Agilent VnmrJ 4.2

Familiarization Guide

Agilent Technologies

Notices

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This guide is valid for 4.2 and later revisions of the Agilent VnmrJ software, until superseded.

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Contents

1 Introduction

This guide provides an overview of the Agilent VnmrJ software and how you use it to acquire and process NMR spectra using Agilent NMR Spectrometers. Descriptions of the VnmrJ program user interface, toolbars, and menu items are included, along with general overview and description of the VnmrJ workflow. For more detailed information on the various workflow steps, see the *Agilent VnmrJ Spectroscopy User Guide* provided with your system.

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Introduction to VnmrJ Workflow

The VnmrJ program is used to acquire and process data from your Agilent NMR spectrometer. Collecting an NMR spectrum requires the following steps. These steps are described in the following sections. For information on the VnmrJ program window, toolbars, and menu items, see "VnmrJ Interface" on page 15.

- Preparing for an Experiment – prepare and load the sample, tune the probe, and shim.
- Acquiring Data – select experiment to be run on the sample and enter sample information, or create a study containing multiple experiments to run on one or more samples.
- Processing Data – use the data processing tools to optimize the spectrum display.
- Plotting Data – use the plotting tools and Graphics Toolbar to adjust the displayed spectrum for the desired output.

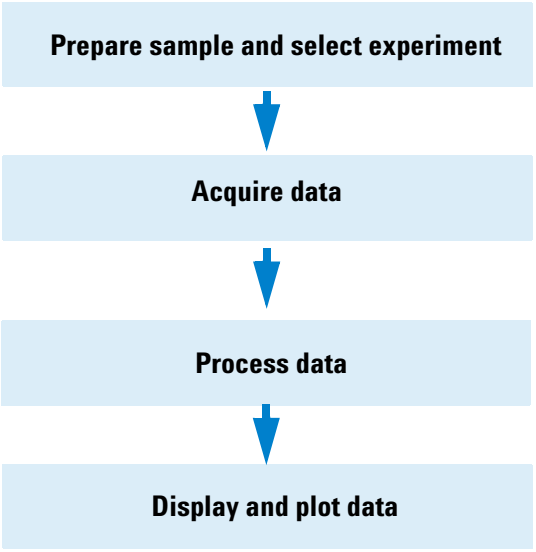

Figure 1 VnmrJ workflow

Commonly Used VnmrJ Terms

The following table lists some common VnmrJ terms that are used in this guide.

Table 1 Commonly used VnmrJ terms

Item	Description
Experiment	Combination of a pulse sequence, a parameter set, and possibly a data set.
Experiment Protocol	Software device that creates an experiment by executing a macro to set up parameters for a given pulse sequence. In Review Mode, a protocol operates in the current workspace and is typically followed by data acquisition. In Submit Mode, a protocol adds a node to the Study Queue for subsequent execution at run-time, followed by the start of data acquisition.
Sample	A physical object, either a tube with liquid or a solid sample in a rotor.
Study	Collection of one or more nodes in the Study Queue. In general, each node represents an experiment. A study is a list of operations to perform; it is not necessarily associated with a specific sample or any other physical object.
Study Queue	Interface feature that is used to display all the various types of queues that are available in VnmrJ. The Study Queue can be configured to show information in several different ways.

Table 1 Commonly used VnmrJ terms (continued)

Item	Description
Submit Mode and Review Mode	When you are interacting with data, processing/plotting data, or collecting data in manual mode, you interact with the software in Review Mode. When you use the Study Queue to load, build, edit, customize, or otherwise work with a study, the software is in Submit Mode. Submit Mode is entered by clicking the **New Study**, **Edit Study**, or **Continue Study** buttons. The interface is moved into Review Mode when you click the **Done** button in the Study Queue window (or it happens automatically upon sample submission).
Viewport	Interface feature that is used to display the contents of a workspace.
Workspace	Directories that can be thought of as digital objects to hold an experiment and/or data set. Equivalent to the idea of exp1, exp2, exp3, exp(n) in older versions of Vnmr.

Where to Find Help

Agilent provides a complete set of documentation to get you started generating quality data as quickly as possible. The following table contains a summary of the manuals and user guides provided, and what kind of information they contain.

Table 2 VnmrJ manuals and their uses

Manual title	Provided as	Information in this manual
VnmrJ Installation Guide	Printed, PDF, and in online help	Instructions on how to install Linux and the VnmrJ software
VnmrJ Administration Guide	PDF, and in online help	How to administer the VnmrJ system, including adding and changing users, and setting permissions and preferences
VnmrJ QuickStart	Printed, PDF, and in online help	Step-by-step overview of how to use Agilent VnmrJ software to collect an NMR spectrum on NMR systems with or without a Robot Sample Changer
VnmrJ Familiarization Guide (this document)	Printed, PDF, and in online help	Overview of the VnmrJ software, including description of the interface, menus, and commonly used tasks
VnmrJ Spectroscopy User Guide	PDF, and in online help	A more in-depth description of using the VnmrJ software to set up studies, perform shimming, and acquire, process, display, and output data
NMR System Calibrations Guide	PDF, and in online help	Use of VeriPulse, Autotest, and system calibrations are described
Basic NMR Experiments Familiarization Guide	PDF, and in online help	Provides a more detailed discussion about some of the most commonly used pulse sequences available in the VnmrJ Experiment Selector
Experiment Reference Guide	PDF, and in online help	Complete descriptions of VnmrJ experiments
Command and Parameter Reference Guide	PDF, and in online help	Comprehensive listing of VnmrJ commands and parameters
User Programming Guide	PDF, and in online help	Comprehensive pulse sequence programming and customization reference

Table 2 VnmrJ manuals and their uses (continued)

Manual title	Provided as	Information in this manual
CRAFT User Guide	PDF, and in online help	Overview and step-by-step instructions for using the CRAFT (Complete Reduction to Amplitude Frequency Table) application within VnmrJ
BioPack Quick Start Guide	Printed, PDF, and in online help	Step-by-step overview of using the BioPack option
BioPack User Guide	PDF, and in online help	Complete information on how to use the BioPack option
BioPack Experiment Guides	PDF, and in online help	Descriptions of BioPack experiments
SolidsPack User Guide	PDF, and in online help	Describes the use of SolidsPack, used to run a solids experiment and control solids console accessories such as shims, variable temperature, and magic- angle spinning
3D Gradient Shimming User Guide	PDF, and in online help	Description of how to use the Agilent 3D Gradient shimming software, used to map and optimize room- temperature, shim systems without additional hardware

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http://www.chem.agilent.com/en- us/ContactUS/Pages/ContactUs.aspx

2 VnmrJ Interface

This section contains descriptions of the main features of the VnmrJ program interface.

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VnmrJ User Interface

The main areas of the user interface for VnmrJ are shown in Figure 2. These areas are described in more detail in other sections of this guide.

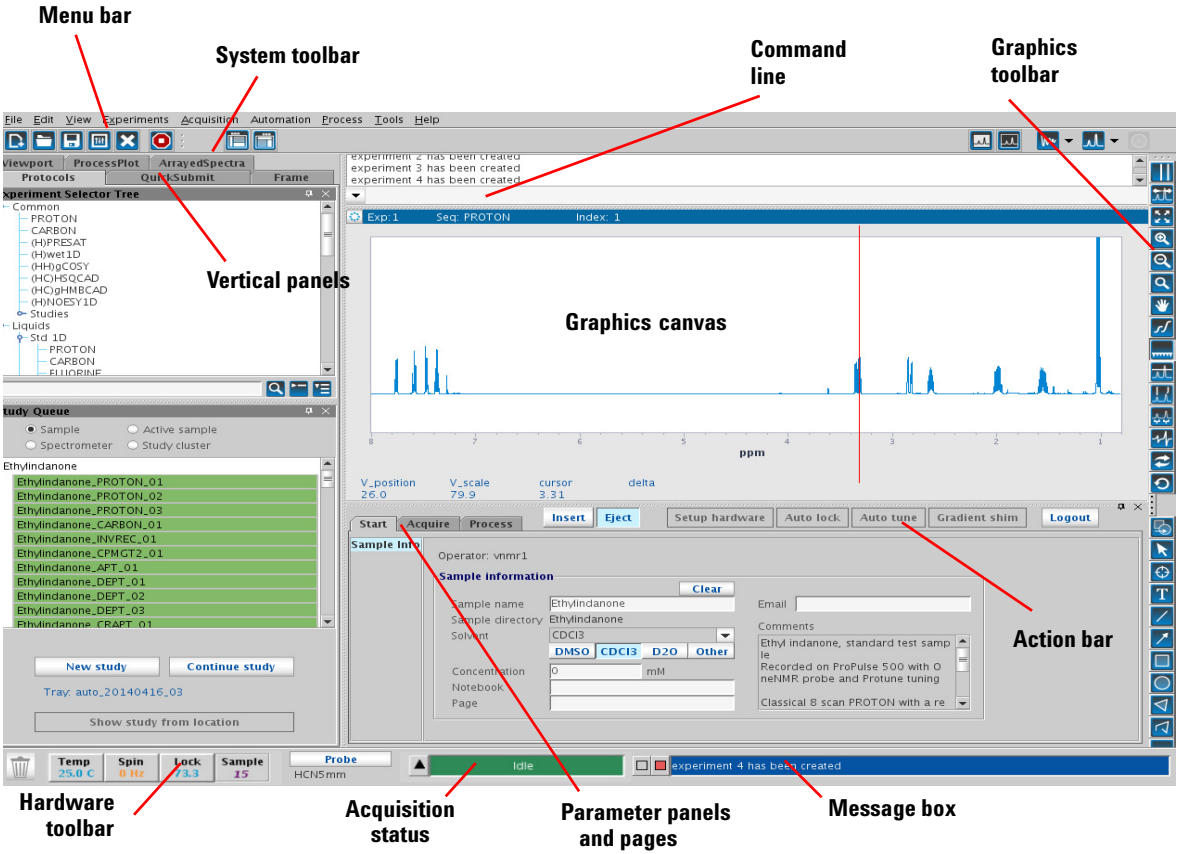


Figure 2 VnmrJ user interface

Toolbars

The VnmrJ toolbars provide quick access to commonly used functions. To view a description of a toolbar icon, move the mouse cursor over the icon until the description appears.

System toolbar

The system toolbar provides access to common system functions. It also lets you show or hide graphics toolbars.

Table 3 System toolbar controls

Icon	Description
	Create a new workspace.
	Opens the File Browser to search for and open a file.
	Opens the File Browser to find a location and save data.
	Opens the Styles and Themes pop-up, where you can select or customize colors or color themes for the VnmrJ user interface.
	Cancel a command.
	Save current screen layout: graphics, parameter panel, locator sizes.
	Save current screen layout: graphics, parameter panel, locator sizes.
	Draw spectral data using a light background. This does not change the User Interface theme.

Table 3 System toolbar controls (continued)

Icon	Description
	Draw spectral data using a dark background. This does not change the User Interface theme.
	Opens the Display FID toolbar controls.
	Opens the 1D display spectrum toolbar controls.
	Opens the nD display toolbar controls.

Hardware toolbar

The Hardware toolbar, located at the bottom of the VnmrJ window, shows a trash can icon and a display area dedicated to real-time hardware information.

Figure 3 Hardware toolbar

Sample temperature, spin rate, lock level, and current sample changer location are displayed to the left of the Hardware toolbar.

Status plots

The status plots provide useful information about sample temperature, spin rate, lock level, and current sample changer location. For more information, see “Status Charts” on page 95.

Acquisition status

Real time events such as system being idle, locking, shimming, or acquiring data are displayed in the field located to the right of the probe file. If the system is active, each event's remaining time is displayed.

Message box

To the right of the Hardware toolbar is a system message box. Error messages and other important system information are displayed in this area.

Graphics toolbar

The Graphics toolbar is used to control the interactive display in the graphics canvas.

See also

"Common graphics display toolbar controls" on page 19

"1D display spectrum toolbar controls" on page 20

"nD display toolbar controls" on page 21

"Display FID toolbar controls" on page 23

For more information on using the graphics toolbar, see "Interacting with the Spectrum Using the Graphical Toolbar" on page 165.

Common graphics display toolbar controls

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

Table 4 Graphic display toolbar controls

Icon	Description
	Reset to full display.
	Zooms in to a region in graphics canvas defined by cursor placement. (Click mouse once to define first cursor and then again to define second cursor.) To zoom further, click to define cursor positions, and then click the zoom icon again.
	Zooms out.
	Pan, or “rubber band” zoom. Click once to define first cursor, then click again and drag.
	Redraw display.
	Return to previous tool menu.

1D display spectrum toolbar controls

The following table shows the icons that appear when you click the 1D Display icon on the graphics toolbar. 

Table 5 1D display Spectrum toolbar

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 region.
	Click to expand to full spectral display.

Table 5 1D display Spectrum toolbar (continued)

Icon	Description
	Display integrals menu.
	Display partial integrals.
	Display full integral.
	Hide integrals.
	Define integrals.
	Adjust integral level/tilt.
	Delete integrals.
	Display or hide scale.
	Pan or move spectral region.
	Toggle threshold on or off.
	Phase spectrum.

nD display toolbar controls

The following table describes the icons displayed when you click the 2D or 3d Display icon on the Graphics toolbar. 

Table 6 nD display toolbar controls

Icon	Description
	Display color map and show common nD graphics tool.
	Display contour map and show common nD graphics tool.
	Display stacked spectra and show common nD graphics tool.
	Display image map and show common nD graphics tool.
	One cursor in use, click to toggle to two cursors.
	Two cursors in use, click to toggle to one cursor.
	Expand to full display.
	Pan and stretch.
	Show trace.
	Show projections.
	Shows horizontal maximum projection across the top of the 2D display.
	Shows horizontal sum projection across the top of the 2D display.
	Shows vertical maximum projection across the top of the 2D display.
	Shows vertical sum projection down the left side of the 2D display.
	Rotate axes.

Table 6 nD display toolbar controls (continued)

Icon	Description
	Increase vertical scale 20%.
	Decrease vertical scale 20%.
	Phase spectrum menu.
	First spectrum selection.
	Second spectrum selection.
	Enter peak pick menu.

Display FID toolbar controls

The following table contains descriptions of the commands available from the menu that appears when you click the Display FID icon in the Graphics toolbar. 

Table 7 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

Table 7 Display FID toolbar controls (continued)

Icon	Description
	Click to show real and zero imaginary
	Click to show real only
	Toggle scale on and off
	Phase FID

Annotation toolbar controls

The following table describes the icons displayed in the graphics toolbar (**View > Toolbars > Graphics Toolbar**) in "ds", "dss", and "dconi" display modes.

Table 8 Annotation toolbar controls

Icon	Description
	Toggle to show or hide annotations in graphics canvas and hard copy plot
	Select annotation for editing. Use this mode to move or delete an annotation, or change properties such as color and line thickness.
	Position – displays the value of the position where it is located, in Hz, PPM, etc. The value is updated automatically as the annotation is moved.
	Text – Text with adjustable font, size, style, color, and transparency.
	Line – Line with a adjustable thickness, color, and transparency.
	Arrow – Arrow with adjustable thickness, color, and transparency.
	Box – Box with adjustable thickness, color, and transparency, with rounded or square corners.

Table 8 Annotation toolbar controls (continued)

Icon	Description
	Oval – Oval with adjustable thickness, color, and transparency.
	Polygon – Polygon with adjustable thickness, color, and transparency.
	Polyline – Connected lie segments with adjustable thickness, color, and transparency.
	X-Bar – displays its width in Hz, PPM. The value is updated automatically as the annotation is resized.
	Y-Bar – displays its height in intensity units, or for 2D data, in Hz, PPM, etc. The value is updated automatically as the annotation is resized.

Command Line

One of the most powerful aspects of the VnmrJ software is the ability it provides to users to execute commands and macros directly using the Command Line. For more information on VnmrJ commands and macros, see the *Agilent VnmrJ Command and Parameter Reference Guide* and the *Agilent VnmrJ User Programming Guide*.

Graphics Canvas

The Graphics Canvas is used to display and interact with graphic and text information. For more information, see "Interacting with the Spectrum Using the Graphical Toolbar" on page 165.

When a spectrum is first displayed on the Graphics Canvas, or the display is refreshed, the bar above the Graphics Canvas displays the functions of the left and right mouse buttons and the scroll wheel:

- Use the left mouse button to set the left cursor,
- Use the right button to set the right cursor
- Use the scroll wheel to adjust the vertical scale of the spectrum

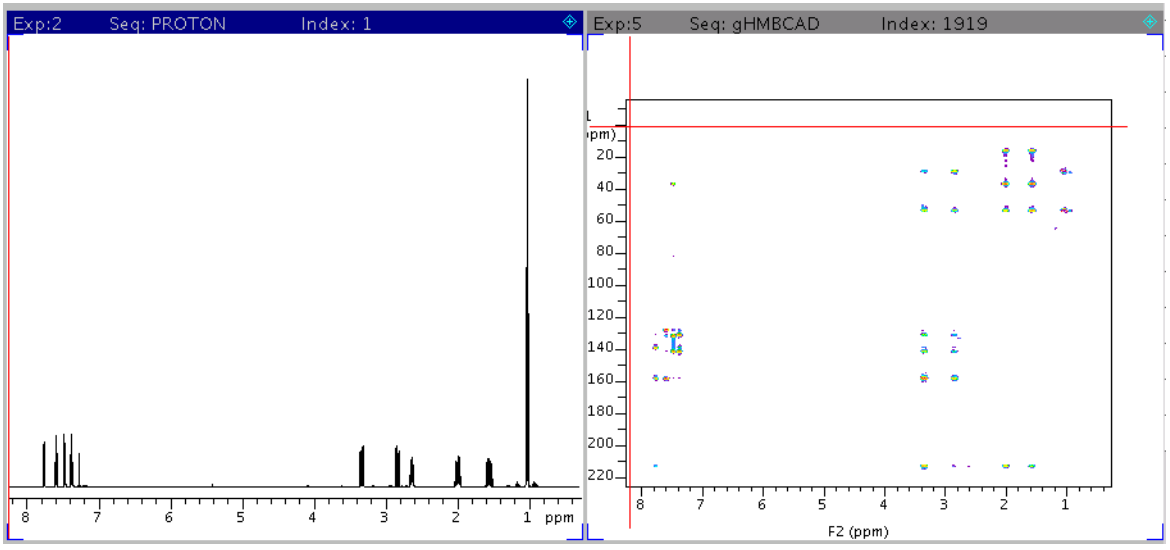


Figure 4 Graphics Canvas

Tray display

If you have a robot sample changer, a graphical display of the changer gives you access to a menu of commands when you right-click the mouse button over the tray display.

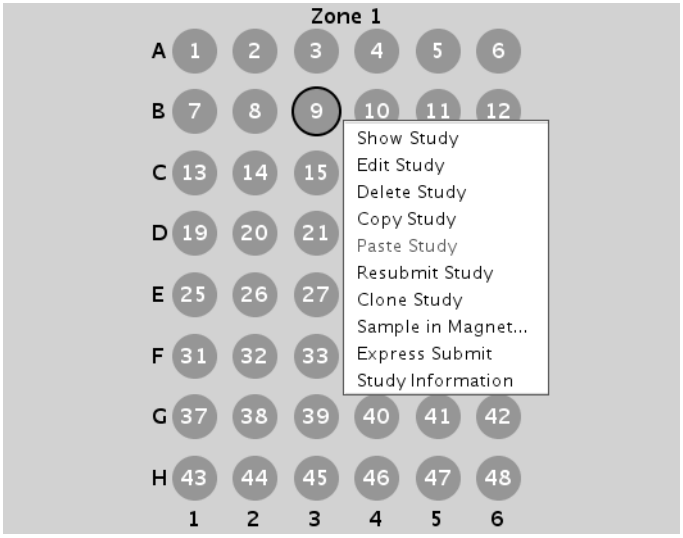


Figure 5 Tray display menu

Table 9 Tray display menu options

Item	Description
Show Study	Displays the queue for the selected location in the Study Queue.
Edit Study	Loads a study into the **Study Queue** from the tray display in preparation for modification of that study.
Delete Study	Deletes the selected location queue.
Copy Study	Copy Study to clipboard.

Table 9 Tray display menu options (continued)

Item	Description
Paste Study	Paste Study from clipboard.
Resubmit Study	Resubmits the selected location to acquisition.
Clone Study	Clones the selected location queue.
Sample in Magnet	Displays the Sample in Magnet popup, preloaded with that location for a sample change operation.
Express Submit	Utility to submit a sample to a specific location using automation, see Using Express Submit with a sample changer.
Study Information	Displays information about Study.
Swap Queue	Swaps experiments queued in the day to night and vice versa. Only displayed if there is an active Study in the selected location.

Vertical Panels

The vertical panels area of the VnmrJ user interface provides quick access to related functions. Each vertical panel contains one or more functional areas where you perform tasks such as selecting experiments and setting up data display.

