VnmrJ Walkup

Varian NMR Spectrometer Systems
With VnmrJ 1.1D

Pub. No. 01-999266-00, Rev. 0604

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Revision history:
A0604 – Initial release for VnmrJ 1.1D

Applicability of manual:
Varian NMR spectrometer systems running VnmrJ 1.1D software

Technical contributors: Frits Vosman, Ghirmai Meresi, Everett Schreiber
Technical writer: Everett Schreiber
Technical editor: Dan Steele

3120 Hansen Way, Palo Alto, California 94304
http://www.varianinc.com

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Chapter 1. *VnmrJ Walkup* Operator

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1.1 Overview of the *VnmrJ* Walkup Operator

The *VnmrJ* Walkup Operator interface provides the user with:

- Protocols are grouped by type, see Table 1, and accessed by clicking on a protocol tab.

Table 1. Experimental Protocols

Protocol Tab	***Protocol***	
Std 1D	Proton	Presat
	Wet1D	Carbon
	Fluorine	Phosphorus
	Apt	Dept
Homo 2D	Cosy	Dqcosy
	Noesy	Rosy
	Tocsy	Gcosy
	Gdqcosy	
Hetero 2D	Hmqc	Hmbc
	Hsqc	Ghmqc
	Ghmqc	Ghsqc
	Hmqctoxy	Hsqctoxy
	Ghmqctoxy	Cigar2j3j

- Optimized parameters for all experimental protocols.
- Selection of multiple experimental protocols for a given sample.
- Submission of the sample study to the acquisition queue by clicking on the Submit button (single sample mode) or either the Submit DayQ or Submit NightQ buttons (sample changer).
- Experimental protocols from each application type are entered into the study queue by selecting the application type and clicking on the desired protocol button.
- 2 D protocols add a proton type protocol (proton, presat, or wet1d with MinSW enabled) if a proton type protocol does not exist ahead of the first 2D protocol in a composite protocol (multiple protocols for a given sample).
- Protocols for 1D experiments not of the proton type can be added to the composite protocol at any time.
- All composite protocols are executed from the top down.
- The protocol is submitted to the acquisition queue when the operator clicks on the Submit (single sample mode) or either the Submit DayQ or Submit NightQ buttons (automated sample changer). Parameters are optimized for each protocol.

1.2 Quick Start

The quick start procedure relies on the following:

- Defaults are set up by the VnmrJ Walkup account owner. Preset defaults include shimming, locking, saving data, and plotting but are not limited to these defaults.
- The *VnmrJ* Walkup Operator interface is active and the switch operator screen is currently displayed.
- A new automation run is started.
- Depending upon the type of sample changer the following are true:

  Single sample operation or sample changer (carousel, SMS 50, or SMS 100)– sample tube is filled to the correct height (approximately 750 µl) and is in the spinner and at the correct height.

  768 AS and Gilson/VAST – racks are installed and configured, refer to 768 AS operations and instructions or the VAST operations and instructions manual for more information..

Switch operator window displays a number or a tray	***Switch operator window does not display a number or a tray***
Note **number** on the screen.	Select **Operator** and enter **Password**.
Place the sample in the **location** indicated by	Click on the **Start** tab.
the number on the screen.	Select the **Study** page.
Select **Operator** and enter **Password**.	Click **Eject.**
Click on the **sample location** in the tray display.	**Remove** the current sample.
Click on the **Start** tab.	**Place** new sample atop the upper barrel.
Select the **Study** page.	Click **Insert**.
Click the **Solvent** drop down menu.	Click on the **Start** tab.
Select the **lock solvent** from the menu.	Select the **Study** page.
Optional: fill in the requested information.	Click the **Solvent** drop down menu.
Click on a **Protocol type** tab.	Select the **lock solvent** from the menu.
Click (once) on each desired **protocol**.	Optional: fill in the requested information.
Click on the **Submit DayQ** or **Submit NightQ** button (long protocols may offer only the Submit NightQ).	Click on a **Protocol type** tab. Click (once) on each desired **protocol**.
Additional sample:	Click on the **Submit** button.
Click on the next **grayed sample position**.	Select **Utilities** from the Menu bar.
Repeat steps beginning at *Click on the **Start** tab.*	Click on **Switch Operators…**.
Select **Utilities** from the Menu bar.	
Click on **Switch Operators…**.	

1.3 Walkup Operator Switch Operators

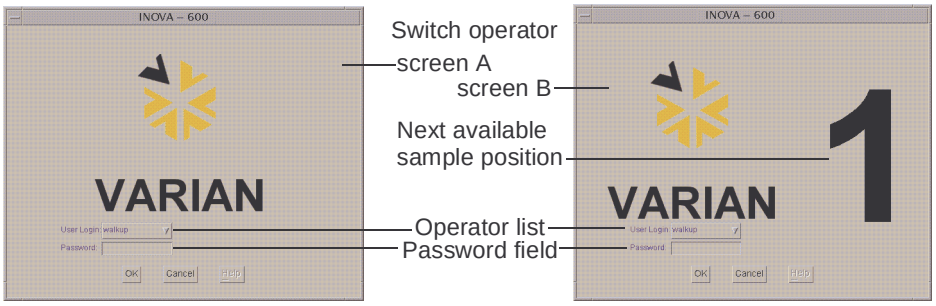
The Switch operator screen shown below should be displayed and *VnmrJ* Walkup running. If this is not true, have the walkup account owner start *VnmrJ* Walkup, see "VnmrJ Walkup Account Owner Interface Description" on page 29.

Systems with a sample changer in use (`traymax>0`) will display a different switch operator screen than a system that either does not have a sample changer or is not in use (`traymax=0`). The value of `traymax`, determines the switch operators windows display.

Switch Operators…
Opens a window for changing walkup operators without exiting *VnmrJ*. The appearance of the switch operator window will change depending upon the value of `traymax`.

· If `traymax=0`,
Switch operator screen A is shown

If `traymax>0`,
Switch operator screen B is show



If `traymax=96` or `768`, switch operator screen B will show five trays with the following color codes:
blue – active tray, black– tray not present, and white – tray present and a configure tray button. Refer to the accessory manuals for the 96 and 768 sample handling systems for more information.
Select an operator from the drop down menu or type the operator name in the field. The operator name will be automatically completed as you type.

Enter a password in the password field

Click **OK** (or press enter after typing the password)

1.4 Starting an Experiment

Proceed as follows based upon switch operator screen.

Switch Operator Screen A

1. **Enter** or **select** operator name and **enter password**.
2. Click on the **Start** tab.
3. Click on the **Eject** button and remove the current sample.
4. Place the sample in the spinner and adjust the position of the sample in the spinner
5. Place new sample atop the upper barrel.
6. Click on the **Insert** button.
7. Select the sample lock solvent from the drop down **Solvent** menu.
8. Place checks in either of the following options: **Find z0** and **Gradient Shim** to enable these options.

Do the following if you did not place checks in Find z0 and Gradient Shim boxes.

a. Establish lock manually or click on the **Find z0 button**.

b. Optimize the magnetic field homogeneity by either clicking on **Gradient shim** button (on the Lock page) or selecting the **Shim** page and manually adjusting the shims.

Refer to the *VnmrJ Liquids NMR User Guide* manual for instructions on locking, lock shimming, and gradient shimming.

9. Place a check in the **Plot all data** to enable this option upon completion of the study or fid acquisition.

10. Enable or disable temperature regulation:

    - Enable – **check** the box next to **Temperature** and enter a **value** in the field next to the check box.
    - Disable – remove the **check** from the box next to **Temperature**.

11. Optional:

    - Fill in the information in the **Sample**, **Notebook**, **Comment**, and **Page** fields.
    - If E-mail is enabled, select either or both of the **Email** options for notification upon completion.

    Refer to the *VnmrJ Liquids NMR User Guide* manual for instructions variable temperature operation.

12. Optional – Select the **Spin/Temp** page.

    The defaults shown on this page are the recommended settings. 1D spectra are acquired with the sample spinning and all 2D spectra are automatically acquire with the sample not spinning.

    Refer to "VnmrJ Walkup Operator Interface Controls and Regions" on page 13 for details about the controls on the Study Spin/Temp page.

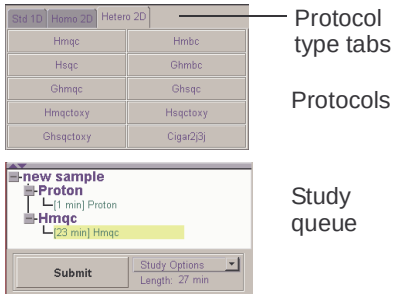
    Refer to the *VnmrJ Liquids NMR User Guide* manual for instructions variable temperature operation, cautions, and warnings.

13. Select a **Protocol Type** tab.

    The options for each menu item are shown in Table 1.

