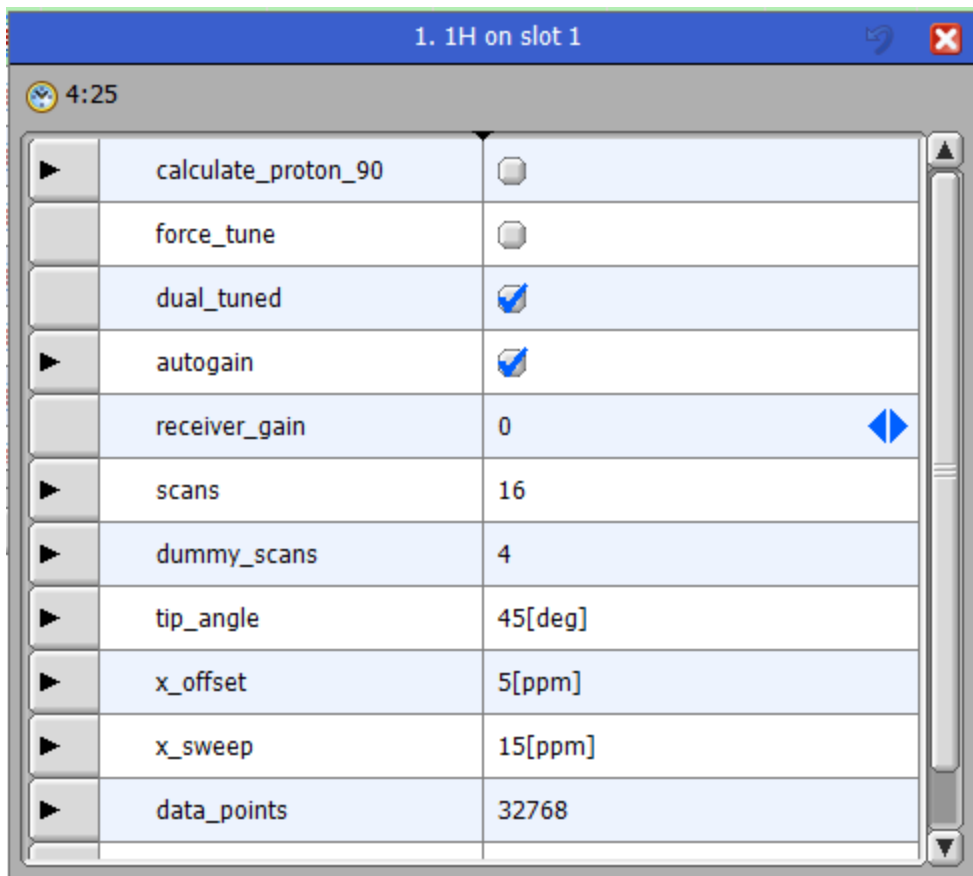


Figure 23

The top left hand corner of the Parameter dialog box displays the estimated run time for the method.

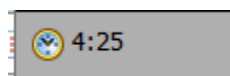


Figure 24

If a change is made to the method, the estimated time will be re-calculated and the value updated.

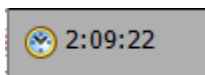


Figure 25

Upon closing the Parameter dialog box, the estimated time will be updated in the main Walkup mode interface.

Method	Est. Time	Force Tune
1. 1H	2:09:22	<input type="checkbox"/>

Figure 26

Submitted jobs appear in the "Job Queue" in the lower pane of the GUI.

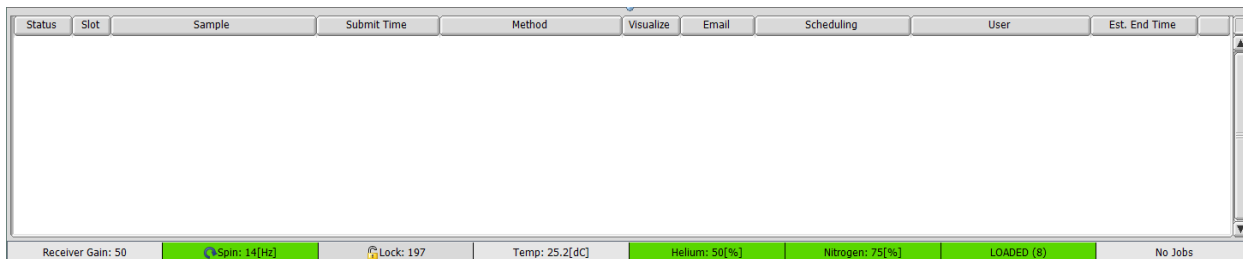


Figure 27

When a job is currently running on a particular slot that slot is “Locked”. This is denoted by the “lock”



icon in the “Status” column

Additional methods can be submitted against the “locked” sample. The fields that **CANNOT** be modified while the current sample is locked/running are