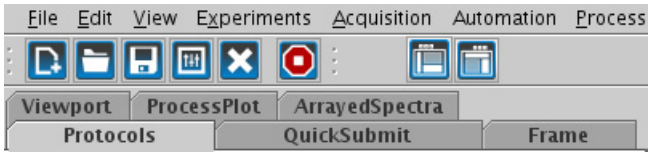


Figure 6 Vertical panel tabs in VnmrJ

For more information, see "Protocols Vertical Panel" on page 31, "QuickSubmit vertical panel" on page 39, "Frame vertical panel" on page 41, "Viewport vertical panel" on page 45, and "ProcessPlot vertical panel" on page 49.

Protocols Vertical Panel

The Protocols vertical panel contains the Experiment Selector, the Experiment Selector Tree, and the Study Queue. To show or hide one or more of these panels, click **View** and then select the item you want to show or hide. See also Experiment Selector, Experiment Selector Tree, and Study Queue.

Experiment Selector

The Experiment Selector can be used to load studies into the Study Queue or the current workspace. When an experiment is selected in Experiment Selector, all submissions to automation can be selected by double-clicking and experiment or dragging and dropping it to the Study Queue. You can configure families of experiments and content by using the Experiment Selector. Simple or complex experiments, based on an account or an operator within an account, are accessible as needed.

Use the Experiment Selector Editor to change the order and display of experiments/protocols within the Experiment Selector. For more information, see "Experiment Selector Editor" on page 90.

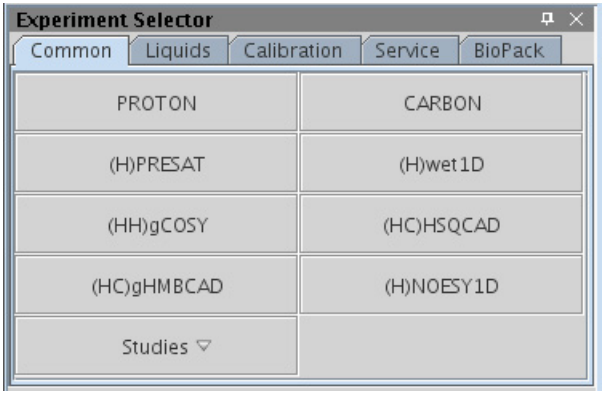


Figure 7 Experiment Selector

Experiment Selector Tree

The Experiment Selector Tree is a convenient way to view the available experiments. Instead of displaying the experiments in tabs (as in the Experiment Selector) experiments are grouped under their respective experiment types. Use the buttons at the bottom of the panel to expand or contract the tree and to search through the tree for an experiment using part or all of the name.

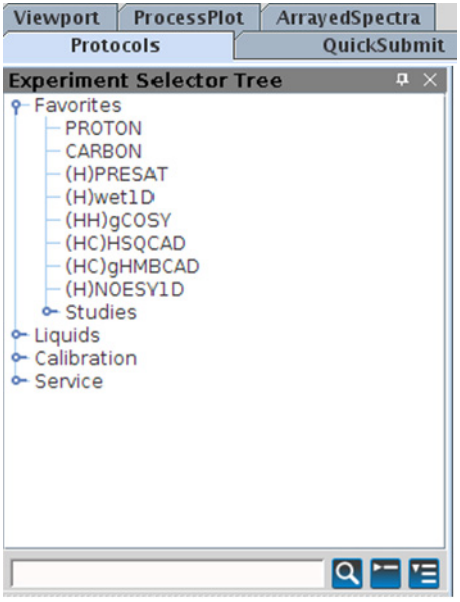


Figure 8 Experiment Selector Tree

Table 10 Experiment Selector buttons

Button	Action
	Type text in this field, and click the search button. The tree view is expanded and selects the first experiment/protocol with a name that contains the text. Click the search button additional times to continue the search further down the tree until the bottom of the tree is reached, at which point the search resumes at the top. Searching for a "Find" text that is not matched anywhere keeps the existing tree view, but does not match a selection.
	Collapses an expanded tree
	Expands the tree view

Study Queue

VnmrJ allows the ability to construct a linked list of experiments as a Study Queue that can be performed on any given sample. The appearance of the Study Queue changes depending on if you have a sample changer installed, or when in Submit mode or Review mode. For more information, see "Build a Study Queue" on page 151.

A Study Queue is used for both data acquisition and processing. Its many functions are described in more detail in the *Agilent VnmrJ Spectroscopy User Guide*.

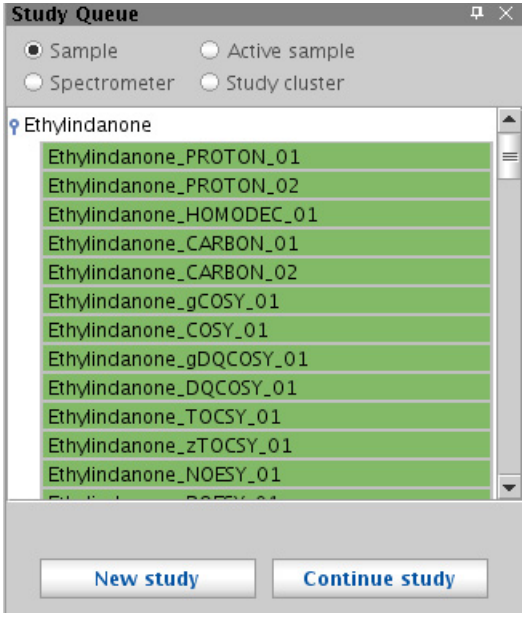


Figure 9 Study Queue—Review mode with no sample changer

Table 11 General Study Queue features

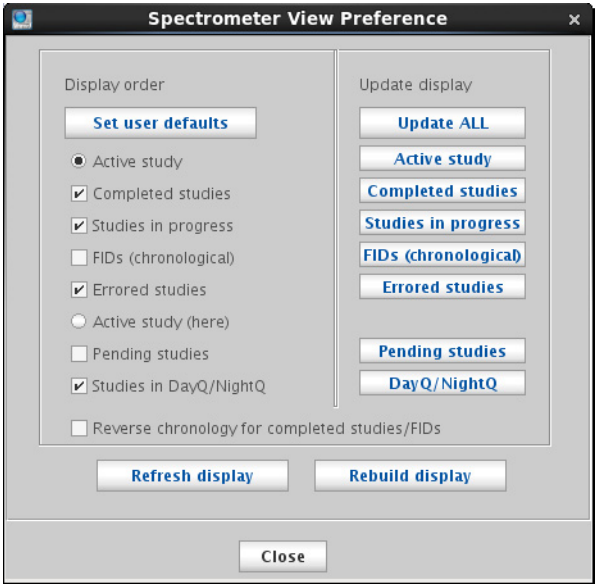
Item	Description
View	Selections that determine what is displayed in the Study Queue: Sample — displays the study linked to the data in the current workspace Spectrometer — displays all studies in the current automation run Active Sample—displays the currently acquiring study Study Cluster—displays study cluster, if one is defined
New Study	Initializes a new study and moves the software to Submit mode
Continue Study	Used to modify the current study displayed in the Study Queue
Show Study from Location (robot changer only)	Loads a study from the tray display

Table 12 Study Queue features — Submit Mode

Item	Description
Cancel	Abandons any changes made to the current study and returns the software to Review mode.
DayQ (robot changer only)	Runs study according to schedule set in DayQ. The schedule is set by the account administrator using the Automation tab of the Edit > Preferences window.
NightQ (robot changer only)	Runs study according to schedule set in NightQ. The schedule is set by the account administrator using the Automation tab of the Edit > Preferences window.
Priority sample (robot changer only)	Allows a sample to be submitted ahead of all other samples in the current automation run. This feature is controlled by the system administrator on an operator-by-operator basis.
Submit	Submits the current study to acquisition, using one of the following choices: Automation–submits the study to the Spectrometer Queue. Foreground exp–submits the study to acquisition in the current workspace. Background–submits the study to a background copy of VnmrJ.
Foreground (shown when not using robot sample changer)	Submits the study to acquisition in the current workspace.
Background (shown when not using robot sample changer)	Submits the study to a background copy of VnmrJ.
Clear Pending Exp from Queue	Deletes all pending experiments from the current Study Queue.

Table 13 Study Queue features — Review Mode

Item	Description
Options	Available when in Spectrometer view. Configure and update display settings on the Spectrometer View Preference window.



Right click over a node to access options, shown below.

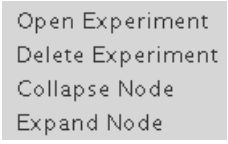


Figure 10 Study Queue node options

Table 14 Node options

Item	Description
Open Experiment	Opens selected experiment and displays parameters in the Parameter Panel.
Delete Experiment	Removes experiment from the Study Queue.
Collapse Node	Collapses selected node so that only experiment name is displayed.
Expand Node	Expands node so that all information is displayed.

QuickSubmit vertical panel

The QuickSubmit panel provides an easy way to quickly submit samples for acquisition.

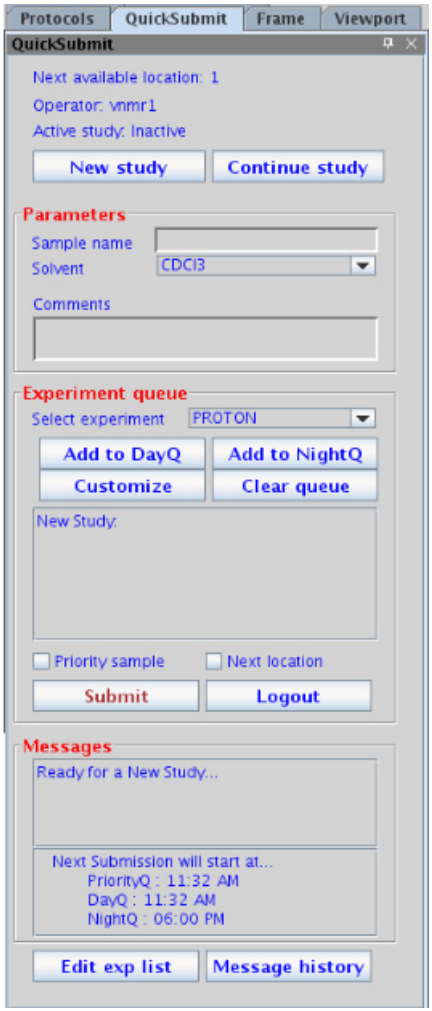


Figure 11 QuickSubmit vertical panel

Table 15 QuickSubmit Options

Item	Description
New study	Click to begin a new study.
Continue study	Click to continue the study currently in the Study Queue.
Parameters	Enter descriptive sample parameters and comments.
Experiment queue	From the Select Experiment drop-down list, select an experiment, then click **Add to DayQ** or **Add to NightQ** to place the experiment in the Study Queue. Continue to add experiments as desired.
Customize	
Clear queue	Clears the experiments from the queue.
Submit	Submits the current QuickSubmit queue for acquisition.
Logout	Click to log out of the VnmrJ system.
Edit exp list	Edit the existing experiment list.
Message history	Click to see a log of previous messages.

Frame vertical panel

Use the Frame vertical panel to create an inset frame. An inset frame initially shares the same workspace and data as the viewport. However, you can change or remove it. For details on creating and working with insets, see the *Agilent VnmrJ Spectroscopy User Guide*.

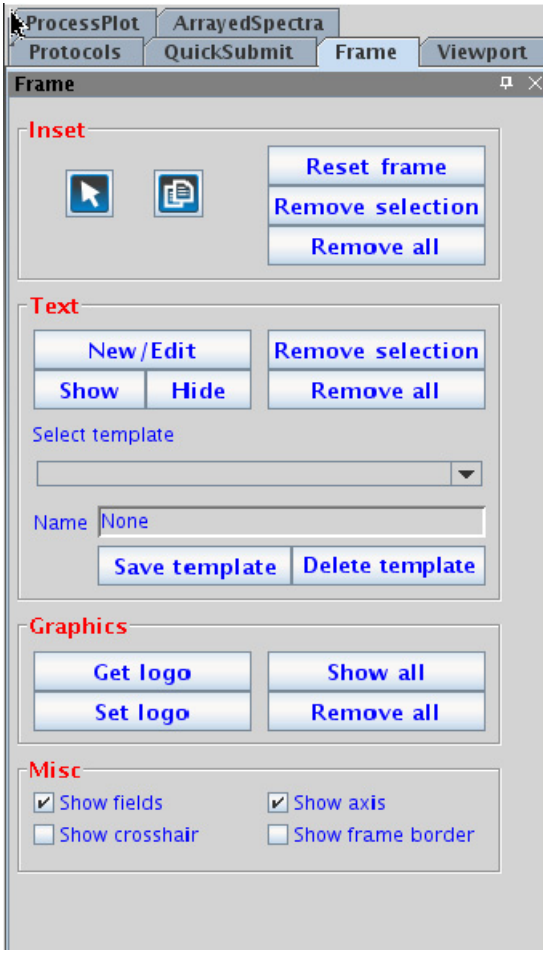


Figure 12 Frame vertical panel

Table 16 Frame vertical panel options

Item	Function
Inset	
	**Default mode** — left mouse click moves the left cursor and right mouse click moves right mouse cursor.
	**Inset mode** — left mouse drag a box over a spectrum region creates an inset frame of the region. A viewport can have multiple inset frames. Exit inset mode — release mouse button.
Reset frame	Resets inset frame to default
Remove selection	Removes selected frame or item
Remove all	Removes all inset frames
Text	Lets you add text to an inset frame.
New/Edit	Create or change a text inset
Show	Show text inset
Hide	Hide text inset
Remove selection	Remove selected text
Remove all	Removes all text
Select template	Select a saved text inset template
Name	Give a name to the text inset
Save template	Save the text inset as a template
Delete template	Delete the selected template

Table 16 Frame vertical panel options (continued)

Item	Function
Graphics	
Get Logo	Lets you select a logo to show in the frame
Set Logo	
Show All	Shows all graphics in the frame
Remove All	Removes all graphics from the frame
Misc	
Show Fields	Display `cr, delta, vp` etc... fields at the bottom of the viewport.
Show Crosshair	Display cross hair and chemical shifts of the cursor position when the mouse is moved over the spectrum. This is a useful function when the fields are not shown, not in cursor mode (default mode), or when chemical shift of a peak without moving the left cursor is required while in the cursor mode.
Show Axis	Show scale of the axis.
Show frame border	Check the box to display a box around the frame. Clear the box to display the four corners of the selected frame as *hot spots* for resizing. No border or corner will be displayed if a frame is not selected. An empty frame is not visible until it is selected.

Inset frame buttons

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

Button	Function
Delete Inset	Delete the selected inset.
Delete all	Delete all inset frames.
Full size	Restore the default frame to its full size.

Display check boxes

The check boxes control optional display features.

Check box	Function
Cross hair	Display cross hair and chemical shifts of the cursor position when the mouse is moved over the spectrum. A useful function when the fields are not shown, not in cursor mode (default mode), or when chemical shift of a peak without moving the left cursor is required 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 if a frame is not selected. An empty frame is not visible until it is selected.

Viewport vertical panel

The Viewport vertical panel is used to set up and customize the display of viewports.

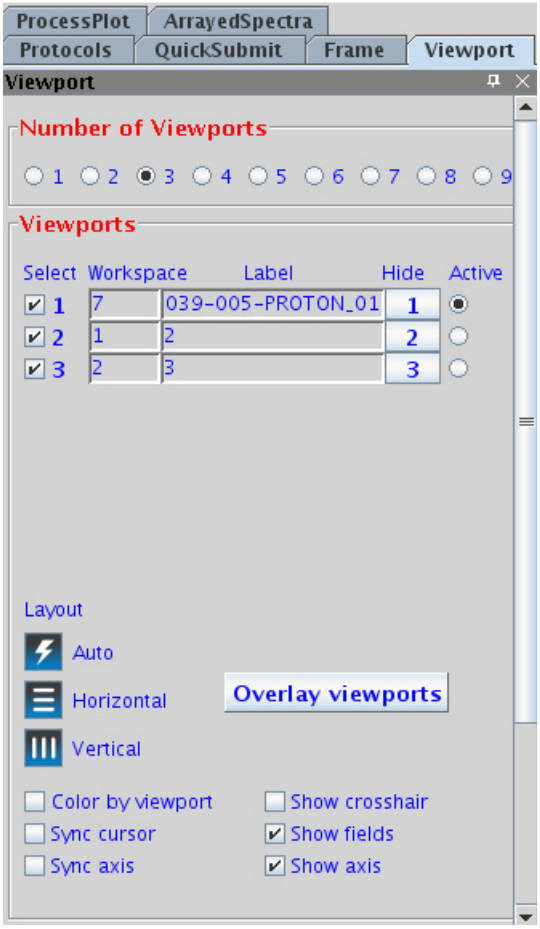


Figure 13 Viewport vertical panel

Table 17 Viewport vertical panel options

Item	Description
Number of viewports	Used to select the number of viewports to display. Available viewports is set in Viewports settings window.
Viewports	Select — When selected, displays that viewport Color — Select color to display data in viewport Workspace — Workspace number (also experiment number shown on upper left corner of viewport) Label — File name or user-defined label Hide — Hide selected viewport Active — Select to make viewport active
Viewport layout	 — Auto mode, let VnmrJ arrange the viewports in an optimized row-by-column matrix  — Stack viewports horizontally  — Arrange viewports vertically
Overlay Viewports	Overlays viewports Stack spectra — show spectra with an offset X — offset in X axis for stacked spectra Y — offset in Y axis for stacked spectra
Color by viewport	Turns on the color option so you can select to display viewports in different colors.
Sync Cursor	Links and synchronizes the cursors and crosshairs in multiple viewports.
Sync Axis	Links and synchronizes axes in multiple viewports. Axis is synchronized to the current active viewport.
Show crosshair	Displays cross hair and chemical shifts of the cursor position when mouse is moved over the spectrum. This is 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 required while in the cursor mode.

Table 17 Viewport vertical panel options

Item	Description
Show fields	Shows information fields at the bottom of the active viewport: vs 111.7 sp(ppm) 35.78 wp(ppm) 65.00 first 1 last 4 step 1
Show axis	Displays axes in the viewports

Contour

The contour sub-panel, Figure 14, appears exclusively for the active viewport with 2D data loaded and displayed in contour mode (dpcon).

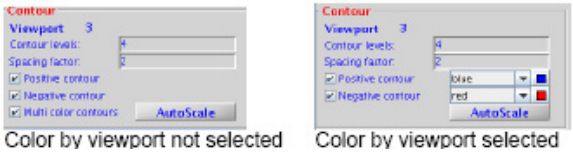


Figure 14 Contour controls

Table 18 Contour panel

Control	Description
Contour levels	Enter a number of contours between 4 and 32 in the text field.
Spacing factor	Enter a number in the text field to specify the spacing between contours. A number between 1.1 and 2 is recommended.
Positive contour	Select this check box to show positive contours using the default color red.
Negative contour	Select this check box to show negative contours using the default color blue.
Color dropdown	Select a color from the menu to use a color other then the default color. Each contour has a color dropdown menu.

Table 18 Contour panel (continued)

Control	Description
Multi color contours	Select this option to use the colors defined in Display Option. If you select the Color by Viewport box, options are not displayed,
AutoScale	Automatically scale the spectrum by clicking.

ProcessPlot vertical panel

The ProcessPlot vertical panel provides quick access to commonly-used options for processing, on-screen display, and plotting. Options in the panel vary depending on current data. Buttons within the panel enable you to open parameter panels that contain more options.

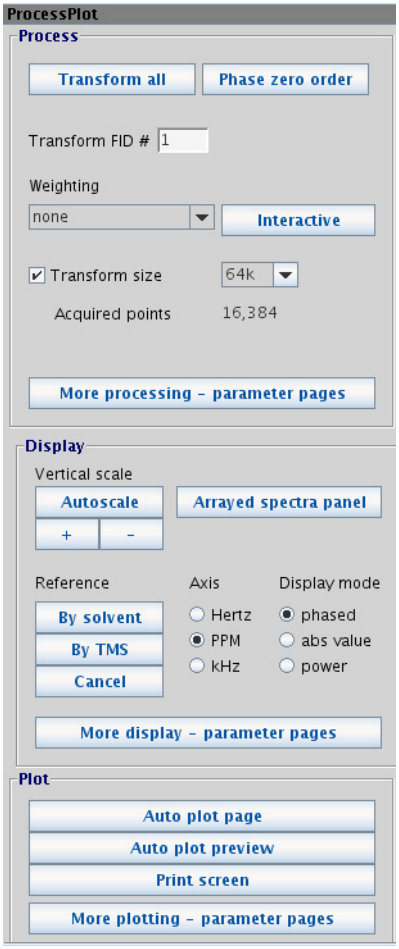


Figure 15 ProcessPlot vertical panel for 1D

Table 19 Options in the ProcessPlot vertical panel

Option	Description
Process	
Transform all	Performs a Fourier transform for all the displayed data.
Phase zero order	Performs a zero order phase correction.
Transform FID #	Select FID # to transform.
Weighting	Select the weighting to be applied to the transform.
Interactive	Select to enter interactive weighting mode.
Transform size	Opens a menu where you can select the number of points to be Fourier transformed (fn).
More processing - parameter pages	Opens the Default page in the Process parameter panel tab for more processing options
Display	
Autoscale	Automatically scales the display vertically.
+/-	Click + or - to increase or decrease the vertical scale.
Arrayed spectra panel	Opens the ArrayedSpectra panel where you can set up display of spectra and FID arrays. See "ArrayedSpectra vertical panel" on page 52.
Reference	By solvent - Reference the spectrum for selected solvent. By TMS - Reference the spectrum to a TMS line. Cancel - Clears the reference line by removing any spectral referencing present, and turns off referencing.
Axis	Select the desired y-axis units: Hertz, ppm, kHz
Display mode	Select the desired display mode: phased, absolute value, or power
More display - parameter pages	Opens the Display page in the Process parameter panel tab for more display options
Plot	
Auto plot page	Executes the `plot` macro; then the `resetplotter` macro.

