VnmrJ Walkup

Varian, Inc. NMR Systems
With VnmrJ 2.2 C / 2.3A
Pub. No. 01-999342-00, Rev. D 1008

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A 1006 initial release for VnmrJ 2.2A
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Varian NMR spectrometer systems running VnmrJ 2.2C / 2.3A software

Technical contributors: Frits Vosman, He Liu, Bayard Fetler, Glenn Sullivan

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Chapter 1. *VnmrJ* Walkup - Account Administrator Functions

Sections in this chapter:

This chapter provides a general overview of the VnmrJ Walkup Account Owner interface, VnmrJ Walkup features, probe calibration (refer to *VnmrJ Installation and Administration* manual for procedures), and account administration tasks. The operating system login account owner is the Walkup administrator.

Procedures for selecting experimental protocols, routine data acquisition, and operations are the same for both the account administrator and operator interfaces. These functions are covered in Chapter 2 “VnmrJ Walkup Operation,” page 19.

Related manuals:

- *VnmrJ Installation and Administration*
- *NMR Spectroscopy User Guide*
- *Sample Management Systems Installation*
- Relevant probe installation manuals.

1.1 Walkup Account Owner and Administrator

The VnmrJ Walkup Account Administrator interface (see Figure 1 through Figure 3) is designed for setting the account functions and options, data acquisition and processing, automation, and plotting tasks. Full access to all menus and functions is provided to the walkup account administrator. All menu and tool bar functions are described in “Walkup Menus and Controls” on page 35.

The VnmrJ Walkup Account Administrator owns of all the files created by operators using the account. Parameters defining the behavior of the walkup session are setup using this interface. Parameters panels and menu options available to the VnmrJ Walkup Operator are determined by the user profile and operator panel level. The default operator user profile is AllLiquids and the default panel level is 10. Account owners have the same default user profile and a default panel level of 30. Refer to “Panel Levels and User Profiles” on page 76 for details on panel levels. Both the operator profile and panel level are set by the VnmrJ Administrator, see *VnmrJ Installation and Administration*.

All operations involving the walkup interface using the Study Queue are treated as automation runs, even if the system does not have or is not using a sample handler. Online help is provided for both the operator and account administrator interfaces.

Walkup Account Owner Interface - Modes

No Sample Handler or Sample Handler Not Used

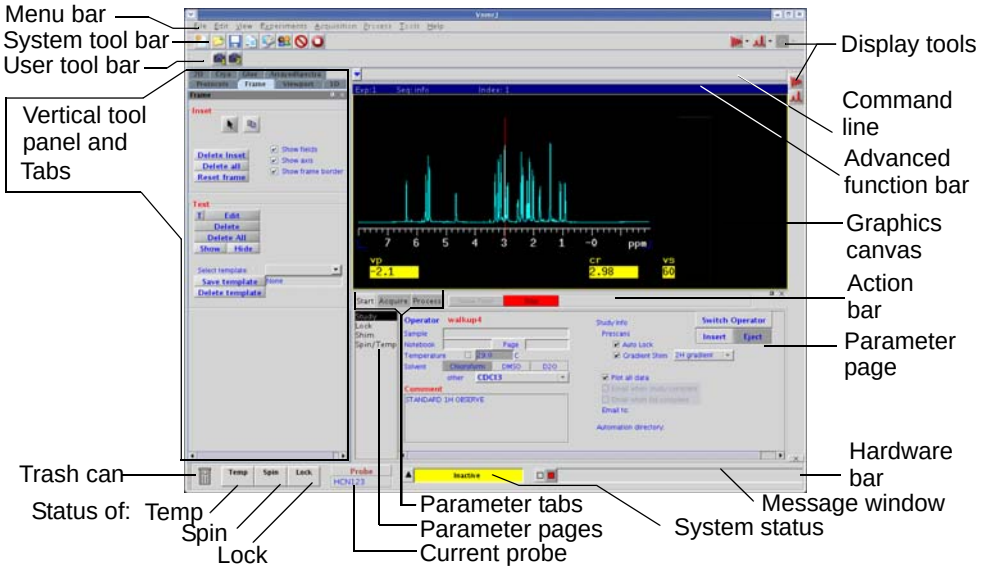


Figure 1. *VnmrJ* Walkup Account Administrator Interface - No Sample Handler

Sample Handler Mode

Toggle between data display canvas (see in Figure 1) and sample position canvas (shown here)

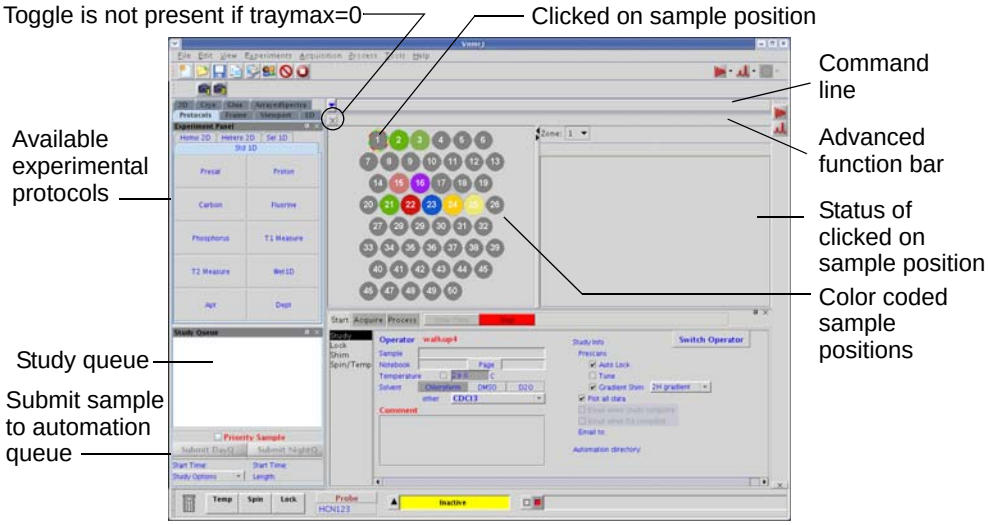


Figure 2. *VnmrJ* Walkup Account Administrator Interface - Sample Handler

Direct Acquisition Mode

The study queue is grayed out (not available or active) and the user selects experiments from the **Experiment** dropdown menu on the main menu.

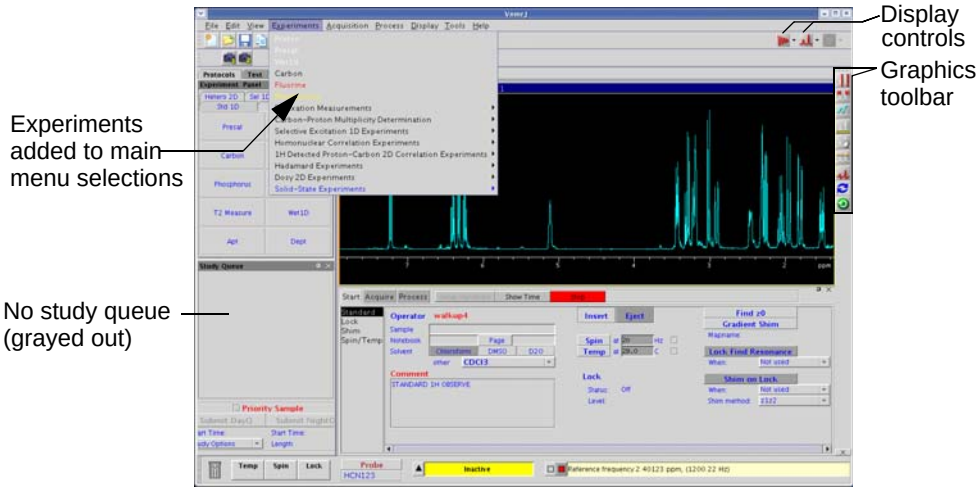


Figure 3. Walkup - Direct Acquisition Mode

Interface Controls

Control	*Description*
Menu bar	At the top of the VnmrJ interface — dropdown menu to access utilities and options usually independent of experiments, see "Main Menu Bar" on page 35.
System tool bar	Below the menu bar — buttons providing access to common functions, see "System Tool Bar" on page 51.
User tool bar	Below the system menu bar — location for user customizable functions, see "User Tool Bar" on page 52.

Vertical Panel Tabs		*Description*
Protocols		
	Experiment panel	Contains a collection of experimental protocols used to set up an experiment. Click on or drag and drop an experimental protocol to place a protocol into the queue, see "Walkup Experiment Protocol Selection" on page 34.
	Study Queue	Used to build a queue of protocols to be applied to a sample or samples. Click on or drag and drop an experimental protocol to place a protocol into the queue. Not used in direct acquisition mode, see "Using Direct Acquisition" on page 27.
Frame		Inset text and spectrum frames tools, see "Frame Panel" on page 66.

Vertical Panel Tabs	*Description*
Viewport	Tools for inset spectrum frames, see “Setting the Number of Available Viewports” on page 60.
Arrayed	Tools for working with arrayed data sets, see “Arrayed Spectra and FIDs” on page 74.
1D	Tools for working with 1D data sets, see “1D” on page 71.
2D	Tools for working with 2D data sets, see “2D” on page 73.

Control	*Description*
Advanced Function bar	Located below the user toolbar — displays basic information about the current experiment and plotting status. If a sample changer is present or being used, a toggle button is presented at the left end of the bar to toggle between the graphics canvas and the sample position canvas, see “Advanced Function Bar” on page 51.
Graphics canvas	Data is displayed on the graphics canvas, see “Graphics Canvas” on page 53.
Sample position canvas	Select position(s) to apply selected experimental protocols which have been placed in the study queue or to display information on a particular position in the sample status window if a sample changer is present and being used.
Graphics toolbar	Icons used to manipulate data in the graphics canvas, see “Graphics Toolbars” on page 54. Icons displayed on the graphics control bar depend on the protocol currently in use and the manipulations occurring in the graphics area. The graphics toolbar can now be dragged.
Action bar	Buttons to performs indicated actions when pressed. The action controls displayed depend on which parameter tab is currently being displayed.
Parameter tabs	The content of the panels associated with the Parameter tabs is determined by the protocol selected. Parameter pages are organized into three categories: Start— display parameter pages associated to the sample Acquire— display parameter pages associated with acquisition Process— access pages associated with processing.
Parameter pages	Parameter pages provide a place for setting parameters and values applied to the study and protocol. Their content depends on the current protocol.
Hardware bar	Displays the current state of the system and any system messages, see “Hardware Bar” on page 58.
Trash can	Study queue or locator data is placed there for disposal. While editing parameter pages and the tool bar, items from these areas can also be placed in the trash can for removal. Items, with the exception of locator data, placed in the Trash can not be recovered. Data from the locator can be retrieved from the Trash can, see “Trash Can” on page 59.

1.2 Using the Walkup Account Administrator Interface

1. Log on to the operating systems as the owner of the Walkup Account (the owner of the account is also the account administrator).
2. Click on the ***VnmrJ*** icon or open a terminal window and enter **`vnmrj`** at the prompt. The Switch Operators screen appears after VnmrJ starts if there are operators assigned to the account in addition to the account administrator. Do the following:
   a. Select (or type the operator name) the walkup account administrator from the **Operator** dropdown menu.
   b. Enter the password in the **Password** field.
   c. Click **OK** (or press enter).

The walkup account administrator interface and operator interface use the default user profile, AllLiquids, giving both interfaces the same experimental functionality, see Chapter 2 “VnmrJ Walkup Operation,” page 19. Command line operation, number of panels, and automation control are the principle differences between the interfaces, see “Walkup Account Owner and Administrator” on page 7. The profile, AllSolids, provides the operator with access to all the solids related experiments in the Experimental panel and removes all the liquids related experiments.

Refer to “Panel Levels and User Profiles” on page 76 for panel level control and the user profile section in the *VnmrJ Installation and Administration* manual. The account administrator has control of the option to provide all or any sub set of the parameters panels and protocols to all account operators.

Refer to the *VnmrJ Installation and Administration* manual for creating and assigning Walkup account operators.

1.3 Walkup Account Administrator Functions

Location of Operator Data

The walkup account administrator (owner) defines where operator data is saved using the Save Data Setup window.

1. Click on **File.**
2. Select **Save data setup…**, see “Setting Up Study Data Directories and Templates” on page 12 for changing and setting directories and templates.

The Save data setup window sets the following parameters:

Directory/Template	*Parameter*
Automation directory	`globalauto`
Study name template	`sqname`
File name template	`autoname`

The `walkup` macro runs and sets `autodir` from `globalauto`, plus the date (`autodir=globalauto +'/auto_' + $date`), when the account administrator starts a new automation run. Parameters such as `operator` are not substituted in the `walkup` macro. Refer to the *Command and Parameter Reference* manual for a more detailed description of these parameters and their arguments.

A user adds protocols and presses the **Submit** button. The **Submit** button uses `autodir+'/'sqname` to create the study name for each sample and set `sqdir` (full path to the study) and `studyid` (a string parameter relative to autodir). The parameters `sqdir` and `studyid` cannot be changed by the user.

Data is saved during an automation run using the `autoname` template. The directory path in the `autoname` template is relative to `autodir`, unless it is redefined as absolute path. The default values of `autoname` in the Save data setup window all start with `$studyid$`, which puts the data within the `studyid` directory. This works whether `studyid` is a relative or absolute path.

Setting Up Study Data Directories and Templates

Use the Save Data Setup window, see Figure 4, to set up directories and templates for saving data.

1. Click on **File**.
2. Select **Save data setup …**
3. Review the current directory and templates selections and do one of the following:
   - Click on the **Cancel** button and continue with “Setting Up for Automated Sample Handling” on page 15.
   - Continue with “Setting Up or Removing a Data Directory” on page 12.

Setting Up or Removing a Data Directory

The automation run data is saved using the controls in the directory set up section of the Save Data Setup window, see Figure 4, using the following procedures as required:

Use an Existing Directory

1. Click on the **Named directories** menu button.
2. Select a named directory from the dropdown menu of named directories.
3. Continue with “Setting Up or Removing a Study Name Template” on page 13.

Creating and Saving a New Data Directory

1. Modify the existing directory path shown in **Current directory** field or enter a new full path in the **Current directory** field.
2. Press **Enter**.

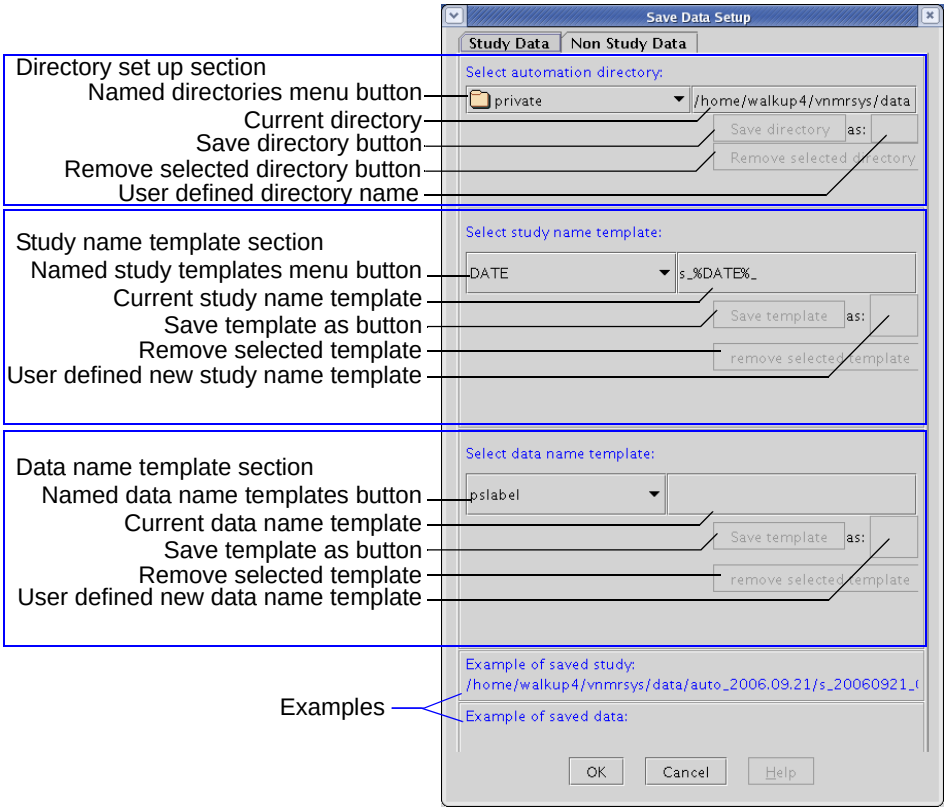


Figure 4. Save Data Setup Window

The Current directory field and Save Directory button are not active until the Enter key is pressed.

3. Enter a name for the new data directory path in the **User defined directory name** field.
4. Click on the **Save directory** button.
5. Continue with "Setting Up or Removing a Study Name Template" on page 13.

Removing a Saved Data Directory

1. Click on the **Named directories** menu button.
2. Select a **named directory** from the dropdown menu of named directories.
3. Click on the **Remove selected directory** button.
4. Continue with "Setting Up or Removing a Study Name Template" on page 13.

Setting Up or Removing a Study Name Template

Automation run data is named using the template set up in the Study Name Template of the Save Data Setup window, see Figure 4, using the following procedures as required:

Use an Existing Study Name Template

1. Click on the **Named study templates** menu button.
2. Select a **named directory** from the dropdown menu of named directories.

3. Continue with "Setting Up for Automated Sample Handling" on page 15.

Creating and Saving a New Study Name Template

1. Modify the existing directory path shown in **Current named study template** field or enter a new study template in the **Current named study template** field. Refer to "Location of Operator Data" on page 11 for a details about the parameter related to this template and the *Command and Parameter Reference* manual.
2. Press **Enter**.

   The Current named study template field and Save templates button are not active until the Enter key is pressed.
3. Enter a name for the new data template in the **User defined new study template name** field.
4. Click on the **Save template** button.
5. Continue with "Setting Up for Automated Sample Handling" on page 15.

Removing a Saved Study Name Template

1. Click on the **Named study templates** menu button.
2. Select a **named directory** from the dropdown menu of named directories.
3. Click on the **Remove selected template** button.

Setting Up Required Parameters

Required parameters are a set of parameters that must be set before submitting a sample, or before an acquisition. Required parameters used to define the sample are; `samplename`, `notebook`, `page`, etc. Empty string parameters are not allowed. Real parameters can not be zero. Do the following to set up required parameters:

Enter an arrayed string for `reqparlist` containing the list of required parameters separated by commas on the command line, e.g.

```
reqparlist='samplename','notebook','page'
```

Enable required parameter checking by:

Entering `reqparcheck='y'` on the command line.

Disable required parameter checking by:

Entering `reqparcheck='n'`on the command line.