Sample

Comment

Solvent

Shown below is an example. The “Sample”, “Comment” and “Solvent” fields are greyed out and cannot be modified while a measurement is in progress.

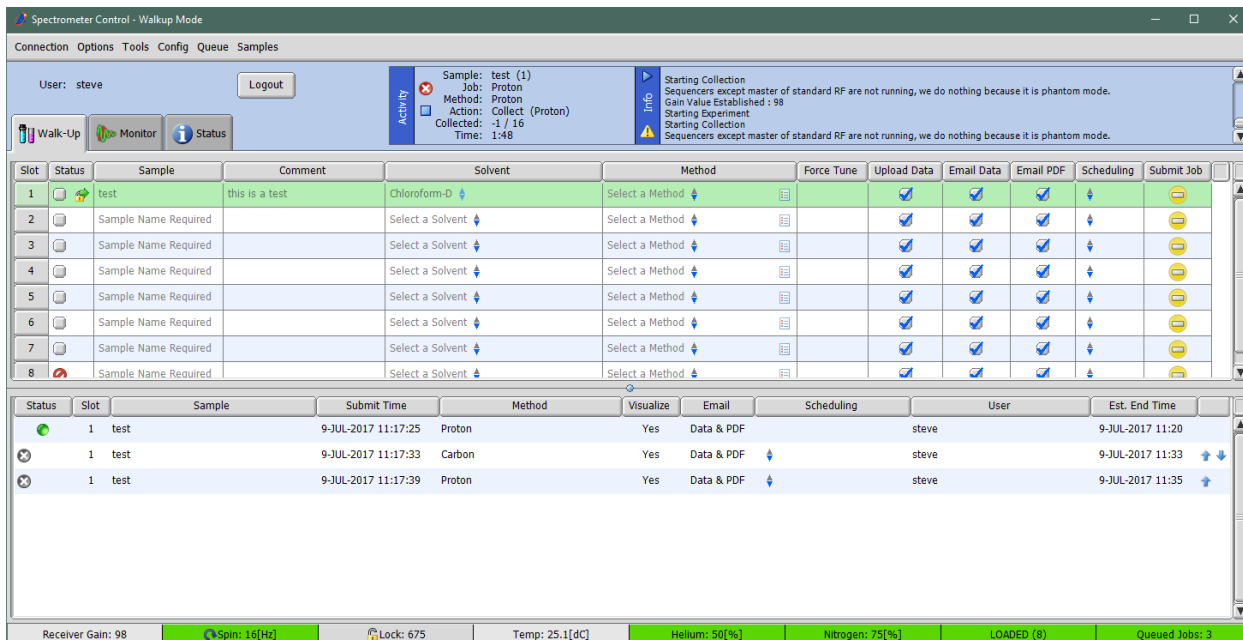


Figure 28

Reserving slots

There are cases when a user may be performing a timed study and needs to leave the sample in the carousel. This user can “block” the use of this slot position in the carousel by checking the box in the “Status” column.

Slot	Status
1	<input checked="" type="checkbox"/>

Figure 29

In the above example, User “Steve” has reserved Slot 1 for his own use.

When another user, for example “Stephanie” logs in, Slot 1 will not be available to her.

Slot	Status
1	<input checked="" type="checkbox"/>

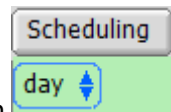
Figure 30

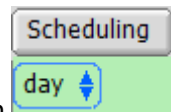
Hovering over the checkbox for popup help will indicate the user who has reserved the slot.

The sample in slot 1 is reserved by user 'steve'.