Table 19 Options in the ProcessPlot vertical panel

Option	Description
Auto plot preview	Opens the Plot View popup and displays the plot in Adobe Reader. Use the Plot View popup to save the plot to a file, send to a plotter, or send to an e-mail address.
Print screen	Opens the Print Screen dialog box, where you can set up and print the VnmrJ window or viewport. See "Saving and Printing a Graphics File" on page 182.
More plotting - parameter pages	Opens the Plot page in the Process parameter panel tab for more display options.

ArrayedSpectra vertical panel

The ArrayedSpectra vertical tab contains parameters for displaying and plotting spectra and FID arrays. This procedure applies equally to the display and plotting of both spectra and FID arrays.

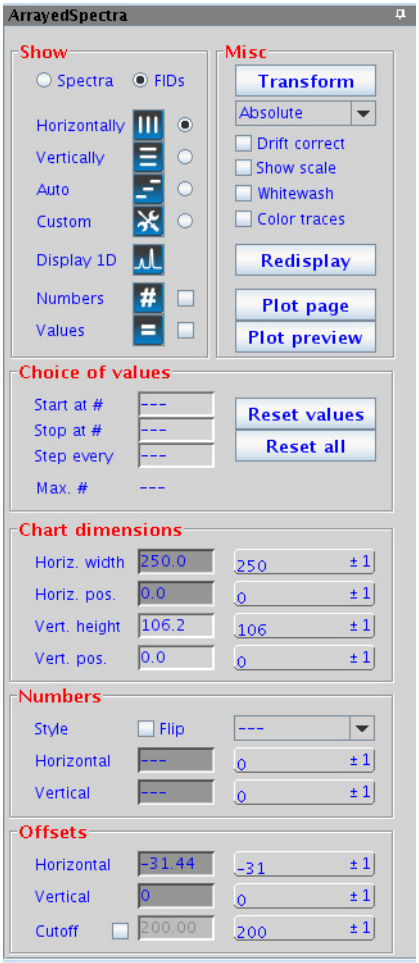


Figure 16 ArrayedSpectra vertical panel

Table 20 Options in the ArrayedSpectra vertical panel

Option	Description
Show	
Spectra or FIDs	Selects to show either spectra or FIDs
Horizontally	Shows the spectra side-by-side
Vertically	Aligns the spectra one above another
Auto	Depends on the previously chosen display mode: • If the previous mode showed the spectra full screen (vertical mode or showing only a single 1D) spectra are aligned vertically, and the vertical offset is chosen such that all spectra together cover the entire vertical space. • If the previous mode was horizontal, a vertical offset is added to show the spectra along a diagonal.
Custom	Takes over the display properties of either horizontal, vertical, or auto modes but allows the choice of horizontal and vertical offsets.
Display 1D	Click the icon to show a single spectrum/FID and use the toolbox to manipulate and zoom.
Numbers	When selected, turns on numbering of the array elements displayed.
Values	When selected, turns on display of values for the array elements displayed.
Misc	
Transform	Fourier transform the current FID data
Drift correct	Apply drift correction (corresponds to "dc" command) to all subspectra of the array.
Show scale	Switch on or off a scale below the first spectrum or FID of the array.

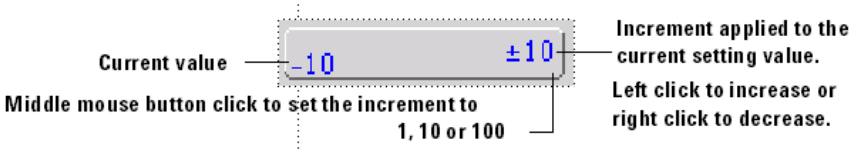
Table 20 Options in the ArrayedSpectra vertical panel (continued)

Option	Description
Whitewash	Aligns the spectra one above another as in the vertical mode, but this mode shows spectra behind each other, avoiding overprinting. Horizontal and vertical offsets can be adjusted.
Color traces	
Redisplay	Refresh the screen.
Plot Page	Send the current array display to the current plotter. Settings on the Plot parameter panel for parameter printing are used. Plotting from the ArrayedSpectra vertical panel does not plot integrals, integral values, and peak frequencies.
Plot Preview	Plot the array to a PDF file and open Acrobat reader with the PDF of the current array. Settings on the Plot parameter panel for parameter printing are used. Plotting from the ArrayedSpectra vertical panel does not plot integrals, integral values, and peak frequencies.
Choice of values	
Start at #	The first element of the array to display
Stop at #	The last element of the array to display
Step every	The element between the beginning and end of the array to display.
Max #	Maximum number of elements to display.
Reset values	Resets just the values to default.
Reset all	Resets all to defaults.
Chart dimensions	Enter the desired values, then 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.
Horiz. width	Enter the horizontal width for the chart.

Table 20 Options in the ArrayedSpectra vertical panel (continued)

Option	Description
Horiz. pos.	Enter the horizontal position for the chart.
Vert. height	Enter the vertical height for the chart.
Vert. pos.	Enter the vertical position for the chart.
Numbers	
Style	Flip — when selected, rotates the numbers 90 degrees counter-clockwise Drop-down menu — Used to select the position of the numbers. Select Custom to specify a horizontal and vertical positioning of the number with respect to the spectrum. Use the horizontal and vertical fields to type the custom positions.
Horizontal	When using Custom style, lets you enter custom horizontal position.
Vertical	When using Custom style, lets you enter custom vertical position.
Offsets	Enabled only for vertical, whitewash, or custom array mode.
Horizontal	Enter horizontal offset. (Note: the horizontal width must be smaller than the screen width in order to apply any horizontal offset.) Use the button to the right of the field to adjust the position. 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.
Vertical	Enter vertical offset. Use the button to the right of the field to adjust the position.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.

Table 20 Options in the ArrayedSpectra vertical panel (continued)

Option	Description
	
Cutoff	Used to avoid overlapping large lines that may reach into the spectra above.

Parameter Panel

The Parameter Panel shows the pulse sequence, context-specific information, menus, and text entry. The panels under the Acquire and Process tabs change depending on the current pulse-sequence. Parameter Panel information is displayed for the current experiment.

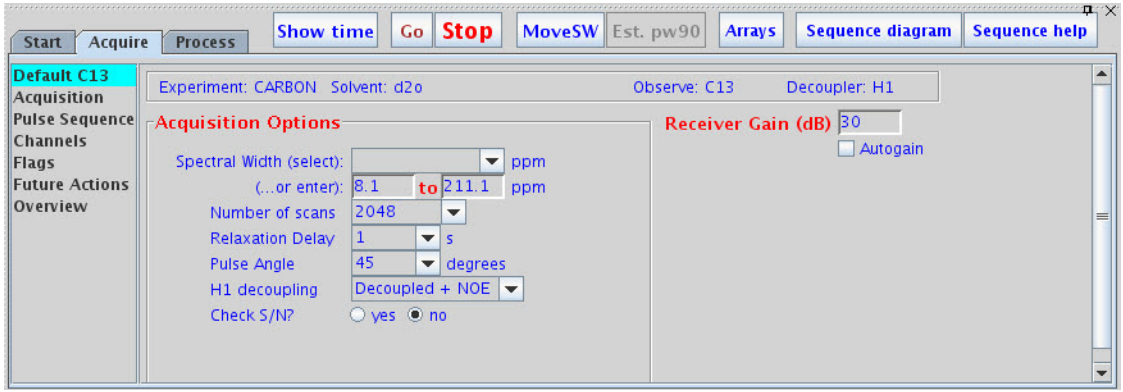


Figure 17 Parameter Panel

Each pane can be resized, reduced to a tab, or closed. Setup, acquire, or process NMR data using the point and click feature of the interface. There are three tabs labeled Start, Acquire, and Process below the graphics window. The top page on each tab displays commonly used functions. Lower pages display detailed functions. Buttons (Action Bar) to the right of the tabs represent tab-specific actions and differ with each tab. The interface can also be accessed using the command line above the Graphics Canvas.

VnmrJ Menus

VnmrJ has an integrated set of tools designed to acquire a series of one and two-dimensional data sets from a library of pulse sequences for any given sample. Access the sophisticated experiments for routine use in a fully automated environment.

Standard menu items are displayed at the top of the VnmrJ window. This section lists menus in alphabetical order rather than in the order they appear in the menu.

Acquisition Menu

The Acquisition menu provides a convenient non-command line access to a number of core VnmrJ commands such as `go`, `ga`, or `au`. The menu option, Parameter Arrays, facilitates the creation of parameter arrays.

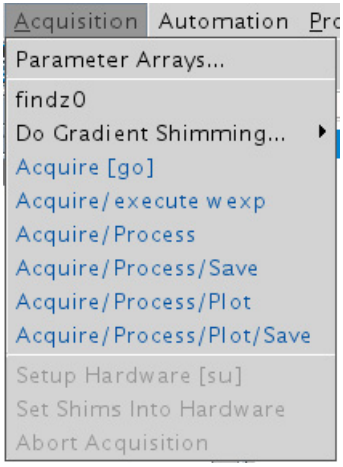


Figure 18 Acquisition menu

Table 21 Acquisition menu

Item	Description
Parameter Arrays...	Opens the Array Parameter window, in which you can create and edit parameter arrays.
findZ0	Find Z0 for locking.
Do Gradient Shimming	Opens the gradient shimming menu where you select the gradient map and execute gradient shimming.

Automation Menu

The Automation Menu provides access to automation start, stop, restart and reset controls not generally used during ordinary sample submission and not accessible from the Study Queue. It also provides access to archive queues and automation logs.

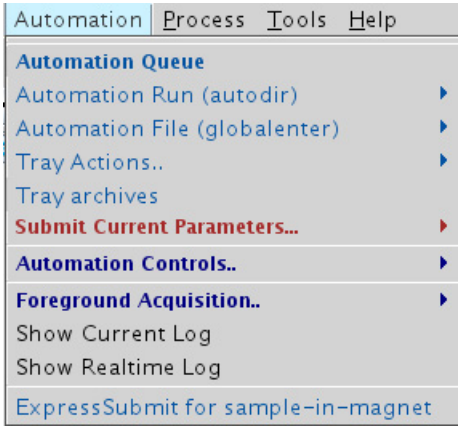


Figure 19 Automation menu

Table 22 Automation menu

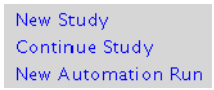
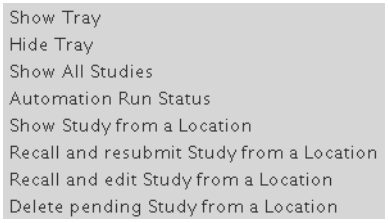
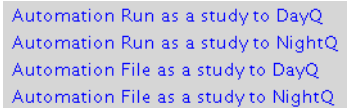
Item	Description
Automation Queue	Select to display Automation Queue.
Automation Run (autodir)	 Start a new study or continue an existing study from an existing automation run. Initiate a new automation run (often done at the start of the day).
Automation File (globalenter)	 Edit, create, display and submit to acquisition the "globalenter" version of a Study Queue.
Tray Actions...	 Provides functionality that is also available on the Study Queue controls or the right-click menu on the tray locations.
Tray Archives...	Tray archives allows the user to browse completed automation runs or automation files from previous dates.
Submit Current Parameters...	 Use to manually build any desired experiment in the current workspace and to submit to an automation queue, both day and night.

Table 22 Automation menu (continued)

Item	Description	
Foreground Acquisition...	Allows user to pause after current acquisition, pause immediately, or resume paused study.	
Automation Controls (visible when autosampler is configured)	Pause after current Study Pause after current Acquisition	To pause the automation run, manually run an emergency sample, resume the automation run, or to pause a run to fill the magnet with cryogens.
	Stop-Save-Resume	Stops the running experiment, process or plot, or save to move on to the next experiment in the chain or queue. For example, if a 4 hour experiment were running in automation and after 30 minutes it was processed and nearly complete, then this action allows you to choose a rational action at that time.
	Stop-Discard-Resume	Stops the running experiment and move on to the next item on the list.
	Stop-Save and Stop-Discard	Functions exactly as the submenus described above except that the queue is not resumed until you select Resume Automation from this submenu.
	Pause NOW	Allows you to pause the experiment immediately.
	Pause at scheduled time	Allows the administrator of the account to define in advance an exact time for the automation run to be paused along with a time for automation to resume.
	Resume Automation	Resumes any paused automation run.
	Abort Automation	Stops automation run.
		During the time of pausing you can use the interface to submit more samples and to acquire NMR data manually. You can also allow time for cryogen fills and the magnet time to recover. The automation run can resume automatically.

Table 22 Automation menu (continued)

Item	Description	
Background Acquisition... (visible when no autosampler is configured)	New background run	Submits a new acquisition run to background.
	Show all studies	Shows status of studies in the Study Queue.
	Pause after current Study Pause after current Acquisition	To pause the automation run, manually run an emergency sample, resume the automation run, or to pause a run to fill the magnet with cryogens.
	Stop-Save-Resume	Stops the running experiment, process or plot, or save to move on to the next experiment in the chain or queue. For example, if a 4 hour experiment were running and after 30 minutes it was processed and nearly complete, then this action allows you to choose a rational action at that time.
	Stop-Discard-Resume	Stops the running experiment and move on to the next item on the list.
	Stop-Save and Stop-Discard	Functions exactly as the submenus described above except that the queue is not resumed until you select Resume Automation from this submenu.
	Pause NOW	Allows you to pause the experiment immediately.
	Pause at scheduled time	Allows the administrator of the account to define in advance an exact time for the acquisition run to be paused along with a time for acquisition to resume.
	Resume Acquisition	Resumes any paused acquisition run.
	Abort Acquisition	Stops acquisition run.
Show Current Log	Displays the current compact acquisition log in a text editor window.	
Show Realtime Log	Displays a compact realtime acquisition log in a popup window.	
ExpressSubmit for sample-in-magnet	Submits default experiment (defined in preferences) to the sample in the magnet.	

Edit Menu

The available commands and options depend on the rights assigned by the VnmrJ Administrator.

Each of the following menu options opens a dialogue that prompts the user to enter the source and destination workspaces of the items. The command and parameter reference refers to these tools as `mp`, `mf`, `mt`, `md`, and `mz`. For more information on commands, parameters, and macros, see the *VmnrJ Command and Parameter Reference Guide*.

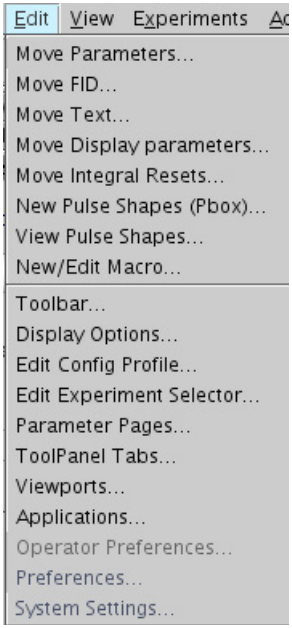


Figure 20 Edit menu

Table 23 Edit menu

Item	Description
Move Parameters...	Opens the Move Parameters window that allows parameters to be moved from one experiment number to another.
Move FID...	Opens the Move FID window to move an FID from one experiment number to another.
Move Text...	Opens the Move Text window to move text from one experiment number / workspace to another.
Move Display parameters...	Opens the Move Display Parameters window to move display parameters from one experiment number to another.
Move Integral Resets...	Opens the Move Integral Resets window to move integral resets from one experiment number to another.
New Pulse Shapes (Pbox)...	Opens the powerful Pbox tool for the creation of pulses and decoupling shapes.
View Pulse Shapes...	Opens the Pulse tool, a Bloch simulator for viewing the effects of any shaped pulse.
New/Edit Macro...	Opens a macro directly in a text editor.
Toolbar...	Enables the addition of a button to the top bar of the user interface with a user-specific function.
Display Options	Opens a graphical interface from which you can modify and save/recall the colors used in every tool used in VnmrJ.
Edit Config Profile...	Allows modification of what experiments are shown in the Experiment Selector tool. The starting point is based on the profile assigned to them by the VnmrJ administrator
Edit Experiment Selector	Enables you to change the way a protocol is displayed in the Experiment Selector. You can add or edit folders, change the order of display, or change displayed names This information is saved separately for each operator.
Parameter Pages	Enables you to build/modify Parameter pages.

Table 23 Edit menu (continued)

Item	Description
ToolPanel Tabs	Opens the Tool Panel Editor, where you can configure what vertical panels are available to view, and move their position in the vertical panel pane. You can also save the configuration in a file.
Viewports...	Enables you to toggle viewports. It is a tool to view multiple workspaces simultaneously, on or off.
Applications...	Enables you to define an account with collections of Applications Directories. An Applications Directory is a specific directory path that could contain macros, parameter, templates, and so on. For example, the AutoTest facility can be toggled on or off with this menu item.
Operator Preferences...	Enables the account administrator to allow the individual operators to manage their own preferences for the interface to automatically preset items as email address, preferred solvent, plotter, or notebook. In this example Operator Preferences is not active because in the Preferences menu, User Remembrance is not enabled. The list of choices for this list is completely general and is defined by the account administrator.
Preferences...	Enables the account administrator to define items such as data saving template and default behaviors for plotting, automatic creation of pdf plot files, and a number of operator privileges. This menu item is discussed in detail in "VnmrJ Preferences" on page 103.
System Settings...	Opens a graphics tool with which system options are defined.

Experiments Menu

Unlike the Experiments Selector which can be configured by both the administrators and individual operators in terms of content, the Experiments menu shows the full selection of experiments accessible for the account. Use the Experiment Selector tool to perform automation submissions.

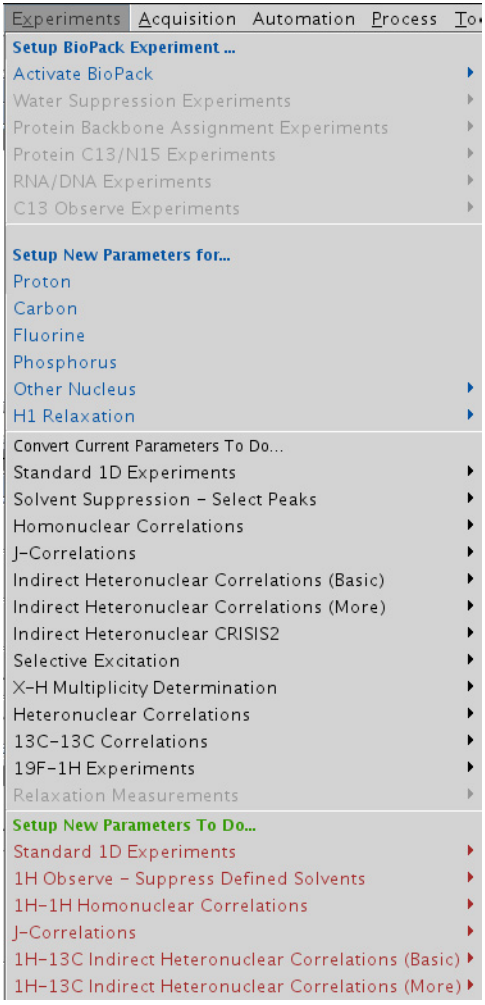


Figure 21 Experiments menu

Table 24 Experiments menu

Item	Description
Setup BioPack Experiment	(Only available when BioPack option is enabled.) For information on using BioPack, see the *Agilent VnmrJ 4 BioPack Users Guide*.
Activate BioPack	(Only available when BioPack option is enabled.) For information on using BioPack, see the *Agilent VnmrJ 4 BioPack Users Guide*.
Setup New Parameters for...	Executes a simple retrieval of standard parameters for the selected experiment and also completely clears all sample tags (parameters used to define a sample's identity).This is a clean slate.
Convert Current Parameters To Do...	Sets up the selected requested experiments but retains all sample tags. If you choose to use the **Experiment** selector without first requesting **New Study** by the **Study Queue** controls the result is the same as this conversion. The conversion of parameters with retention of sample identification parameters is the modality of "more on this sample." The acquired data is auto saved and added to the pre-existing data acquired the current study
Setup New Parameters To Do...	Allows a simple retrieval of default parameters for all 2D and a few 1D experiments, according to your need.
Hadamard Experiments	Provides access to all of the Hadamard Fast methods 2D experiments.
Solid-State Experiments	Allows access to all routine Solids NMR experiments

File Menu

Figure 22 File menu

Table 25 File menu

Item	Description
New Workspace	Creates a new workspace for use. Workspaces are called exp1, exp2, and so on, up to exp9999. A workspace is a directory where data is acquired or processed.
Join a NEW Workspace	Creates a new workspace and then actively joins the workspace in the interface. Following is an example of the command line equivalent: `cexp(7) jexp7` will create a new workspace and join exp7.
Open...	Accesses the Open window (also called the Experiment Selector Editor) where you can browse for and open files.
Save As...	Opens the File Browser window where you can specify the location and name for saving the data in the current workspace.