14. Select a **protocol** or series of **protocols** from the display of protocols by single clicking on each desired protocol (or drag and drop the protocol into the study queue).

    The study protocol for the current operator's samples appears in the study queue window. Each time a protocol is clicked it is added to the study queue list.



switch operator screen A

Hetero 2D and Homo 2D protocols run two experiments. Selecting Hsqc will automatically add the Proton protocol ahead of the Hsqc protocol to the study queue if a Proton type protocol is not already present. If another experiment is added, such as Cosy which includes a Proton type protocol as part of the protocol, only one spectrum using a Proton type protocol is acquired.

Proton, Presat, and Wet1d are Proton type protocols.

15. Refer "Customizing Acquisition Parameters" on page 12 to change acquisition parameters.
16. Refer to "Removing a Protocol from a Composite Protocol in the Study Queue" on page 12 if a protocol is to be removed from the study queue.
17. Click the **Submit** button to add the study to the queue.
18. Click on **Utilities**.

    Select **Switch Operators…**

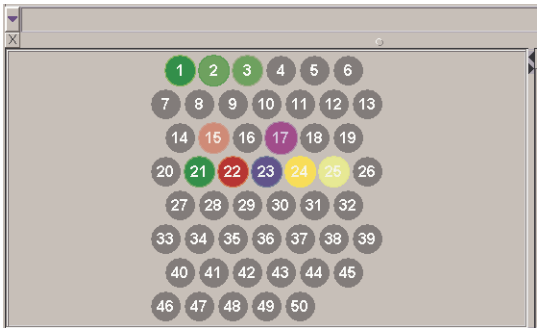
Switch Operator Screen B

1. Place the sample in the spinner and adjust the position of the sample in the spinner.
2. Place the sample and spinner in the location shown on the log in screen (or other available location — switch operators to see the available locations).
3. **Enter** or **select** operator name and **enter password**.
4. Click on a **gray sample position** — available sample positions are gray.

   The number displayed on the switch operator window is the next available position but any grayed position can be used. Samples are run in the order in which they are submitted to the queue. The location of the sample in the sample changer does not determine when a sample will be run. The status of occupied sample positions is indicated by the color displayed at the position. Dimmed colors indicate the sample is owned or belongs to a another operator, not the current operator.

   Sample reuse option – refer to the *VnmrJ Installation and Administration* manual for instructions on setting this option. If this option is enabled, any sample position that is indicated as completed (green), error (red), or available (gray) can be used.

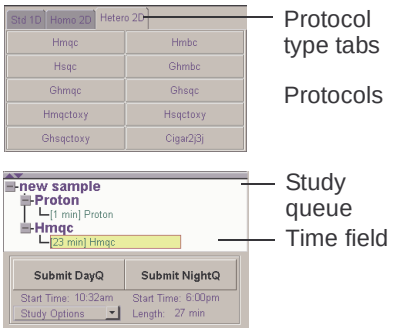
   An example is shown here with a SMS 50 sample tray.

Item	*Description*
Available sample positions. The colors of the sample position indicate the status of that sample position as follows:	
Gray	Available
Green	Completed
Blue	Active
Yellow	Submitted - Day queue
Purple	Submitted - Night queue
Red	Error
Faded or grayed out colored sample position	Sample submitted by an operator other than the operator that is currently logged in to the walkup interface.

5. Select the sample lock solvent from the drop down **Solvent** menu.

6. Place checks in either of the following options: **Find z0** and **Gradient Shim** to enable these options.
7. Place a check in the **Plot all data** to enable this option upon completion of the study or fid acquisition.
8. Enable or disable temperature regulation:
   - Enable – **check** the box next to **Temperature** and enter a **value** in the field next to the check box.
   - Disable – remove the **check** from the box next to **Temperature**.
9. Optional:
   - Fill in the information in the **Sample**, **Notebook**, **Comment**, and **Page** fields.
   - If E-mail is enabled, either or both of the **Email** options for notification upon completion.
10. Select a **Protocol Type** tab protocol from the drop down menu.

    The options for each menu item are shown in Table 1.



switch operator screen B

11. Select a **protocol** or series of **protocols** from the display of protocols by single clicking on each desired protocol (or drag and drop the protocol into the study queue).

    The study protocol for the current operators samples appears in the study queue window. Each time a protocol is clicked it is added to the study queue list.
12. Refer "Customizing Acquisition Parameters" on page 12 to change acquisition parameters.
13. Refer to "Removing a Protocol from a Composite Protocol in the Study Queue" on page 12 if a protocol is to be removed from the study queue.
14. Click on either the **Submit DayQ** or **Submit NightQ** to submit the study to the queue.

    The study can be submitted to either the DayQ or NightQ provided the time allocated for data acquisition during either the DayQ or NightQ is longer than total experiment time. If either the Submit DayQ or Submit NightQ button is grayed out, the total experiment time exceeds the time allocation for that queue. DayQ and NightQ time periods are set by the VnmrJ administrator using VnmrJ Admin functions (refer to the *VnmrJ System Administration* manual).
15. Add the next sample to the automation run.
16. Repeat the steps beginning at step 4 through step 15 for each additional sample.
17. Click on **Utilities**.
18. Select **Switch Operators…**

1.5 Customizing Acquisition Parameters

Must be done before the experiment is submitted to the queue.

1. Double click with the left mouse button on the time field for the experiment in the protocol (or click drag and drop the protocol onto the graphics canvas) – the text will change bold when it is selected.
2. Click on the **Acquire** tab.
3. Make adjustments to the acquisition as required.
4. Repeat the preceding steps for each experiment in the protocol.

If the sample is submitted and changes in the acquisition parameters are required, delete the sample from the queue, see “Removing a Sample from the Queue” on page 12.

1.6 Removing a Protocol from a Composite Protocol in the Study Queue

Must be done before the composite protocol associated with the current sample is submitted to the queue.

- Do the following to remove all protocols:

1. Clicking on the **Study Options** drop down menu button
2. Select **New Sample**.

   This will remove all the protocols for the sample and clear the study queue. A new study protocol can be created.

- Do the following to remove one protocol from the composite protocol:

  Drag and drop an individual protocol for a sample in to the trash can, see Figure 1.

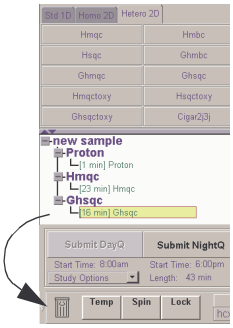


Figure 1. Removing a Protocol from a Composite Protocol

1.7 Removing a Sample from the Queue

The only users that can remove samples from the queue are the owner of the sample (operator that submitted the sample to the queue) and the VnmrJ Walkup account owner. The Walkup Operator can see the status and position in the sample tray of the samples from other operators (the status is indicated by a the dimmed color code) but cannot view protocols in the study queue that belong to other users.

Individual parts of an experimental protocol for a sample can not be removed, that entire sample must be removed from the queue, a new experimental protocol list created and the sample re-submitted to the queue.

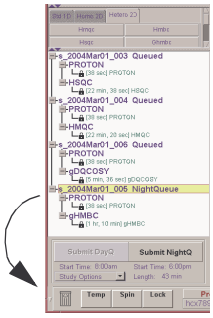


Figure 2. Removing a Sample from the Study Queue

Remove a sample from the queue as follows:

1. Click on sample - it will become high lighted in yellow.
2. Hold the left mouse button down.
3. Drag the sample to the trash can and release the mouse button, see Figure 2.

1.8 *VnmrJ* Walkup Operator Interface Controls and Regions

The *VnmrJ* Walkup Operator interface, see Figure 3, and Figure 4, has the following controls and regions:

- "VnmrJ Walkup Operator Interfaces" on page 14
- "Walkup Operator Menu Bar" on page 15
- "Tool Bar" on page 16
- "Locator" on page 16
- "Graphics Controls Bar" on page 17
- "Hardware Bar" on page 18
- "Function Bar" on page 19
- "Graphics Canvas" on page 17
- "VnmrJ Walkup Operator Start Panel," page 20
- "VnmrJ Walkup Operator Acquire Panel" on page 22
- "VnmrJ Walkup Operator Process Panel" on page 22