Figure 31

Scheduling



The Scheduling column  is controlled by using the “Scheduling” tool.

Workstation Data Storage Locations

Data Storage locations in general has been improved (this is not only applicable to Walkup mode).

In the “User Account” management tool a default sub-folder to the “root” data directory defined in Delta can be assigned per logged in user.

Shown below is an example for User “Steve”. The “Default Folder” is set to “steve/data”. This means that when the data returns to the workstation the data will get stored in “ROOT DATA PATH/steve/data”.

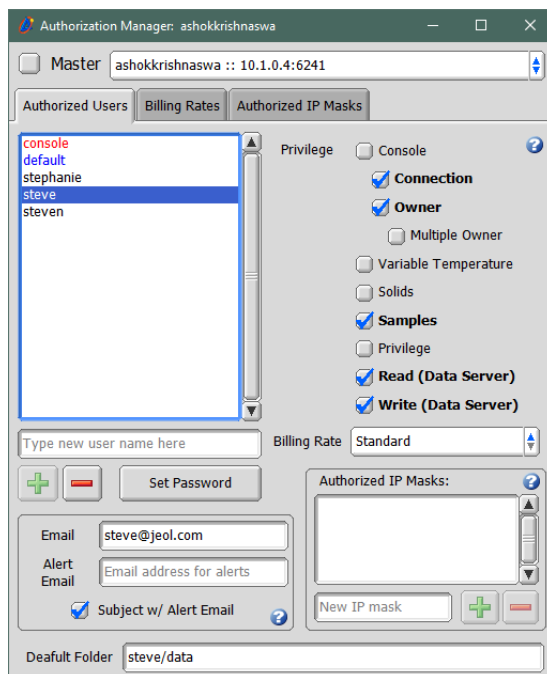


Figure 32

Note: If a “Default Folder” is not specified in the “Authorization Manager” then when the data returns to the workstation it will be placed in a folder based on the “login name”.

Walkup mode enhancements

Additionally segregate data files based on “Projects”. This choice is available under the “Options” menu of Spectrometer Control.

Initially if the user has no “Projects” the list of prior projects will be blank. The user can select “Add New Project” from the menu.

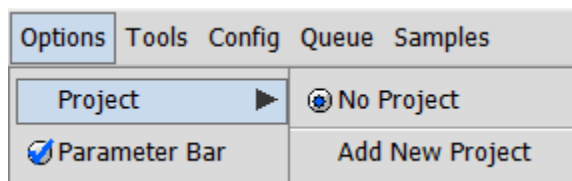


Figure 33

A dialog box appears for “Project name” entry.



Figure 34

Hit OK for the Project name to be created.

The new project will be automatically associated with the sample. On completion of the job when the data returns it will be placed in

ROOT DATA PATH/<PROJECT NAME>/<FOLDER NAME>

Note 1: Projects are NOT a delta feature but is stored on the data server. If a user creates a project and does not submit a job which results in a data set being saved to the data server, the project does not exist. The next time the user logs in the project will not be displayed.

Note 2: Projects are user specific. The list of displayed projects depend on the logged in user.

Note 3: The storage path is in the following order – ROOT DATA PATH/PROJECT PATH/FOLDER PATH. This is the current order as defined in Delta. There could be situations where one would prefer ROOT DATA PATH/PROJECT PATH/FOLDER PATH. There is a plan to have a preference to allow the order to be flipped.

Default Automation File (JAF)

Due to the fact that in “Walkup” mode a JOB can only contain single methods requires that methods become more complex to contain multiple experiments within a single method.

For this reason a separate JAF file is used. The name of this file is “Standard_walkup.jaf”. If “Standard_walkup.jaf” is not found or has errors, “Standard.jaf” will be loaded.

Note: Error messages are sent to the main Delta window of errors are encountered.

Samples Menu

The “Samples” menu in Spectrometer Control provides a quick mechanism to

Reload Method List – If an automation template is modified while connected to the spectrometer in “Walkup Mode” this provides a method to reload the file without disconnecting and re-connecting to the spectrometer.