Setting Applications Directories

Operator access and permissions to change applications directories are set by the VnmrJ administrator, refer to the *VnmrJ Installation and Administration* manual for instructions on setting permission. The Applications directory interface, Figure 5, is accessible to the operator if permissions are granted by the administrator.

Applications Directories

VnmrJ application directories (`appdir`) can include subdirectories: `templates`, `maclib`, `manual`, `menulib`, `parlib`, `probes`, `seqlib`, `shims`, `tablib`, `shapelib`, `gshimlib`, and `mollib`. These are directories that VnmrJ uses during its normal operation. The `exists` command searches for other files and directories in the

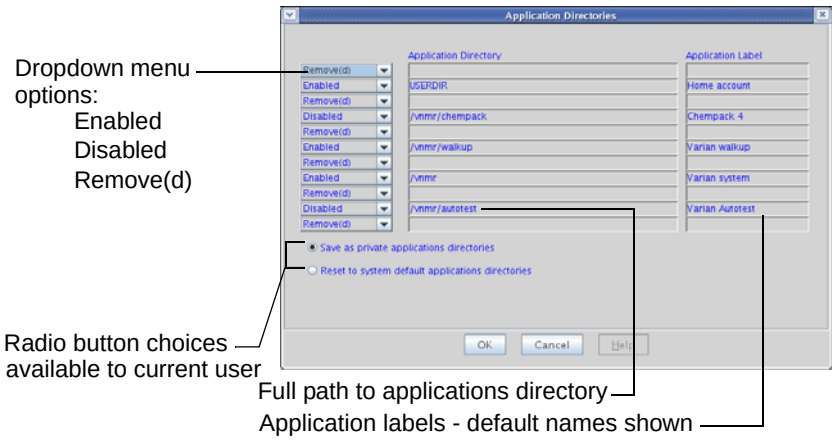


Figure 5. Applications Directory Interface

applications directories and provides users with flexibility to customize their applications. VnmrJ does not look for `expN` directories, `global`, `psg`, `psglib`, or other files or directories.

The `appdir` is an ordered list of paths to search for a specific item. Applications directories may be updated at any time. Operator specific applications directories are set when a new operator logs into the walkup interface.

Applications Directory Interfaces

Applications directory interface, Figure 5, is available if the VnmrJ administrator has set permission to allow the operator to edit the applications path. The editor for applications directories is available to an operator with this permission. This editor popup has entry boxes for defining the paths, labels, and active/nonactive field for the applications directories. Operator with system write permissions can set applications directories for all users. Operator that do not have system write permissions can edit only their private applications directories.

Setting Up for Automated Sample Handling

Set up for automated Sample Handling mode:

1. Set up the following defaults:
   - Lock, Shim, and Temperature – see **Study page** in “VnmrJ Walkup Tabs and Panels” on page 78.
   - Select a **printer** and **plotter** from the File menu option.
   - Verify that the parameter `traymax` is set to the tray size of the sample changer.

     If needed set the parameter to the correct value by setting the hardware as (if the currently logged in walkup account owner is vnmr1 it is not necessary to log out), see “Setting Traymax to the Correct Value or Disabling the Sample Handler” on page 16.
   - Setup directories for saving data during an automation run.
   - Set data saving options.
2. Configure ProTune for systems equipped with AutoX probes and ProTune.

   Refer to “Configuring ProTune” on page 18 for instructions.

3. Click on **File** menu and select **New automation run…**

   Opens the sample tray and creates an automation directory in the account administrator's directory.

4. Click on **File** on the main 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 resizable switch operator banner. The general operator can then enter the operator name and a password and *VnmrJ* will display the operator interface, see "Operator Log In and Log Out" on page 20.

Setting Traymax to the Correct Value or Disabling the Sample Handler

1. Log **out**.
2. Log **in** as the hardware administrator, typically vnmr1.
3. Click on **Edit** on the main menu.
4. Select **System stettings**.
5. Click on **System Config**.
6. Do one of the following:
   - Select the **sample changer** from the dropdown menu.
   - Select none from the sample changer dropdown menu.
7. Select the **sample changer port,** if a sample changer is used, from the dropdown menu.
8. Click **OK**.
9. Log **out**.
10. Log **in** as the **walkup account owner**.

Setting Up Sample Changer Not Used Mode

Single-sample mode 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 directories for automatically saved data (refer to "Setting Up Study Data Directories and Templates" on page 12).
2. Set printer and plotter defaults.
3. Do one of the following:
   - Systems with a sample changer — Set the parameters `traymax`=0 and `loc='n'` or disable the sample changer in the hardware config, see "Setting Traymax to the Correct Value or Disabling the Sample Handler" on page 16 and continue with step 4.
   - Systems without a sample changer — continue with step 4.
4. Configure ProTune for systems equipped with AutoX probes and ProTune.

   Refer to "Configuring ProTune" on page 18 for instructions.

5. Click on **File** menu and select **New automation run…**
6. Click on **File** menu and select **Switch Operators…**.

The resizable switch 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 “Operator Log In and Log Out” on page 20.

Automated Sample Handling vs Manual Single-Sample Mode

The Walkup account administrator can switch between automated sample handling and single-sample mode by setting the `traymax` parameter on the command line.

Mode	*traymax value*	*Sample Handler Selected in Config*	*When/Why/What*
Automated sample handling	`traymax>0` The `traymax` default is the maximum number of sample positions for the sample handler system specified in config: Carousel=9 SMS 50=50 SMS 100=100 768AS=768 VAST=96 LC-NMR=1	`Yes`	A sample changer is installed and is used to insert samples. Set `traymax` to a value up to the number of positions available, see “Setting Traymax to the Correct Value or Disabling the Sample Handler” on page 16. The interface displays non-interactive panels at login and when switching operators. The panel level by VnmrJ Admin as required for the account administrator, see “Panel Levels and User Profiles” on page 76. Enter `traymax?` on the command line to return the current value of `traymax` in the message display box. The panel level and other operator specific parameters are set after switching operators.
Single-Sample	`traymax=0` Set by the account administrator to override the default value set by config.	`Yes`	Samples are inserted directly into the magnet and the sample handler, though present, is not used. Operator panel level determines the panels displayed, see “Panel Levels and User Profiles” on page 76, and are not interactive while switching operators.
Single-Sample	`traymax=0`	`No`	A sample handler is not installed. Operator panel level determines the panels displayed, see “Panel Levels and User Profiles” on page 76 and are not interactive while switching operators. Operator interface panellevel is set by the VnmrJ administrator, see *VnmrJ Installation and Administration* for more information.

Configuring ProTune

- Applies to systems equipped with ProTune and AutoX probes.
- The system must be properly configured and ProTune calibrated. Refer to the *VnmrJ Installation and System Administration* manual for configuring the software and calibrating ProTune.

1. Log in and start VnmrJ as the walkup account administrator (or switch operators to the walkup account administrator).
2. Click on the **Tools** button on the main menu bar.
3. Select **Probe Tuning**.
4. Select **Auto tune setup …** from the pop-out menu.

   The Autotune Setup window is displayed.

5. Specify when ProTune automatically tunes the probe.

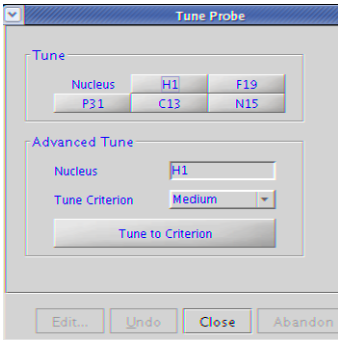
   Placing a check in the box next to each change in condition results in automatically tuning the probe. Click the **Reset** button to return to the default conditions.

6. Check the box next to **Do not tune** if no tuning by walkup operators is allowed.
7. Selecting any option aside from **Do not tune** places a check box on the study panel and selecting **Do not tune** removes the check box from the study panel.

   Gradient shimming will start after each auto tune event if both auto tune and gradient shimming are selected.

8. Click on **Close** to save the changes and exit the Setup Autotune window.

Running ProTune



1. Click on the **Tools** button on the main menu bar.
2. Select **Tune Probe…** from the popout menu.
3. Click on a **nucleus button** next to Nucleus in the Tune region to set the tune frequency.
4. Select a criteria from the dropdown menu next to Tune Criterion in the Advanced Tune section:

   Coarse – within 5 percent of optimum `pw`

   Medium – within 2 percent of optimum `pw`

   Fine – within 0.5 percent of optimum `pw`

5. The criteria function is available to the walkup operator depending on the panellevel setting.
6. Click on **Tune to Criterion** button.
7. Click on **Close** to save the changes and exit the Tune Probe window.

Chapter 2. VnmrJ Walkup Operation

Sections in this chapter:

2.1 VnmrJ Walkup Operator Overview

The walkup account owner has set up the system for walkup operation and clicked on the switch user icon. The walkup login screen is displayed. VnmrJ is running and is waiting for an operator assigned to the account to login.

The tools, rights, protocols, and content of the menu and panel selections available to the user working within the Walkup Operator environment are determined by the value of the parameter `panellevel` and the `user profile` set up by the system administrator using the VnmrJ Admin interface. Operators have a default user profile of AllLiquids and `panellevel=10` and no advanced function bar. The user profile, panel level, and the presence of the advanced function bar, “Advanced Function Bar” on page 51, are set by the VnmrJ administrator, see *VnmrJ Installation and Administration* manual. The walkup account owner can set the panel levels from the command line of the advance function bar for the current login session, see “Panel Levels and User Profiles” on page 76. Panel level defaults to the panel level set for the operator through the VnmrJ Adm interface the next time the account owner initiates a login. This chapter describes the default walkup operator interface that provides the user with:

- Protocols are grouped by type, see Table 1on page 34, and accessed by clicking on a protocol tab.
- Optimized parameters for all experimental protocols.
- Selection of multiple experimental protocols for a given sample.
- Submission of the sample to the acquisition study queue by clicking on the Submit button (single sample mode) or either the DayQ or NightQ buttons (sample changer) (the StudyQ mode only).
- Walkup Operator Login and Logout (switch operator) functions.

2.2 Starting an Experiment

Running experiments differs slightly between no sample handler and sample handler modes, follow the appropriate procedure for system configuration.

- "Operator Log In and Log Out" on page 20
- "No Sample Handler Mode" on page 21
- "Sample Handling Mode" on page 22
- "Running Solids Experiments" on page 25

Running an experiment requires the following:

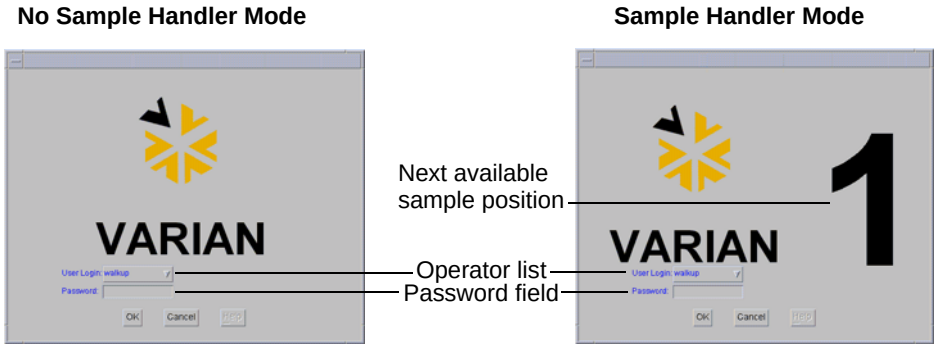
- Defaults are set up by the VnmrJ Walkup account administrator and will be used by each operator. Preset defaults include shimming, locking, saving data, and plotting but are not limited to these defaults.
- The VnmrJ Walkup Operator interface is active and the login screen is currently displayed.
- A new automation run is started.
- The sample tube is filled to the correct height (approximately 750 µl).

Operator Log In and Log Out

The operator Log In window is re-sizable and appears only if an operator is assigned to the account.

- "Log In" on page 20
- "Log Out" on page 20

The Walkup operator logs in using the VnmrJ Walkup login screen. If a sample handler is active, the login screen shows the next available sample position.



Log In

1. Select an **operator** from the dropdown menu or enter an operator name in the field.
2. Enter the **password** for the operator.
3. Click **OK** or press **Enter**.

Log Out

1. Click **File** menu.

2. Select **Switch Operators**. The login screen appears.

No Sample Handler Mode

The interface shown in these procedures is the operator interface defaults; user profile of AllLiquids, `panellevel=10`, and no advanced function command line.

Operators set up with panellevel>29, see "Panel Levels and User Profiles" on page 76, have more panel choices. Operators with a user profile of BasicLiquids will have fewer menu choices.

See "Walkup Menus and Controls" on page 35 for a list of menu and function bar options.

1. **Login** as described in "Operator Log In and Log Out," page 20.
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. Optional – Fill in the information in the **Sample**, **Notebook**, and **Page** fields.
8. Select the sample lock solvent from the solvent buttons or dropdown **Solvent** menu.
9. Place checks in any of the following options: **Find z0**, **Gradient Shim**, and **Tune** (if available) 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. Click on **Tools**, select one of the following:

      Auto Tune Probe

      Manual Tune Probe
   c. Optimize the magnetic field homogeneity by either clicking on **Gradient shim** button or selecting the **Shim** page and manually adjusting the shims.

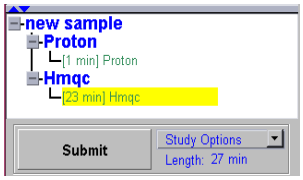
   Refer to the *NMR Spectroscopy User Guide* manual for instructions on locking, fid or lock shimming, and gradient shimming.
10. Place a check in the **Plot all data** to enable this option upon completion of the study or fid acquisition.

    Select either or both of the **Email** options for notification upon completion if email is enabled.
11. Place a check in the temperature **check box** and enter a temperature in the **temperature field** to control the sample temperature during the experiment.

Leave the box unchecked if no temperature regulation is required.

12. Select a **Protocol Type** tab.

13. Select a **protocol** or series of **protocols** from the protocols list by single clicking on the protocol or dragging and dropping the it into the study queue.



A protocol contains one or more NMR experiments. The protocols 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.

Some protocols run two experiments. The Hsqc protocol is an example. Selecting the Hsqc protocol automatically adds a required Proton protocol to the study queue. Adding another protocol that requires Proton as part of the protocol, such as Cosy, uses the Proton protocol brought in by Hsqc and adds the Cosy experiment without adding an additional Proton experiment. The composite protocol of; Proton, Hsqc, and Cosy, is created in the study queue. Required parameters from the Proton experiment are incorporated into both the Hsqc and Cosy experiments without operator intervention.

The Proton protocol is a member of the proton type protocol. Other members of this set are Presat and Wet1D. When Presat or Wet1D is the first protocol, it is used as the required experiment by protocols requiring running a Proton protocol first.

Refer to "Removing a Protocol from the Study Queue" on page 27 to remove a protocol from the Study Queue.

14. Adjust acquisition parameters as necessary as described in "Customizing Acquisition Parameters" on page 26.
15. Click the **Submit** button to add the study to the queue.
16. A pop-up window is displayed if required parameters are enabled, see "Setting Up Required Parameters" on page 14.
    a. Enter the required parameters. All fields must have an entry, either a text string or a value.
    b. Click **OK** after all the fields are filled.
17. Log out as described in "Operator Log In and Log Out" on page 20.

Sample Handling Mode

The interface shown in these procedures is the default operator interface; user profile of AllLiquids, `panellevel=10`, and no advanced function command line.

Operators set up with panellevel>29 see "Panel Levels and User Profiles" on page 76, have more choices.

The full list of menu and function bar options are provided in "Walkup Menus and Controls" on page 35.

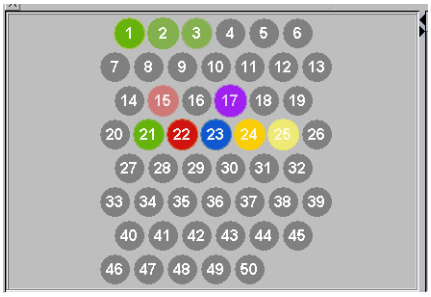
1. Place the sample in the spinner and adjust the position of the sample in the spinner.

2. Place the sample and spinner in the location shown on the log in screen (or another available **gray sample position** location).
3. **Login** as described in "Operator Log In and Log Out," page 20.
4. Click on the **gray sample position** corresponding to the placement of the sample in step 2.

   All sample positions are available if the option for sample reuse is selected, see *VnmrJ Installation and Administration* manual.

   The number displayed on the login window is the next available position but any 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 another operator, not the current operator.

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

Item	***Description***
Sample positions. The colors of the sample position indicate the status of that sample position as follows:	
Gray	Empty
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 then the currently logged in operator to the walkup interface.

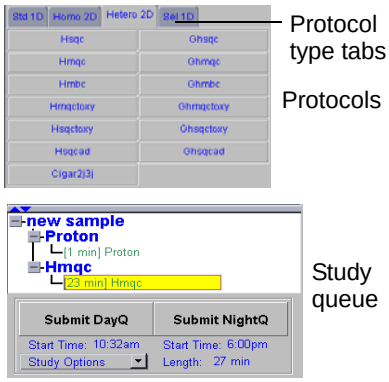
5. Select the sample lock solvent from the **Solvent** buttons.
6. Place checks in any of the following options: **Find z0**, **Gradient Shim**, and **Tune** (if available) to enable these options.
7. Place a check in the **Plot all data** to enable this option upon completion of the study or fid acquisition.
8. Optional – Fill in the information in the **Sample**, **Notebook**, and **Page** fields.

If E-mail is enabled, either or both of the **Email** options for notification upon completion.

9. Select a **Protocol Type** tab.

10. 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). A protocol contains one or more NMR experiments.

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



    Some protocols run two experiments. Hsqc protocol is an example. Selecting the Hsqc protocol automatically adds a required Proton protocol to the study queue. Adding another protocol that requires Proton as part of the protocol, such as Cosy, uses the Proton protocol brought in by Hsqc and adds the Cosy experiment without adding an additional Proton experiment. The composite protocol of; Proton, Hsqc, and Cosy, is created in the study queue. Required parameters from the Proton experiment are incorporated into both the Hsqc and Cosy experiments without any operator intervention.

    The Proton protocol is a member of the proton type protocol. Other members of this set are Presat and Wet1D. When Presat or Wet1D is the first protocol, it is used as the required experiment by protocols requiring running a Proton protocol first.

    Refer to "Removing a Protocol from the Study Queue" on page 27 to remove a protocol from the Study Queue.

11. Adjust acquisition parameters as necessary as described in "Customizing Acquisition Parameters" on page 26.

12. Click on either the **Submit DayQ** or **Submit NightQ** to submit the sample to the queue.

    The sample 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 DayQ or 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 Installation and Administration* manual).

13. A pop-up window is displayed if required parameters are enabled, see "Setting Up Required Parameters" on page 14.

    a. Enter the required parameters. All fields must have an entry, either a text string or a value.

    b. Click **OK** after all the fields are filled.