VnmrJ Walkup Operator Interfaces

Walkup Operator - No sample changer and traymax=0

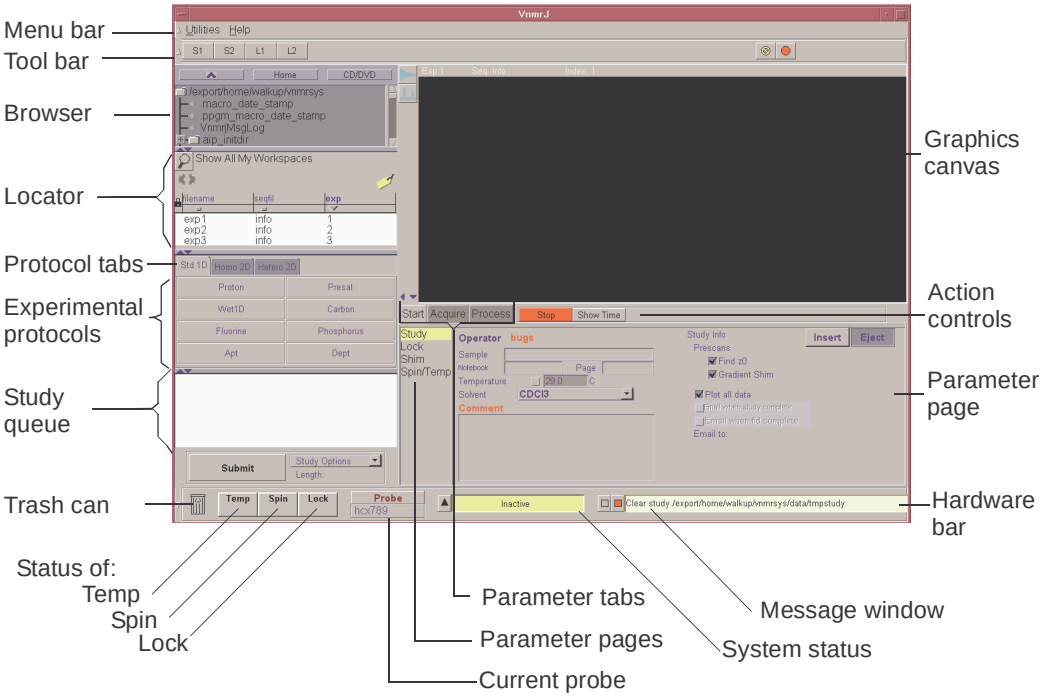


Figure 3. *VnmrJ* Walkup Operator Interface - No Sample changer

Walkup Operator - Sample changer and traymax=50

Toggle between data display canvas (shown in Figure 3) and sample position canvas (SMS 50 shown here as an example). The display will reflect the type of sample

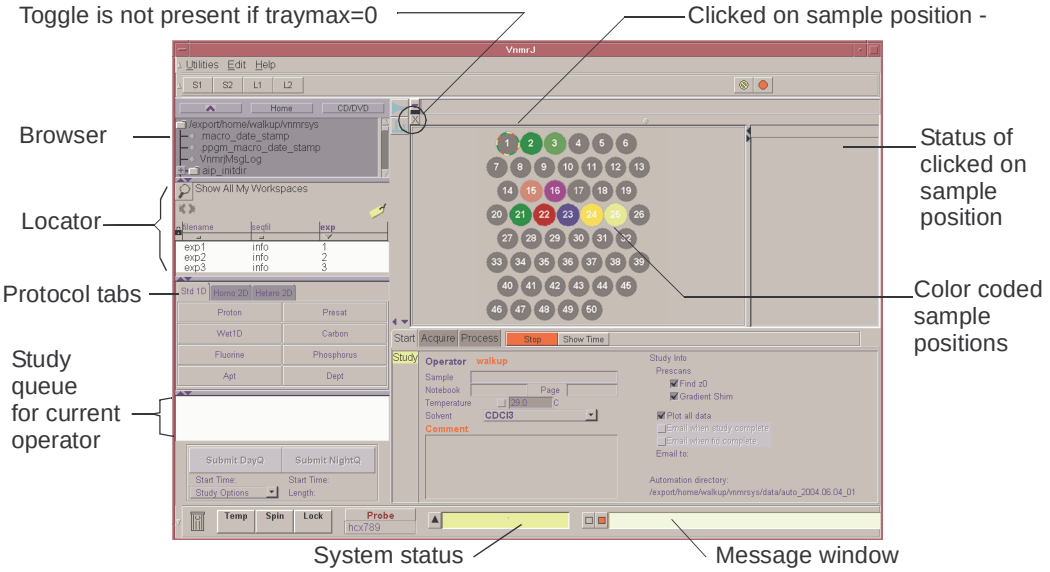
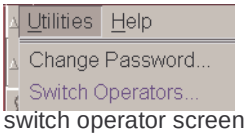


Figure 4. *VnmrJ* Walkup Operator Interface - Sample Changer operation

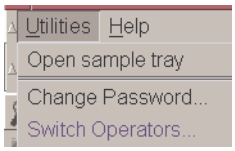
Walkup Operator Menu Bar

Menu bar selections are:

- "Utilities Menu," next
- "Help," next



switch operator screen A



switch operator screen B

Utilities Menu

Utilities Menu selections change based upon the switch operator screen, see "Switch Operators…" on page 15. The Walkup Operator menu bar choices are:

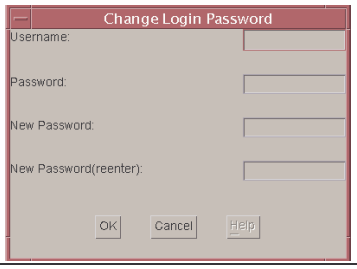
- "Open sample tray," next — Appears only for switch operator screen B.
- "Change Password …," next
- "Switch Operators…," next

Open sample tray

Changes the canvas to display the sample positions, see Figure 3 as an example.

Change Password …

Change Password...
Opens a window for changing Walkup operator (user) password. The walkup operator having a UNIX login account uses the same password for both the walkup and UNIX login. Changing the walkup password changes the UNIX login password.

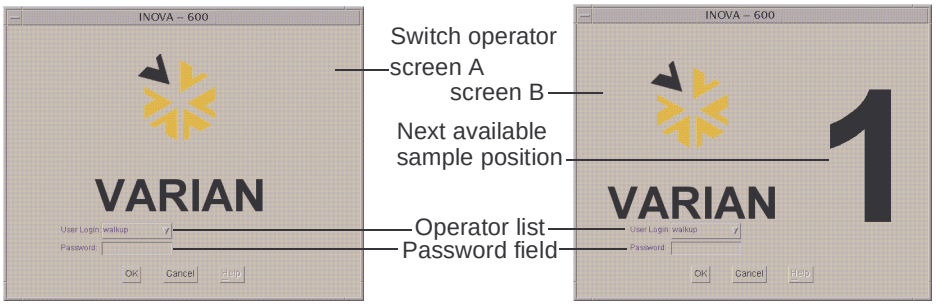


Switch Operators…

Opens a window for changing walkup operators without exiting VnmrJ. The appearance of the switch operator window will change depending upon the value of `traymax`.

If `traymax=0`,
Switch operator screen A is shown

If `traymax>0`,
Switch operator screen B is showr



Select an operator from the drop down menu or type the operator name in the field.

Select an operator from the drop down menu or type the operator name in the field. The operator name will be automatically completed as you type.

Click **OK** (or press enter after typing the password).

Help

Start HTML browser based online help.

Tool Bar

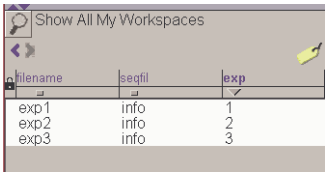
The tool bar is directly below the menu bar. These buttons provide quick access to common functions. The following tools are the default available in this tool bar:

Button	*Function*
	Save the current locator data sort display. To save the display, click on one of the buttons and press the mouse button for five seconds. To return to the saved display, click again on the button.
	Save the current screen layout (graphics, a parameter panel, locator sizes). To save the layout, click on one of the buttons and press the mouse button for five seconds. To return to the saved layout, click again on the button.
	Cancels commands.
	Stops acquisition.

Hiding and Showing the Tool Bar

To hide the tool bar, click the left mouse button on the arrowhead in the menu bar. The tool bar closes and the arrowhead changes to a rectangular box. To show the tool bar, click the left mouse button on the box.

Locator



The Locator provides access to data sets and experiments.

Clicking the magnifying glass with the left mouse button opens a menu of searches. Selecting one changes the *search sentence* (next to the magnifying glass). The results of the search are displayed in the list. Those items in the white part of the list satisfy the search sentence. Those in the gray part do not. For each item that is found by the search, three attributes are displayed. These correspond to the three columns in the list. Clicking on the attribute name at the top of the list with the left mouse button opens a menu of attribute choices.

Clicking on an item in the Locator list selects that item. That item can then be dragged to the graphic area or the parameter panel area to cause the appropriate action. For example, dragging a data set to the graphic canvas retrieves that data set into the current workspace (experiment) and displays the spectrum. Dragging a workspace to the graphic canvas causes that workspace (experiment) to be *joined* with the graphic area. Double-clicking on an item performs the same action as dragging the item to the graphics canvas.

Graphics Controls Bar

The graphics control bar is to the left of the graphics canvas. Use the buttons in the bar to control the interactive display in the graphics canvas. A full description of all the graphics control bars is provided in *VnmrJ Liquids NMR User Guide* manual.