Inactive Sample

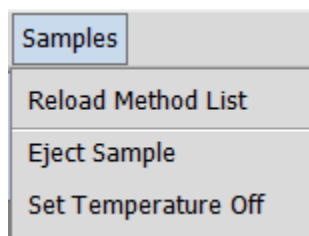


Figure 35

Active Sample

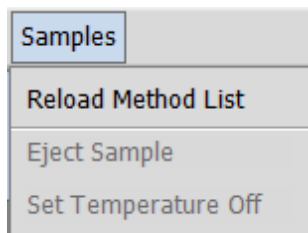


Figure 36

Eject Sample – Provides a mechanism to force eject the sample. This feature is greyed out when the spectrometer is busy collecting data on the loaded sample.

If the Instrument Preference “Job Queue: Sample Parking Slot” is set to 0

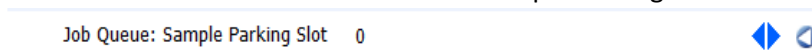


Figure 37

then the menu entry will display “Eject Sample”.

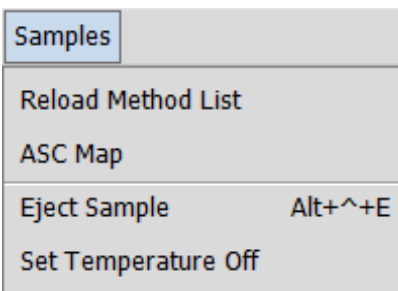


Figure 38

If the Instrument Preference “Job Queue: Sample Parking Slot” is set a non-zero value within the allowable range that the current sample changer supports then the menu entry will display “Park Sample”. During a Park operation the currently loaded sample will be ejected and the assigned “Parking” sample will be loaded.

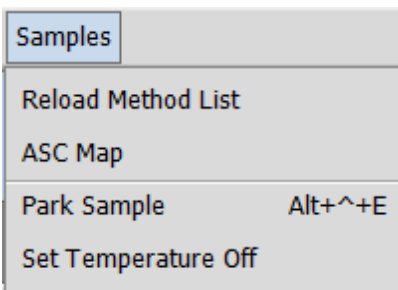



Figure 39

Set Temperature Off – Turn off VT. This feature is greyed out when the spectrometer is active collecting data on the loaded sample.

Appendix

After the first successful login to “Walkup” mode a table consisting of all available slots is automatically created. Samples that have been created in other modes (Advanced/Smart) that are “verified” are not available in “Walkup” mode. Un-available samples are indicated by the  icon next to the slot position.

All samples created in “Walkup” mode are owned by a pseudo account named “walkup”. All samples are created with the “Shared” flag set to TRUE and the “Verified” flag set to FALSE. **On Job submission the “Verified” flag is set to TRUE.** The “Verified” flag remains set to TRUE even after the Job may have ended as there may be other pending jobs against that sample.

Because “walkup” is a pseudo account, samples created by “Walkup” do not appear by default in “Advanced” mode. There are 2 ways to manipulate samples that were created by user “Walkup”.

Login as user “Console”

Switch connection mode from “Walkup mode” to “Advanced mode” using Delta Preferences. Connect to the spectrometer as user “console”.

From the “Samples” menu select “Show Walkup Samples”.

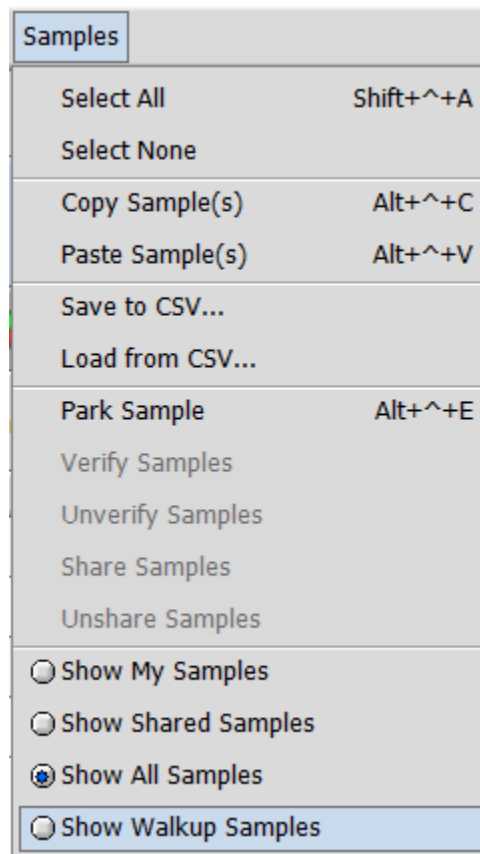


Figure 40

Samples created by “Walkup” will be displayed.