14. Add the next sample to the automation run.

15. Repeat the steps beginning at step 4 through step 14 for each additional sample.

16. Log out as described in "Operator Log In and Log Out" on page 20.

Running Solids Experiments

All of the Solids sequences use a new set of consistent parameter definitions. These experiments can be set up from either set-up macros or protocols on the command line, set up from the Experiments pull-down menu, Figure 6, (Study Q turned off) or by drag-and-drop from protocols in the Experiment Panel, Figure 7, (requires AllSolids user profile). Refer to the solids chapter of the *NMR Spectroscopy User Guide* for instructions on running solids experiments.

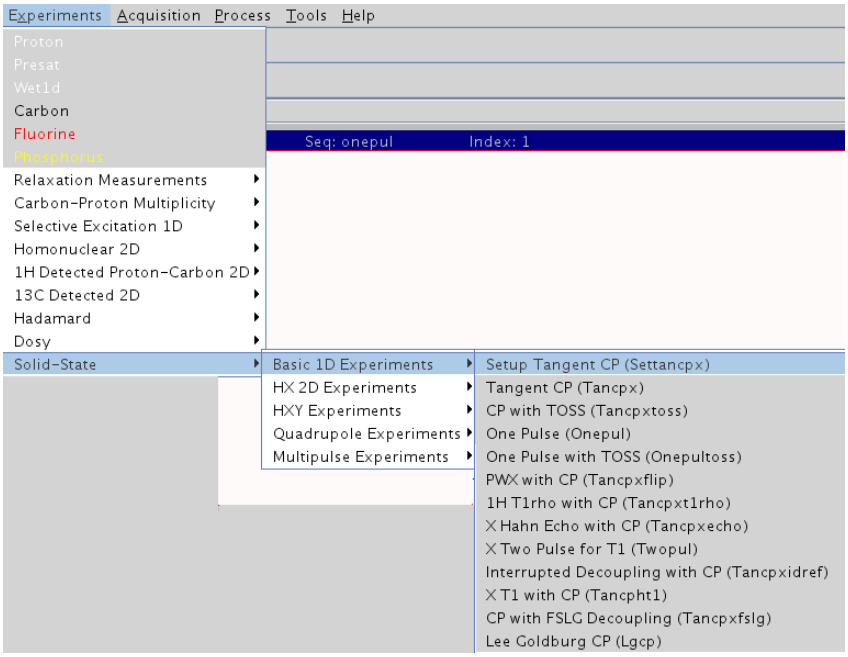


Figure 6. Solids Experiments and Menus

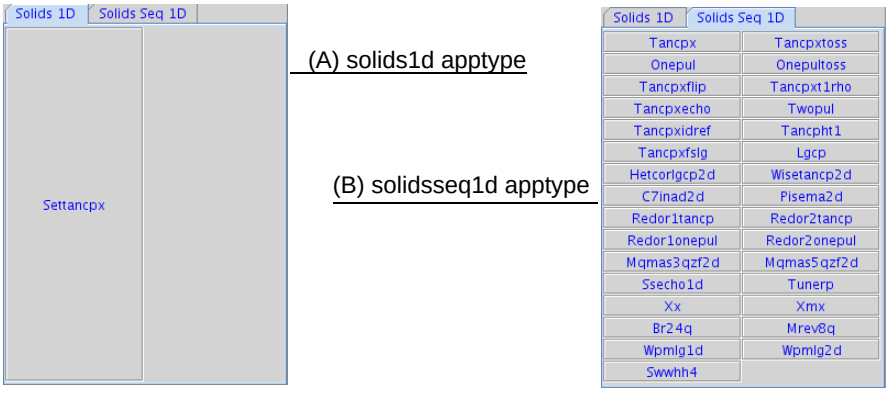


Figure 7. Solids Protocols Tabs

2.3 Working with Protocols in the Study Queue

Adding a Protocol to a Queued Sample

Adding protocols to a queued sample in either the DayQ or NightQ must be done prior to the sample becoming active.

1. Click on a protocol with the left mouse button.
2. Drag the protocol to sample position in the study queue.
3. Drop the protocol into the study queue.

   The protocol is added to the list and run if there is time (there is a maximum time limit per sample) or skipped if there is not enough time to run the experiment.
4. See "Customizing Acquisition Parameters" on page 26 to edit a skipped protocol.

Customizing Acquisition Parameters

Customizing acquisition parameters must be done either before the sample is submitted to the queue or before the sample becomes active.

1. Double click with the left mouse button on the time field for the experiment in the protocol – the text will change bold when it is selected and the parameter pages for the experiment are displayed.
2. Click on the **Acquire** tab.
3. Make adjustments to the acquisition parameters as required.
4. Do one of the following:
   - Samples not yet submitted — continue with step 5
   - Samples submitted to the queue — Click on either Submit DayQ or Submit NightQ button. The protocol is run if there is time (there is a maximum time limit per sample) or skipped it there is not enough time to run the experiment.
5. Repeat the preceding steps for each experiment in the study as required.

Moving a Protocol within the Study Queue

Moving a protocol in queued sample in either the DayQ or NightQ must be done prior to the sample becoming active and is limited to protocols within a sample. A protocol can not be moved from sample to sample.

1. Click on a protocol with the left mouse button.
2. Drag the protocol to the new position within the sample's protocol list.

Removing a Protocol from the Study Queue

A protocol must be removed either before the sample is submitted to the queue or before the sample becomes active. Remove a protocol using either of the following procedures:

- Remove an individual protocol within a protocol list for a sample as follows.
  Drag and drop an individual protocol for a sample into the trash can.
- Remove all the protocols before a sample is submitted as follows:
  Click on the **Study Options** dropdown menu button and select **New Sample**.

Removing a Sample from the Study Queue

Users and the VnmrJ Walkup account administrator can remove samples from the queue.The Walkup Operator can see the status and position of the samples from other operators (the status is indicated by a dimmed color code).

The default user profile allows any visible protocol can be edited by other users. Refer to the *VnmrJ Installation and Administration* manual for more details on operator profiles.

Remove a sample from the queue as follows:

1. Click on the **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 8.

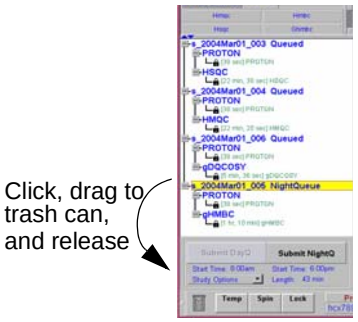


Figure 8. Removing a Sample from the Study Queue

2.4 Using Direct Acquisition

Only applicable if the Use Study Queue option in the Acquisition Menu is available.

Sample Handler Not Used or Not Present

Running a Protocol in Foreground on the Current Sample

Pause an Active Study Queue to Run a Protocol in Foreground on the current sample as follows:

1. Click on the **Acquisition** menu and select **Pause Automation**.

   The current acquisition will pause at the end of its current acquisition. An acquisition in the Study Queue may be `findz0`, automatic tuning, gradient shimming, autolocking and automatic gain adjustment in addition to the acquisition of experimental data itself. Clicking on Pause Automation may pause at the end any of these acquisitions.

2. Wait until the status bar reads **Idle**.
3. Click on the **Acquisition** menu and **remove** the check from the **Use Study Queue** check box.

   The Acquisition menu is populated with a selection of experiments for both liquids and solids. The Study Queue is grayed out.
4. Select an experiment using either of the following methods:
   - Using the **Protocols** vertical panel:

   a. Select a the **Protocols** tab from the vertical panel tabs.

   a. Click on a **Protocol Type** type on the Experiment Panel.

   b. Select a **Protocol**.

      This retrieves an experimental protocol into the foreground.

   c. Continue with step 5.

   - Using **Experiments** on the main menu.

   a. Click on **Experiments** on the main menu.

   b. Select a **protocol** or **protocol type** from the drop down list.

   c. Select a **protocol** from the **protocol type** if a pop-out is presented.

      This retrieves an experimental protocol into the foreground.

   d. Continue with step 5.
5. Adjust the acquisition parameters as necessary.
6. Click on the **Acquisition** menu and select **Acquire Data**, **Acquire and WFT** or **Acquire and Process**.
7. A pop-up window is displayed if required parameters are enabled, see “Setting Up Required Parameters” on page 14.

   a. Enter the required parameters. All fields must have an entry, either a text string or a value.

   b. Click **OK** after all the fields are filled.
8. When acquisition is complete, click on **File** menu and select **Save As…**
9. Choose a directory and provide a **File Name**, then press **Save**.
10. Click on the **Acquisition** menu and **check Use Study Queue**.
11. Click on the **Acquisition** menu and select **Resume Automation**.

Running a Protocol in Foreground on a Different Sample

Pause an Active Study Queue to run a protocol in foreground on a different sample then resume the study queue and automation with the original sample as follows:

1. Click on the **Acquisition** menu and select **Pause Automation**.

   The current acquisition will pause at the end of its current acquisition. An acquisition in the Study Queue may be `findz0`, automatic tuning, gradient shimming, autolocking and automatic gain adjustment in addition to the acquisition of experimental data itself. Clicking on Pause Automation may pause at the end any of these acquisitions.
2. Wait until the status bar reads **Idle**.

3. Click on the **Acquisition** menu and remove the check from the **Use Study Queue** check box.

   The Acquisition menu will be populated with a few more options and an Experiments menu choice will appear between the Edit and Acquisition menu choices.

4. Press **Eject** in the **Study** page under the **Start Tab**.

5. Follow the procedure in section 2.2 “Starting an Experiment,” page 20 under “No Sample Handler Mode” on page 21 step 4 through step 12.

6. Select an experiment using either of the following methods:

   - Using the **Protocols** vertical panel:

   a. Select a the **Protocols** tab from the vertical panel tabs.

   a. Click on a **Protocol Type** type on the Experiment Panel.

   b. Select a **Protocol**.

      This retrieves an experimental protocol into the foreground.

   c. Continue with step 5.

   - Using **Experiments** on the main menu.

   a. Click on **Experiments** on the main menu.

   b. Select a **protocol** or **protocol type** from the drop down list.

   c. Select a **protocol** from the **protocol type** if a pop-out is presented.

      This retrieves an experimental protocol into the foreground.

   d. Continue with step 5.

7. Adjust the acquisition parameters as necessary.

8. Click on the **Acquisition** menu and select **Acquire Data**, **Acquire and WFT** or **Acquire and Process** or click on the **Acquire** button on the action bar.

9. A pop-up window is displayed if required parameters are enabled, see “Setting Up Required Parameters” on page 14.

   a. Enter the required parameters. All fields must have an entry, either a text string or a value.

   b. Click **OK** after all the fields are filled.

10. When acquisition is complete, click on **File** menu and select **Save As…**

11. Choose a directory and provide a **File Name**, then press **Save**.

12. Press **Eject** in the **Study** page under the **Study Tab** and return the previous sample to the magnet.

    The lock, shimming, and tuning, may have changed and need adjusting for the sample. Refer to the *NMR Spectroscopy User Guide* manual for instructions on locking, lock shimming, gradient shimming and tuning.

13. Click on the **Acquisition** menu and **check Use Study Queue**.

14. Click on the **Spin/Temp** page.

15. Set spinning options (spin or non-spin requirements that are integrated into the protocols override the selections on this page).

a. Turn on the spinner by clicking the **Spin On** button or to run non-spinning, click the **Spin Off** button.

b. Select spinner control setup and error handling options.

16. Set temperature control options.

- Enable VT regulation:

a. Enter a temperature in the **temperature field** or move the slider bar until the desired temperature appears in the temperature field.

b. Click on the **Regulate Temp** button.

c. Select temperature control setup and error handling options.

- Disable VT control:

Click on the **Temp Off** button.

17. Click on the **Acquisition** menu and select **Resume Automation**.

Sample Handler Present

Run a Protocol in Foreground on a Different Sample

Pause the Active Study Queue to run a protocol in foreground on a different sample then resume study queue and automation with the original sample as follows:

1. Click on the **Acquisition** menu and select **Pause Automation**.

   The current acquisition will pause at the end of its current acquisition. An acquisition in the Study Queue may be `findz0`, automatic tuning, gradient shimming, autolocking and automatic gain adjustment in addition to the acquisition of experimental data itself. Clicking on Pause Automation may pause at the end any of these acquisitions.

2. Wait until the status bar reads **Idle**.

3. Click on the **Acquisition** menu and remove the check from the **Use Study Queue** check box.

   The Acquisition menu is populated with a more options and an Experiments menu choice appears between the Edit and Acquisition menu choices.

4. Optional: place the sample in the desired position of the sample changer (i.e. 7) and in the advanced function bar type **`loc=7 change`**.

   The sample changer will remove the current sample (i.e 2) and insert the new sample (i.e. 7).

5. Follow section 2.2 “Starting an Experiment,” page 20 under “No Sample Handler Mode” on page 21 step 4 through step 12.

6. Select an experiment using either of the following methods:

- Using the **Protocols** vertical panel:

a. Select a the **Protocols** tab from the vertical panel tabs.

a. Click on a **Protocol Type** type on the Experiment Panel.

b. Select a **Protocol**.

   This retrieves an experimental protocol into the foreground.

c. Continue with step 5.

- Using **Experiments** on the main menu.

a. Click on **Experiments** on the main menu.

b. Select a **protocol** or **protocol type** from the drop down list.

c. Select a **protocol** from the **protocol type** if a pop-out is presented.

This retrieves an experimental protocol into the foreground.

d. Continue with step 5.

7. Adjust the acquisition parameters as necessary.
8. Click on the **Acquisition** menu and select **Acquire Data**, **Acquire and WFT** or **Acquire and Process**.
9. A pop-up window is displayed if required parameters are enabled, see "Setting Up Required Parameters" on page 14.

a. Enter the required parameters. All fields must have an entry, either a text string or a value.

b. Click **OK** after all the fields are filled.

10. When acquisition is complete, click on **File** menu and select **Save As…**
11. Choose a directory and provide a **File Name**, then press **Save**.
12. Optional: return the original sample (i.e. 2) to the magnet by typing **`loc=2 change`**.

    The sample changer will remove the current sample (i.e 7) and insert the original sample (i.e. 2).

    The lock, shimming, and tuning, may have changed and need adjusting for the sample. Refer to the *NMR Spectroscopy User Guide* manual for instructions on locking, lock shimming, gradient shimming and tuning.
13. Click on the **Acquisition** menu and **check Use Study Queue**.
14. Click on the **Acquisition** menu and select **Resume Automation**.

Chapter 3. *VnmrJ* Walkup - Interface Menus and Controls

Sections in this chapter:

This chapter provides an overview of the VnmrJ Walkup interface, menus, and controls. Features that are not available to walkup operators are noted.

Related manuals:

- *VnmrJ Installation and Administration*
- *NMR Spectroscopy User Guide*
- *Sample Management Systems Installation*
- Relevant probe installation manuals.

3.1 Walkup Experiment Protocol Selection

The walkup account administrator and walkup operator interfaces access application types from a protocol type tab selection menu on the vertical panel, see Figure 9. A full list of

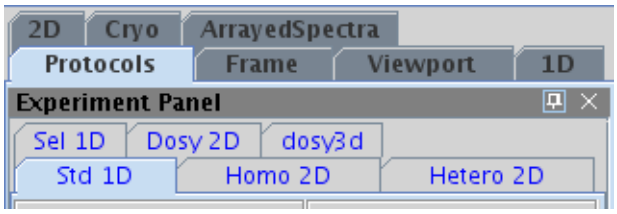


Figure 9. Vertical Panel Tabs

protocols is given on Table 1. Experimental protocols from each application type are entered into the study queue by selecting the application type and clicking on a protocol button. The 2D protocols require a proton type protocol (Proton, Presat, or Wet1d with MinSW enabled) as the first protocol and will add a Proton protocol if a proton type protocol does not exist ahead of the first 2D protocol for a given sample. Placing a Presat or Wet1d first in the protocol list satisfies this requirement and a Proton protocol is not added. Protocols for 1D experiments not of the proton type can be added at any time.

All 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. All operation involving the walkup interface using study Q are treated as automation runs, even if the system does not have or is not using a sample handler. Online help is provided for both the operator and account administrator interfaces.

Table 1. Experimental Protocols

Protocol Tab	*Protocol*	
Std 1D	Proton	Presat
	Wet1D	Carbon
	Fluorine	Phosphorus
	T1 measure	T2 measure
	Apt	Dept
Homo 2D	Cosy	Gcosy
	Dqcosy	Gdqcosy
	Noesy	Rosy
	Tocsy	
Hetero 2D	Hsqc	Ghsqc
	Hmqc	Ghmqc
	Hmbc	Ghmbc
	Hmqctoxy	Ghmqctoxy
	Hsqctoxy	Ghsqctoxy
	Hsqcad	Ghsqcad
	Cigar2j3j	Ghmbcad
Sel 1D	Noesy 1d	Roesy1d
	Tocsy1d	

Table 1. Experimental Protocols

Protocol Tab	*Protocol*	
Dosy 2D (option - requires license and password)	DgcsteSL Doneshot DgsteSL_cc	DgcsteSL_cc Dbppste Dbppsteinept Dbppste_cc
Dosy 3D (option - requires license and password)	Dgestecosy Dgestehmqc	

3.2 Walkup Menus and Controls

The operator interface on systems that do no use a sample changer is the same as the walkup account administrator interface but, by default, does not have an command line.