Icon	*Description*
	Displays the FID
	Toggles the graphics control tool bar to interactive mode.
In the interactive mode the tool bar actions are:	
	Place cursors on screen - two if two bars are shown, one if one bar is shown on the icon
	Zoom out if (-) shown in magnifier, zoom in if (+) shown in magnifier
	Integral displays. This buttons change depending on the type of data that is displayed in the graphics canvas.
	Display scale
	Scan zoomed region
	Threshold adjustments, and other actions.
	Apply interactive phase correction
	Refresh the display
	Toggle back to the minimal tool bar

Graphics Canvas

This portion of VnmrJ, shown in Figure 5, is used to display and interact with graphic information.

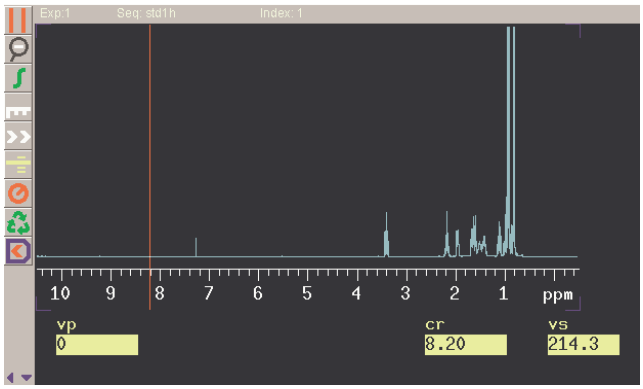
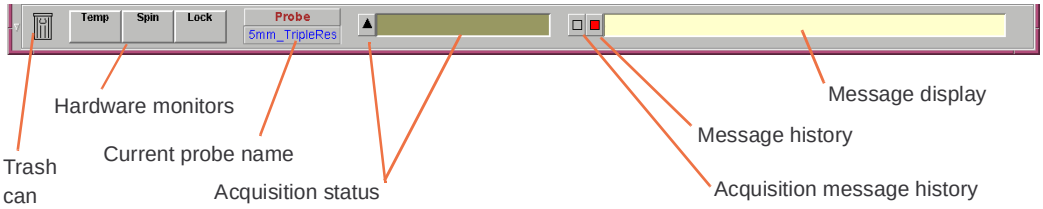


Figure 5. Graphics Canvas

- Resize the graphics canvas by clicking on the canvas boundary line with the left mouse (the cursor changes form) and dragging the line (e.g., between graphics and parameter pages or between graphics and Locator).
- Toggle the graphics canvas to show or hide the parameter templates area by clicking the small arrow between the graphics canvas and templates with the mouse button.

- Flip the parameter templates behind the graphics canvas without resizing the graphics canvas by clicking the small arrow with the middle mouse button.
- Toggle the parameter area to maximum height required to remove the parameter template scroll bar by clicking on the small arrow with the right mouse button.
- Toggle the graphics canvas to show or hide the Locator area by clicking the small arrow between the graphics canvas and Locator with the left mouse button.
- Flip the Locator area behind the graphics canvas without resizing the graphics canvas by clicking on the small arrow with the middle mouse button.
- Toggle the Locator area to maximum by clicking on the small arrow with the right mouse button.

Hardware Bar



The hardware bar contains the following:

- “Trash Can” on page 18
- “Hardware Monitors” on page 19
- “Probe Selection” on page 19
- “Acquisition Status Details” on page 19
- “Acquisition Status Display” on page 19
- “History of Acquisition Messages” on page 19
- “History of All Messages” on page 19
- “Message Display” on page 19

The right portion displays the current state of the acquisition system and system messages:

Hiding and Showing the Hardware Bar

To hide or show the hardware bar, click on the arrow icon  to the left of the trash can with the left mouse button.

Trash Can

Dragging an item to the trash can from the Locator or other area generally removes the item and adds it to the trash can.

Double-clicking on the trash can enables you to view items in the trash can area. In this mode, you can restore objects from the trash can by selecting them and then clicking the **Restore items** button. To exit this mode, double-click on the trash can.

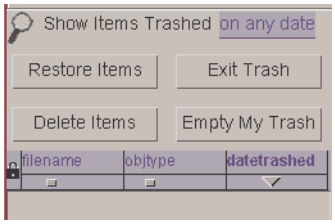


Figure 6. Trash Can Mode

CAUTION: **Data is deleted from the disk upon emptying the trash can.**

Hardware Monitors

When you click Temp, Spin, or Lock, a window appears with a line graph showing the history of the relative hardware function. To close the window, click the icon again.

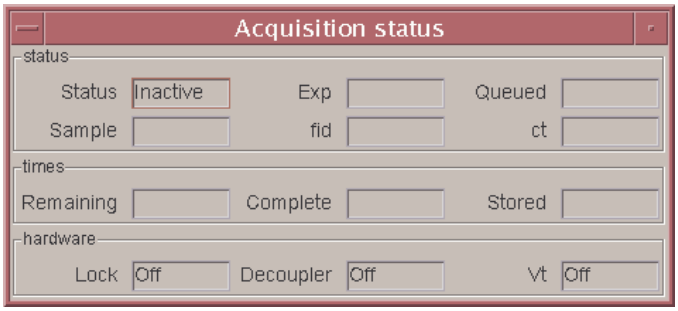
Button	*Description*
Temp	Shows a history of the sample temperature
Spin	Shows a history of the sample spin rate
Lock	Shows of a history of the sample lock level

Probe Selection

Probe selection is not active in the Walkup Operator interface. Access to probe selection and calibration is limited to the Walkup account owner.

Acquisition Status Details

To open a window showing acquisition status details, click on the  icon. To close the window, click on the icon again.



Acquisition Status Display

The acquisition status bar  is always visible in the hardware bar. During an acquisition, the bar shows the remaining experiment time as a thermometer display. Click the right mouse button inside the bar to change the displayed text.

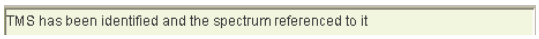
History of Acquisition Messages

To see a history of all acquisition messages, click on the  icon. To close the window, click on the icon again. Click the right mouse button within the scrolling message window to change the text view options.

History of All Messages

To see a history of all spectrometer messages, click on the  icon. To close the window, click on the icon again. Click the right mouse button within the scrolling message window to change the text view options.

Message Display

The message display 

shows the last message that occurred. Messages can be informational, a warning, or an error message.

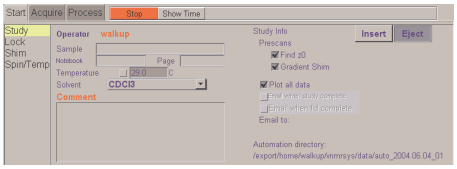
Function Bar

The function bar in the VnmrJ Walkup Operator interface display basic information about the current experiment.

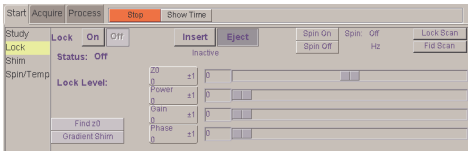
VnmrJ Walkup Operator Start Panel

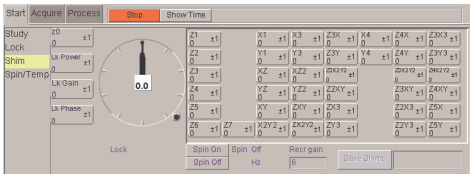
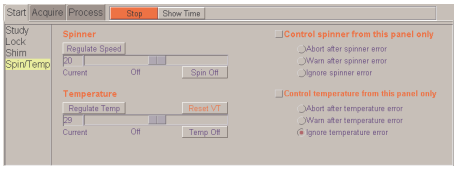
Depending upon the switch operator screen (sample change not active or present, switch operator screen A, or sample change present and in use, switch operator screen B) the pages that are displayed when the Start tab is selected will vary. These panels are defined by the default panel level settings. Refer to the *VnmrJ System Administration* manual for setting panel levels.

Panels Always Displayed

Description	*Panel*
Study page—All protocols have this page. Insert and Eject—present *only for switch operator screen A (traymax=0)* Sample field – enter sample information Notebook field – enter notebook information	
Solvent drop down menu	Select lock solvent
Place a check in box to enable Prescans options:	Find z0 — finds lock frequency Gradient Shim— adjust homogeneity using preset gradient shimming method
Plot all data option	Check box to enable
If E-mail is enabled, place a check in one or more of the operations:	Email when study complete or Email when fid complete

Panels Displayed When Sample Changer is Not Used (traymax=0)

Description	*Panel*
Lock page *Present only if for switch operator screen A (traymax=0)* Lock ON and Off buttons and spin status Insert and Eject sample buttons	
Spin On and Spin Off buttons	Turn sample spinning on or off
Lock Status and Lock Level	Value are reported in this window
Lock Scan button	Display interactive lock in display canvas
Fid Scan button	Display interactive fid in display canvas
Find z0 button	Finds lock frequency
Gradient Shim button	Adjust homogeneity using preset gradient shimming method
Manual lock Z0, Power, Gain, Phase controls:	Button (click or hold down) Right mouse button to increase left mouse button to decrease, middle mouse button to set increment. Entry field — enter a value Slider bar — move until desired value is displayed in the Entry field.