Table 25 File menu (continued)

Item	Description
Auto Save	Saves the data that has been acquired in an experiment workspace using the template set up in User Preferences. See Templates Tab. The location and file name are automatically set based upon the values defined in the Preferences Templates tool.
Printers...	Allows you to select a valid printer and/or plotter for output.
Print Screen...	Allows you to print the current screen.
Auto Plot	Calls the appropriate automatic plotting routine for any type of data in the current workspace.
Create a Plot Design...	Opens Plot Designer to create plot designs or output.
Review PDF Plots...	Allows you to review the PDF plot in Adobe Acrobat. You can set the user preference to create a pdf plot automatically for data that has been acquired of a given sample.
Switch Operators...	Allows the current operator of the system to logout during automation thereby freeing the system for use by another operator.
Exit VnmrJ	Executes an exit of the VnmrJ program. It is equivalent to typing `exit` in the command line.

Help Menu

The Help menu provides links to help and reference information.

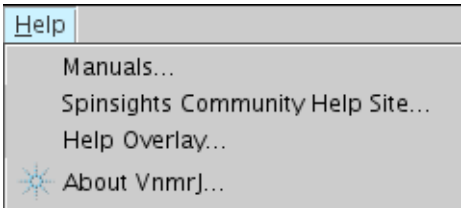


Figure 23 Help menu

Table 26 Help menu

Item	Description
Manuals...	Opens online help where you can view manuals in html or PDF format.
Spinsights Community Help Site...	Opens the Agilent Spinsights home page, where you can find resources such as community forums, downloads, and news.
Help Overlay...	Opens the Help Overlay, which gives you a visual overview of the VnmrJ user interface.
About VnmrJ ...	Opens information about the VnmrJ 4 software.

Process Menu

The Process menu provides tools for common tasks as an alternative to the command line

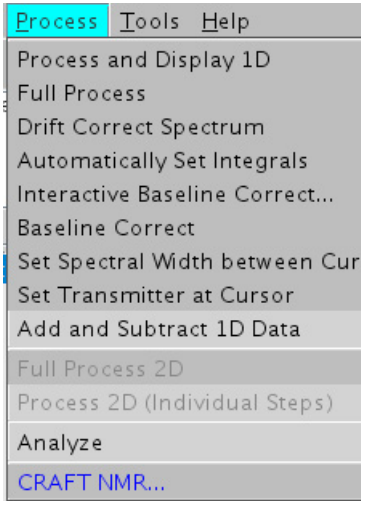


Figure 24 Process menu

Table 27 Process menu

Item	Description
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.
Full Process 2D	Process and display 2D data using the processing and display parameters associated with the protocol.

Table 27 Process menu (continued)

Item	Description
Process 2D (Individual Steps)	Step by step processing of 2D data.
Analyze	Use to analyze COSY correlations, spin simulation, deconvolution, and regression.
CRAFT NMR	Opens the CRAFT application, (Complete Reduction to Amplitude Frequency Table). CRAFT lets you convert an FID or a collection of FIDs into the component NMR signals in the form of a chemicalshift (frequency) / amplitude / linewidth table. For more information, see the *VnmrJ CRAFT User Guide.*

Tools Menu

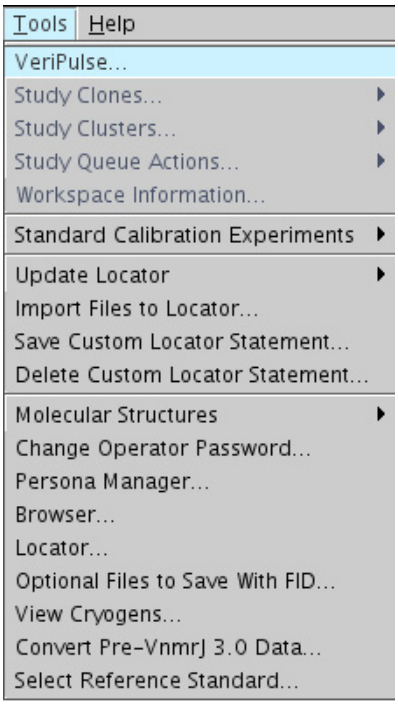


Figure 25 Tools menu

Table 28 Tools menu

Item	Description
VeriPulse...	If VeriPulse is enabled, opens the VeriPulse window that enables you to perform automated testing and calibration. See the *Agilent NMR System Calibrations User Guide* for information.
Study Clones...	See "Study Clones submenu" on page 77

Table 28 Tools menu (continued)

Item	Description
Study Clusters...	Opens menus with commands that let you create study clusters. A study cluster lets you treat a set of FIDs (from different studies) as a single group. For details, see the *VnmrJ Spectroscopy User Guide*.
Study Queue Actions...	Displays two menu options: Refresh Study Queue—Updates the study information in the **Study Queue** window. Clear Study Queue—Clears the **Study Queue** window.
Workspace Information...	Opens a window that displays the status of all workspace ongoing processes.
Probe Tuning	May display two menu options: Auto Tune Probe...—Opens the ProTune auto-tuning dialog window. Appears only if ProTune accessory is installed and configured. Manually Tune Probe...—Opens the "mtune" panel.
Enforce ProbeID	For installed probes with ProbeID, once ProbeID is configured in System Configuration, this selection enables the ProbeID function. ProbeID prepopulates calibration target values appropriate for the current probe and ensures that the probe file selected in the Probe popup matches the probe that is currently attached to the system.
Disable ProbeID	Disables ProbeID functions.
Standard Calibration Experiments	See "Standard Calibration Experiments submenu" on page 82.
Update Locator	Opens a submenu that provides choices for updating the different parts of the Locator database.

Table 28 Tools menu (continued)

Item	Description
Import Files to Locator...	Opens a window for importing files to the Locator database.
Save Custom Locator Statement...	Opens a window to save custom Locator statements.
Delete Custom Locator Statement...	Opens a window for deleting custom Locator statements.
Molecular Structures	Display all—Display all molecular structures. Plot all—Plot all molecular structures. JChempaint...—Opens the open source application JChempaint (molecular drawing program) in a separate window. Select the Help menu for an online manual. Jmol—Opens the open source application Jmol (3D molecular viewing program) in a separate window. Select the Help menu for an online manual.
Change Operator Password...	Opens a window for changing operator passwords. If the operator has an operating system login account, the password will also be changed.
Persona Manager...	Opens the Persona Manager, where the administrator adds and configures system operators and personas.
Browser...	Opens a file browser window.
Locator...	Opens a Locator window.
Optional Files to Save With FID	Choose additional files that can be automatically saved in the .fid directory.
Sample in Magnet...	Tool to command the sample changer to change samples and to assign the sample position currently in the magnet.

Table 28 Tools menu (continued)

Item	Description
View Cryogens	Opens the CryoMonitor pop-up where you can read the current levels of cryogens and see the level history. This option requires that a cryogen monitor is installed and configured in system configuration.
Convert pre-VnmrJ 3.0 data...	Tool to convert pre-VnmrJ 3 data for use in VnmrJ 3.x.
Select Reference Standard...	Choose the reference compounds used for chemical shift referencing.

Study Clones submenu

The Study Clones submenu is a group of convenience utilities.

A Study Clone is a set of experiments built in the Study Queue with any desired parameter customizations. This set of experiments is automatically represented as a new button in the Experiment Selector. After creation, the user can repeat the exact set of experiments simply by selecting that button either in or out of automation and with or without a sample changer. One use of a Study Clone is to set the desired parameters for a very fast PROTON spectrum, such as `nt=1 ss=0 gain=4` and Clone current Exp with a button label Fast_H. It might also be useful to set parameters for a slow quantitative PROTON experiment such as `d1=60 pw(90) ss=2 nt=8` and Clone current Exp with a label as Quant_H. The user can use the Study clones to recall complex sets of multidimensional experiments or to simply establish a convenience button for commonly done tasks. Clones from other clones can also be created by adding more experiments in any desired fashion.

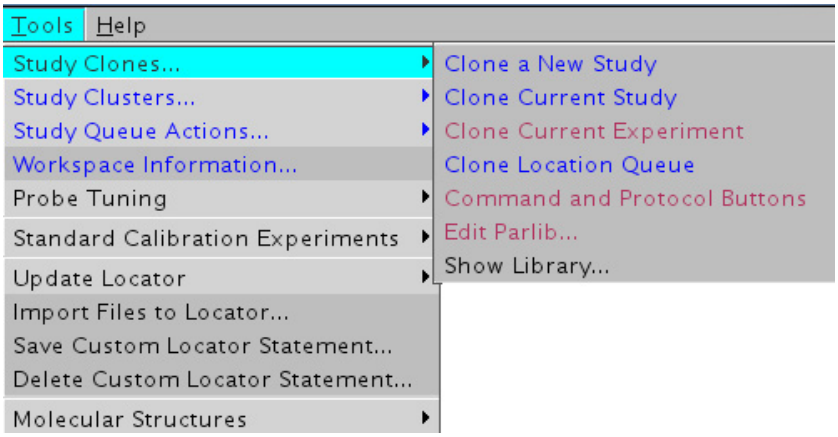


Figure 26 Study Clones submenu

Table 29 Study Clones submenu

Item	Description
Clone New Study	Enters the Study Queue mode to create a new Study that shall be saved as a new clone. Presents a "**Save Study**" button on the Study Queue window to save the new Study.
Clone Current Study	Use to assign a name for the button associated with a study of a list of experiments assembled in the Study Queue.
Clone Current Experiment	Allows user to assign a name for the button option associated with the currently loaded or displayed experiment. For example, use this option if an FID from a previous study is retrieved in the current workspace, and the user wants to create a clone of the single experiment that had been acquired on that sample.
Clone Location Queue	Allows creation of a button associated with the study completed for the selected tray sample location.

Table 29 Study Clones submenu (continued)

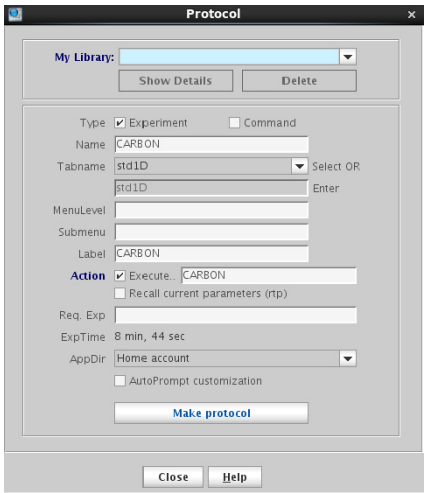
Item	Description
Command and Protocol Buttons	Use the Protocols menu option to devise a method to create a button to run a macro to setup an experiment.  In the Type field, select either **Experiment** or **Command**. If **Command** is selected, a button option is created to call a macro that, for example, analyzes the lineshape. Based on the result, the user can decide to call a group of non-spin shim routines. A Study Clone could then be composed of a PROTON experiment customized appropriately for running 1H lineshape, followed by the command protocol to analyze lineshape in the Study Clone. This Study clone can be submitted at any time and automates the task of refining shims.

Table 29 Study Clones submenu (continued)

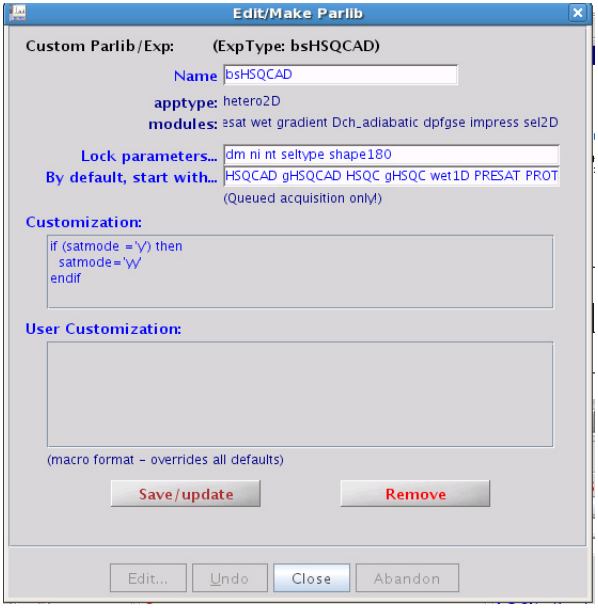
Item	Description
Edit Parlib...	Enables users to view the details of any valid VnmrJ protocol. Edit/Make parlib can also create new protocols based on the contents of the parameter set in the current workspace. Use the Study Clones tool to create a modified version of an already existing protocol, such as PROTON or CARBON experiments with specific parameters for a quick or long experiment. Do not use Edit/Make Parlib. In order to properly utilize the tool, the user must have a basic understanding of the concept of modules and locked parameters (Plock). The following is an example view of Edit/Make parlib for a band-selected 2D experiment. 

Table 29 Study Clones submenu (continued)

Item	Description
	Both the apptype and the list of modules are different from the PROTON protocol. The user can query the values and modules for the apptype parameter by using the `apptype?` and `modules?` commands before creating a new protocol from a pulse sequence and parameter set that originated from outside VnmrJ, such as the user library. Assign the value for modules to the Lock parameters list and add any parameter needed to be kept at setup time. In the above PROTON experiment, basic protocols include the following key concepts: • Name—Displays the name of the set parameter and the protocol's button. • apptype—Displays a generic helper macro name for setting up a group of protocols. In VnmrJ apptype is optional. Common apptypes are std1D, homo2D, hetero2D, and lstd1Dmodules. (The names for the little min-parameter sets that are combined to create the existing parameter set.) • Module—Displays a module and all of the values for the parameters in that module, type on the command line module ('popup','modulename'), for example module ('popup','presat'). • Default Starting Experiment—Define a default experiment as a starting point to morph the default experiment into the desired experiment. Type `REQexp?` from the command line to query the value for the default starting experiment. • Customization—Shows the contents of the macro name_setup or in the case of this example PROTON_setup. Not editable in this tool but it can be edited in a text editor. • User Customization—Creates a macro from the text typed in this field. userprotocolname or for this example userPROTON.
Show Library	Opens a graphical tool to backup then remove old buttons and to review the executable actions of buttons.
Show Library	Opens a graphical tool to backup then remove old buttons and to review the executable actions of buttons.

Standard Calibration Experiments submenu

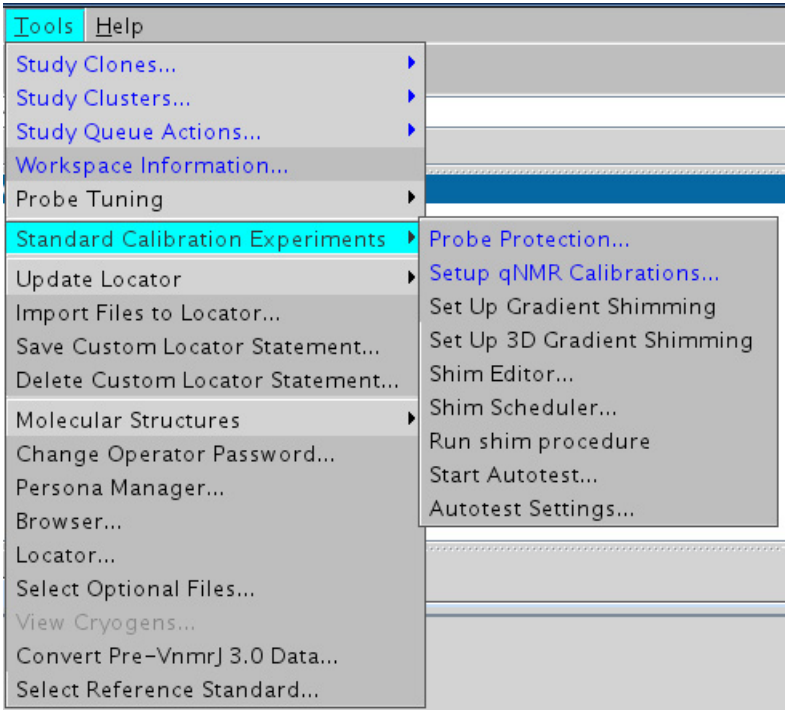


Figure 27 Standard Calibration Experiments submenu

Table 30 Standard Calibration Experiments submenu

Item	Description
Probe Protection...	Opens a window to set up maximum allowed power values for probe protection. See below.
Setup qNMR Calibrations...	Setup qNMR Calibrations-Opens a window to calibrate and set up quantitation tools.
Setup Gradient Shimming	Setup Gradient Shimming-Loads the pulse sequence and panels for making a shim map for gradient shimming.
Shim Editor	Opens the Shim Menu Editor, where you set up or change shim menus.

Table 30 Standard Calibration Experiments submenu

Item	Description
Shim Scheduler	Opens the Shim Maintenance Scheduler, where you set up and schedule shim service.
Run Shim Procedure	Executes the shim procedure.
Start Autotest	Opens the Auto Test window, where you can configure and run an autotest. For more information, see the *Agilent AutoTest User Guide*.
Autotest Settings	Opens the Autotest settings window, where you select the parameters for AutoTest. For more information, see the *Agilent AutoTest User Guide*.
Setup 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.

Probe Protection

Probe Protection settings are global parameters used for sample protection. Recommended settings are to leave power protection on and using default settings.

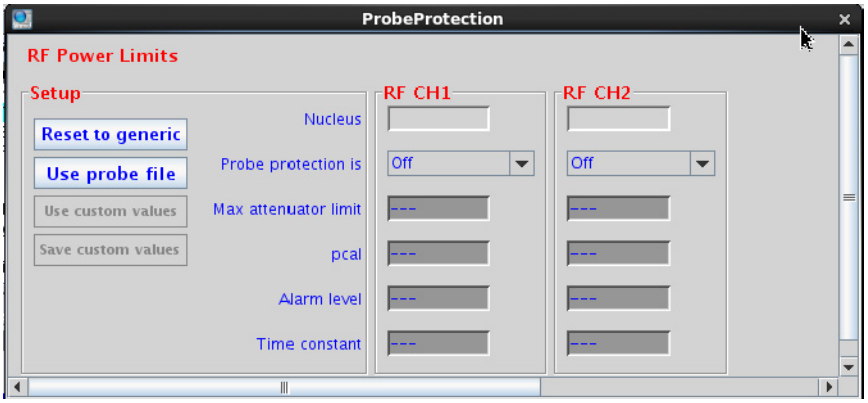


Table 31 Probe Protection

Item	Description
Use probe file	Updates pcal, alarm level, and time constant values using values from the probe.
Use custom values	Use for advanced sample protection.
Save custom values	Saves advanced sample protection values from the interface.
Nucleus	Displays channels with associated nuclei.
Probe protection is:	• On—Default state terminates experiments that are predicted to exceed the alarm level. When this happens, PSG prints the relevant rf channel on line 3 and the error window. • Verbose—Same settings as "on" and prints diagnostic messages in process>text. • Warn verbose—Alerts when 90% of alarm is reached and terminates when alarm is reached. • Warn only (off)—Alerts when 90% of alarm is reached and will not terminate. • Off-Will not terminate when the alarm level is reached.
Max. attenuator limit	Displays associated maxattench value for each channel.
pcal	Tpwr level associated with 2 watts of power at the probe.
Alarm level	An energy (power * time) value at which the probe may be damaged or the sample may be overheated.
Time constant	The length of time, typically 5 seconds, for the probe cooling processes.

View Menu

Use this menu to access parts of the interface and restore the interface elements. Close the window by clicking the **Close** button in the upper right hand corner of each window. Access the hardware or graphics toolbars using the Toolbars submenu.

Figure 28 View menu

Changing Display Colors

Using the Styles and Themes window, you can change the colors used for the display and printing of various items in VnmrJ. To open the Styles and Themes window, click the Display Options icon.

There are four user interface styles available (Default, Classic, Dark and Light), and several look and feel (LAF) choices to customize the interface.

You can also set default colors for drawing 1D and 2D spectral graphics and labels (Display). 1D and 2D spectral drawing have adjustable line thickness for better visibility and report generation. And, when zooming 1D and 2D data, VnmrJ can automatically switch to thicker lines.

The Plot functions let you set up defaults for printing and plotting.

To change the look and feel of the VnmrJ user interface

1 On the System Toolbar, click the Display Options icon.

The Styles and Themes window opens.