- "Main Menu Bar" on page 35
- "Advanced Function Bar" on page 51
- "System Tool Bar" on page 51
- "User Tool Bar" on page 52
- "Locator" on page 52
- "Graphics Canvas" on page 53
- "Graphics Toolbars" on page 54
- "Hardware Bar" on page 58
- "Graphics Toolbars" on page 54

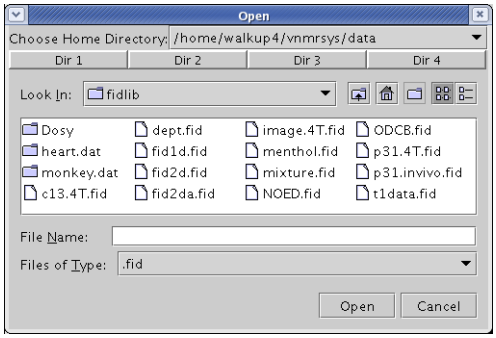
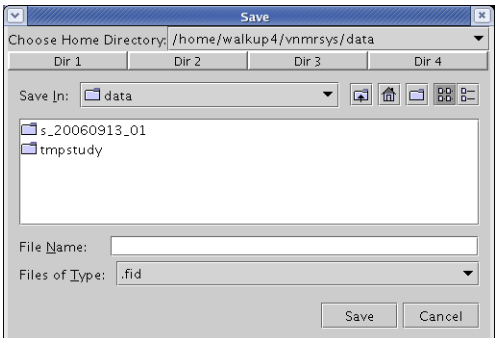
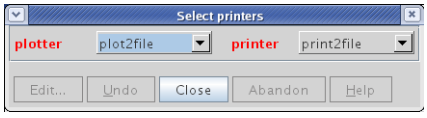
Main Menu Bar

The main menu bar for the account administrator provides the following items:

- "File Menu Selections" on page 36
- "Edit" on page 38
- "View" on page 40
- "Experiments - Direct Acquisition Mode Only" on page 41
- "Acquisition" on page 43
- "Process" on page 45
- "Tools" on page 47
- "Help" on page 50

File Menu Selections

The menu selections are for the File menu are:

Menu Items	*Descriptions*
New Workspace	Make and join the next available workspace.
Open	Opens the file navigation window to the locate the required file. Click the **file** and click on the **Open** button to open. 
Save as …	Opens the file navigation window to the locate the required directory. Enter a **file name** in the Save as field and click **OK** to save. 
Save data setup …	Opens the Save Data Setup window — customize where data is saved and customize the file naming for automation runs, see “Setting Up Study Data Directories and Templates” on page 12.
New automation run	Sets *VnmrJ* foreground and background operations for all walkup acquisitions. Creates an automation directory in the account administrator’s directory, within globalauto. Opens the sample tray.
Printers...	Opens a window for selecting printers and plotters.
	Only printers and plotters defined through VnmrJ Admin are displayed, see the *VnmrJ Installation and Administration* manual for information about connecting printers and plotters. 
Print Screen …	Prints part or all of the VnmrJ screen to either a file or printer using the options selected.

Printer Region of window

Printer radio button – sends output to printer

File radio button - save output to the file named in the File field

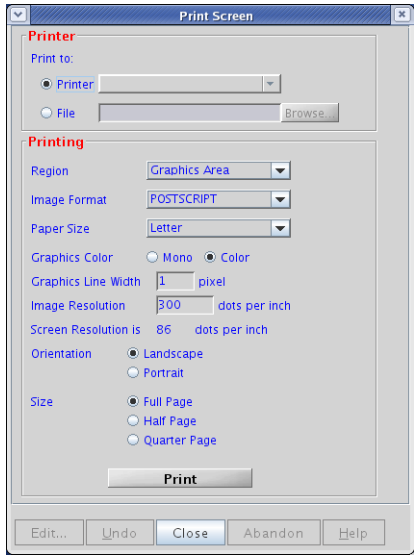
Printing Region of window

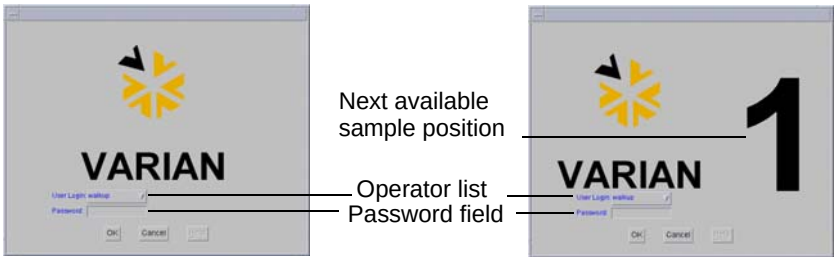
Select Region dropdown menu choices:

Graphics Area

VnmrJ Screen

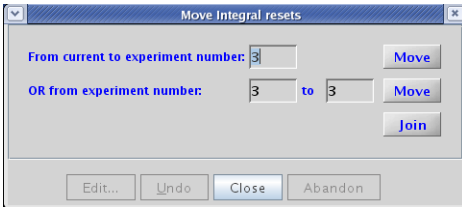
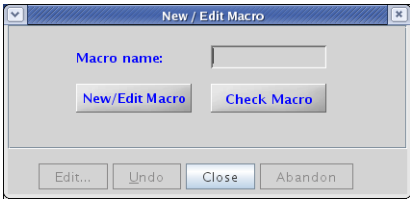
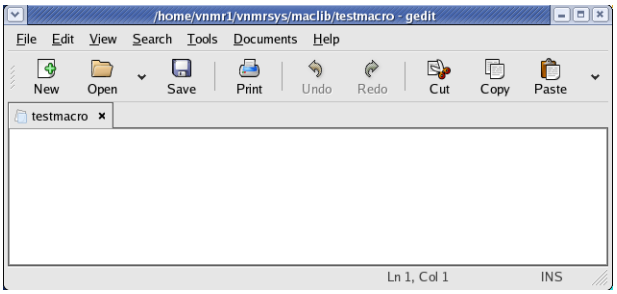
Menu Items	*Descriptions*
	Format dropdown menu choices: JPEG, GIF, TIFF, or BITMAP **Page Size** – click on a radio button for: Full, Half, or Quarter page **Graphics Color** — click on a radio button to select Mono or Color **Graphics Line Width** — enter a line width in pixels **Image Resolution** — enter an image resolution in dots per inch **Screen Resolution is** — displays current screen resolution in dots per inch **Orientation** – click a radio button for: Landscape or Portrait **Size** — Click a radio button for: Full Page, Half Page, or Quarter Page **Print** button – sends screen to default printer **Close** button – close the Print Screen window
Auto Plot	Plots current data using protocol plotting and printing defaults.
Create a Plot Design…	Opens Plot Designer, see *NMR Spectroscopy User's Guide* manual for description and how to use Plot Designer.
Switch Operators	Opens the window for changing walkup operators. The appearance of the login/logout window will change depending upon if automation is active or not. **Select** an operator from the dropdown menu or type the operator name in the field. **Select** an operator from the dropdown 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).
Exit VnmrJ	Exits VnmrJ.

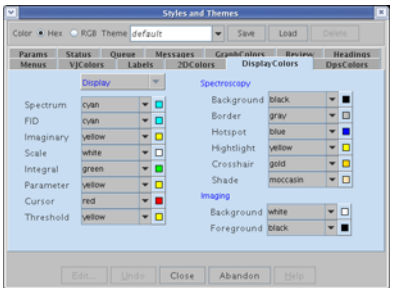




Edit

The Edit menu selections are:.

Edit Menu Items	*Descriptions*
Move Parameters… **Move FID…** **Move Text…** **Move Display parameters…** **Move Integral resets…**	All the **Move …** selections open a pop up window similar to the Move Integral resets window shown.  Do either of the following or click **Close**: • Enter a target experiment number in the field next to **From current to experiment number:** to move the selection from the current experiment. Click the **Move** button. • Enter the number of the source experiment in the field next to **OR from experiment number:** and the number of the target experiment in the **to** field. Click the **Move** button. Click the **Join** button. Click **Close.**
New Pulse Shapes (Pbox)…	Opens Pbox window, see *NMR Spectroscopy User's Guide* manual for description and how to use Pbox.
Pbox Window tab	
Make Waveform:	Click on the **New Wave Form** button to display the wave form parameter fields.
Update Parameters	Update the various parameters associated with the current wave form.
View Pulse Shapes…	Opens Pulse Tool window, see *NMR Spectroscopy User's Guide* manual for description and how to use Pulse tool.
New/Edit Macro…	Opens a dialog window to create a new macro, edit and existing macro, or test a specific macro.  1. Enter the name of a new or existing macro in the field next to **Macro name**. 2. Click on the **New/Edit Macro** button to open the **gedit** tool. . 

Edit Menu Items	*Descriptions*
	Instruction for using the gedit tool are access by clicking on Help button on the tool's menu bar. 3. Edit or write the new macro, refer to the section in the *VnmrJ User Programming* manual for Guide for instructions on writing macros using the Magical II language. 4. Save the new or edited macro or abandon the new or changed material. 5. Click on the **Check Macro** button to test the macro. 6. Click on the **Close** button to exit the New/Edit Macro dialog window.
Tool Bar	Opens the tool bar editing tool. Refer to the *VnmrJ Installation and Administration* manual for more details.
Display options...	Opens a window for setting symbolic colors and fonts in the interface. 
Edit config profile…	Opens the Edit User Config Profile window, see "Panel Levels and User Profiles" on page 76.
Parameter Pages…	Opens the parameter panel editing tool. Refer to the *User Programming* manual section on panel editing.
Viewports	Opens the Viewport Settings panel to set the number of viewports. Select a radio button from 1 to 9 to set the number of viewports, see "Setting the Number of Available Viewports" on page 60 for more details.
Applications…	Opens Applications Directories editor, see "Setting Applications Directories" on page 14, if the operator has rights to edit the contents of `appdir` file, see *VnmrJ Installation and Administration* manual for more information on appdir and rights.
System Settings...	Opens the System Settings window, which enables you to set system parameters. **System** tab — provides system-level settings. **Display/Plot** tab — provides display and plot settings. **Display configuration check box** — displays system hardware configuration in the text output panel (config).
System Settings Window tabs	
System	**Application mode** — Walkup, Standard, Imaging, LC, or Autotest. **Gradient amplifier** — On/Off selection for each gradient axis that is installed. **Hardware Z1 Shimming** dropdown menu: none, delay, and presat

Edit Menu Items	*Descriptions*
	Probe protection check box — check to enable. **Solids VT system** check box — check to enable.
	VT cutoff (0 – 50) entry field — enter value above which the VT air flow will not use the heat exchanger.
Display/Plot	**Set display from plotter aspect ratio (wysisyg)** — check to enable.
	Spectrum updating during phasing (0-100) — set the percentage of the display that is updated during interactive phasing. 100 is recommended.
	Max # of pens — specify the number of plotter pens to use.
	Show Tooltips — check to enable.
	Max # of items to show in Locator - Set the number of items to show in the locator. Setting this to greater than 2000 starts to diminish the performance. **Display only matching items in locator** — check to enable. **Day Limit of files in Locator (neg = forever)** — Enter the cutoff age in days for keeping `.fid` and `.fdf` files in the locator database. Files are only removed from the database after reaching this age. Files remain on the disk and are not removed. A negative number means keep all files forever. Zero, means do not keep any `.fid` nor `.fdf` files except Varian files. An entry of 30 means remove files older than 30 days from the database. Refer to *VnmrJ Installation and Administration* manual for more information on working with the locator. **Turn Locator Off** - check to completely disable the Locator. **Process data on drag-and drop** — check to enable. **Show last spectrum of submitted sample**— check to enable. **Trash study node preferences** — set options from dropdown menu: **Customized study nodes:** deleted, skipped, or not allowed. **Completed study nodes:** not allowed, remove data, delete **Display configuration** — check box to display

View

View Menu Items	*Descriptions*
Command Line	Displays the command line if it is hidden — default is account owner only.
Experimental Panel	Adds the experiment panel to the vertical panel protocol tab.
Parameter Panel	Opens the horizontal parameter panels if they are hidden.
Study Queue	Adds the study queue panel to the vertical panel protocol tab.
Toolbars	Opens a pop-out menu. Place check next to a tool bar to show the tool or remove the check to hide the tool bar.
Frame	See “Frame Panel” on page 66.
Viewport	See “Viewport Panel and Controls” on page 61.
1D	See “1D” on page 71.

View Menu Items	*Descriptions*
2D	See "2D" on page 73.
Cryo	Controls for cryogenic system and probe. Refer to the related manuals for instructions.
Arrayed Spectra	See "Arrayed Spectra and FIDs" on page 74.
Graphics Toolbar	 Tool bar for spectra Tool bar for fids See "Graphics Toolbars" on page 54
Hardware Toolbar	
System Toolbar	 See "System Tool Bar" on page 51.
User Tool bar	

Experiments - Direct Acquisition Mode Only

Not all experiments are available on all spectrometer systems. System configuration and options selected at installation determine the available experiments. This menu shows only if **Use Study Queue** in the **Acquisition** menu is deselected. Refer to *NMR Spectroscopy User Guide* for explanations of all supported experiments.

Experiments Menu Items	*Sub menu choices*	
Proton **Presat** **Wet1D** **Carbon** **Fluorine** **Phosphorus**		
Relaxation Measurements	T1 Measure	T2 Measure
Carbon-Proton Multiplicity	Apt	Dept/DeptQ
Selective Excitation 1D	Noesy1d Tocsy1d	Roesy1d
Homonuclear 2D	Cosy Dqcosy	Gcosy Gdqcosy
	Noesy	Roesy
	Tocsy	Homo2dj
1H Detected Proton-Carbon 2D	Hsqc Hmqc	Ghsqc Ghmqc
	Hmbc	Ghmbc
	Hsqctoxy	Ghsqctoxy
	Hmqctoxy	Ghmqctoxy
	Hsqcad	Ghsqcad
	Ghmbcad	Cigar2j3j
	AdequateAD	
13C Detected 2D	Hetcor	Ghetcor

Experiments Menu Items	*Sub menu choices*
Hadamard Experiments	Setup Hadamard HsqcHT TocsyHT
Dosy	
	2D DOSY
	Bipolar Pulse Pair Stimulate Echo
	Bipolar Pulse Pair STE with Watergate 3-9-19 Solvent Suppression
	Gradient Compensated Stimulated Echo
	Gradient Compensated STE with DPFGSE Solvent Suppression
	ONESHOT-DOSY
	DOSY-INEPT
	2D DOSY with Convection Compensation
	Bipolar Pulse Pair Stimulated Echo
	Gradient Stimulate Echo
	Gradient Compensated Stimulate Echo
	PFG Double Stimulated Echo
	Absolute Value 3D DOSY Sequences
	Gradient Compensated Stimulate Echo COSY
	COSY-IDOSY
	Gradient Compensated Stimulate Echo gHMQC
	HOM2J-IDOSY
	Phase Sensitive 3D DOSY Sequences
	Sensitivity Enhanced gHSQC-DOSY
	Gradient Stimulated Echo HMQC
	gHMQC-IDOSY
Solid-State Experiments	
	Basic 1D Experiments
	Setup Tangent CP (Settancps)
	Tangen CP (Tancpx)
	CP with TOSS (Tancpxtoss)
	One Pulse (Onepul)
	One Pulse with TOSS (Onepultoss)
	PWX with CP (Tancpxflip)
	1H T1rho with CP (Tancpxt1rho)
	X Hahn Echo with CP (Tancpxecho)
	X Two Pulse for T1 (Twopul)
	Interupted Decoupling with CP (Tancpxidef)
	X T1 with CP (Tancpht1)
	CP with FSLG Decooupling (Tnacpxfslg)
	Lee Golburg CP (Lgcp)

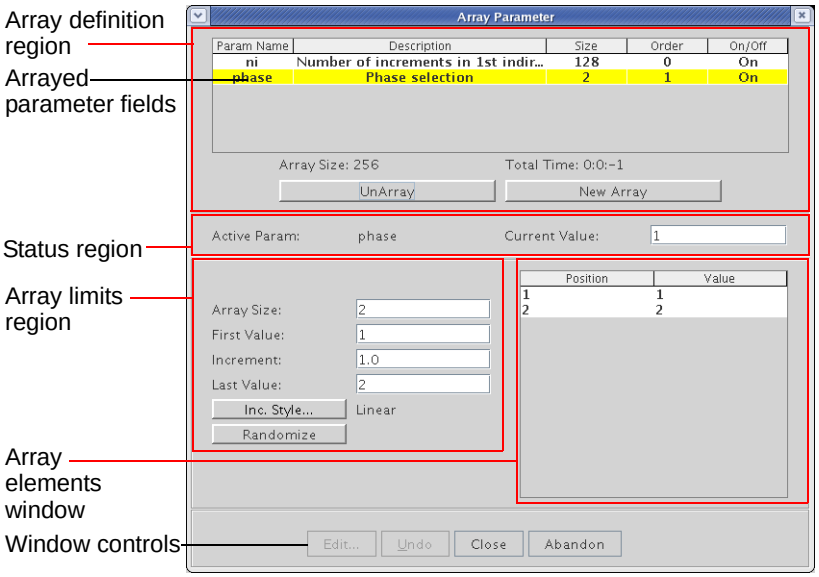
Experiments Menu Items	*Sub menu choices*
	HX2D Experiments
	FSLG with Lee-Goldburg CP (Hetcorlgcp)
	WISE (Wisentancped)
	2Q-1Q with CP and C7 Mixing (C7inad2d)
	PISMA using FSLG
	HXY Experiments
	CP REDOR with XY8 on X and Y (Redor1tancp)
	CP REDOR with XY8 Y and X inversion (Redor2tancp)
	One Pulse REDOR with XY8 on X and Y (Redor1onepul)
	One Pulse REDOR with XY8 Y and X inversion (Redor2onepul)
	Quadrupole Experiments
	Quadrupole Echo (Ssecho1d)
	3Q-1Q MQMAS with Z-filter (Mqmas3qzf2d)
	5Q-1Q MQMAS with Z-filter (Mqmas5qzf2d)
	Multipulse Experiments
	High Power Pulse Tuning (Tunexp)
	XX Tuneup (Xx)
	XmX Tuneup (Xmx)
	BR24 with Quad Detection (BR24q)
	MREV8 with Quad Detection (Mrev8q)
	Semiwindowless WaHuHa (Swwhh4)
	Windowless PMLG-N (Wpmlg1d)
	2D F1 and Windowed PMLG-N (Wpmlg2d)

Acquisition

The Acquisition menu selections are:.

Menu Items	*Descriptions*
Use Study Queue check box	Check this box to enable the study queue and to facilitate submitting a sample. Uncheck this box to access experiments using the experiments menu and run experiments without using the study queue, see “Using Direct Acquisition” on page 27.
Parameter arrays…	Open Array Parameter window.

Menu Items *Descriptions*



Array Parameter Window Regions

Array definition

Arrayed parameter field columns:

Param Name – enter name of arrayed parameter.

Description – displays text description of array.

Size – displays number of steps or increments in the array.

Order – displays precedence for running the array – double click in the field and enter the array order. Arrays with sequential numbers create a full matrix (array A x Array B) and each array can be a different size. Arrays with the same order number (and the same size) create a diagonal array.

On/Off – Array is used / array not used.

Fields and buttons

Array Size field – shows size of selected array.

Total Time field – shows estimated time to complete the array.

UnArray button – remove selected parameter from the list of arrayed parameters.

NewArray button – add new row to list of arrayed parameters.

Status – show active parameter during acquisition and parameter's current value.

Array limits

Array Size field – enter the size of the array and press return.

First Value – enter the starting value of the array and press return.

Increment – enter the array increment and press return.

Last Value – enter the ending value of the array and press return.