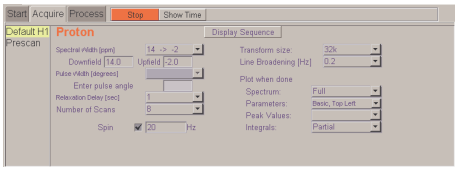
Description	*Panel*
Shim page *Present only if for switch operator screen A (traymax=0)* Lock Level meter display Spin On and Spin Off buttons to turn sample spinning on or off while adjusting shims	
Lock Recr gain	Enter new value and display current value
Button control for lock Z0, Power, Gain, Phase, and each configured shim	Button (click or hold down) Right mouse button to increase left mouse button to decrease, middle mouse button to set increment.
Save Shims button	Enter a name in the entry field to active the Save Shims button then click on the button to save the shims using the name in the entry field
Spin/Temp page *Present only if for switch operator screen A (traymax=0)* Spin On / Off button — turn sample spinning on or off during data acquisition Spin Entry field — enter a value	
Slider bar	Move until desired value is displayed in the Entry field
Regulate Speed button	Regulate spinning speed at set value
	Enable (checked box) disable (unchecked box) Control spinner from this panel only.
Radio button selection for spinner error handing	Abort after spinner error
	Warn after spinner error
	Ignore spinner error
	For more details see the *VnmrJ Liquids NMR* manual.
Temp On / Off button to turn sample temperature regulation on or off during data acquisition.	Spin Entry field — enter a value Slider bar — move until desired value is displayed in the Entry field.
Regulate Temp button	Regulate sample temperature at set value
	Enable (checked box) disable (unchecked box) Control temperature from this panel only
Radio button selection for VT error handing	Abort after temperature error
	Warn after temperature error
	Ignore temperature error
	For more details see the *VnmrJ Liquids NMR* manual.

VnmrJ Walkup Operator Acquire Panel

Panels Always Displayed

Description	*Panel*

Default page
The full name of this page and the controls on the page will change depending upon the experiment. The experiment, in this example, is a proton 1D, the default page label is Default H1, and the panel title is Proton.

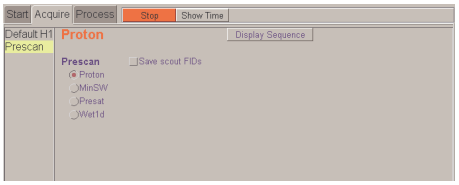


All default pages have a **Display Sequence** button. Click on this button to display the pulse sequence on the graphics canvas.

Acquisition parameters that are typically customized by an operator for a sample are accessed from the default page. The parameters presented on the page change according to the experiment. Parameters are customized by either entering a value in the field next to the parameter name or selecting a value from the drop down menu. The 1D protocols have a spin option – on by default. All 2D protocols have spinning turned off.

Some options must be enabled by checking a box. The options in the Default H1 page to spin the sample and plot the results must be enabled by placing a check in the box next to the option. The field next to the option and the fields associated with the options must also have values entered or selected. If no value is entered or no selection is made then that setting for the option is not used.

Prescan page — Proton only
Prescan option, Proton, Presat, Wet1D, and Save Scout FID, are presented as buttons or check boxes. Click or check the prescan options of choice.



Selecting MinSW results in the acquisition of an additional proton spectra to minimize the spectral width. The MinSW option is selected by default when any 2D experiment is selected.

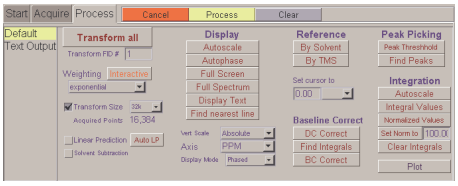
All prescan pages have a **Display Sequence** button. Click on this button to display the pulse sequence, associated with the selected experiment, on the graphics canvas.

VnmrJ Walkup Operator Process Panel

Panels Always Displayed

Description	*Panel*

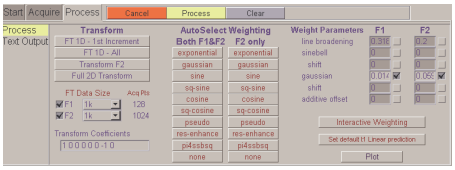
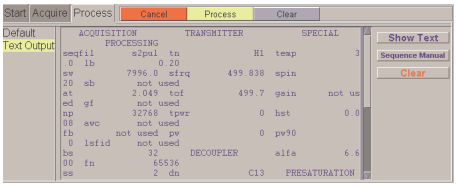
Defaults page — 1D Protocols Only
The **Process** button on the action bar processes the data (linear prediction, weighting, and any other selected processing and referencing options).



The **Transform all** button processes a weighted transform of the data. Processing and display choices are presented as push buttons. In some cases a drop down menu is present. The value or selection from this menu is applied when the associated button is clicked.

Value entry fields are associated with some buttons and the value in the field is applied when the data is processed.

Check boxes are associated with some buttons. The options are active if a check present in the check box.

Description	*Panel*
The graphics control bar functions work along with the choices on Process Defaults page, see "Graphics Controls Bar" on page 17 and the *VnmrJ Liquids NMR* manual.	
Process page — 2D Protocols Only All 2D processing options for the current 2D experiment are available on this page. The **Process** button on the action bar processes the data (linear prediction, weighting, and any other selected processing options). Refer to the *VnmrJ Liquids NMR Users Guide* for details on the application of the various processing options.	
Text Output page — all protocols Displays various text outputs. There are three buttons on this page: **Show Text** – show text associated with the file. **Sequence Manual** – online sequence manual. **Clear** – Clears the text window.	

Chapter 2. *VnmrJ* Walkup - Account Owner

Sections in this chapter:

- 2.1 “Overview of the VnmrJ Walkup Account Owner Interface,” this page
- 2.2 “Starting the VnmrJ Walkup Account Owner Interface,” page 26
- 2.3 “Setting up an Automation Run,” page 26
- 2.4 “VnmrJ Walkup Account Owner Interface Description,” page 29

This chapter provides a general overview of the *VnmrJ* Walkup Account Owner interface, features of the *VnmrJ* Walkup buttons, probe calibration, and administration tasks.

Selecting experimental protocols, all routine data acquisition procedures, and operations are the same for both the account owner and operator interfaces. These functions are covered in Chapter 1 “VnmrJ Walkup Operator,” page 5.

Related manuals:

- *VnmrJ System Administration*
- *VnmrJ Liquids NMR*
- *Sample Management Systems Installation*
- Relevant probe installation manuals.

2.1 Overview of the *VnmrJ Walkup* Account Owner Interface

The *VnmrJ* Walkup Account Owner interface (Figure 7) is designed to automate setting up, acquiring, processing, and plotting tasks for single sample walkup and sample changer operation. Both single sample walkup and sample changer operation function as automation runs and the data files are treated identically. All files are owned by the *VnmrJ* Walkup Account Owner. Parameters defining the behavior of the walkup session are setup using this interface, these parameters are not available to the *VnmrJ* Walkup Operator.

Both the walkup account owner and walkup operator interfaces access application types from a protocol type tab selection menu, see Table 2. Experimental protocols from each application type are entered into the study queue by selecting the application type and clicking on the desired protocol button. The 2D protocols add a proton type protocol (proton, presat, or wet1d with MinSW enabled) if a proton type protocol does not exist ahead of the first 2D protocol in a composite protocol (multiple protocols for a given sample). Protocols for 1D experiments not of the proton type can be added to the composite protocol at any time. All composite protocols are executed from the top down. The protocol is submitted to the acquisition queue when the operator clicks on the Submit (single sample mode) or either the Submit DayQ or Submit NightQ buttons (automated sample changer). Parameters are optimized for each protocol. Online help is provided for both the operator and account owner interfaces.

The *VnmrJ* Walkup interface provides limited access to acquisition parameters. The walkup interface, operations, calibrations, and customization are covered in this chapters.

Table 2. Experimental Protocols

Protocol Tab	*Protocol*	
Std 1D	Proton	Presat
	Wet1D	Carbon
	Fluorine	Phosphorus
	Apt	Dept
Homo 2D	Cosy	Dqcosy
	Noesy	Rosy
	Tocsy	Gcosy
	Gdqcosy	
Hetero 2D	Hmqc	Hmbc
	Hsqc	Ghmqc
	Ghmqc	Ghsqc
	Hmqctoxy	Hsqctoxy
	Ghmqctoxy	Cigar2j3j

2.2 Starting the *VnmrJ* Walkup Account Owner Interface

1. The walkup account owner must log in to UNIX.
2. Click on the *VnmrJ* icon on the CDE bar or open a UNIX terminal window and type `vnmrj` at the prompt.