2 Select the **UI** button.

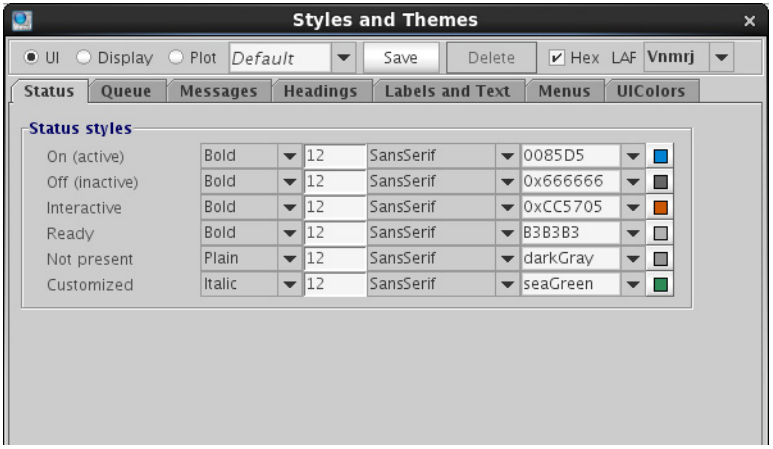


Figure 29 Styles and Themes window with UI selected

3 From the drop-down menu, select **Default**, **Classic**, **Light** or **Dark** to change the interface color theme. You can also customize further using the tabs and selections available.

To change color options for spectral drawing

1 On the System Toolbar, click the Display Options icon.

The Styles and Themes window opens.

2 Select the **Display** button.

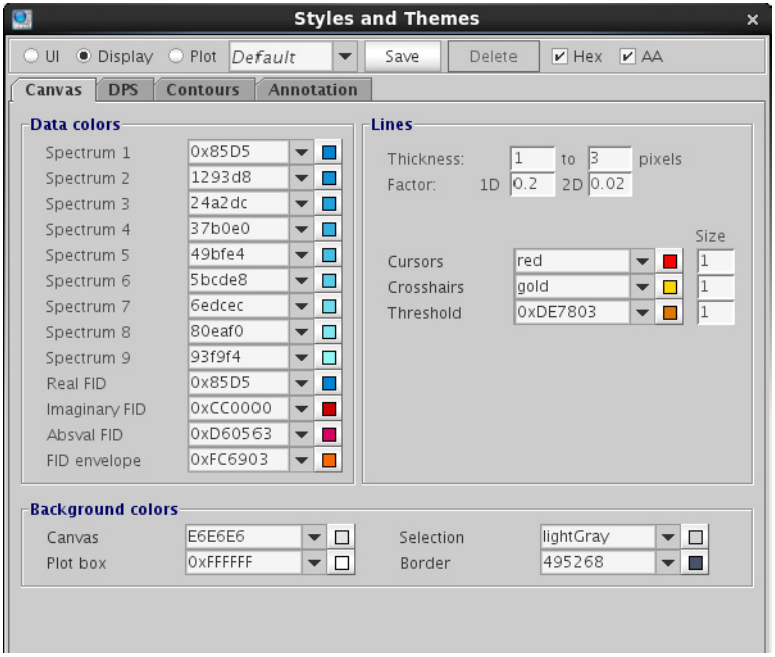


Figure 30 Styles and Themes with Display selected

3 Set the widths of lines used to draw 1D and 2D spectral graphics.

There are two Line Thickness settings, used depending on whether the number of points in the spectral region is much smaller than the number of pixels in the spectral drawing canvas. The corresponding

Factor parameter controls when the thicker lines will be used. For example, if the Factor parameter is set to 0.2, the thicker lines will be used whenever the ratio of points to pixels is 0.2 or less. If desired, you can set both Thickness values to the same number, so that line drawing will not change when spectra are zoomed.

4 Use the other tabs and selections to customize the display of pulse sequence (DPS), Contours, and Annotations.

To change color options for plotting

1 On the System Toolbar, click the Display Options icon. 

The Styles and Themes window opens.

2 Select the **Plot** button.

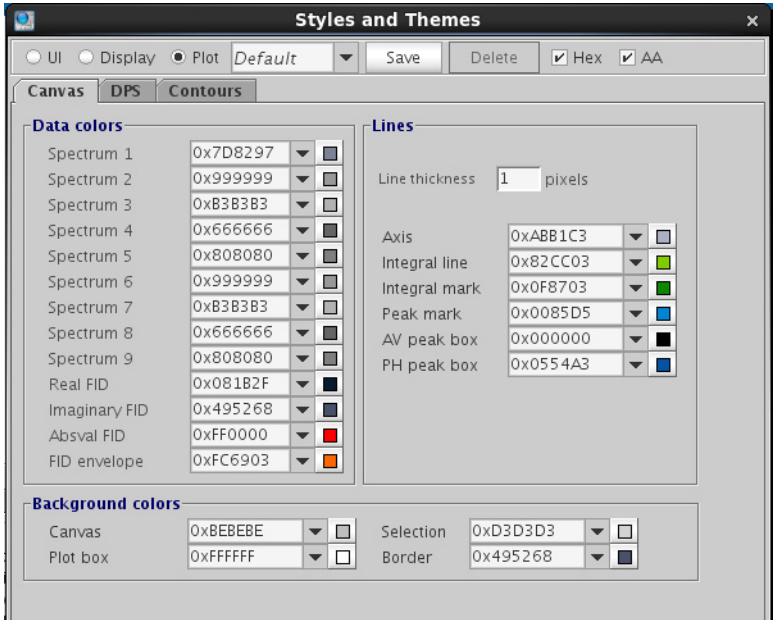


Figure 31 Styles and Themes with Plot selected

3 Set the widths of lines and colors to be used to plot 1D and 2D spectral graphics.

The Line thickness sets the same line thickness to all lines associated with the spectral drawing.

4 Use the other tabs and selections to customize the plotting of pulse sequence (DPS), Contours, and Annotation.

Experiment Selector Editor

The Experiment Selector Editor lets you customize how protocols are displayed in the Experiment Selector in the Protocols vertical panel. To open the Experiment Selector Editor, on the main menu click **Edit > Edit Experiment Selector**.

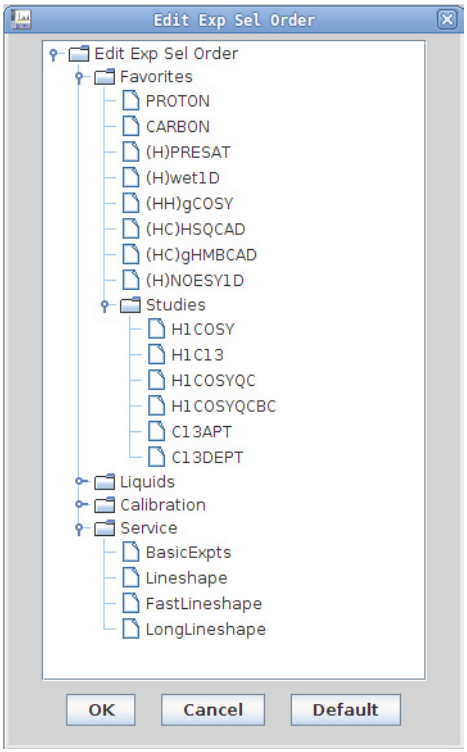


Figure 32 Experiment Selector Editor

The Experiment Selector has the following capabilities.

Table 32 Features of the Experiment Selector Editor

Feature	Action
Drag a protocol or folder to a new location.	Changes the order in which folders and protocols are displayed
OK	Closes the panel and updates the Experiment Selector
Cancel	Discards any changes and keeps the Experiment Selector unchanged
Default	Reverts to the Agilent default order and names
Click 3rd mouse button on an item	Opens a menu
Copy	Copies selected item to clipboard
Paste	Pastes the "copied" item to the position above the location selected
Delete Entry	Deletes selected entry
New Folder	Creates a new Folder (or Node) in the tree. Type in the desired name and then hit the "Enter" key. Failing to hit the enter key causes the folder name to revert to "New Folder". In that case, click on the name and edit the name, then press Enter.
Add to Favorites	Copies the selected item to the Favorites node. Note: The menu item will show the name of the first Folder/Node displayed in the Experiment Selector. Normally, the first Node is called "Favorites", however, this is not required. If the first Node is called "Common", then the menu will display "Add To Common" and the selected item will be copied to the "Common" Folder/Node.
Change the name for an item	Click on the name and type a new name, then press Enter. Failing to press the Enter key will cause the name to revert to its original name.

NOTE Duplicate names are not allowed in the same folder/node. If you try to paste or rename an item in a folder/node where an identical name exists, an error appears and the action is aborted.

NOTE

Experiment Selector information contained in a protocol .xml file is always active and cannot be overridden by this Editor. Therefore, if (for example) a user has a protocol in his vnmrsys directory area which puts that protocol into a tab named ABC, that tab (or first level in the tree) cannot be permanently renamed, moved, or deleted. Nor can the protocol entry be permanently deleted or removed from its defined location. A warning will appear if one of these actions is attempted for information defined in the protocol.xml file.

File Browser

The file browser opens when you select **File > Open** from the menu bar.

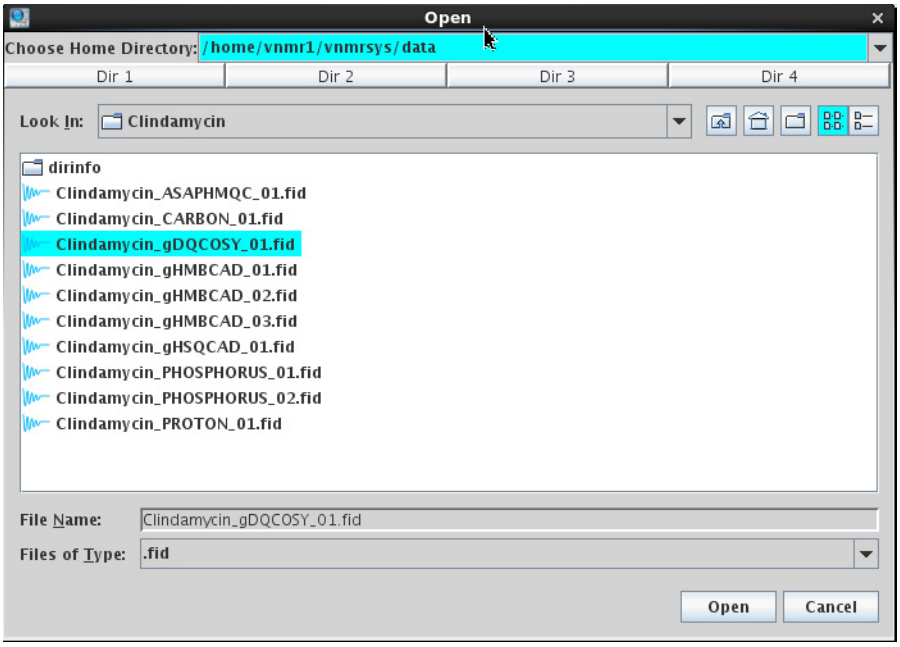


Figure 33 File browser — Open

Table 33 Icons and buttons in the file browser

Button	Description
	Go up one level in the directory tree.
	Go to user's home directory.
	Make a new folder in the current directory.

Table 33 Icons and buttons in the file browser

Button	Description
	Show a list of files and directories at the current directory level.
	Show the details of files and directories at the current directory level.
	Open selected file. Load into current experiment if it is a VnmrJ 3 data file, sequence, or parameter set.
	Save file with the name shown in the **File Name:** field using the extension shown in the **Files of Type:** field.
	Cancel selection and close the file browser.
	Click and hold to assign current directory to this button.

Status Charts

The Status charts are accessed from the Hardware Toolbar at the bottom of the VnmrJ main window.

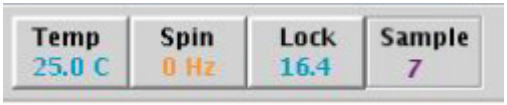


Figure 34 Hardware toolbar in VnmrJ

When you click one of the status plot buttons, a window appears that enables you to log and examine status data.

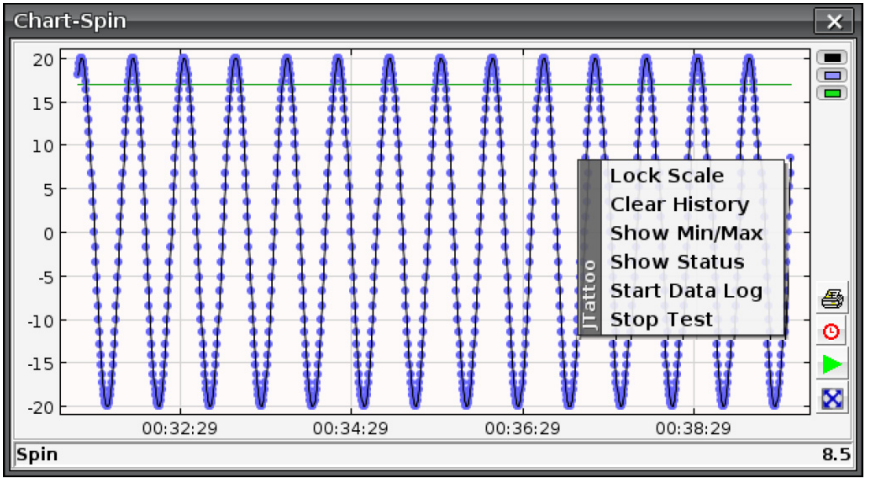


Figure 35 Example of Chart-Spin window with right-click menu

Features of the status chart window

Table 34 Features of the Status Plot windows

Item	Description
	Select color to show/hide the associated element in the chart.
	Opens the Plot Format window. Here, you can • Choose the orientation mode (Portrait, Landscape) The plot will be scaled to fit a full page either vertically or horizontally depending on the chosen orientation mode. • Click **print** in the plot format window to cause the currently displayed data to be printed at the selected printer.
	Toggles the x-axis units between “time-of-day” and “elapsed-time” formats. Initial format is “time-of-day”.
	Click to zoom to display only the most recent data (“Tail” mode). • The amount of data displayed will be set to the x-range selected from most recent mouse “zoom-in” operation (or last 10 seconds if zoom-in action has not yet occurred). • After clicking, any new plot data will be automatically added to the end of the visible region.
	Zoom out to fit data in the display (“Fill” mode).
Right-click menu items	
Lock scale	Lock the scale to the current y axis scale. (Click tail or fill button to remove scale lock.)
Clear history	Removes all collected plot data.
Show Min/Max	Displays the maximum and minimum values observed since the start of data collection. (Does not appear in the printer output.)

Table 34 Features of the Status Plot windows

Item	Description
Show Status	Shows the current status of the relevant status variable. (Does not appear in the printer output.)
Start Data Log	Opens a Save dialog box where you can specify a file into which the plot data will be saved.

Using the status chart

This section describes the components of the status chart window, and what you can do with them.

Data Area

Data area where data traces and the grid are drawn.

Toolbar

A set of buttons in a right-side vertical panel (for descriptions, see Table 34.)

Popup menu

Used to select various options (right-click in data area to open the menu)

Axis Area

Values and tick marks shown to the left and below the data area, along with an x-y grid. The Horizontal axis units are displayed in either "Time-of-day" or "Elapsed-time" format. Initial format is "Time-of-day".

- Elapsed time units are Hours:minutes:seconds measured from the time that VnmrJ is started or from when "Clear Data" is selected from the pull-down menu.
- Time of Day units are "month/day hours:minutes:seconds" in local time.

Status line

Shows variable type and value (drawn below x-axis area).

Zooming

The following modes of zooming are provided:

- Click and drag the left mouse button down and right to zoom in. Click and drag the left mouse button up and left to zoom out.
- Zoom in using the green arrow "tail" button in the toolbar. 
  - Click the green arrow "tail" icon in the toolbar  to display only the most recent data. The amount of data displayed will be set to the x-range selected from most recent mouse "zoom-in" operation (or last 10 seconds if zoom-in action has not yet occurred).
  - After you click the "tail" icon, any new plot data will be automatically added to the end of the visible region.
- Zoom out using the "fill" button 
  - Click the "fill" button in the right-side toolbar. This action sets the plot y and x range to show all current data scaled to fit within the display.

Scale locking/unlocking

- In "zoom-in" mode, the x and y ranges will be "locked" to the boundaries set by the selected "zoom-box".
- In "Fill" mode, the x and y ranges will autoscale to make sure that all of the data in the plot buffer is displayed (ranges are "unlocked").
- In "Tail" mode the x range will normally be locked to show only the most recently collected data and the y range will be "unlocked" so that all of the displayed data is shown.
- In any mode scaling can be "locked" to the current y values by selecting **Lock scale** from the chart popup menu.
- Scale-locking is removed by selecting either the fill or tail button in the interface

Data collection

- The amount of data that is buffered and displayed in the status plots is controlled by the "values" attribute in the "`statusbutton`" sections of `HardwareBar.xml` (a system resource file).
  - The Current default is 1000 points. For example, `values="1000"`.

  - If more points than “values” are collected earlier points are discarded from the plots.
  - Setting “values” to -1 will cause all data to be retained.
- All collected Plot data can be removed by selecting “Clear History” from the chart popup menu.

Data display

Status plots can show the following “traces”

- “Lines” a set of connecting lines drawn between successive data points
- “Points” individual “dots” displayed for each collected point
- “Set Value” The “target” or setpoint value for the relevant status variable type

Each display trace can be made visible or hidden by selection the associated color toggle button in the right-side toolbar.

Data Logging

A text file containing status history can be generated as follows:

- Right-click in the chart area, and then select **Start Data Log** from the display popup menu.

  This opens a standard system “save” dialog window (see Figure 36). Browse to an existing file or type the name of a new file to save the log data. Click **Save File Path**. When the file dialog closes, new data will automatically be written to the specified file. Any old data in the file will be discarded (That is, a new file will be created each time).

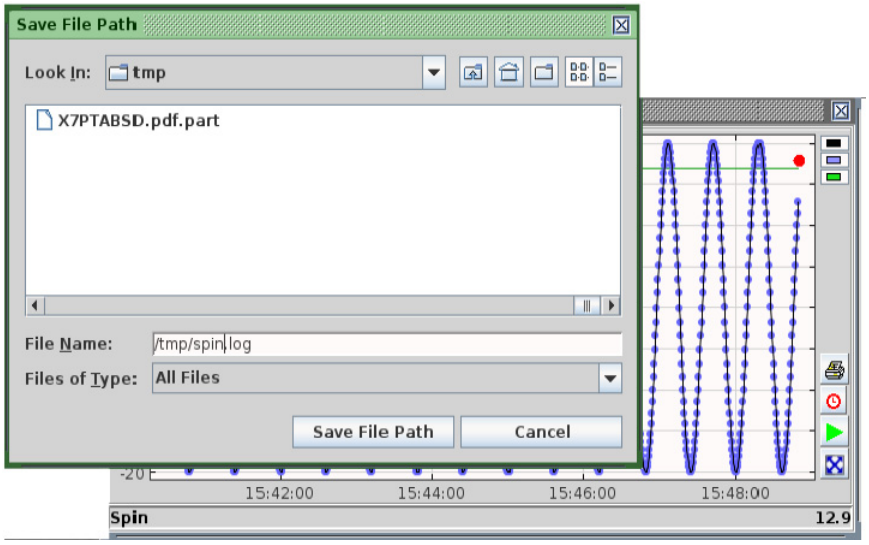


Figure 36 Status chart with save window

  - Only new data acquired in the plot after logging starts will be added to the file.
- If logging is active a red “recording dot” will be displayed in the upper right area of the plot (see Figure 36).

To stop data logging, right-click in the data area to open the chart popup menu and select **Stop Data Log**.

Log file data format is:

“Time-of-day” “elapsed-time” “value”

Example output

DATE TIME VALUE

10/01 11:33:14 000:00:45 -17.3

10/01 11:33:15 000:00:45 -16.4

10/01 11:33:15 000:00:46 - 15.3

Plotting

1. Click the “printer” icon in the right-side toolbar to open a system Print dialog box.
2. Select the printer, orientation, and appearance in the General, Page Setup, and Appearance tabs.
3. Click **Print** in the plot format dialog to cause the currently displayed data to be printed at the selected printer. The plot will be scaled to fit a full page either vertically or horizontally depending on the chosen orientation mode.

Annotation

To include optional text information, right-click in the data area, and select the following options from the popup menu:

Show Min Max will show the maximum and minimum values observed since the start of data collection.

Show Status will show the current status of the relevant status variable.

Note: Annotation text does not appear in the “printer” output.

3 VnmrJ Preferences

The default behavior of VnmrJ at the user account level has several customizable options. These options are different from those that can be accessed by the administrator of VnmrJ. The optimal operation of these customization options requires a properly set up probe file for the probe in use.

Select **Preferences** from the **Edit** menu on the main VnmrJ window to access the VnmrJ preferences setup window. Note that some of the options appear only if the **Enable Email Options** check box has been selected. Ensure that an email server has been properly configured on the host computer.