Menu Items	*Descriptions*
	Inc. Style … button – click and select linear or exponential.
	Randomize button – click to create a random array.
Array elements	
	Change the value of the array element by double clicking on the value of the array element associated with the array position, entering a new value, and pressing **Enter**.
Window buttons	
	Edit—Not active.
	Undo—Click to undo click again to restore the change.
	Close—Closes the window.
	Abandon—Closes the window and makes no changes.
Options available for direct acquisition only. **The Use Study Queue box is not checked.**	
Acquire Data	Acquire data only. No post acquisition processing.
Acquire and WFT	Acquire and process data post acquisition using current weighting functions and values.
Acquire and Process	Acquire and process data post acquisition using the current settings.
Pause Automation	Halt automation at the end of the current sample protocol.
Resume Automation	Resume Automation with the next sample in the queue
Abort Acquisition	Abort data acquisition for the current sample. Sample handlers systems remove the sample, insert the next queued sample in the magnet, and start data acquisition.
Abort Automation	Abort the current automation run. The current sample remains in the magnet.

Process

The Process menu selections are:.

Menu Items	*Descriptions*
Process and Display 1D	Process and display 1D data.
Full Process	Process and display 1D data using the processing associated with the protocol.
Drift Correct Spectrum	Apply drift correction along both axes of a 2D data set.
Automatically Set Integrals	Automatically find and set integral regions.
Baseline Correct	Apply baseline correction.
Set Spectral Width between Cursors	Mark new spectral width on the graphics screen using the left and right cursors and set the new spectral width.
Set Transmitter at Cursor	Mark new transmitter location on the graphics screen and set the transmitter.
Add and Subtract 1D Data	Results are shown displayed in current when second spectrum is selected.
Sub-menu item	

Menu Items	*Descriptions*
Clear Buffer and Add Current Spectrum	Clears buffer (experiment 5) or creates experiment 5 (if necessary) and places current spectrum in experiment 5.
Add Second Spectrum into Buffer	Adds current spectrum (algebraically) to buffer.
1D FDM	Only available if FDM option is loaded.
Full Process 2D	Process and display 2D data using the processing and display parameters associated with the protocol.
Process 2D (Individual Steps)	Step by step processing of 2D data

Sub-menu Choices

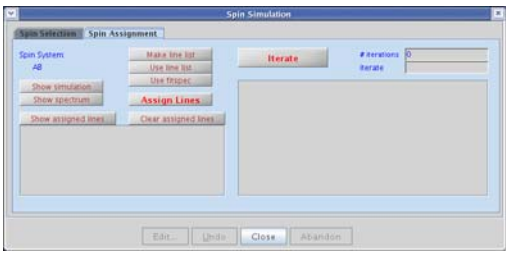
Phase and Set Weighting F2
Do first FT (t2 Domain)
Adjust Weighting in F1 (must do first FT)
Baseline Correct F2
Full 2D-FT (t1, t2 domains)
Baseline Correct F1

Analyze

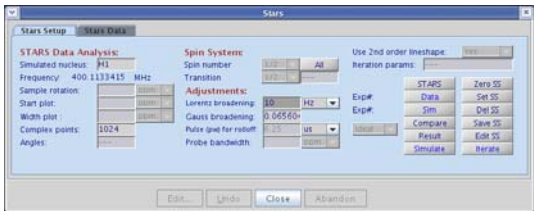
Sub-menu Selections

Cosy Correlations…
opens Cosy Correlations window if current viewport contains an appropriate data set.

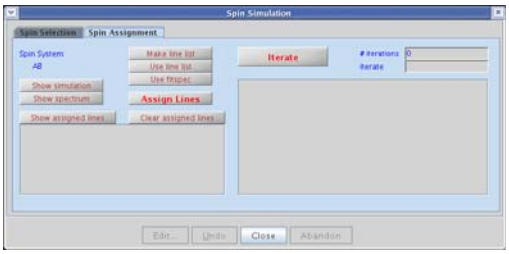
Spin Simulation… opens Spin Simulation window:
Refer to *NMR Spectroscopy User Guide* manuals.



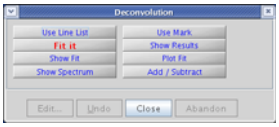
Stars… opens the Stars window:
This window is only available if the optional Stars software module was installed.



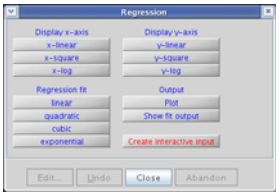
Menu Items	*Descriptions*



Deconvolution… opens the Deconvolution window:



Regression… opens the regression window:



Tools

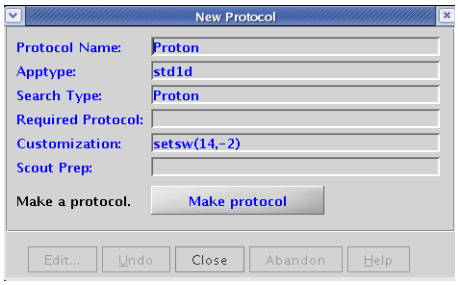
The tools menu selections are available only if viewport 1 is active:

Menu Items	*Descriptions*
Update night queue start time	Menu selection available only if the viewport 1 is active. Used by the admin after setting the night queue start time, see *VnmrJ Installation and Administration* manual.

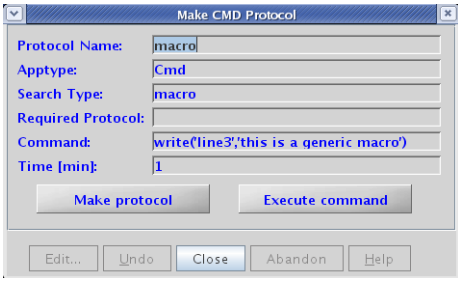
Create Protocols menu selection is only available if the viewport 1 is active.

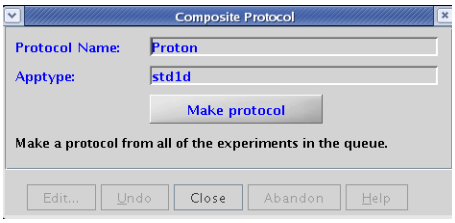
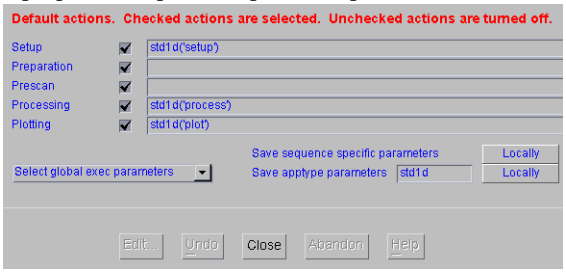
Sub-menu items

Make a New Protocol Opens a window for saving the current parameter set as a new protocol.

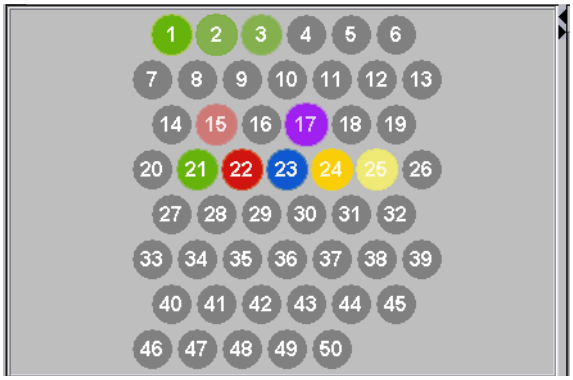


Make a Command Protocol… Opens a command protocol window. A command protocol is a method for running a command or macro in the study queue.

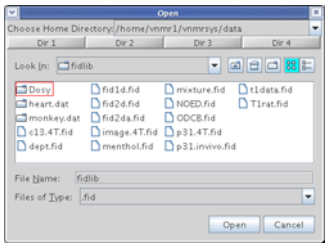
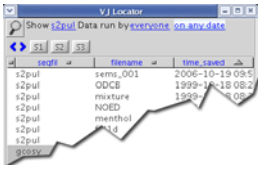


Menu Items	*Descriptions*
Make a Composite Protocol	Opens a window for making a protocol from the experiments in the new sample area of the Study Queue. 
Configure EXEC parameters	Opens a window to access parameters controlling generic acquire, preparation, process, plot, and prescan functions. 
Select global exec parameters	Dropdown menu of application types. The **Setup**, **Preparation**, **Prescan**, **Processing**, and **Plotting** fields are filed in or remain empty as appropriate. The default action is active if check mark appears in the box next to the action. The fields are editable.
Save sequence specific parameters	The **sequence specific parameters** are saved when button labeled **Locally** is clicked. If the account administrator has permission, a button is labeled **Globally** appears next to the Locally button, to save the parameters globally.
Save apptype parameters field	Specify an application type. The save process occurs when button labeled **Locally** is clicked. If account administrator has permission, a button labeled **Globally** appears next to the Locally button, to save the parameters globally.

The tools menu selections are available at all times:

Menu Items	*Descriptions*
Sample Tray	Opens sample tray window if the system is configured to run a sample changer . 

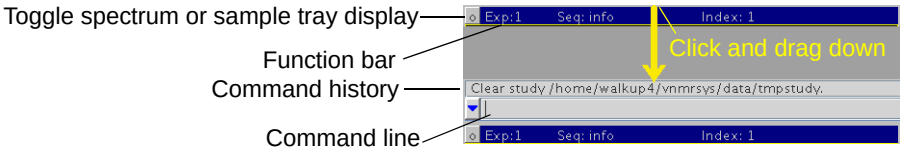
Menu Items	*Descriptions*
Open	Select **Open** to display sample tray: The sample position colors the indicate the availability of the position and status of that sample position as follows: Gray - empty Green - completed Blue - active Yellow - submitted to day queue Purple - submitted to night queue Red - error Faded or grayed out - Sample submitted by an operator other than the currently logged in operator.
Close	Closes the sample display and show spectrum
Probe Tuning	Option is displayed if hardware and software are installed.
Sub-menu items	
Auto tune setup…	Opens the Setup AutoTune window if ProTune present, see “Configuring ProTune” on page 18.
Tune probe…	Opens the Tune Probe window if ProTune present, see “Configuring ProTune” on page 18.
Manual Tune Probe	Loads manual tuning parameters and panels.
Do Gradient Shimming	Starts the gradient shimming using the gradient shim map associated with the current probe and the gradient shimming parameters set when **Set Up Gradient Shimming** was last run.
Standard Calibration Experiments	Provides the interfaces for probe calibration and gradient shimming setup:
Sub-menu items	
Probe Calibration	Opens a window for running a series of experiments to calibrate the probe. Refer to the *VnmrJ Installation and Administration* manual and the *NMR Spectroscopy User Guide* manual for descriptions of the probe calibration experiments. 
Set Up Gradient Shimming	Loads the pulse sequence and panels for making a shim map for gradient shimming
Set Up 3D Gradient Shimming	Selection appears only if this option is installed. Loads the pulse sequence and panels for making a 3D shim map for gradient shimming.
Applications directory Enabled/Disabled Sub-menu selections (refer to “Setting Applications Directories” on page 14):	
Start AutoTest	Starts AutoTest, see *AutoTest* manual for a description of the AutoTest.
AutoTest Settings	Opens the AutoTest test settings window, see the *AutoTest* manual for a description of settings and options.

Menu Items	*Descriptions*
Update locator	Opens a submenu that provides choices for updating the different parts of the Locator.
Import files to locator	Opens a window for importing files to the locator.
Save custom locator statement	Opens a window for saving the current locator view.
Delete custom locator statement	Opens a window for deleting custom locator statements.
Molecular Structures	
Sub-menu items	
Display all	Display all molecular structures.
Plot all	Plot all molecular structures.
JChempaint…	Opens the open source application JChempaint in a separate window. Refer to the online manual provided with JChempaint.
Jmol…	Opens the open source application Jmol in a separate window. Refer to the online manual provided with Jmol.
Change Password	Opens a window for changing Walkup operator (user) passwords. If the walkup operator has an operating system login account, that password is also changed.
Browser…	Opens a file browser window refer "Browser" on page 53. 
Locator…	Opens Locator "Locator and File Browser" section of the *NMR Spectroscopy User's Guide* manual and "Locator" on page 52. 

Help

Menu Items	*Descriptions*
Online Manuals (PDF)	Opens manuals on line in PDF format. The help files must be loaded from the VnmrJ Manuals CD. Or, the CD must be left in the CD-ROM drive.
Varian NMR Home Page	Opens the Varian NMR home page if internet access is permitted.
About VnmrJ	Opens a window to display current software version.

Advanced Function Bar



The advanced function bar is available to operators assigned to the account.

Access to the command line is available to the account administrator only by default. Dragging down the advanced function bar opens a command, macro, and parameter entry field and a text output field. The default settings make the click and drag down feature to display the command line available to the account owner but not to operators, see *VnmrJ Installation and Administration* manual for changing this default. Open or close the field by clicking once on the button, which restores it to its most recent view. Error and information messages are displayed in the scrolling text window above the command line in addition to the hardware bar. Click on the arrow with the left mouse button to view the command history. Select a command from the command history by highlighting it and pressing **Return** to execute it.

System Tool Bar

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

Button	*Function*
	Create a new work space.
	Open the file browser to locate a directory, select a file, and load the file. Click on the file to load and click on the **Open** button to load the file into the current workspace (experiment).
	Save As… Opens a file browser to locate a directory, name a file, and save a data set. Enter a file name in the **File Name:** field, select the **file type** from the dropdown menu, and click on the **Save** button.
	Open the display options Styles and Themes window.
	Cancel command.
	Stop acquisition.
	Show the fid display toolbar, see “Display FID Toolbar Controls” on page 56.
	Show the spectrum display toolbar, see “1D Display Spectrum Toolbar Controls” on page 55.
	Show the contour controls (grayed out if the data set is 1D), see “nD Display Toolbar Controls” on page 57.
	Select a view port from the drop down list. Menu names are the same as the names entered for the view port labels in the Viewport vertical panel

User Tool Bar

The tool bar and buttons can be edited. Save the current screen layout (graphics, a parameter panel, locator sizes).

Button	*Descriptions*
	Save layout view 1.
	Save layout view 2.

Save a view as follows:

1. Place cursor over the view button.
2. Hold the left mouse button down.
3. Wait for *layout saved* to appear in the message box on the hardware bar (approximately five seconds). The same message appears on the command line if the command line is visible.
4. Release the mouse button.

Click on a saved layout button to return to the saved layout.

Hiding and Showing the Tool Bars

Hide or show a tool bar from the main menu:

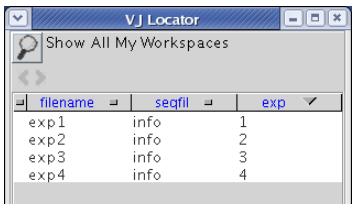
1. Click on **View** from the main menu.
2. Select **Toolbars**.
3. Check on a **toolbar name** to toggle the tool bar on (place a check mark to the left of the toolbar name) or off (remove the check mark to the left of the toolbar name).

A tool bar with an **X** at the bottom can be hidden or closed by clicking on the **X**.

Locator

The Locator provides access to data sets and experiments. Open the VJ Locator popup as follows:

1. Click on **Tools** on the main menu.
2. Click on **Locator…**



Click the magnifying glass with the left mouse button to open 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. Three attributes are displayed for each item that is found by the search. The attributes 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.

Click on an item in the Locator list to select that item. The selected item can 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). 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.

Browser

Browser Buttons and Drop Down Menus

Button	*Description*
	Go up one level in the directory tree.
	Go to user's home directory.
	Make a new folder in the current directory.
	Show list of files and directories at the current directory level.
	Show details of files and directories at the current directory level.

Graphics Canvas

This portion of VnmrJ, shown in Figure 10, is used to display and interact with graphic and text information.

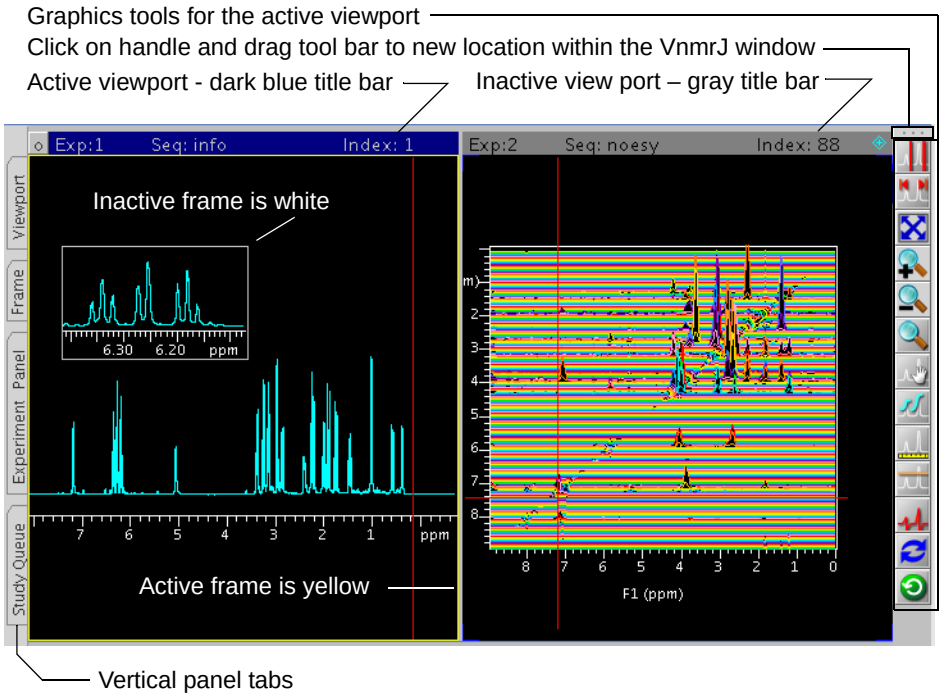


Figure 10. Graphics Canvas and Two Viewports

- Turn viewports on and off using the controls in the Viewport tab, see "Setting the Number of Available Viewports" on page 60.

- Make a viewport active by clicking on the viewport's title bar.
- Make an inactive frame active by double clicking inside the frame.
- Turn graphics tools on and off, see "Hiding and Showing the Tool Bars" on page 52.
- 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 vertical panel on the left side of the graphics canvas).
- Expand the graphics canvas to hide the parameter templates area by clicking on the **X** in the upper right hand corner of the parameter panel. Show the parameter panels by clicking on **View** from the main menu and selecting **Parameter Panel**.
- Flip the parameter panels behind the graphics canvas by clicking the push pin. The parameter panel tab appears on the right side of the canvas. **Click** on the parameter tab or **hover over** the parameter tab with cursor to show the parameter panel without resizing the graphics canvas.
- Flip vertical panels to tabs along the left side of the graphics canvas by clicking on the push pin on each of the vertical panels.
- Close the vertical panels by clicking on the **X** in the upper right hand corner of the panel. Show the vertical panels by clicking on **View** from the main menu and selecting each vertical panel to view.

Graphics Toolbars

The graphics control bar for the active viewport is to the right of the graphics canvas. Use the buttons in the bar to control the interactive display in the graphics canvas.