   The Switch Operators screen, see "Switch Operators…" on page 39, appears after VnmrJ starts if there are operators assigned to the account in addition to the account owner.
3. Select (or type the operator name) the walkup account owner from the **Operator** drop down menu.
4. Enter the password in the **Password** field.
5. Click **OK** (or press enter).
6. Continue with "Setting up an Automation Run," next.

   All operation involving the walkup interface are treated as automation runs, even if the system is operating in the single sample mode with or without a sample changer.

2.3 Setting up an Automation Run

Required *VnmrJ* Hardware Administrator Actions

This is required if *VnmrJ* is not currently configured to use the sample changer.

1. All hardware, including sample changer type, must be configured by the system hardware administrator, typically vnmr1 and the *VnmrJ* Experimental Interface.
2. Login as the system hardware administrator (typically vnmr1).
3. Select **Utilities** from the main menu.

4. Select **System Settings**.
5. Click on **System config** button.
6. Click **OK**.
7. Configure the sample changer.
    a. Click on the **Sample Changer** drop down menu and select the sample changer type from the choices:

        — None
        — Carousel
        — SMS 50 Sample
        — SMS 100 Sample
        — VAST
        — NMS
        — LC-NMR
        —768 AS

    b. Click on the **Sample Changer Comm Port** drop down menu and select the sample changer type from the choices.

        — Not Used
        — Port A
        — Port B
        — Ethernet
8. Click on **Exit and Save**.
9. Select **Utilities** from the main menu.
10. Select **Exit** *VnmrJ*.

Walkup Account Owner

1. Set up the following defaults:
    - Lock, Shim, and Temperature– see **Study page** in “VnmrJ Walkup Operator Start Panel” on page 20.
    - Select a printer and plotter – see “Printers …” on page 37.
    - Verify that the parameter `traymax` is set to the tray size of the sample changer. If needed set the parameter to the correct value.
    - Setup directories for automatically saved data – see “Save data setup …” on page 33.
    - Data saving – see “System settings…” on page 30 and “System tab” on page 31
    - Data processing – see “System settings…” on page 30, “System tab” on page 31, and “Display/Plot tab” on page 32
2. Click on **Utilities** menu and select **New automation run…**

    Refer to “New automation run” on page 33 for more information.
3. Click on **Utilities** menu and select **Open sample tray…**

    Refer to “Open sample tray” on page 34 for more information.
4. Click on **Utilities** menu and select **Switch Operators…**. The switch operator banner will cover the *VnmrJ* interface. The next available sample changer position will be indicated by the number displayed on the switch operator banner. The general

operator can then enter the operator name and a password and *VnmrJ* will display the operator interface, see "VnmrJ Walkup Operator" on page 5.

Single Sample Operation – Sample Changer Not Used

Single sample operation applies to systems that do not have a sample changer or the sample changer is not used to insert the sample into the magnet.

1. Set up the following defaults:
   - Select a printer and plotter – see "Printers …" on page 37.
   - Setup directories for automatically saved data – see "Save data setup …" on page 33.
   - Data saving – see "System settings…" on page 30 and "System tab" on page 31
   - Data processing – see "System settings…" on page 30, "System tab" on page 31, and "Display/Plot tab" on page 32
2. Set the parameter `traymax`=0.
3. Click on **Utilities** menu and select **New automation run…**

   Refer to "New automation run" on page 33 for more information.
4. Click on **Utilities** menu and select **Switch Operators…**. The select operator banner will cover the *VnmrJ* interface. The general operator can then enter an operator name and password and *VnmrJ* will display the operator interface, see "VnmrJ Walkup Operator" on page 5.

2.4 *VnmrJ* Walkup Account Owner Interface Description

Walkup account owner interface, see Figure 7, functions are accessed from the menu bar and associated drop down and pop out menus. Functions unique to the walkup account owner interface are shown here.

All functions in common with the operator interface are described in "VnmrJ Walkup Operator Interface Controls and Regions" on page 13.

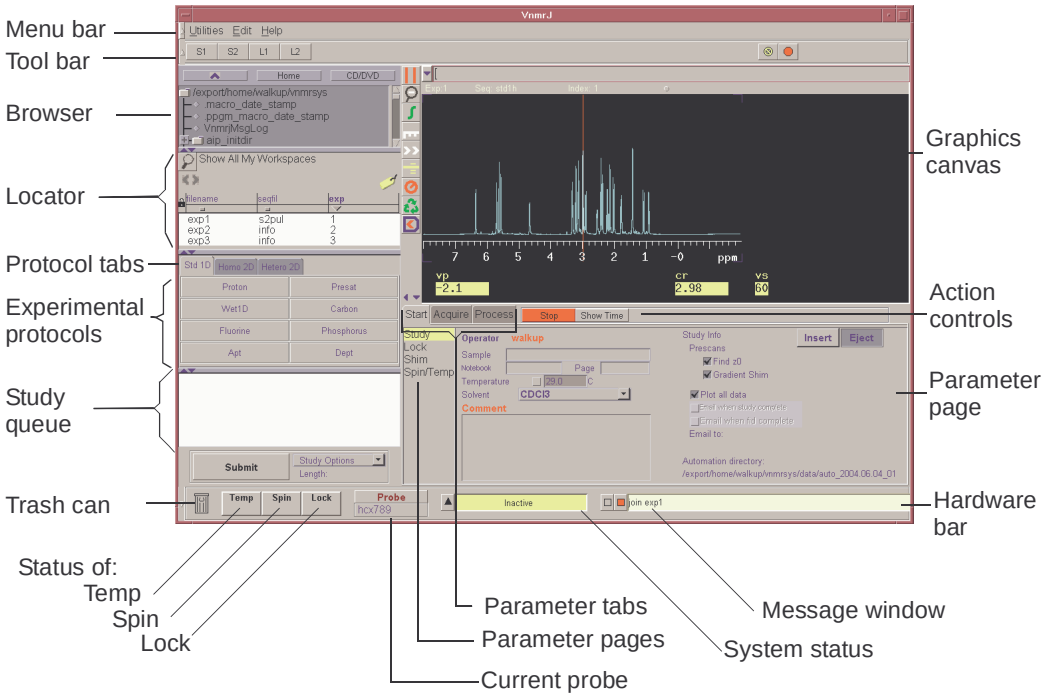


Figure 7. *VnmrJ* Walkup Account Owner Interface - Traymax=0

Menu Bar, Walkup Account Owner Interface

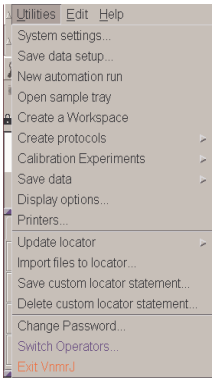
The four drop down menus :

- "Utilities Menu Selections" on page 30
- "Edit" on page 40
- "Help" on page 40

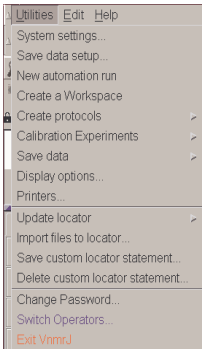
Utilities Menu Selections

Utilities drop down menu selections are determined by the value of the parameter `traymax`. The value of `traymax` will also affect the switch operator screens, see "Switch Operators…" on page 39. Determine or set the value of the parameter by accessing the command line, see "Advanced Function Bar" on page 40, and entering `traymax=?` to return the current value of `traymax` in the message display box. The Utilities Menu selections available in the account owner interface are:

- "System settings…" on page 30
- "Save data setup …" on page 33
- "New automation run" on page 33
- "Open sample tray," page 34
  Appears only if `traymax>0`
- "Create a Workspace" on page 34
- "Create protocols" on page 34
- "Calibration Experiments" on page 36
- "Display options …." on page 37
- "Printers …" on page 37
- "Change Password …" on page 39
- "Switch Operators…" on page 39
- "Exit VnmrJ" on page 40



Traymax>0



Traymax=0

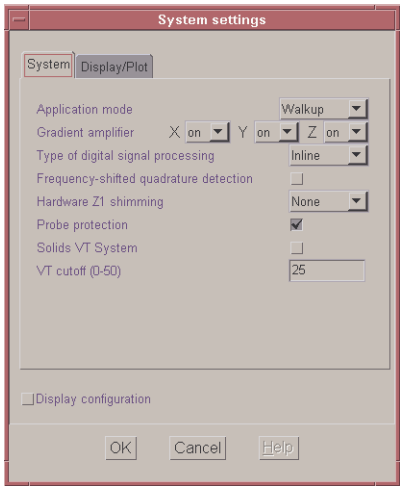
System settings…

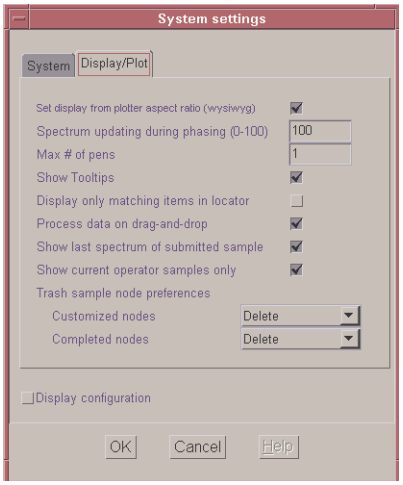
Opens the Systems settings window to access system, display, and plotting parameters. Click on the specific tab to open.