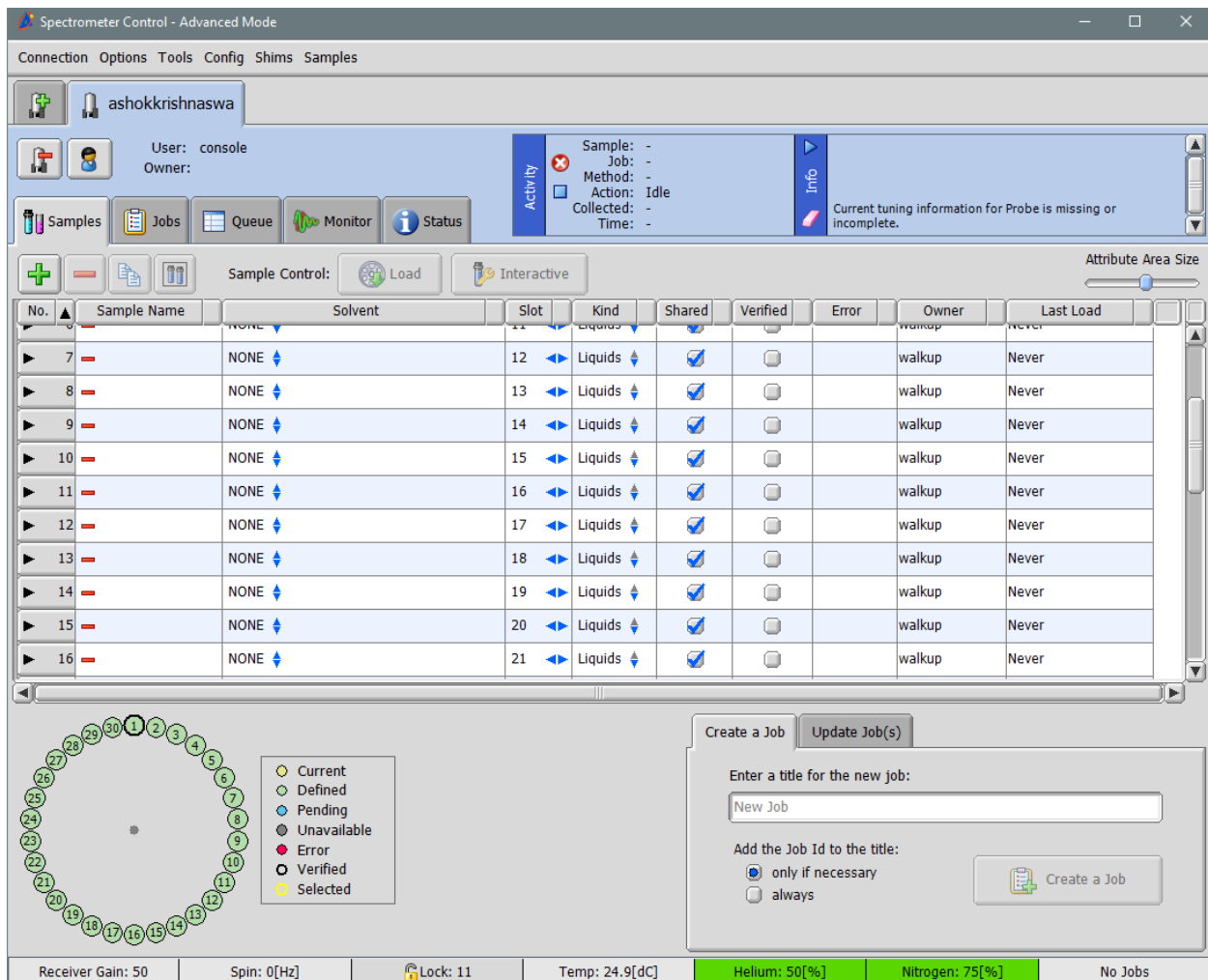


Figure 41

Login as user “walkup”

Even though user “Walkup” does not exist, connection can be established to the spectrometer as user “walkup”. This provides another way to display and manipulate samples owned by user “walkup”.