Templates Tab

The **Edit > Preferences > Templates** tab can be used to select where the data is saved and how data is to be named.

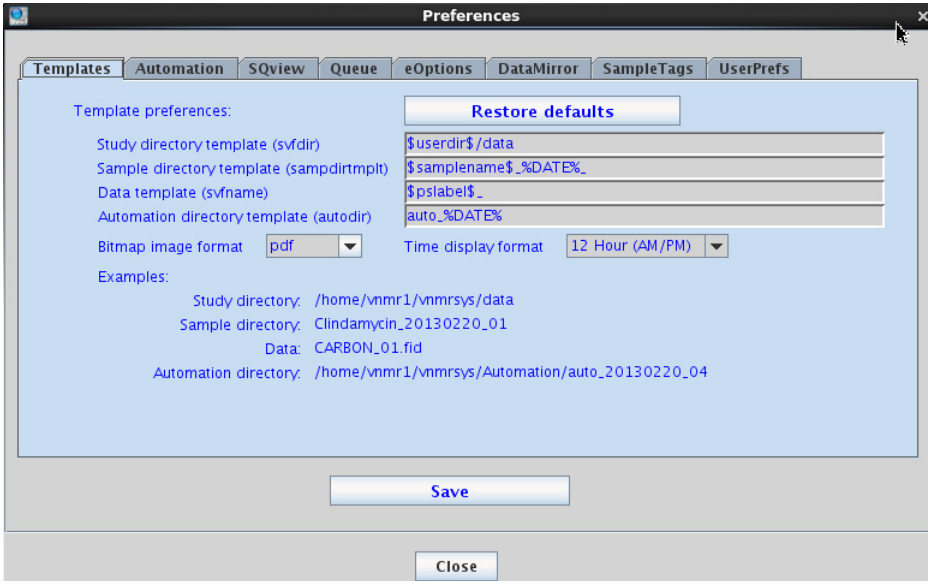


Figure 37 Preferences—Templates tab

The following describes the options for the Templates tab:

Table 35 Options in the Preferences—Templates tab

Item	Description
Study Directory Template	Defines where the data for all the samples is stored. It defines the parameter `svfdir`. Refer to Format of the Entry Level for the exact format of this entry.
Sample Directory Template	Defines the directory inside the study directory where all the data for any sample are stored. It defines the parameter sampdirtmplt. This is always a subdirectory for the study directory, `svfdir`. Refer to Format of the Entry Level for the exact format of this entry.
Data Template	Defines the actual name that is given to the individual fid files. It defines the parameter `svfname`. This file is saved inside `sampdirtmplt`. Refer to Format of the Entry Level for the exact format of this entry.
Automation Directory Template	Defines location of the automation directory, where the system stores all the information to do the automation run. It defines the parameter `autodir`. Refer to Format of the Entry Level for the exact format of this entry.

Table 35 Options in the Preferences—Templates tab

Item	Description
Bitmap Image Format	Drop-down menu with the following selections: **tif**–This creates a TIFF format document, typical for accurate representation of bitmap images. A TIFF document can be read with most common image and word processing programs. **pdf**–This creates a document according to the Adobe PDF™ document format. A PDF document can be read using Adobe Acrobat Reader. The PDF documents created from VnmrJ require Adobe Reader version 5 or higher. **pcx**–This creates a document using the PCX protocol, adequate for representations of bitmap images. PCX documents can be read with most common image and word-processing documents. **jpg**–This creates a JPEG format document accurate for the representation of real-life photos. JPEG documents can be read with most common image and word processing programs.
Time display format	Select the desired format for displaying time from the drop-down menu.

Format of the Entry Level

The format used to enter the directories in the first three fields is the same as was used previously for "autoname". A detailed description of it appears under the description of "autoname" in the *Command and Parameter Reference Manual* for VnmrJ. A brief description is shown here.

There are three types of text that can be entered in these fields. All the options can be mixed together generating very powerful saving options.

1 Fixed text, such as "*/home/vnmr1/data*." This is interpreted as is without any special translations. If the text defines an absolute directory path then this path will be used (example */vnmr/data*). If there is no absolute path then the directory will be created as a subdirectory of the previously defined directory path. So if sample

directory is defined as "*mysamples/today*" then the subdirectory will be created for the study directory.

2. Text enclosed in "$" signs. This will substitute the enclosed text with the value of the VnmrJ parameter with the same name. For example **$samplename$** will be substituted with "mysample" if **samplename**='mysample'. Any VnmrJ parameter can be used for this. The most useful ones will be the ones defining sample parameters (**studyowner, samplename, solvent**, etc.) and experiment parameters (**pslabel** which shows what experiment is run for example). So "**$samplename$/$pslabel$**" will translate into "mysample/PROTON" in the case of a proton spectrum.
3. Text enclosed in "%" signs. This will substitute the enclosed text with the entry on the actual enterQ file being used. This can be very cryptic but some useful options are outlined here. For more detailed description the user is referred to the *Command and Parameter Reference Manual*.
   a. %DATE%: This will be substituted with the date that the spectrum is acquired. Other allowed entries are %DAY%, %MO%, %MOC%, %YR%, %YR2%, %HR%, %MIN% and %SEC%.%RX% where X is a number: This will be substituted with a numerical extension in the form "00", "01", "02" etc. The number X defines the number of digits that will be used for the extension, so %R2% will generate "01" while %R3% will generate "001" etc. This ensures that a unique name is generated for every directory created. A %R2% will be appended automatically to the study, sample and automation directory templates if no "%RX%" is explicitly defined. One can suppress the numbering entirely using %R0%". This is, however, not recommended for the Data Template as it may accidentally overwrite data. When using %R0% at the end of the "Sample Directory Template", all data on the same sample but from different Automation Runs (typically from two or more consecutive days) will be saved into the same sample directory, which may be desirable.

The examples at the bottom of the **Templates** tab show what each of the strings entered translates to. Some useful examples are displayed below.

The example shown in Figure 38 on page 108 will direct all study data to *home/chemp/vnmrsys/data/*<operator name>. This is accomplished by the use of the **$operator_$** argument. Note that the more proper parameter to use in VnmrJ would be **$studyowner$**. The data for each sample will further be saved in a directory named <notebook>_<page>, where notebook and

page are the notebook and page numbers that were entered in the Start tab of the parameter panel. The revision number is suppressed here. The actual FIDs will be saved as <experiment>_<samplename> with a three digit revision after it.

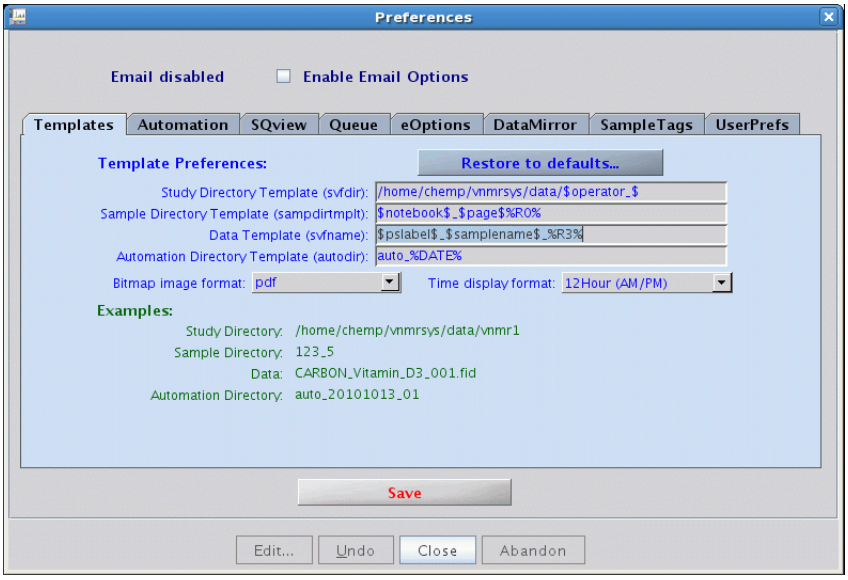


Figure 38 Data saving templates

The example shown in Figure 39 on page 109 illustrates the inclusion of a fixed text in the sample directory name (Book_<notebook>).

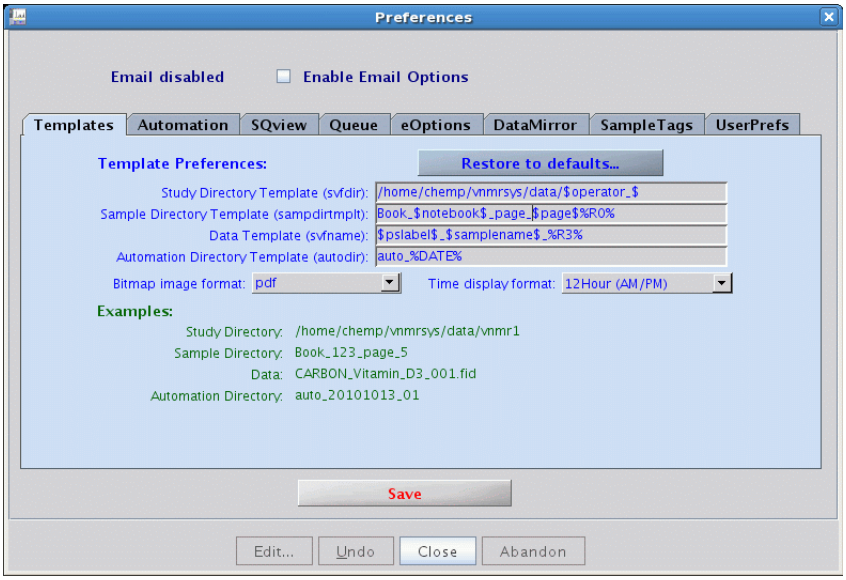


Figure 39 Example–Inclusion of text in Sample Directory Template

The example in Figure 40 on page 110 shows the date is part of the directory name.

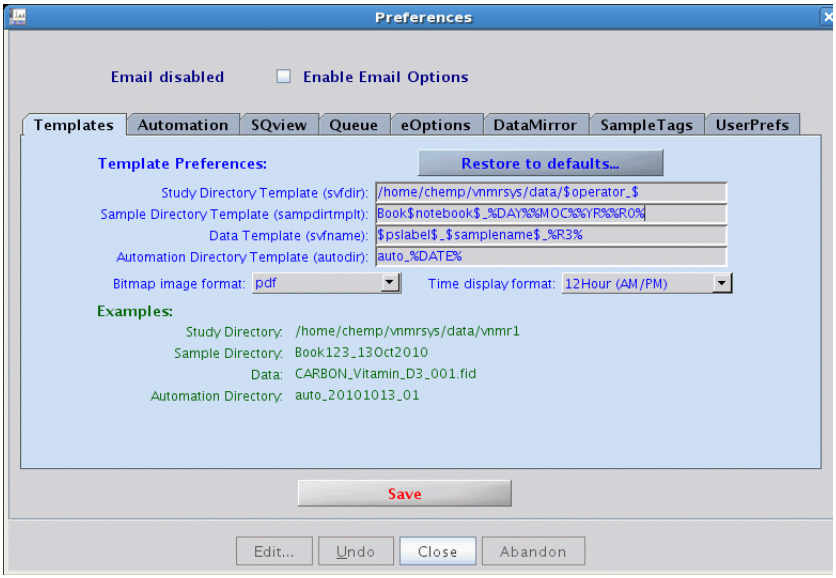


Figure 40 Example—Inclusion of date in Sample Directory Template

Data from one operator can be sorted to different subdirectories according to the date the data was recorded.

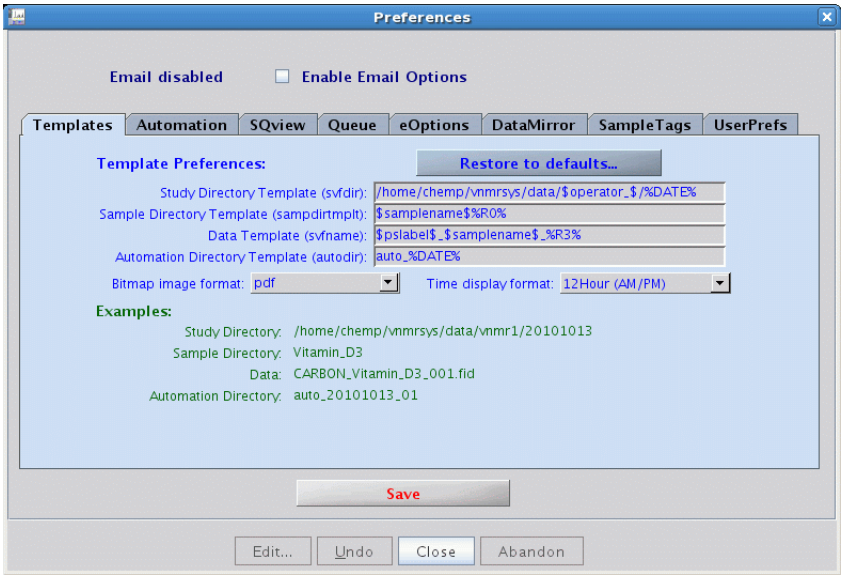


Figure 41 Example—Inclusion of date in Study Directory Template

NOTE Any changes done on this window should be saved before exiting the window. Otherwise, changes are lost. The changes require the creation of a new automation run to become active.

Automation Tab

Automation preferences are set in the **Edit > Preferences > Automation** tab.

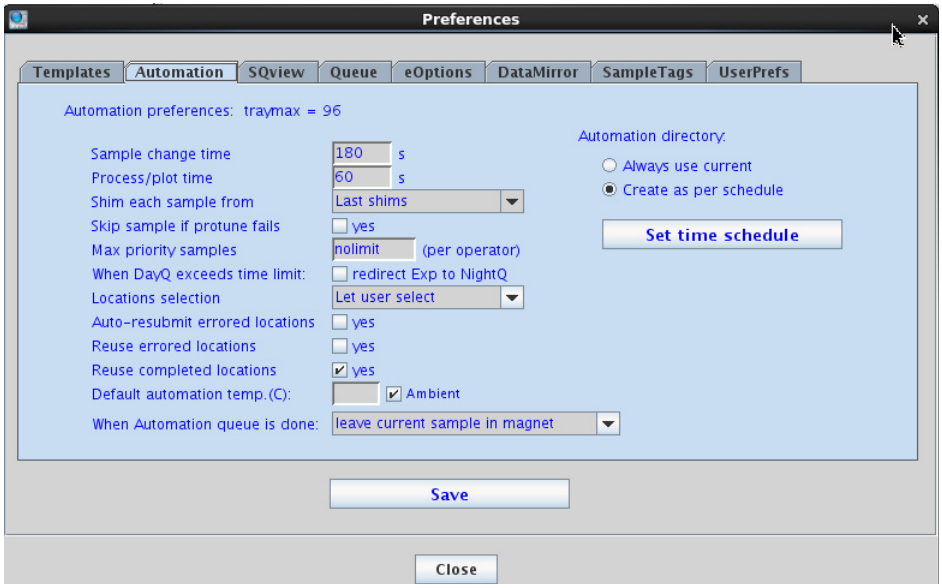


Figure 42 Preferences–Automation tab

The **Automation** tab defines the defaults that will be used for automation experiments. Defaults are described in the following table.

Table 36 Preferences — Automation tab

Item	Description
Traymax	This parameter indicates what type of autosampler is actually used. If this is not set up properly then it needs to be changed in the **System Preferences** window. Only vnmr1 can make this change.
Sample Change Time	This is the approximate time required for the sample change using the autosampler, the finding of the z0 value for the automatic locking, the automatic tuning (ProTune) and the automatic shimming. The default value is 120 seconds which should be sufficient for most cases. It is generally advised to round the time rounded up, so if the system needs 100 seconds to enter instead 120. This ensures that the time calculations will not fall off because of too short estimates.
Process/Plot Time	This is the time required to process, plot and save the spectrum. The default value of 10 seconds should be sufficient. Use a longer value only if you are using a slower computer.
Shim Each Sample From	This defines the shims started by the system when the shim tries to shim a new sample. There are two options: **1** Last shims: Last shims use the shims from the previous sample run **2** Default shims: Default shims load the shim file that is in the probe file. In actual operation with properly prepared samples the outcome should be equivalent. If however that range of samples and tubes used varies widely then the use of Default shims give more consistent results.
Skip Sample if Protune Fails	This check-box appears only if ProTune is installed. If checked then the system skips the sample in the unlikely event that the automatic tuning fails. When the check box is not selected, the data acquisition proceeds.
Maximum Priority Samples	This defines the maximum priority samples an operator can submit in each automation run. The right to have priority samples is granted from the VnmrJ administrative interface.
When DayQ Exceeds Time Limit	By default, with "redirect Exp to NightQ" unselected experiments that are attempted to be added to the DayQ but exceed the DayQ limit result in an error and are not added to the StudyQ. With this option selected, such Experiments are added to the NightQ instead, Select redirect Exp to NightQ if the DayQ has exceeded it's time.
Locations Selection	This drop-down menu defines whether users will be allowed to choose the sample location manually (Let User Select option) or not (Next Available option). The Next Available option will ignore the user input and submit the experiment queue for the next available sample position in the autosampler.
Auto-Resubmit Errored Locations	Select yes to automatically resubmit samples back into the queue that have errorred.

Table 36 Preferences — Automation tab (continued)

Item	Description
Reuse Errored Locations	Select yes to automatically reuse samples that have errored.
Reuse Completed Locations	Select yes to automatically reuse samples that have completed.
Default Automation Temp. (C)	Defines the temperature default for all samples run in automation. If at the time New Automation run is started, the temperature control is enabled in the account, a new temperature can be specified at customization time. The software checks if the chosen temperature is safe given the choice of solvent for that sample. In addition, if variable temperature is allowed in sample changer automation, it is important to set the value for the **tin** (temperature interlock) parameter contained in *~/vnmrsys/modules/cpQdefaults* be set to "w" so that the sample changer will not insert any sample until the probe has reached the requested temperature.
When Automation Queue is Done	This dropdown menu defines what should happen when the last sample of a StudyQ is done and there are no more sample in the queue: • put standby sample (loc=>traymax>) into magnet. This removes the last sample run from the magnet thus allowing its owner to retrieve it from the autosampler tray. The standby sample needs to be placed in the position indicated in the field, position 96 in the case of the figure above. That particular sample location is not available for use. • leave current sample in magnet. This leaves the last sample of the StudyQ in the magnet for further use. • remove current sample from magnet. Only removes the current sample from the magnet without inserting a (standby) sample. This option is only available with 7600AS and 7510AS sample changers.
Automation Directory	Determines when a new automation directory shall be created: • Always use current. The current automation directory is used until the user creates a new one by selecting "Automation Run (autodir) -> New Automation Run" from the "Automation" menu. • Create as per schedule. A new automation directory is created on each day on which a previous NightQ ended as defined with the "**Set Time Schedule**" window.
Set Time Schedule	Opens the Automation Schedule window to set time schedules for automation runs. See "Automation Schedule" on page 114.