- "System tab" on page 31
- "Display/Plot tab" on page 32

All tabs have the following buttons and one check box:

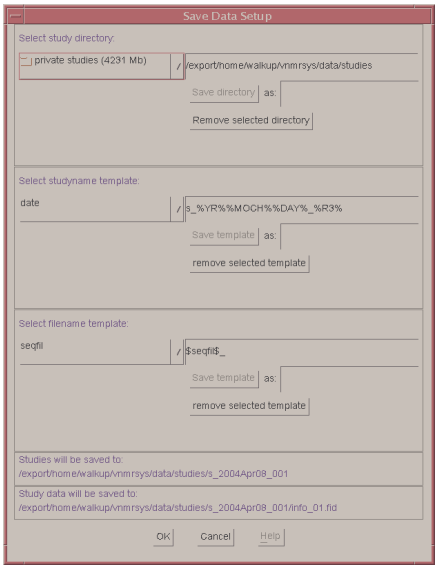
- OK — accept changes and close
- Cancel — close and make no changes
- Help— open online help

Item	*Descriptions*
System tab	
Application mode	Drop down menu selection of Standard (liquids) or Imaging mode for the Walkup interface.
Gradient amplifier	On/Off selection for each gradient axis that is installed.
Type of digital signal processing	Drop down menu, select one of the following choices: None— no digital signal processing Inline — software implemented digital signal processing Real time —hardware implemented digital signal processing — INOVA only
Frequency-shifted quadrature detection	Check box, enables frequency-shifted quadrature detection if the box is checked — INOVA only.
Hardware Z1 shimming	— INOVA only Drop down menu , select one of the following choices: None — no Z1 shimming Delay — Z1 shimming enabled during delay time Presat — Z1 shimming enabled during delay time proceeding presat
Probe protection	Enabled if the box is checked — INOVA only
Solids VT System	Enabled if the box is checked — INOVA only
VT cutoff (0 - 50)	Specify VT cutoff temperature, 25^{o}C recommended
Display configuration	Displays current system hardware configuration on the text page of the process panel for Inova systems and start a popup window for Mercury. Changes in the configuration can be made for Mercury systems only and remain active only while the current account owner is logged one and are not stored for later retrieval. Click on the **Process** tab and, if multiple pages are present, select **Text Output** page. If the current user is also the system hardware administrator, the system configuration window is displayed, refer to *VnmrJ System Administration* manual for more details. If the Walkup Account owner and the hardware system administrator are the same OS login, this box will appear as a button. Refer to *Vnmr Installation and Administration* for more information on Config and setting the user interface.

Item	*Descriptions*
Display/Plot tab	
Set display from plotter aspect ratio (wysiwyg)	Enabled (default) if the box is checked.
Spectrum updating during phasing (0-100)	Enter value in field (100 recommended).
Max # of pens	Number of plotter pens to use.
Show Tooltips	Enabled (default) if the box is checked.
Display only matching items in locator	Enabled if the box is checked.
Process data on drag-and-drop from locator	Enabled (default) if the box is checked.
Show las spectrum of submitted sample	Enabled (default) if the box is checked.
Show current operator samples only	Enabled (default) if the box is checked. All operators sample are shown in the study queue if this option is disabled.
Trash sample node preferences	Specify options: Customized nodes — Drop down menu selection: Delete Not allowed Skip Customized nodes — Drop down menu selection: Delete Not allowed Remove data

Save data setup …

Opens the save data setup window. These options determine how the data is handled for the current user's account. Click on the specific tab to open the menu.

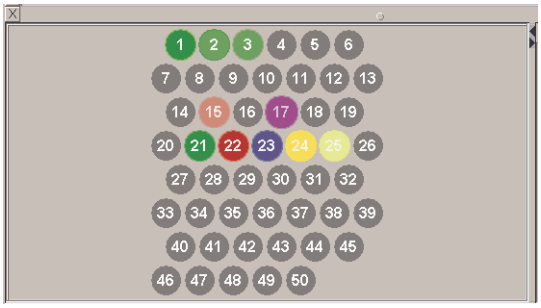
Item	*Description*
All tabs have the following buttons: OK — accept changes and close Cancel — close and make no changes Help— open online help	
Select study directory	Sets the globalauto parameter that determines where all automation runs are stored.
Select studyname template	Sets the sqname template parameter that determines where the sample studies are stored.
Select filename template	Sets the autoname template parameter that determines where all data is stored. To store data in the sample study,. autoname must begin with `$studyid$`, refer to the *VnmrJ Command and Parameter Reference* manual for more information.
Create a new directory or template	Enter change in the field next to the a menu and press Enter. Enter a name in the box next to **Save directory** or **Save template** button: and press return. Press **Save directory** or **Save template** button.
Deleting a directory or template	Select a directory or template from the drop down menu and press the **remove selected directory** or **remove selected template** button. Only user created directories and templates can be removed.

New automation run

Sets *VnmrJ* foreground and background operations for all walkup acquisitions. Creates an automation directory in the account owner's directory, within globalauto. Opens the sample tray.

Open sample tray

This option is displayed only when the parameter `traymaxy>0`.

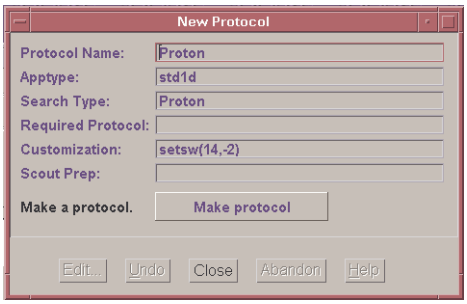
Item	*Description*
Available sample positions. The colors of the sample position indicate the status of that sample position as follows:	
Gray	Available
Green	Completed
Blue	Active
Yellow	Submitted - Day queue
Purple	Submitted - Night queue
Red	Error
Faded or grayed out colored sample position	Sample submitted by a operator other then the operator that is currently logged in to the walkup interface.

Create a Workspace

Create a Workspace— Creates a new work space within the current user account.

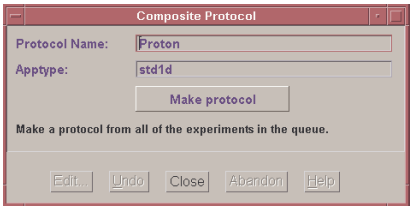
Create protocols

Make a New Protocol…

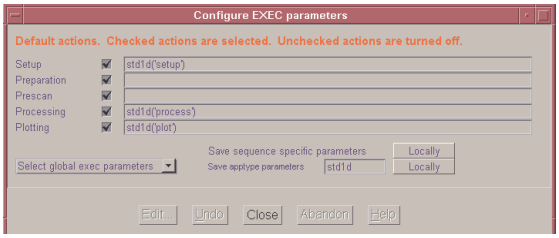
Item	*Description*
Make a New Protocol... opens a window for saving the current parameter set as a new protocol. A protocol consists of an XML file, parameter set, and the associated apptype macro.	
Protocol Name	Name for the new parameter set
Apptype	Group of protocols accessed from the Application Type Selection drop down menu, see Figure 7.
Search Type:	Specifies the type of protocol. This is the key word used when the study queue is searched.
Required Protocol	Specify the protocol that must precede the new protocol for proper setup of the experiment.

Item	*Description*
Customization	Customize any parameter used in the standard protocol to meet the requirements of the new protocol
Scout Prep	Specify the scout macro executed before the main protocol
Make protocol button	Click this button to make the new protocol.
Update protocol button	Click this button to update an existing protocol.

Make a Composite Protocol…

Item	*Description*
Make a Composite Protocol... opens a window for saving the current set of protocols in the new sample area of Study Queue area as a composite protocol. A protocol consists of an XML file, parameter set, and the associated apptype macro.	
Protocol Name	Enter a name for the protocol
Apptype	Specify the group of like protocols with which the new protocol will be grouped.
Make protocol button	Click this button to make the new protocol.