- "Common Graphics Display Toolbar Controls" on page 54
- "1D Display Spectrum Toolbar Controls" on page 55
- "Integration and Graphics Controls" on page 55
- "Display FID Toolbar Controls" on page 56
- "nD Display Toolbar Controls" on page 57

Common Graphics Display Toolbar Controls

The following tools are common to 1D, nD, and fid display toolbars.

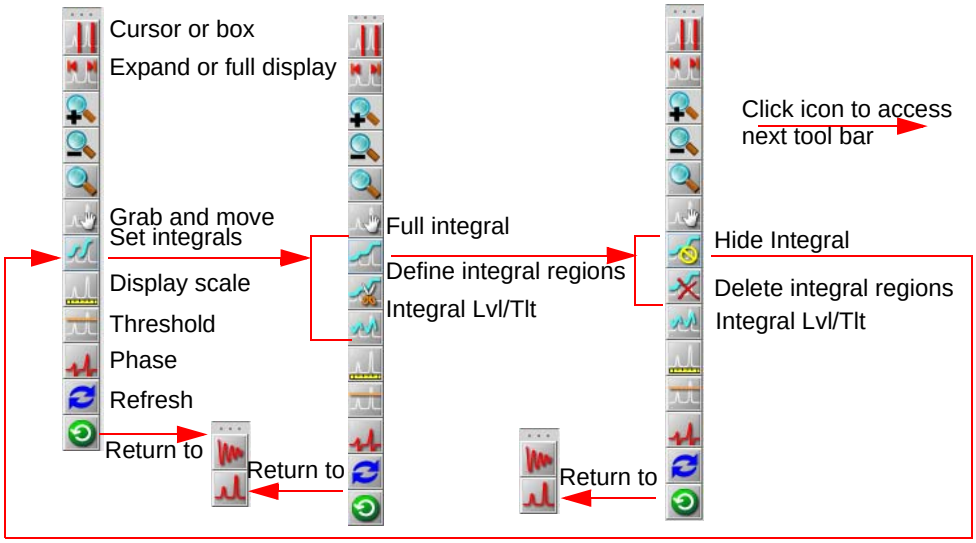
Icon	*Description*
	Reset to full display.
	Zoom in.
	Zoom out.
	Select zoom region.
	Redraw display.
	Return to previous tool menu.

1D Display Spectrum Toolbar Controls

Icon	Description
	One cursor in use, click to toggle to two cursors.
	Two cursors in use, click to toggle to one cursor.
	Click to expand to full spectral display.
	Pan or move spectral region.
	Display integral.
	Display scale.
	Toggle threshold on or off.
	Phase spectrum.

Integration and Graphics Controls

This section describes methods and tools for displaying and plotting integrals.



Display FID Toolbar Controls

Icon	*Description*
	One cursor in use, click to toggle to two cursor.
	Two cursors in use, click to toggle to one cursor.
	Click to expand to full fid display.
	Pan and stretch.
	Click to show real and imaginary.
	Click to show real and zero imaginary.
	Click to show real only.
	Toggle scale on and off.
	Phase fid.

nD Display Toolbar Controls

Main nD Display Bar Tools

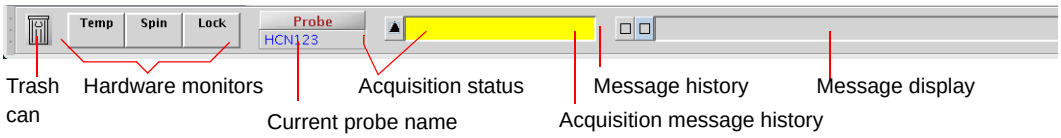
Icon	*Description*
	Display color map and show common nD graphics tools.
	Display contour map and show common nD graphics tools.
	Display stacked spectra and show common nD graphics tools.
	Display image map and show common nD graphics tools.

nD Graphic Tools

Icon	*Description*
	One cursor in use, click to toggle to two cursors.
	Two cursors in use, click to toggle to one cursor.
	Click to expand to full display.
	Pan and stretch.
	Show trace.
	Show projections.
	Click on  to show horizontal maximum projection across the top of the 2D display.
	Click on  to show horizontal sum projection across the top of the 2D display.
	Click on  to show vertical maximum projection down the left side of the 2D display.
	Click on  to show vertical sum projection down the left side of the 2D display.
	Rotate axes.
	Increase vertical scale 20%.
	Decrease vertical scale 20%.

Icon	*Description*
	Phase spectrum tool bar selection.
	Click on  One cursor in use, click to toggle to two cursors.
	Click on  Click to expand to full display.
	Click on  Show trace.
	Click on  Redraw display.
	Click on  Rotate axes.
	Click on  to select the first spectrum.
	Click on  to select the second spectrum.
	Click on  Phase spectrum tool bar selection.
	Click on  to select the first spectrum.
	Click on  to select the second spectrum.
	 Return to previous tool menu.
	Enter peak pick menu.

Hardware Bar



The hardware bar contains the following:

- “Hiding and Showing the Hardware Bar” on page 59
- “Trash Can” on page 59
- “Hardware Monitors” on page 59
- “Probe Selection” on page 59
- “Acquisition Status Details” on page 60
- “Acquisition Status Display” on page 60
- “History of Acquisition Messages” on page 60
- “History of All Messages” on page 60
- “Message Display” on page 60

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

Hiding and Showing the Hardware Bar

1. Click on **View** on the main menu bar and Select **Toolbars**.
2. Click on **Hardware Toolbar** to **check**, show the hardware tool bar, or **uncheck**, to hide the Hardware Toolbar.

Trash Can

Dragging an item to the trash can from the Locator or other area removes the item and adds it to the trash can, see Figure 11. Double-click on the trash to view locator items in the trash can area when the locator is open. Restore deleted objects from the trash can by selecting them and then clicking the **Restore items** button before clicking on the **Empty My Trash** button. Double-click on the trash to exit the Trash Can mode.

Figure 11. Trash Can Mode

Emptying the trash can (clicking on the Empty My Trash button) deletes the data from the disk - there is no restore function.The Locator must be running to use the trash can.

Dragging an icon to trash from the Study Queue deletes the item from disk by default. Check the Trash mode preferences in the System Setting dialog in the **Edit** menu to set the trash mode behavior.

Hardware Monitors

Click on Temp, Spin, or Lock to open a window with a line graph showing the history of the relative hardware function. Click the icon again to close the window.

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

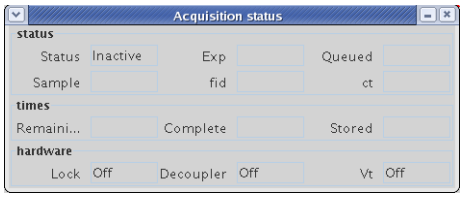
Probe Selection

Available only to the walkup account administrator. A probe cannot be selected by operators that are not the account administrator. The currently selected probe is shown on the button. Access to probe selection and calibration is limited to the Walkup account administrator. Refer to the *VnmrJ Installation and Administration* manual for probe selection and calibration.

Acquisition Status Details

Click on the icon to open a window showing acquisition status details.

Click on the icon again to close the window.



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

Click on the icon to see a history of all acquisition messages.

Click on the icon again to close the window.

Click the right mouse button within the scrolling message window to change the text view options.

History of All Messages

Click on the icon to see a history of all spectrometer messages.

Click the right mouse button within the message window to change the text view options.

Message Display

The message display TMS has been identified and the spectrum referenced to it shows the last message that occurred. Messages can be informational, a warning, or an error message.

3.3 Setting the Number of Available Viewports

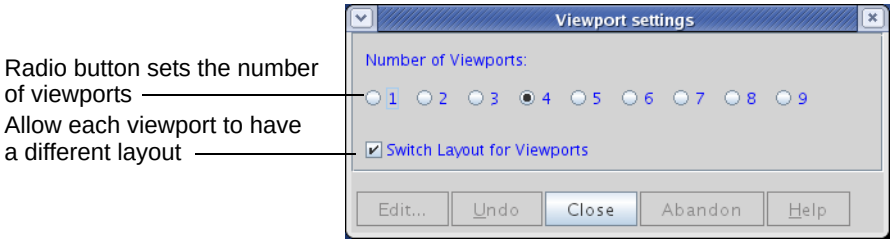


Figure 12. Viewport settings window

1. Click on **Edit** on the main menu.
2. Select **Viewports…** to open the Viewports settings window, see Figure 12.
3. Click on a **radio button** under **viewports** next to the number of viewports to create.

   A maximum of nine viewports can be created. Each viewport created is added to the vertical tool bar Viewport tab.

4. Check the box next to **Switch Layout for Viewport** to allow each viewport to have a different layout.

3.4 Vertical Panels

Viewport Panel and Controls

Click on the **Viewport** tab to display the viewport controls.

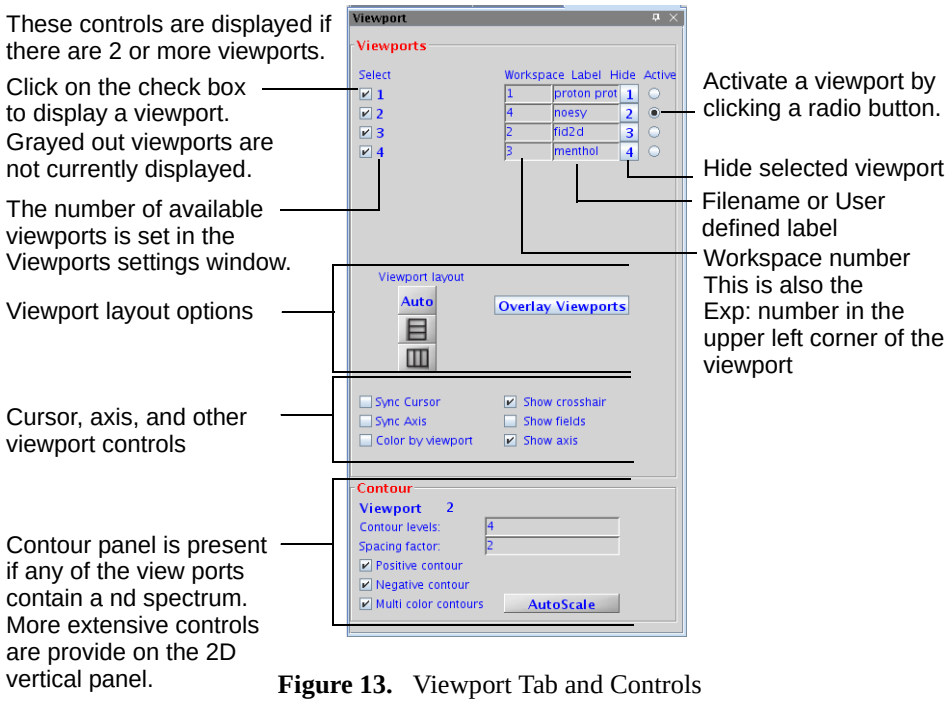


Figure 13. Viewport Tab and Controls

Using Viewports Region Controls

The viewport controls are present if there are two or more view ports (see "Setting the Number of Available Viewports" on page 60).

Showing and Hiding Viewports

The selected viewports are arranged on the graphics canvas based the layout selection, see "Setting Viewport Layout" on page 62.

1. Place a check in the check box next to each viewport to show on the graphics canvas.
2. Remove the check from a check box next to a view port to hide the viewport.
3. Temporarily hide a viewport by placing the cursor over the box next to the viewport label and holding down the left mouse button. Release to mouse button to show the viewport. The viewports do not change their layout on the graphics screen. This tool is used when overlay viewports is selected.

Making a Viewport Active

1. Click on the radio button associated with a viewport to make the viewport active. The title bar of the active viewport is colored. The inactive viewports have gray title bars.
2. Use the horizontal and vertical panel tools to work on the data in active viewport or begin data acquisition using the active panel. Experiments started from the current active panel are run in the order of submission. Systems running an automated sample changer use only experiment 1 (which is in viewport 1) to submit samples to the automation queue. All other viewports are used for data processing and analysis.

Adding a Label to the Viewport

The default label for a viewport is the currently loaded experiment's file name.

1. Click inside a viewport's label box (viewport does not have to be active).
2. Select the contents of the box and overwrite the text with new text.
3. Click outside the text box. The new label associated with this viewport.

Setting Viewport Layout

Select a layout icon to arrange the view ports on the graphics canvas. Click on the Overlay Viewports to stack viewport on view port. The overlay is useful for placing high resolution 1D spectra on the appropriate 2D axes.

Icon	*Function*
	Auto layout arranges viewports in an optimized row by column matrix
	Horizontal layout of viewports
	Vertical layout of viewports

Aligning and Stacking Spectra

Requirements for Aligning and Stacking Spectra

Spectra can be a mixture of 1D and 2D data sets, all 2D data sets, or all 1 D data sets provided these requirements are met:

- All selected viewports need to use a common scale.

Data in the viewports may have different nuclei, different spectrum width, or different spectral regions. The common scale is determined based on data in all selected viewports and determines if alignment or stacking is possible. Overlaid and stacked spectra are drawn based on the common scales.

- Alignment is enabled if more than one axis in more than one viewport have the same axis (H1, C13 etc.).
- Stacking is enabled when data in all viewports have the same axis/axes.

Setting up Stacked Aligned Spectra

1. Select the **Viewport** tab from the vertical tabs panel.
2. Load each data set into a different viewport and process the data. Data must meet the the requirements for aligning and stacking spectra as described in the *NMR Spectroscopy User Guide* manual.
3. Select viewports containing spectra to overlay by placing a check in the check box under select.
4. Click on the **Overlay viewports** button to overlay all selected viewports.

The **Stack Spectrum** button, Figure 14, is displayed below **Overlay viewports** button if all spectra have the same dimension (all 1D or all 2D) and all axis/axes (nuclei) match. Stacked spectra are aligned and each spectrum is shifted along x and y. The shift between spectra is specified by **x** and **y** offset in the entry fields below **Stack Spectrum** button. Spectral axes are also synchronized to enable zoom and pan of the spectrum without losing the alignment.

Figure 14. 1D Stacked Spectra

The **Align spectra** button, Figure 15, is available if it is a mix of 1D and 2D spectra when multiple spectra are overlaid. All 2D spectra must have matching axes. All 1D data must

match one of the 2D axes. 1D spectra are aligned and displayed at the margins of the 2D

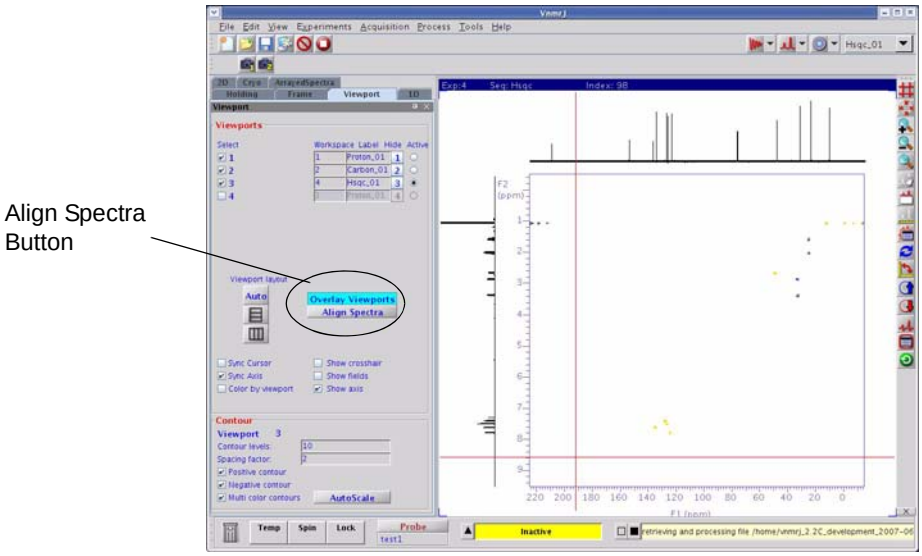


Figure 15. 2D Spectra with Overlaid 1D's

spectrum. 1D spectrum will be rotated if necessary to align with the 2D spectrum. Zoom and pan are synchronized when the spectra are aligned.

The stacked spectrum button for 2D's, Figure 16, is displayed below Overlay Viewport if all 2D spectra axes and nuclei match. Spectral axes are synchronized to enable zoom and pan of the spectra without losing alignment.

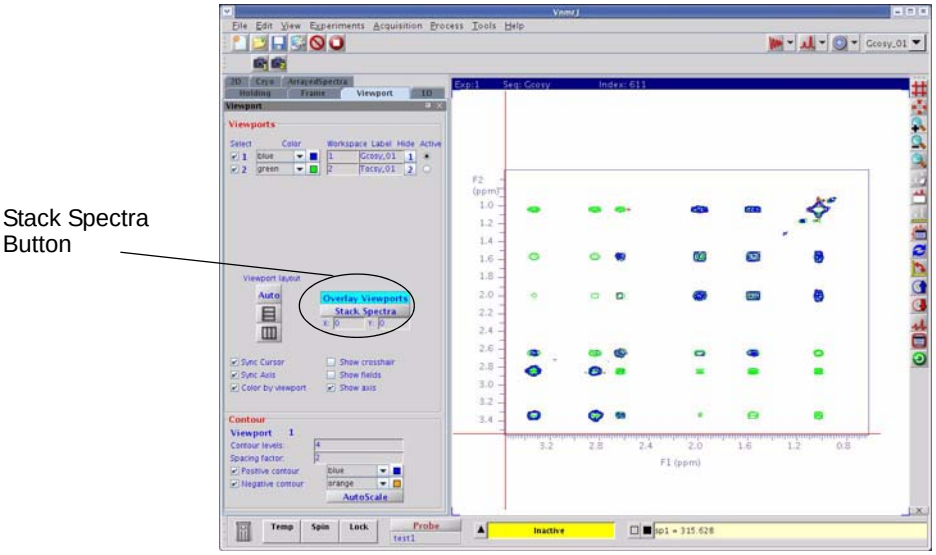


Figure 16. Stacked Overlaid 2D Spectra

Synchronizing Cursors and Axes

Check Box	*Function*
Sync cursor	Check this box to link and synchronize the cursors and cross hairs in multiple viewports.
Sync Axis	Check this box to link and synchronize axes in multiple viewports.Axis are synchronized to the current active viewport.

Setting Crosshair, Fields, and Axis Display Options

Check Box	*Function*
Show crosshair	Check this box to show crosshairs and display current position.
Show fields	Check this box to show information fields at the bottom of the active viewport canvas: vs 111.7 sp(ppm) 35.78 wp(ppm) 65.00 first 1 last 4 step 1
Show axis	Check this box to show the axis or remove the check to hide the axis.

Assigning Colors to Spectra by Viewport

Check Box	*Function*
Color by viewport	Check this box to display the spectral data using colors assigned by the viewport, see Figure 17. **Default color assignment**: spectra are displayed using a different color for each viewport if the box is checked. The spectra a displayed using the defaults assigned in the Display options window if this box is not checked **Change a color assignment:** Click on the dropdown color menu for a viewport and select a color for the spectral display in the viewport.