Note: For user “walkup” to connect to the spectrometer, “Connection” privilege must be enabled for user “default”.

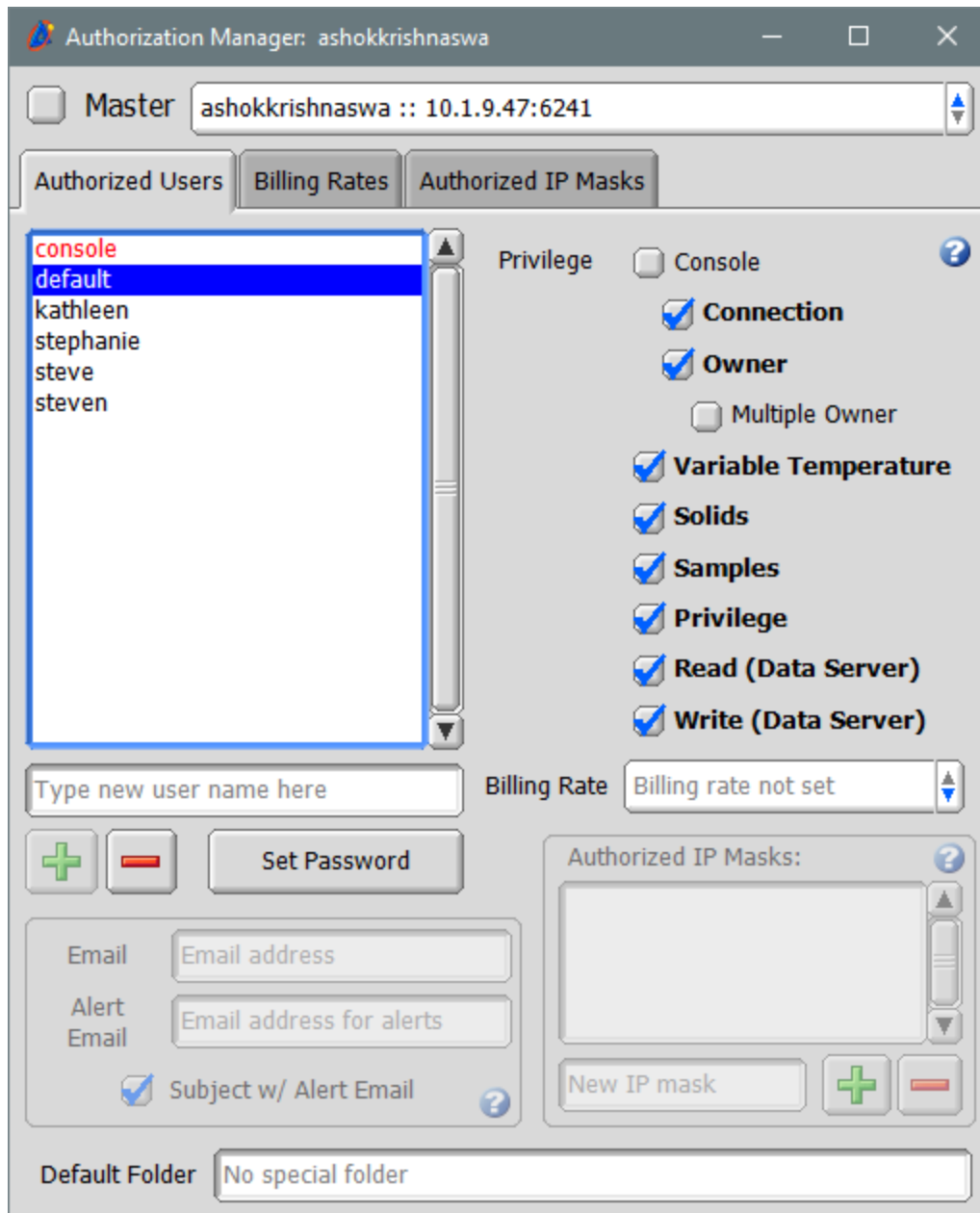


Figure 42