Configure EXEC parameters…

Item	*Description*
Configure EXEC Parameters opens the window shown and provides access to the parameters used to control the generic acquire, prep, process, plot, and prescan functions	

The EXEC parameters concept provides setup, preparation, prescan, processing, and plotting customization based on the type of NMR data. This selection is based on the value of the `apptype` parameter.
This panel allows you to view and/or to set the EXEC parameters.

Check boxes	Enables the action as the default action
Setup	Specify the setup action with any required arguments
Preparation	Specify the preparation action and requirements
Prescan	Specify the prescan action and requirements
Processing	Specify the processing actions with any required arguments
Plotting	Specify the plotting actions with any required arguments
Select global exec parameters	Drop down menu of exec parameters that are available to all users (global: `/vnmr/execpars`).

Item	Description
Save sequence specific parameters - button	Save the sequence specific parameters locally (as indicated on the button)
Save apptype parameters - field	Specify the application type to apply the new EXEC parameters
Save apptype parameters -button	Save the apptype parameters locally (as indicated on the button)

Calibration Experiments

Calibrate Probe

Item	Description
	 Opens a window for running a series of experiments to calibrate the probe. Refer to the *VnmrJ System Administration* manual for instructions on running calibration experiments.

Set Up Gradient Shimming

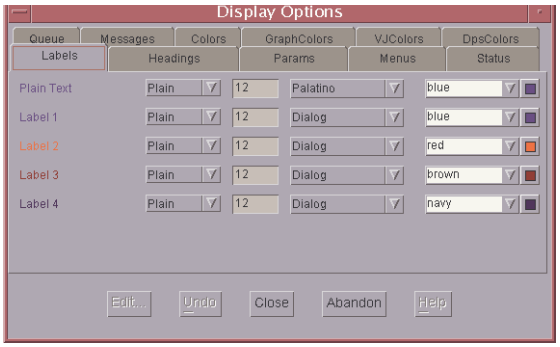
Item	Description
Loads the pulse sequence and panels for making a shim map for gradient shimming.	

Save data

Item	Description
	
Save current fid	Saves the current FID with a filename constructed from the `svfdir` and `svfname` parameters.
Save process as…	Saves reprocessing to given record.

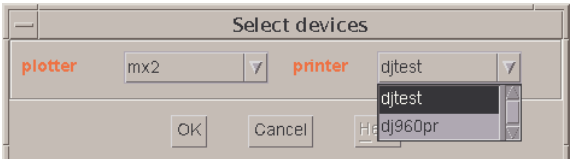
Display options ….

Display options...
Opens a window for setting symbolic colors and fonts in the interface.
Select the tab and color options to customize the user environment

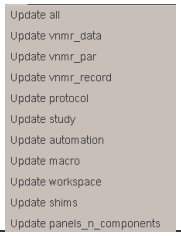


Printers …

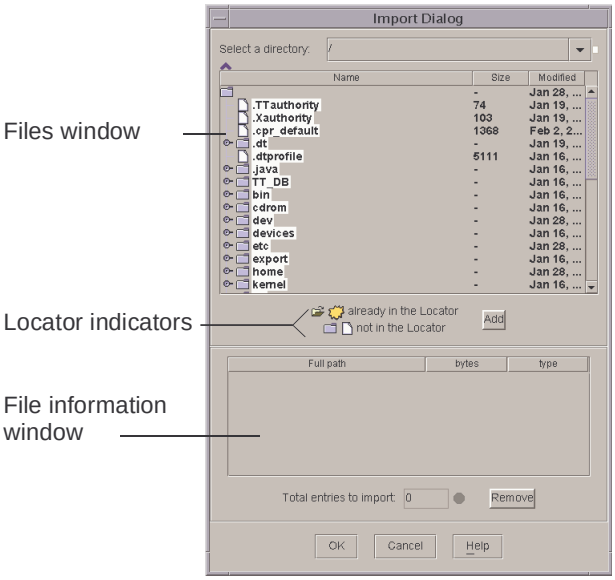
Printers...
Opens a window for setting printers and plotters from previously defined printers and plotters. For information about connecting printers, refer to *VnmrJ Administration* manual.



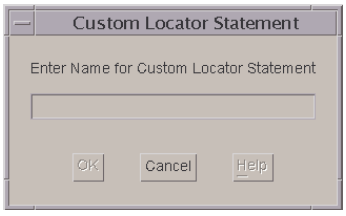
Update locator…

Item	***Description***	
Opens a submenu that provides choices for updating the different parts of the Locator.	Click on any item in the menu to update a single item or click on Update all to update all listed items.	

Import files to locator…

Item	*Description*
Import files to locator… opens a window for importing files to the locator	
Select a Directory	Drop down menu of directories - select a directory by clicking on it or enter the full path beginning at root (/).
Files window	Select a file by clicking on the file
Locator indicators	Icons appearing next to files and folders to indicate if the file or folder is currently in the locator or is not in the locator.
File information window	Displays the full path, size and type of file to be added to the locator
Total entries to import	Number of items in the file information window to be imported when the OK button is clicked
Remove - button	Click on a file or folder and click on Remove to remove the item from the list of items to be imported into the locator
OK - button	Adds selected items to locator and closes the window
Cancel	Exits the window - no items are added to the locator

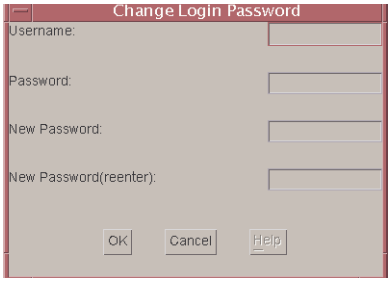
Save customer locator statement…

Item	*Description*
	Opens a window for saving the current locator view. 
Enter Name for Custom Locator Statement	Enter statement in the field, click on OK to save, Cancel to exit this window.

Delete custom locator statement…

Item	*Description*	
Delete custom locator statement… opens a window for deleting custom locator statements		
Items listed in window	Click on item to select Click on Delete to remove the item from the list	

Change Password …

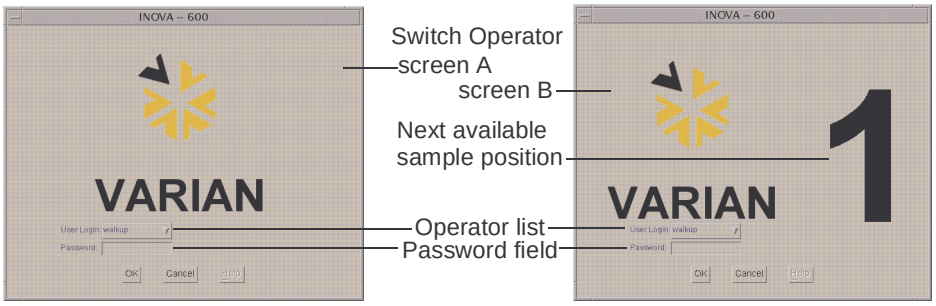
Change Password... Opens a window for changing Walkup operator (user) passwords. If the walkup operator has a UNIX login account, that password is also changed.	

Switch Operators…

Opens a window for changing walkup operators without exiting *VnmrJ*. The appearance of the switch operator window will change depending upon the value of `traymax`.

- If `traymax=0`,
  Switch operator Screen A is shown

If `traymax>0`,
Switch operator screen B is show



Select an operator from the drop down menu or type the operator name in the field.

Enter a password in the password field

*Click **OK** (or press enter after typing the password)*

Exit VnmrJ

Exit VnmrJ	exits VnmrJ.

Edit

The Edit menu selections available *VnmrJ Walkup* account owner interface are:

- “Tool bar…,” next
- “Pulse Sequence,” next
- “Parameter Panels…,” page 40

Tool bar…

Item	***Description***
Tool Bar…	Opens the tool bar editing tool
Refer to the *VnmrJ System Administration* manual for details on how to use this tool.	

Pulse Sequence

Item	***Description***
Pulse Sequence…	Opens the Spin Cad tool
Refer to the *Spin CAD* manual for details on how to use this tool.	

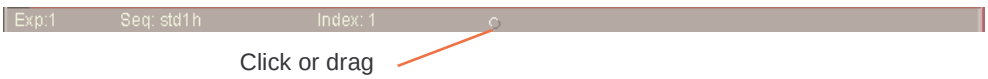
Parameter Panels…

Item	***Description***
Parameter Panels…	Opens the parameter panel editing tool.
Refer to the *VnmrJ System Administration* manual for details on how to use this tool.	

Help

Starts on line help

Advanced Function Bar



Dragging down the button in the advanced function bar opens a command entry field and a text output field. Open or close the field by clicking once on the button, which restores it to its most recent view. Any command or macro can be entered into this command window. Error and information messages are displayed in the scrolling text window above the command line in addition to the hardware bar. Command history can be shown if you click on the arrow with the left mouse button. Select a command from the command history by highlighting it and pressing **Return** to execute it.

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