Automation Schedule

To open the Automation Schedule tool, click **Edit > Preferences** to open the **Preferences** window. Then select the **Automation** tab and then click **Set Tine Schedule.**

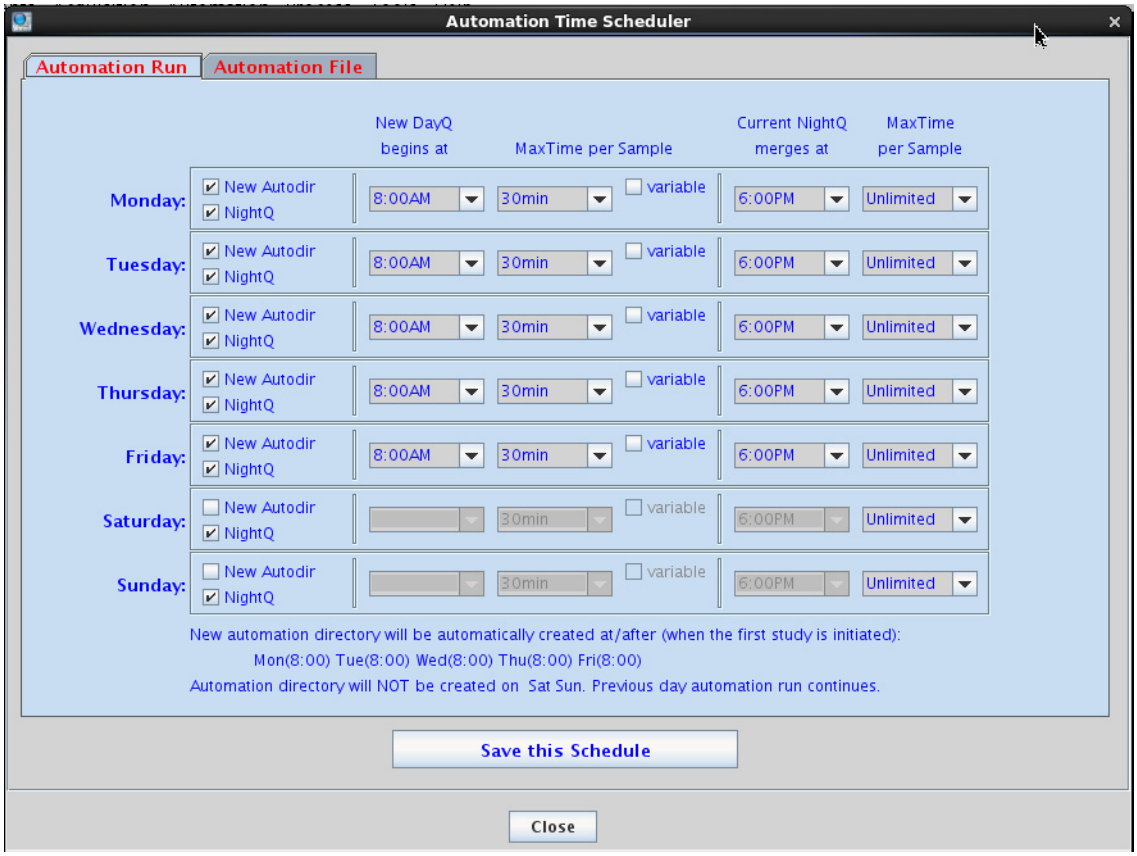


Figure 43 Automation Schedule window—Automation Run tab

Figure 44 Automation Time Scheduler—Automation File

The **Automation Schedule** tool allows the account administrator to define how time is allocated during the day or night for Automation Runs (AutoRuns, typically on demand sample automation) and Automation Files (AutoFiles, sample queues built for submission at a time chosen by the account administrator). Selecting the All Day check simply turns off time management and is a better choice for a research environment as opposed to an open system being accessed by a large number of chemists. Using the **Automation Schedule** tool, the user can define different queue times for

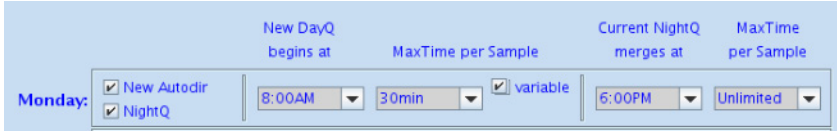
different times of the day as well as after hours' queues. At sample submission time with the NightQ enabled, a chemist can submit certain experiments to the day and others to the night.

There are definitions for each day of the week. The first two columns define when the day and night starts. They are only active if the "All day" option is not selected. The third column, Max Time per Sample, defines how much experiment time will be allocated per sample during the day. The column with the same name further to the right defines the maximum time per sample during day and night runs.

The definitions for the AutoFiles are similar, with the fields defining how long the total time for short and long queues should be and how long the maximum time per sample allowed for short and long queues should be.

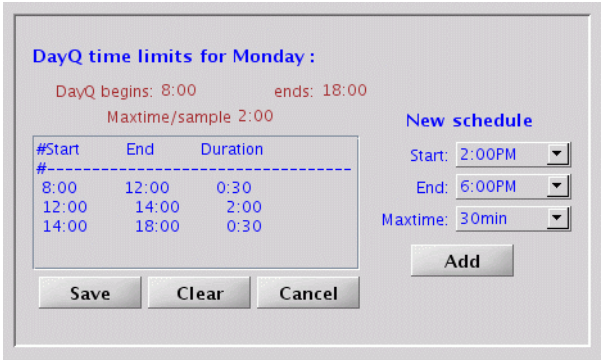
The maximum time per DayQ sample can also be made variable, for example, to allow users longer runs during lunchtime. To do this:

1 Select the **variable** check box. A new button **set/view** appears.



2 Select a longer MaxTime per Sample to accomodate the longer allowed "lunch queue".

3 Click it to see and/or edit the detailed DayQ time limits for that day.



4 Enter the new, "split" DayQ limits by adding pieces of schedule:

- **a** Start with first schedule part: Select the **DayQ start** (here 8:00 AM), select the **End** (to the beginning of "lunch", here noon) and select **Maxtime** (here the default 30 min). Click **Add**.
- **b** Now enter the start and end times during which longer DayQs are allowed (here 2 h). Click **Add** again.
- **c** Finally, enter the second **normal** time period (afternoon). Click **Add**.
- **d** Click **Save** to keep this variable schedule. The variable time limits schedule can be erased to start afresh by clicking **Clear**. Click **Cancel** if you want to exit this panel without saving.

A variable schedule may have more than three entries.

Note that any changes done on the automation schedule need to be saved (red **Save** button) before exiting the window, otherwise they will be lost. The changes will usually require the creation of a new automation run in order to become active.

SQview Tab

The **Edit > Preferences > SQview** tab allows the user to change the Study Queue display order or restore the display order to default.

Select the **Show Scout Fids** check box to display all prescan FIDs in the Study Queue.

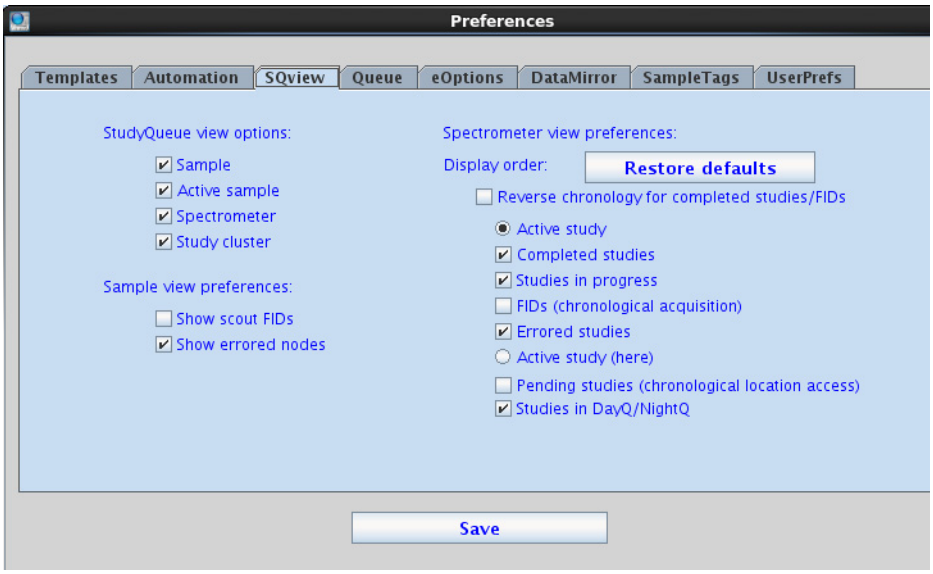


Figure 45 Preferences-SQview tab

Queue Tab

The **Edit > Preferences > Queue** tab offers options for the actual automation queue. All settings at this page are default settings. Each sample submission will start with these default settings. They can be overwritten during the sample submission.

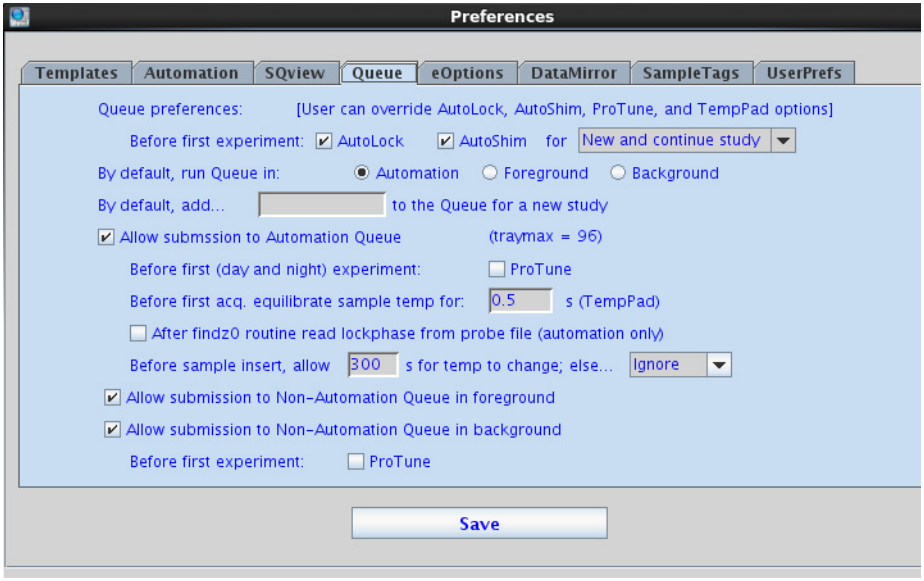


Figure 46 Preferences–Queue tab

Table 37 Preferences — Queue tab

Item	Description
Before First (Day and Night) Experiment	Defines whether the system will automatically lock and shim before the first experiment of a sample queue.
By default run queue in	Select whether to run the queue automatically, in the foreground, or in the background.
By default, add...	This option allows for an experiment to be automatically added by default to each new queue. For example, "PROTON".

Table 37 Preferences — Queue tab (continued)

Item	Description
Allow Submission to Automation Queue	This setting activates the automation queue. If this is not desired then this should be unchecked.
Before First (Day and Night) Experiment	If the system is equipped with a ProTune module, this selection defines whether the system will automatically run ProTune before the first experiment of a sample queue.
Before first acquisition equilibrate sample Temp for ___seconds (TempPad)	This sets the amount of time that the system will wait for the temperature to equilibrate after it inserts the sample into the magnet but before recording any spectra. The default value is 2 seconds which should be sufficient for experiments conducted at or near ambient temperatures. Increasing this value has got the advantage of having the temperature better equilibrated in the sample but the disadvantage of increasing the time required for each sample.
After findz0 routine read lockphase from probe file (automation only)	This is a setting for optimizing the lock system before spectra are recorded. If selected then the lock phase is set to the value in the probe file overwriting any value that has been set manually. The normal value for this box is unchecked. It should only be checked if there is a suspicion that the lock phase is not set properly. In this case the probe file should be updated with the correct value for the lock phase.
Before sample insert, allow ___seconds for Temp to change; Else...	This value selects the amount of time the system waits after retrieving a completed sample but before inserting the next sample for the temperature to equilibrate. This is a useful feature when operators are allowed to run samples in automation at different temperatures. It can be used to avoid the case where a sample was run at a temperature higher than the boiling point or lower than the freezing point of the next sample's solvent. The time defined here is the maximum time that the system will wait for the temperature to equilibrate. If the temperature equilibrates faster, the run continues. The actions in the pull-down menu define what will happen if such a condition is met and there is no waiting time defined. The possible actions are: "Ignore", which causes the system to ignore the condition and proceed with the sample submission, "Abort", which causes the system to abort the automation run and "Alert" which gives a warning to the operator.
Allow submission to Non-automation Queue in Foreground	Select to allow users to run manual Study queues on one sample in the foreground. The foreground option will run all of the StudyQ's experiments in the current VnmrJ experiment.

Table 37 Preferences — Queue tab (continued)

Item	Description
Allow submission to Non-automation Queue in Background	Select to allow users to run manual Study queues on one sample in the background. The background option runs the single Study queue in the same way as a standard automation run; by holding all the information in the autodir directory.
Before First Experiment	If the system is equipped with a ProTune module, the option for automatic tuning before the first experiment appears here If automatic tuning before the first experiment is not desired then this box should be unchecked.

NOTE Any changes done on this window need to be saved (red button **Save**) before exiting the window, otherwise they will be lost. The changes will require the creation of a new automation run in order to become active.

eOptions Tab

Electronic options are set in the **Edit > Preferences > eOptions** tab.

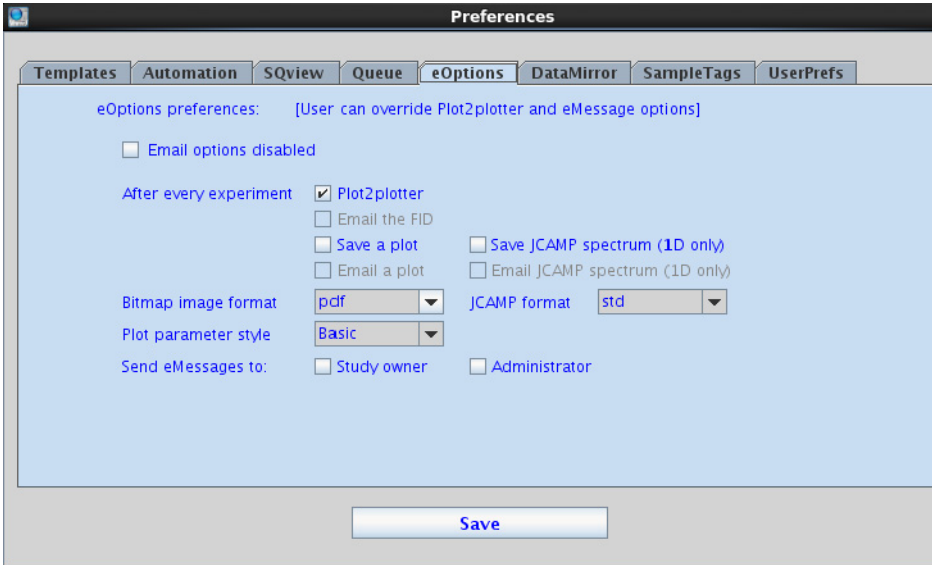


Figure 47 Preferences-eOptions tab

The **eOptions** tab defines actions that will be taken to produce an electronic output of the recorded spectra. The default options set on this tab will be the default option with every new study queue. Each operator has the option to override these in the **Start** parameter panel during the submission of the queue. The available options define what happens after every experiment.

Table 38 eOptions tab

Item	Description
Plot2plotter	Select to produce a hardcopy output to a defined plotter.
Save a plot	Select to save the plot in the format defined in the Bitmap Image Format field.

Table 38 eOptions tab (continued)

Item	Description
Email a plot	This option is enabled only if the "Enable Email Options" is checked at the top of the window. If it is, then the system will send a plot of the recorded spectrum as an e-mail attachment to the e-mail address of the operator who submitted the sample.
Save JCAMP spectrum (1D ONLY)	Select to save a 1D JCAMP Spectrum in the format defined in the JCAMP Format field.
Email JCAMP spectrum (1D ONLY)	Select to email a 1D JCAMP Spectrum as an e-mail attachment to the e-mail address of the operator who submitted the sample. This option is enabled only if the "Enable Email Options" is checked at the top of the window.
Email the fid	This option is also enabled if the "Enable Email Options" is checked at the top of the window. If it is then the system will send the entire fid of the recorded spectrum as an e-mail attachment to the e-mail address of the operator who submitted the sample. This option should be used with care as NMR spectra, especially multidimensional ones, can grow to very large sizes which may not be accommodated by the available capacity and bandwidth of the e-mail servers.
Bitmap image format	This pull-down menu defines the format of the plot that will be saved or e-mailed. Options are: • tif. This creates a TIFF format document, typical for accurate representation of bitmap images. A TIFF document can be read with most common image and word processing programs. • pdf. This creates a document according to the Adobe PDF™ document format. A PDF document can be read using Adobe Acrobat Reader. The PDF documents created from VnmrJ require Adobe Reader version 5 or higher. • pcx. This creates a document using the PCX protocol, adequate for representations of bitmap images. PCX documents can be read with most common image and word-processing documents. • jpg. This creates a JPEG format document accurate for the representation of real-life photos but are less recommended for line-art pictures. JPEG documents can be read with most common image and word processing programs.
JCAMP Format	This pull-down menu defines the JCAMP format for 1D that will be saved or e-mailed: • std. Contains the processed spectrum in binary encoded text format. • xy. X-Y ASCII text table of the processed spectrum that can be read by spreadsheet programs like Excel or mathematical software.

NOTE

Any changes done on this window need to be saved (red button **Save**) before exiting the window, otherwise they will be lost. The changes will require the creation of a new automation run in order to become active.

Data Mirror Tab

VnmrJ provides the option to automatically store another copy of the data recorded in automation on a local or remote disk. Use the **Edit > Preferences > Data Mirror** tab to set up this feature.

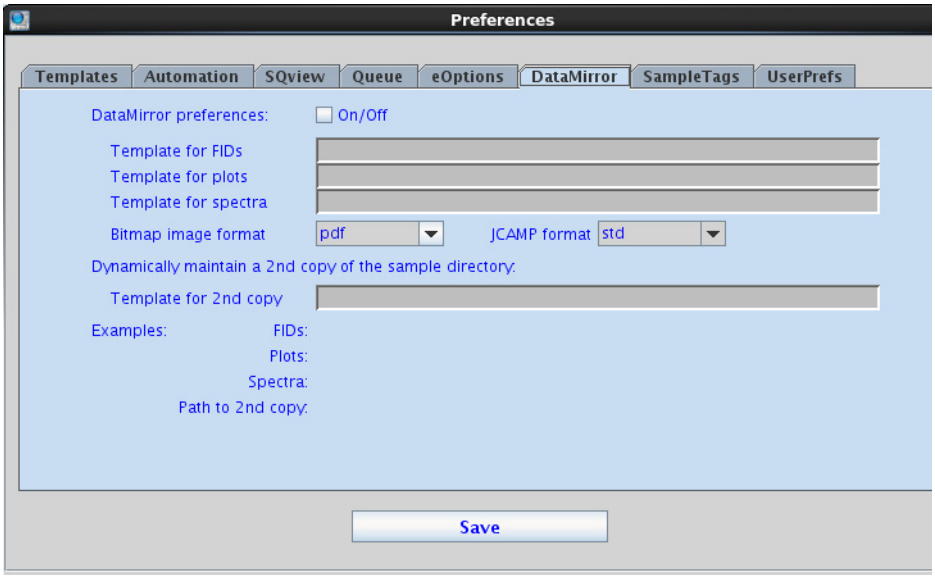


Figure 48 Preferences — DataMirror tab

If the option is turned on (**ON/OFF** check box at the top of the window) the feature is activated and each dataset is saved twice: first at the locations defined in the **Templates** tab, second at the locations defined on this tab. The syntax for the templates is identical to the ones in the "Templates Tab" on page 104.

There are three types of files that can be mirrored: FIDs, Plots and Spectra. The entire sample directory can be mirrored as well which is defined in the last field on this tab.

Data mirroring can be useful for backup. When used with externally mounted or network drives, users can access data at other systems. This can have several benefits, reducing the load on the spectrometer computer host and reducing the need for extensive network transfers of data.

A complementary tool to this is the UNIX function of rsync. The way to setup rsync is described in the *User Programming Guide*.

NOTE Any changes done on this window need to be saved (red **Save** button) before exiting the window, otherwise they will be lost. The changes will require the creation of a new automation run in order to become active.

SampleTags Tab

The **Edit > Preferences > SampleTags** tab allows the system administrator to define which parameters required for each sample will be recorded and transferred to all experiments in one sample queue.

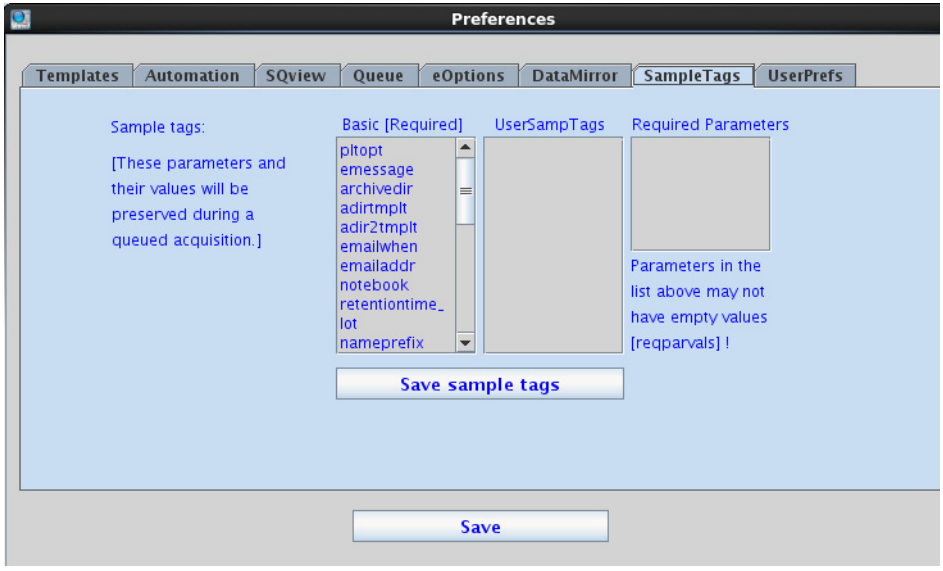


Figure 49 Preferences — SampleTags tab

The window displays three lists of parameters.

Table 39 Preferences — Sample Tags tab

Item	Description
Basic	These are parameters are the standard set captured by default with every parameter set, such as samplename, the data directory where data are saved, etc.

Table 39 Preferences — Sample Tags tab (continued)

UserSamp Tags	Any parameters that the account owner has created and wants to have available for all spectra. For example, a string variable named `charge_code` could be created and then added to this list. That variable would then be captured with every spectrum and would be available for use in the data save templates.
reqparvals	This column contains the parameters that will be absolutely required to be entered, otherwise the automation run will not be able to proceed. Note that any parameter appearing as data saving parameter in the Templates tab will automatically be required and does not need to be entered again here.