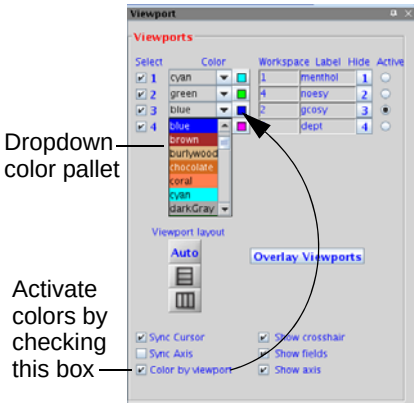


Figure 17. Setting Spectra Colors by Viewport

Display Check Boxes

The check boxes control of optional display features.

Check box	*Function*
Cross hair	Display cross hair and chemical shift(s) of the cursor position when mouse is moved over the spectrum. A useful function when the fields are not shown, not in cursor mode (default mode), or chemical shift of a peak without moving the left cursor is require while in the cursor mode.
Fields	Display cr, delta, vp etc... fields at the bottom of the viewport.
Axis	Show scale of the axis.
Show frame border	Check the box to display a box around the frame. Un-check the box to display the four corners of the selected frame as *hot spots* for resizing. No border or corner will be displayed for if a frame is not selected. An empty frame is not visible until it is selected.

Contour

The contour sub-panel, see Figure 18, appears exclusively for the active viewport with 2D data loaded and displayed in contour mode (`dpcon`).

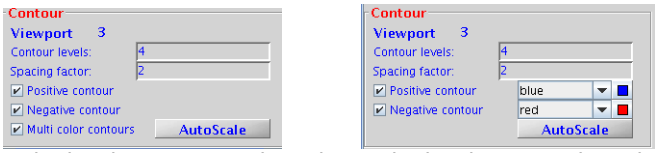


Figure 18. Contour Controls

The Contour panel has the following controls

Control	*Function*
Contour levels	Enter a number of contours between 4 and 32 in the field.
Spacing factor	Enter a number in the field to specify the spacing between contours. A number between 1.1 and 2 is recommended.
Positive contour	Check this box to show positive contours using the default color red.
Negative contour	Check this box to show negative contours using the default color blue.
Color dropdown	Each contour has a color dropdown menu.Select a color from the menu to use a color other then the default color.
Multi color contours	Options is not displayed if the Color by viewport box is checked.Check this option to use the colors defined in Display Option.
AutoScale	Automatically scale the spectrum.

Frame Panel

- “Text Insert” on page 67

Text Insert

Text Frame Tools

Text is placed into a text frame within the default frame of the active viewport using the tools on the Text tab, see Figure 19. The text frame can be selected, moved and resized in the same way as an inset or default spectrum frame. The content of each text frame is defined by a file.

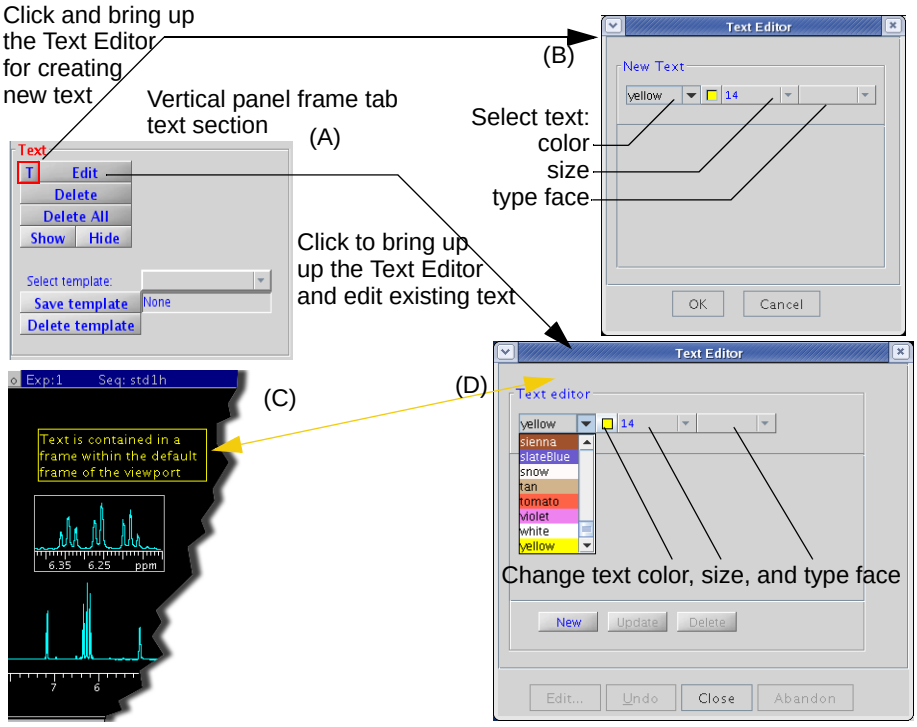


Figure 19. Text Panel Controls and Text Editor

Creating a Text Frame with Text

1. Do the following if the Text tab is not displayed to the left of the graphics canvas:
   a. Click on **View** on the main menu bar.
   b. Select **Text**.

2. Click on the **Text** tab, see Figure 19 (A).
3. Click on the **T** button, see Figure 19 (A).
4. The Text Edit window, see Figure 19 (B), appears.
5. Use the default text colors, text size, and type face or select a different text colors, text size, and type face using the dropdown menus.
6. **Enter the text** in the text box.

   The frames do not have a word wrap feature.

   Press the **Enter** key to create a new line of text within the same text frame.
7. Click the **OK** button to place the text and text frame on the graphics canvas and close the window.

   Click the **Cancel** button to close the window without placing any text on the graphics canvas.

Editing Text Inside a Text Frame

1. **Double click** inside the frame to make the frame active, see Figure 19 (C).

   An active frame has a yellow border.
2. Click on the **Text** tab, see Figure 19 (A).
3. Click on the **Edit** button on the Text tab.

   The Edit Text window is displayed, see Figure 19 (D).
4. Click a text frame to edit or change the type color, size, and or type face style.
5. Click **Update** to apply and display the changes to the text in the active text frame.

Moving a Text Frame

1. **Double click** inside the frame to make the frame active, see Figure 19 (C).

   An active frame has a yellow border.
2. Move the mouse cursor to an edge of the inset frame.

   The cursor changes from a single headed arrow to a four headed arrow.
3. Hold down the left mouse button and grab the edge of the frame.
4. Drag the frame to the new position.
5. Release the mouse button when the frame is at the desired position.

Resizing a Text Frame

1. **Double click** inside the frame to make the frame active, see Figure 19 (C).

   An active frame has a yellow border.
2. Move the mouse cursor to a corner of the inset frame.

   The cursor changes from a single headed arrow to a double headed arrow.
3. Hold down the left mouse button and grab the corner of the frame.
4. Drag the corner to resize the frame.
5. Release the mouse button when the frame is at the desired size.

Deleting One Text Frame

1. **Double click** inside the text frame to make the frame active.

   An active frame has a yellow border.

2. Click on the **Delete** button.

Deleting All Text Frames

- Click on the **Delete All** button.

Hiding and Showing Text Frames

- Hide — click on the **Hide** button.
- Show — click on the **Show** button.

Creating, Deleting, and Using Text Templates

- "Creating a Text Template" on page 69
- "Using a Text Template" on page 69
- "Deleting Text Template" on page 69

The supplied default template, `sampleInfo`, displays the content of the text file, in current `exp` directory, created from the comment text field in Study panel under the Start tab.

Creating a Text Template

1. Create one or more text frames on the graphics canvass.
2. **Enter a name in the field** next to the Save template button.
3. Click the **Save template** button.

   A template may contain one or more text frames. The current text display layout is saved as new template using the name entered in the field next to the Save template button. The template will be overwritten if the name already exists in template menu.

Using a Text Template

1. Click on the **dropdown menu** next to Select Template:
2. Select a **named template**.
3. Click on the a text frame to edit the content.

   The Edit Text window is displayed, see Figure 19(D).

4. Edit the text or change the type color, size, and or type face style.
5. Click **Update** to apply and display the changes to the text in the active text frame.

Deleting Text Template

1. Click on the **dropdown menu** next to **Select Template:**
2. Select a **named template**.
3. Click on the **Delete from menu** button.

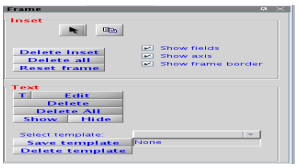
Creating a Spectrum Inset Frame

- "Inset Frame Buttons and Tools" on page 70

Inset Frame Buttons and Tools

The buttons delete one or all inset frames and restore the default frame to full size.

Buttons and Tools	*Function*
Delete Inset	Delete the selected inset.
Delete all	Delete all inset frames.
Full size	Restore default frame to full size.
 .	Select the inset mode tool
 .	Default mode tool



Creating the Inset Frame

An inset frame has the full capability of the default frame. The only difference is that the default always exists, while as an inset frame can be created and removed. Colors may vary depending upon color scheme used. Colors used here are for illustration of function only.

Create an inset frame within the default viewport frame as follows:

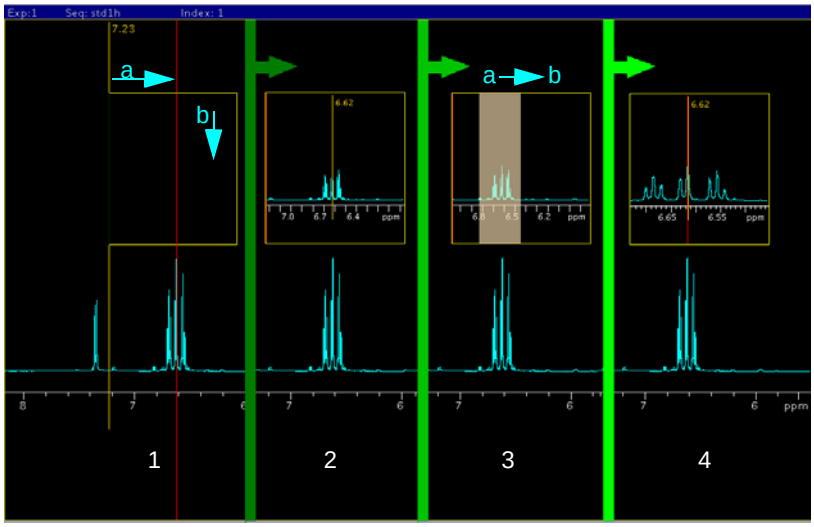


Figure 20. Creating an Inset Frame

1. Select the Frame vertical panel.
2. Select the inset mode tool  .
3. Place the cursor at the low field (left) side of the region to be expanded as shown in Figure 20 frame 1a.
4. Hold the left mouse button down and drag the inset window to the high field (right) side of the region.
5. Drag the cursor down to set the height of the inset frame as shown in Figure 20 frame 1b.

6. Release the mouse button to create the inset frame, see Figure 20 frame 2.

Zooming in on a Region Within an Inset Frame.

1. Select the default mode tool  .
2. Click inside the frame to make the frame active.

   A frame has a yellow border when it is active and white boarded when it is inactive (these are the default colors of inactive and active frames).
3. Select the zoom mode tool  .
4. Place the cursor at the low field (left) side of the region to be expanded as shown in Figure 20 frame 3a.
5. Hold the left mouse button down and drag the inset window to the high field (right) side of the region, Figure 20 frame 3b.

   The region selected is indicated by a transparent gray rectangle.
6. Release the mouse button and the selected region expands to fill the inset box, Figure 20 frame 4.

Resizing an Inset Frame

1. Select the default mode tool  .
2. Click inside the frame to make the frame active. An active frame has a yellow border.
3. Move the mouse cursor to a corner of the inset frame. The cursor changes from a single headed arrow to a double headed arrow.
4. Hold down the left mouse button and grab the corner of the frame.
5. Drag the corner to resize the frame.
6. Release the mouse button when the frame is at the desired size.

Moving an Inset Frame

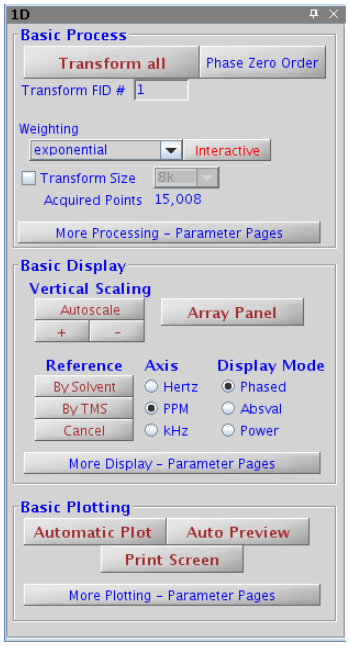
1. Select the default mode tool  .
2. Click inside the frame to make the frame active. An active frame has a yellow border.
3. Move the mouse cursor to an edge of the inset frame. The cursor changes from a single headed arrow to a four headed arrow.
4. Hold down the left mouse button and grab the edge of the frame.
5. Drag the frame to the new position.
6. Release the mouse button when the frame is at the desired position.

1D

Panel provides a reduced set of the full 1D process, display, and plot parameters available on the parameter pages of the process tab.

Control	*Description or Function*	*1D Vertical Panel*

Basic Process Controls



Transform all Button — Transforms the data displayed in the active view port using the parameters specified on the parameter pages and the values of the processing parameters in the Basic Process region.

Transform FID # — Enter a value corresponding a FID in an arrayed data set.

Transform Size — Check the box and select a transform size from the drop down menu. The number of acquired points is shown below the drop down menu.

More Processing – Parameter pages — Opens Default page of the Process tab.

Basic Display

Vertical Scaling buttons: Autoscale, (+), and (-). — Autoscale optimizes the display to utilize the available display area. The (+), and (-) buttons increase or decrease the vertical scale by a factor of 2.

Reference buttons

- By Solvent — Use the standard chemical shift of the solvent as reference.
- By TMS — Uses TMS at 0.0 PPM as the chemical shift reference.
- Cancel — Cancels either of the above two choices.

Axis radio buttons

- Hertz — Sets axis scale in Hz
- PPM — Sets axis scale in PPM
- kHz — Sets axis scale in kHz

Display Mode radio buttons

- Phased — Displays a phased spectrum
- Absval — Displays an absolute value spectrum.
- Power — Displays a power spectrum.

More Display – Parameter Pages button — Opens Display page of the Process tab.

Opens Display page of the Process tab.

Basic Plotting buttons

Automatic Plot Uses current plotting parameters and plots to the current plotter

Auto Preview Same as Automatic plot but creates a PDF and starts a PDF reader

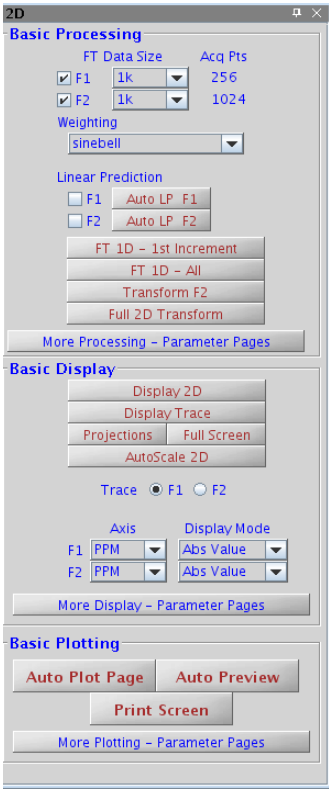
Print Screen Prints the current screen to the current output device

More Plotting – Parameter Pages button — Opens Plot page of the Process tab

2D

Panel provides a reduced set of the full 2D process, display, and plot parameters available on the parameter pages of the process tab.

Control	*Description or Function*	*2D Vertical Panel*
Basic Process Controls		
F1 check box	Check box to make F1 FT Data Size drop down menu active. Select the size of the F1 data set. F1 Acquired points are shown to the right of the menu.	
F2 check box	Check box to make F2 FT Data Size drop down menu active. Select the size of the F2 data set. F2 Acquired points are shown to the right of the menu.	
Weighting	Select a weighting function from the drop down menu	
Linear Prediction	Click on either or both the Auto LP F1 and Auto LP F2 buttons to enable or disable linear prediction during data is process. Placing or removing a check mark from a box is the same as clicking on a button.	
Processing Buttons	Data is processed as stated on the button using the processing parameters in the Basic Processing frame and on the parameter pages	
FT 1D - 1st Increment		
FT 1D - All		
Transform F2		
Full 2D Transform		
More Processing – Parameter Pages button	Opens the Default page of the Processing tab	
Basic Display		
Display 2D	Displays a contour plot of the 2D	
Display Trace	Displays a trace based on the Trace F1 F2 radio button selection.	
Projections		
Full Screen	Display data using the full size of the active viewport	
AutoScale 2D	Scales tallest peak to maximum color level, calculates the noise threshold, and optimizes the vertical scale.	
Axis	F1 and F1 drop down menus for selection of scale in PPM, Hz, or KHz.	
Display move	F1 and F1 drop down menus for selection Phased, Abs Value, or Power	
More Display – Parameter Pages button		



Opens the Display page of the Processing tab

Basic Plotting buttons

Automatic Plot Uses current plotting parameters and plots to the current plotter

Auto Preview Same as Automatic plot but creates a PDF and starts a PDF reader

Print Screen Prints the current screen to the current output device

More Plotting – Parameter Pages button — Opens Plot page of the Process tab

Arrayed Spectra and FIDs

The procedure here applies equally to the display and plotting of both spectra and FID arrays.

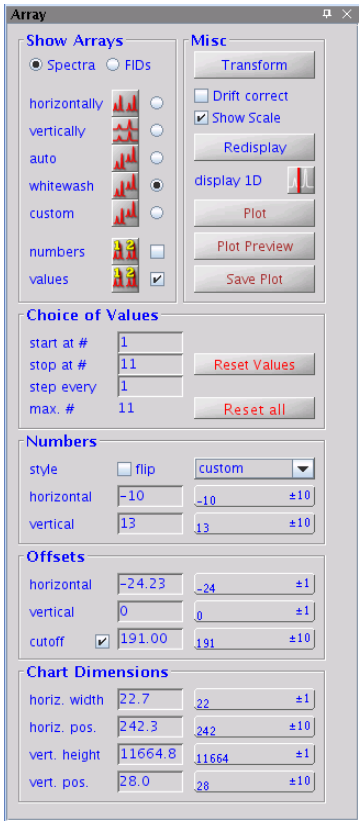
1. Select the type of presentation by selecting form the following choices of display modes for the arrayed spectra or FID:

- **horizontally** shows the spectra side-by-side.
- **vertically** aligns the spectra one above another.
- **auto** depends on the previously chosen display mode:

  Spectra are aligned vertically and the vertical offset is chosen such that all spectra together will cover the entire vertical space if the previous mode showed the spectra full screen (vertical mode or showing only a single 1D).

  A vertical offset is added to show the spectra along a diagonal if the previous mode was horizontal.
- **whitewash** aligns the spectra one above another like the vertical mode but this mode shows spectra behind each other, avoiding overprinting. Horizontal and vertical offsets can be adjusted.
- **custom** takes over the display properties of either horizontal, vertical, or auto modes but allows the choice of horizontal and vertical offsets.

2. Specify the elements of the arrayed data that are displayed by entering the following information in the **Choice of Values** region:



   a. Enter a starting value (the first element of the array to display) in the field next to **start at #**.

   b. Enter a stop value (the last element of the array to display) in the field next to **stop at #**.

   c. Enter a step value (to skip elements between the beginning and end of the array) in the field next to **step every**.

   d. Enter a maximum number of elements to display in the field next to **max #**.

   e. Use the **Reset Values** and **Reset all** buttons to return to the default settings

   Optional: turn on numbering of the array elements displayed by placing a check in the check box next to **number** or **values** in the **Show Arrays** region. Suppress all numbering by leaving the check boxes next to **number** and **values** in the **Show Arrays** region un-checked.

   a. Specify the orientation of the numbers; up-right or place a check in the check box (flip) to display the numbers rotated 90 degrees counter clockwise.

   b. Specify the position of the numbers from the options on the drop down menu next to the flip check box.

   c. Specify a horizontal and vertical positioning of the number with respect to the spectrum by selecting **custom** for the drop down menu and entering the positions of the numbers in the fields next to **horizontal** and **vertical**.

3. Specify the vertical and horizontal offsets for the display of the array in the vertical, whitewash, or custom array mode (Offsets entries are enabled only for these modes) as follows:

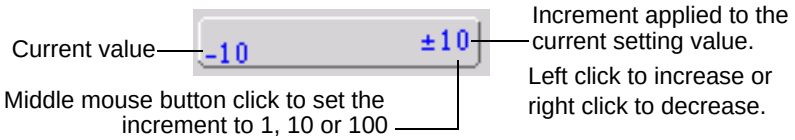
   a. Enter a value for horizontal offset in the field next to **horizontal**.

   The horizontal width (see below) must be smaller than the screen width to apply any horizontal offset.

   b. Enter a value for vertical offset in the field next to **vertical**.

   c. Adjust the positions as needed using the buttons next to each field.

   Right mouse click on the button to increase the value or left mouse click on the button to decrease the value the increment shown on the left side of the button.



d. Switch on or off a cutoff to avoid overlapping large lines that may reach into the spectra above.

4. Set the chart dimensions as follows:
   a. Enter a value for horizontal width in the field next to **horiz. width**.
   b. Enter a value for horizontal position in the field next to **horiz. pos**.
   c. Enter a value for vertical height in the field next to **vert. height**.
   d. Enter a value for vertical position in the field next to **vert. pos**.
   e. Adjust the positions as needed using the buttons next to each field.
5. Use the functions in the Misc region to do the following as needed:
   - Click on the **Transform** button to Fourier transform the current FID data.
   - Check the **Drift box** to apply drift correction (corresponds to "dc" command) to all subspectra of the array.
   - Check the **Show scale** box to switch on or off a scale below the first spectrum or FID of the array.
   - Click on the **Redisplay** button to refresh the screen.
   - Click on the display 1D icon  to show a single spectrum/FID and use the toolbox to manipulate and zoom.
   - Click on the **Plot** button to send of the current array display to the current plotter
   - Click on the **Plot Preview** button to plot the array to a PDF file and open Acrobat reader with the PDF of the current array.
   - Click on the **Save Plot** button to save a plot file in the format as chosen on the Plot parameter panel.
   - Settings on the Plot parameter panel for parameter printing are used. Plotting from the ArrayedSpectr vertical panel controls does not plot integrals, integral values, and peak frequencies.

3.5 Panel Levels and User Profiles

Panel Levels

The panel level value determines what panels are displayed. The panel level defaults to the value set for the operator through the VnrmJ Adm interface, see *VnmrJ Installation and Administration* for details.

<value>	*Display for panellevel=<value>*
0-9	Show minimum number of pages – used for automated sample handling No shim, lock, or processing, and minimal parameter control is available.
10-29	Default for Walkup operator. Shim and lock are available if a sample handler is not present or `traymax`=0. Basic processing is available. Pages are not fully populated, allowing control of a few basic parameters.
30-100	Default for the account administrator. All pages are available and fully populated.

User Profiles

The walkup account owner user profile is set by the system administrator, see *VnmrJ Installation and Administration*. The default for the walkup account owner permits the account owner to allow editing of protocols by operators assigned to the account.

Set the user profile for the operators as follows:

1. Login to the system as the walkup account owner.
2. Click on **Edit** on the main menu.
3. Select **Edit config profile…**

   The Edit User Config Profile window is displayed.
4. Place a **check in a box** to grant permission or **remove the check** to withdraw permission to show the protocols.
5. Click on **Save** to save the changes and exit the window or Close to exit the window without applying any changes.

3.6 Setting Colors in VnmrJ

Using Standard Styles and Themes

Access the Styles and Themes window as follows:.

1. Click on **Edit** on the main menu.
2. Click on the **Display Colors** tab to show the colors of the current color scheme, see Figure 21.

   Styles and themes supplied with VnmrJ are displayed in italics: *classic*, *default*, and *beach_house*.

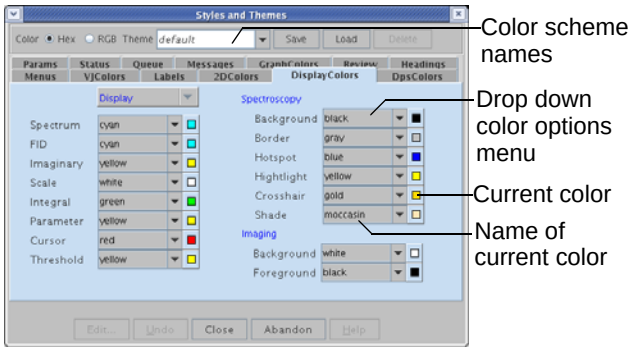


Figure 21. Setting Display Colors

3. Select a theme.
4. Click on Load to apply the theme.
5. Click on **Close** to exit the window or **Abandon** to exit and make no changes in the current display.

Creating, Editing, and Applying Styles and Themes

1. Click on **Edit** on the main menu.

2. Click on the **Display Colors** tab to show the colors of the current color scheme, see Figure 21.
3. Do one of the following:
   - Enter a name in the color scheme field and click **Save**.
   - Select a theme to edit from the list of themes.

   Names of user defined styles and themes are listed in a bold regular type face.
4. Click a radio button next to Color to show color definitions in either **HEX** or **RGB**.
5. Click on a tab and edit colors and type faces as required using the dropdown menus.
6. Click on **Save** to save the changes to the file named in the theme field.
7. Click on **Load** to load the new color scheme.
8. Click on **Close** to exit the window.

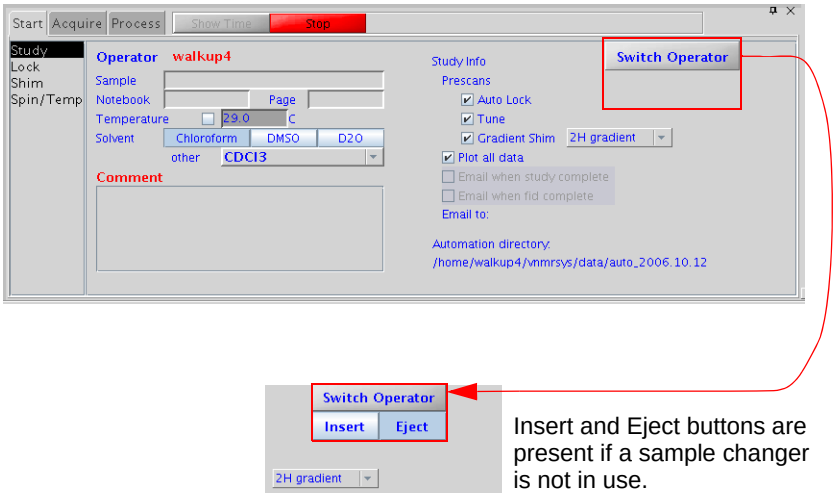
Deleting Styles and Themes

1. Click on **Edit** on the main menu.
2. Click on the **Display Colors** tab to show the colors of the current color scheme, see Figure 21.
3. **Select** a theme to delete from the list of themes.
4. Click on **Delete** to remove the theme.
5. Click on **Close** to exit the window.

3.7 VnmrJ Walkup Tabs and Panels

The default operator panels listed under the Start tab depend on whether or not a sample handler is active. The default operator panel level is `panellevel=10`, see “Panel Levels” on page 76. Additional panels are displayed depending upon the panel level set by the VnmrJ system administrator for the operator. The walkup account owner has the full set of panels available.

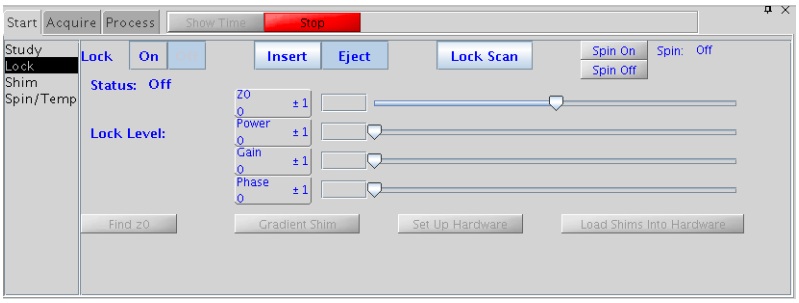
Study Page -- Always Displayed



Insert and Eject buttons are present if a sample changer is not in use.

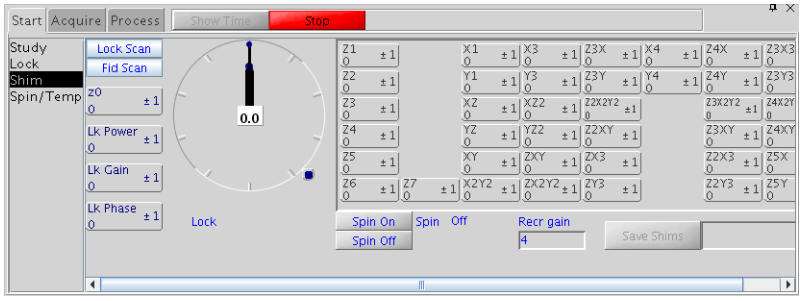
Operator	Identifies the name of the operator that is logged in.
Sample	Enter sample information (optional).
Notebook	Enter notebook information (optional).
Temperature	Enter a sample temperature value. Check the box to select variable temperature operation.
Solvent	Click on a lock solvent button or select a solvent from the drop-down menu of solvents.
Comment	Enter additional information (optional).
Prescans options	Find z0 — find lock frequency. Tune — use ProTune to tune the probe prior to running the sample. Gradient Shim— use preset gradient shimming method and adjust homogeneity. Select either deuterium or proton gradient shimming from the dropdown menu.
Plot all data	Plot all data at the end of the acquisition.
Email to:	Select Email when study is complete or Email when fid is complete

Lock Page -- Displayed if Sample Handler is Not Active



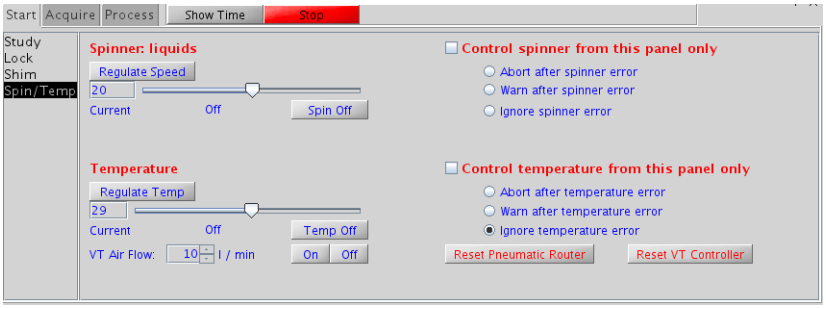
Lock	Turn lock on or off. Status shows the current lock status. Lock Level displays the current lock level.
Find z0	Find the lock frequency.
Gradient Shim	Adjust homogeneity using preset gradient shimming method.
Set Up Hardware	Downloads values to hardware.
Load Shims Into Hardware	Loads the current shims into hardware.
Spin On and Spin Off	Turn sample spinning on or off.
Lock Scan	Display interactive lock in display canvas.
Fid Scan button	Display interactive fid in display canvas.
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 shown in the Entry field.

Shim Page -- Displayed if Sample Handler is Not Active



Lock Recr gain	Enter new value and display current value.
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	Enter a name in the entry field and press return to activate the Save Shims button then click on the button to save the shims using the name in the entry field.

Spin/Temp Page -- Displayed if Sample Handler is Not Active



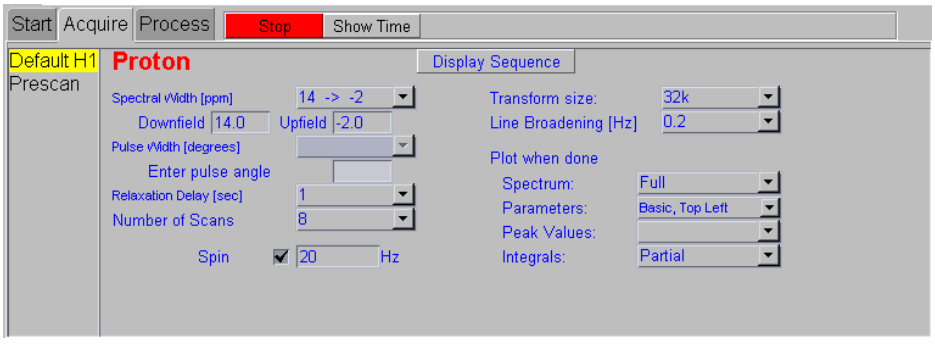
Spinner	Regulate Speed – click to regulate spinning speed and the set value. Slider – move until desired value is displayed in the Entry field. Entry field – Regulate spinning speed at set value. Spin Off – click to stop spinning.
Temperature	Regulate Temp – click to regulate sample temperature at set value. Entry field — enter a value. Slider — move until desired value is displayed in the Entry field. Temp Off – click to stop temperature regulation.
Error handling	Select how spinning or temperature errors are handled and reported.
Reset Pneumatic Fault	Click to clear pneumatic fault.

VnmrJ Walkup Operator Acquire Tab and Pages

The Default and Prescan pages available to automation and single-sample users.

- “Default Experiment Page” on page 81
- “Prescan Page” on page 82

Default Experiment Page



The full name of this page changes to correspond to the experiment. The experiment, in this example, is a proton 1D, the default page label is Default H1, and the panel title is Proton.

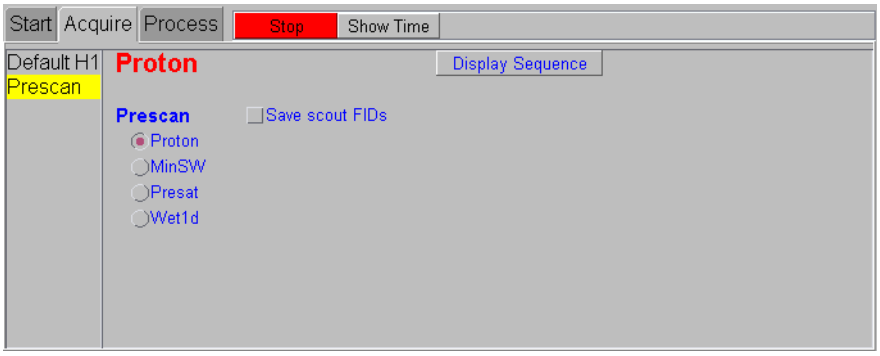
Click the **Display Sequence** button to display the pulse sequence on the graphics canvas.

Acquisition parameters that are typically customized by an operator for an 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 dropdown menu.

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 the default setting for the option is used.

Prescan Page



This page is present only if it is relevant to the experiment. Only Proton, Presat, and Wet1d protocols have a Prescan page.

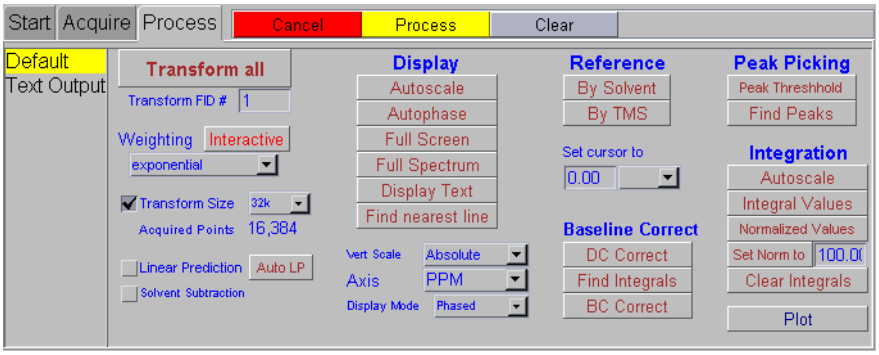
Prescan options are typically presented as radio buttons. Click the prescan options of choice. Some options are enabled by checking a box, selecting a menu, or entering a value into an input field.

VnmrJ Walkup Operator Process Tab and Pages

The Defaults and Text Output pages are available to automation and single-sample users.

- “Defaults Page” on page 82
- “Text Output Page” on page 83

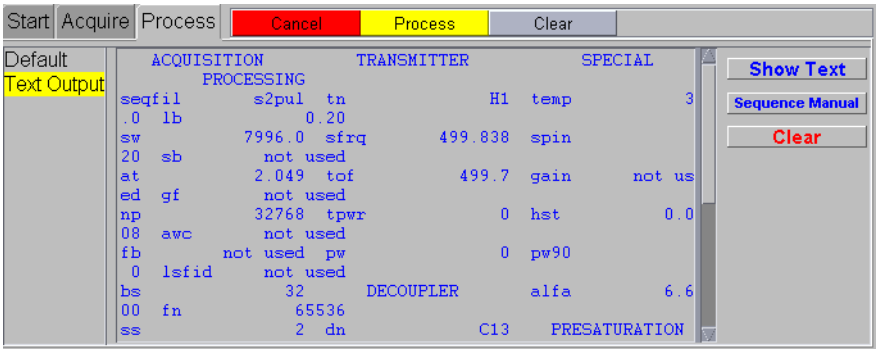
Defaults Page



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

Text Output Page

The Text Output page displays various text outputs. There are three buttons:



Show Text	Show the text associated with the experiment file.
Sequence Manual	Online pulse sequence manual.
Clear	Clear the text window

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