NOTE Any changes done on this window need to be saved (red **Save Sample Tags** button) before exiting the window, otherwise they will be lost. The changes will require the creation of a new automation run in order to become active.

UserPrefs Tab

The **Edit > Preferences > UserPrefs** tab allows the account administrator to set up operator options.

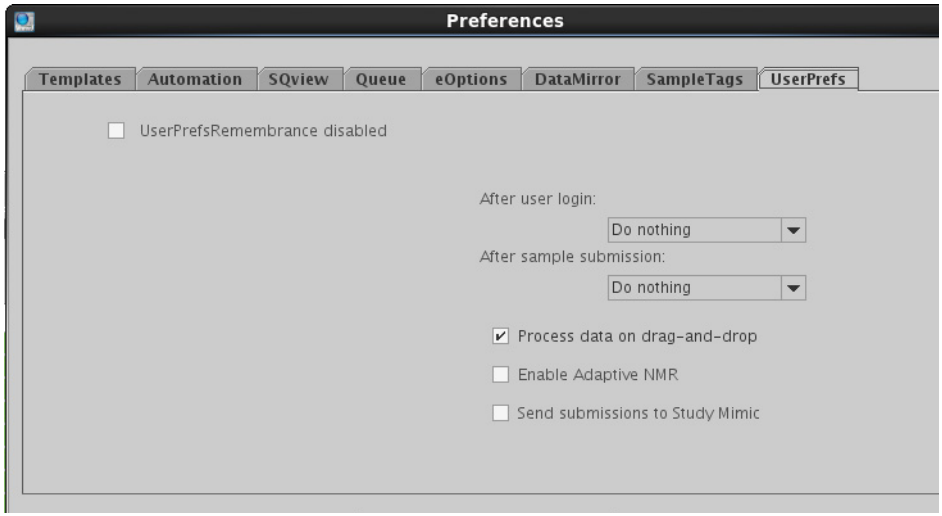


Figure 50 Preferences — UserPrefs tab

The first task the account administrator should perform using the **UserPrefs** tab is to decide the action to be taken after sample submission.

Table 40 Preferences — UserPrefs tab options

Item	Description
Do nothing	Enables the user to leave the list of experiments in the StudyQueue in place for submission in full or in part to another location.
Clear Queue	Clears the experiment list while leaving the interface in submission mode for easy creation of a new queue for other sample locations.
Quit Submit mode	Automatically "clicks" the **Done** button, exits the sample submission mode and leaves the operator in Data Review mode.

Table 40 Preferences — UserPrefs tab options (continued)

Item	Description
Operator logout	Quits the submit mode and logs that operator out automatically. This may be useful for a high-volume NMR service lab with lots of operators who tend to generally submit one sample at a time.

The account administrator should next define the interface personality at the time of operator login.

The choices are as follows:

Table 41 Options for defining user interface at login

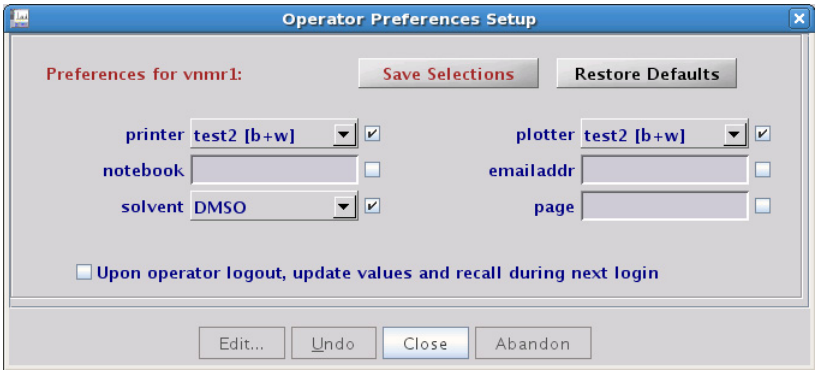
Choice	Description
Do nothing	Displays the manual/sample review mode - the user must click **New Study** to begin an Automation.
Show Tray	Displays the manual/sample review mode showing the automation tray
Ready for submit	Automatically "clicks" **"New Study"** button to enable the submission mode of the interface

In the **UserPrefs** tab, the option **UserPrefsRemembrance** enables the user to set values for any desired parameters that can be pre-set upon entry of sample submission mode. The parameters can be unique for each operator, allowing users to easily manage pre-filling of items such as preferred solvent, notebook, email address, and so on.

NOTE

Any changes done on this window need to be saved (red button **Save**) before exiting the window, otherwise they will be lost. The changes will require the creation of a new automation run in order to become active.

Once **UserPrefsRemembrance** is enabled and the parameter list for remembrance is defined by the account administrator, individual operators can manage their own preferences for those parameters via the menu **Edit> Operator Preferences:**



In this example, the operator choices for printer, plotter, and solvent have been defined by the account administrator by entering those checks or parameter names into the entry box. After the first time, the account administrator must select the **Setup Default** values button to assign defaults for the user to start modifying values.

The menu for plotter and printer read valid devices known to the NMR spectrometer and each operator can choose the location where the data hard copy is plotted. The userRemembrance tools help prevent keying errors of items such as a laboratory notebook and preferred solvents. In this example the email address is controlled by the operator and not an administrative task for the account administrator. An operator can choose to direct PDF plot emails to any desired email address.

4
Preparing for an Experiment

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Starting VnmrJ

1. Log in to the workstation.
2. Double-click the VnmrJ icon.

   The VnmrJ program window opens. See Figure 2 on page 16.

Preparing for an Experiment

Before you can acquire a spectrum, prepare the sample and set up the experiment using the following steps.

After you complete these steps, go to Chapter 5, "Acquiring Data" to review how to acquire the data.

Prepare the sample

1 Prepare the NMR sample by dissolving the analyte in a deuterated solvent.

   Use a concentration that will completely dissolve the sample, usually between ~1 mg/mL and ~50 mg/mL.

2 Transfer between 600 µL and 750 µL of the solution into a 5-mm NMR tube.

3 Positioning the NMR tube:

   a Insert the NMR tube into a spinner turbine.

   b Carefully place the spinner turbine into the top of the sample depth gauge.

Depth gauge

   c Carefully center the sample on the thick black line in the middle of the depth gauge window

   d Remove the spinner-turbine from the depth gauge.

   This step insures that the sample is positioned in the probe coil after insertion into the magnet.

Load the sample

For systems without a robot sample changer: Load the sample into the system.

1 Click **Eject** on the VnmrJ **Start > Standard** parameter panel to lift the current sample to the top of the magnet bore.

2 Carefully remove the current sample and replace it with the new sample.

3 Click **Insert** on the **Start > Standard** parameter panel to lower the sample into the magnet.

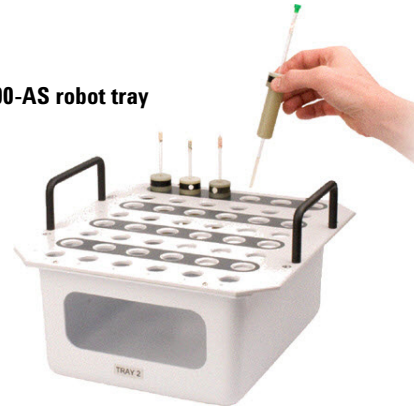
For systems with a robot sample changer:

- Load your sample into the robot tray and note the location.
  Avoid blocking the location of the sample currently in the magnet.

  7600/7620-AS: The current location is displayed on the LCD information panel.

7510-AS: The location directly over the magnet bore is reserved for the sample currently in the magnet.

7600-AS robot tray



7510-AS robot tray

Tune the Probe

Probe tuning is required when there is a significant change in the polarity of the solvent. Changing from a non-polar organic solvent to a more polar organic solvent or aqueous solvent generally requires retuning the probe. Changes in the ionic strength of the solution (for example, low salt to high salt) also require retuning of the probe.

Tuning probes on systems with ProTune

Agilent NMR Systems spectrometers equipped with ProTune provide the features described in Table 42. To open the ProTune window, click **Tools > Probe Tuning > Auto Tune Probe**. For details on tuning a system using ProTune, see the *Agilent VnmrJ Spectroscopy User Guide*.

Table 42 ProTune features and functions

Feature	Button, label, or message	Description
Diagnostic and tuning	Motor Communication OK, Sweep Communication OK	Status of Ethernet communications between the module and the workstation
	Abort Command	Stops current command
	Drop-down list	Probe name and channel number
	Corrected Data/Raw Data	Toggles window to display corrected or raw data
	Tune Probe (MHz)	Tunes frequency
	Threshold (dB)	Criteria for successful tuning
	Refresh (times)	The number of times the plot should update with new data
	Center (MHz)	Sets center value of the sweep range
	Span (MHz)	Sets span value of the sweep range

Table 42 ProTune features and functions (continued)

Feature	Button, label, or message	Description
	Absval Plot/Polar Plot	Toggles between polar plot (imaginary and real reflection) and absolute value plot (reflection v. frequency).
	Cmd	Executes the ProTune command in the field.
Settings	Tune/Match Backlash	Difference between the number of steps traveled from the tune frequency and the number of steps traveled back to the tune frequency.
	Tune/Match KHz/Step Size	Number of KHz the dip moves in 1 step
	Tune/Match Reflection/Step	Minimum dip movement in one step with no regard to frequency. Positive values are inside the circle of origin, and negative values are outside the circle of origin.
	Dip Frequency	Frequency the dip occurs
	Dip Reflection	Reflection value at the dip
	Match at Freq MHz	Reflection at the desired frequency
Controls and output	Tune	Tune motor control
	Match	Match motor control
		Displays the graph in full scale view.

Manual tuning using mtune

If your system does not include ProTune, you can manually tune the system using **Tools > Manual Tune Probe**. The mtune routine runs in the graphics canvas and uses VnmrJ panels. You can also run manual tuning from the command line. For details on manually tuning the system, see the *Agilent VnmrJ Spectroscopy User Guide*.

Optimize the Lock

Under computer control, the lock system maintains a constant field at the sample as the static field generated by the superconducting magnet drifts slowly with time or changes due to external interference. Locking makes the resonance field of the deuterium in the deuterated solvent coincide with the lock frequency.

The lock level can be viewed by clicking on the **Lock** button on the hardware bar.

For information on how to perform lock optimization, see the *Agilent VnmrJ Spectroscopy User Guide*.

Shim the System

There are various ways to shim the system, either manually or using an automated Proshim method. For details on all shimming methods, see the *Agilent VnmrJ Spectroscopy User Guide*.

Shimming on the lock signal manually

Monitor the intensity of the lock signal while adjusting the shim settings. Each shim setting controls the current through shim coils that control magnetic field gradients in different directions. The Z direction must be parallel to the vertical direction of the probe, and it is for this reason that the height of the sample in the NMR tube affects the Z shim settings rather dramatically. For details on how to manually shim the system, see the Agilent VnmrJ Spectroscopy User Guide.

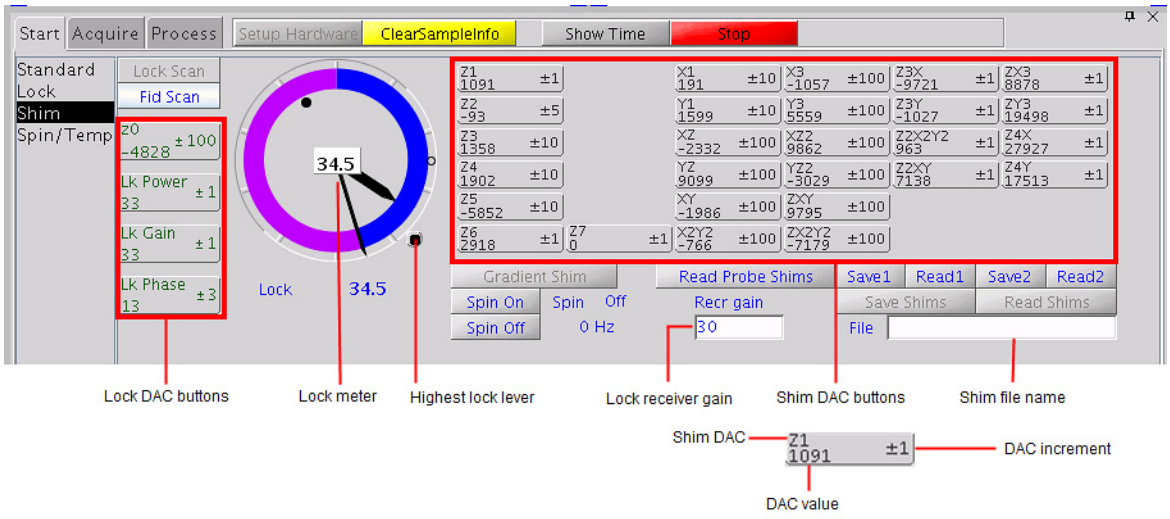


Figure 51 Location of shim buttons and controls

Proshim

With VnmrJ, you can create shim methods that can be saved and used again. The Proshim editor is used to create or modify shim methods.

To open the Proshim window to build or edit Proshim methods, click **Tools > Standard Calibration Experiments > Shim Editor.** For details on using Proshim, see the *VnmrJ Spectroscopy Users Guide*.

Use the Proshim editor (Figure 52) to:

- Display the method selected in the Current Method group
- Edit the method selected in the Current Method group
- Build a new method
- Save changes to a shim method

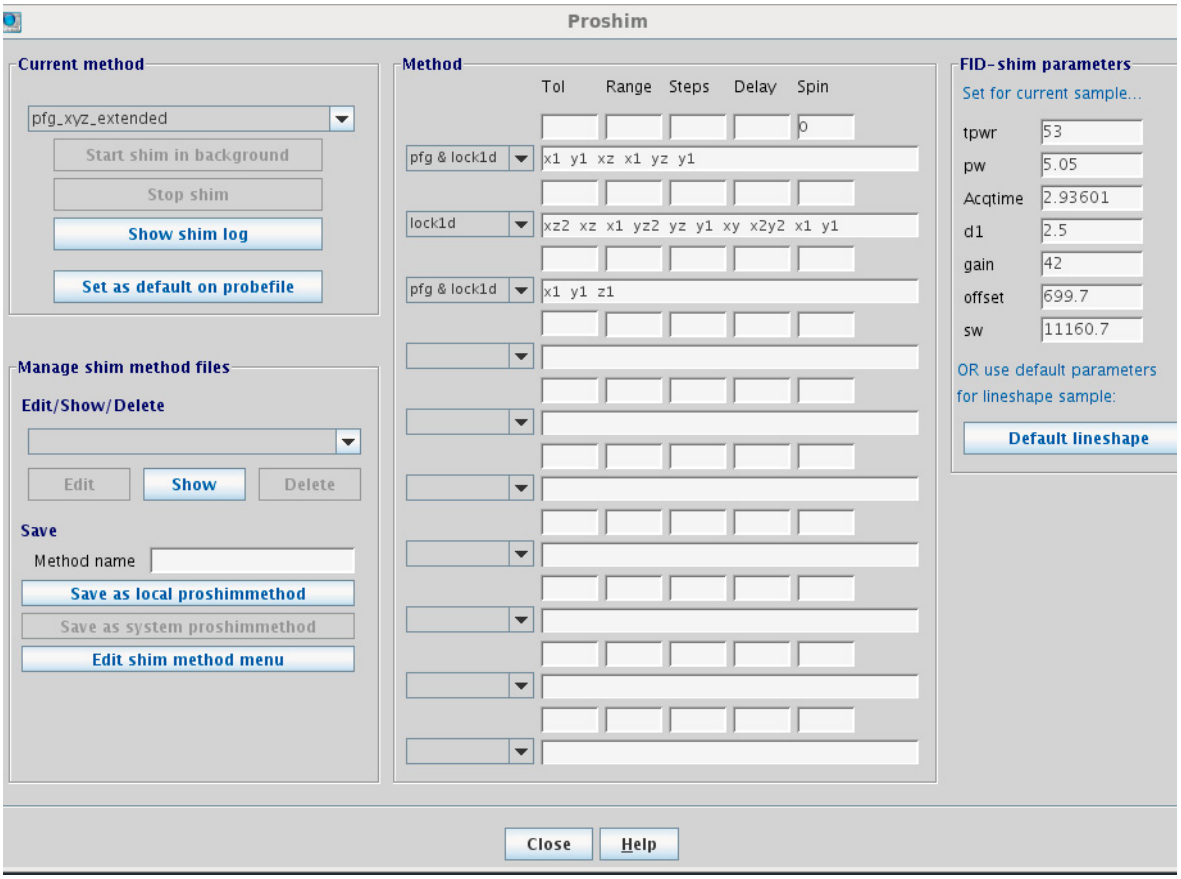


Figure 52 Proshim window

Manage shim method files

After making edits to the shim method and Start shim is run, you can save the edited Shim.

Use Manage shim method files to

- Save the edited shim method as a local or system shim method
- Display a shim method
- Edit a shim method

- Delete a shim method

Use a Proshim method in automation

Once a Proshim method is created, it can be used to shim a sample as part of an automated study.

1. Create a New Study and add the desired experiments to the Study Queue.
2. On the Sample Info page, use the Select shim map pull-down to choose a Proshim method.
3. The specified Proshim method will now be used when the study is submitted to acquisition.

Set up the Experiment

Set up the experiment using the pages in the **Start** tab in the Parameter Panel.

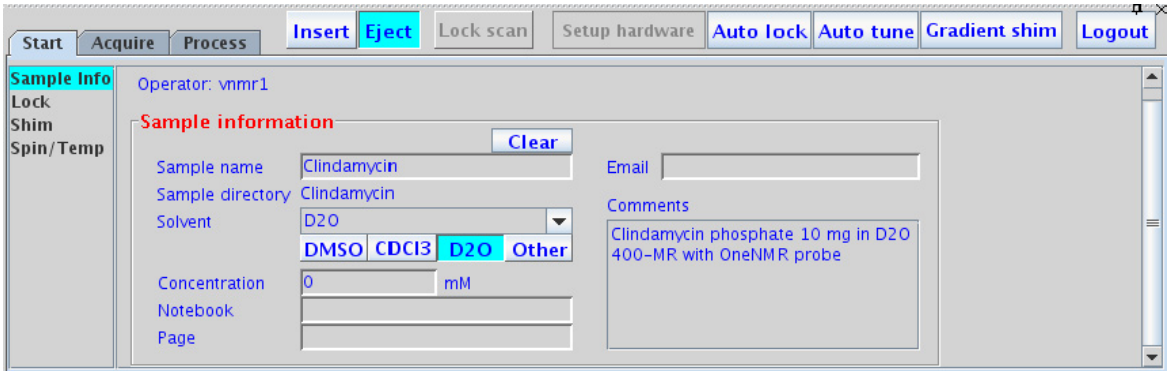


Figure 53 Sample Info tab of the Parameter Panel

1 Under the **Start** tab, select the **Sample Info** page.
   - **a** Fill in the information for the sample, select a **Solvent**, and enter the comments.
   - **b** Enter a name in the **Sample Name** field to name the sample.
   - **c** Define the sample, if desired, by filling in the optional **Email**, **Concentration**, **Notebook**, **Page**, and **Comment** fields.
2 Insert the sample (if not already loaded).
3 Regulate spinning and temperature on the **Spin/Temp** page.
4 Find Z0 and adjust the lock using the **Shim** and **Lock** pages.
5 Shim the system to adjust the field homogeneity using the controls provided on the **Shim** page.

5 Acquiring Data

Using VnmrJ, spectra are typically acquired using a Study (with or without a robot sample changer). A Study is a collection of one or more experiments that you want to perform on one or more samples. However, you can also acquire a single spectrum manually. This section contains information on how to acquire spectra using VnmrJ.

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Acquire a Spectrum Manually

For manual acquisition,

1. Use the Experiment Selector or the Experiment Selector Tree in the Protocols vertical panel to select an experiment.
2. Use the pages in the Start and Acquire tabs of the Parameter Panel to view and change parameters. See the *Agilent VnmrJ Spectroscopy User Guide* for details on acquisition settings and pages.
3. When ready, click the green Acquire button at the top of the Parameter Panel to start acquisition.

Using a Study Queue to Acquire Data

A study is a ordered list of experiments that can be performed on any given sample. When data is collected using the Study Queue, information regarding that sample, including raw data, processed data, and plots, are linked together and automatically collected into a Sample Directory. These links allow customized information from one experiment (for example, calibrated pulse widths, optimized sweep widths, and solvent suppression conditions) to be automatically incorporated into subsequent acquisitions, and the automatic addition of high-resolution reference spectra to 2D plots.

Build a Study Queue

The Study Queue contains an ordered list of experiments you want to perform on one or more samples (with or without a robot sample changer). To create a study and add experiments to the Study Queue, use the following steps.

1 **Protocols** vertical panel, under **Study Queue**, click **New Study**. This puts the Study Queue in Submit mode, where you can build a study and submit it to acquisition.

2 Double-click to select experiments from the Experiment Selector or the Experiment Selector Tree to add to the Study Queue.

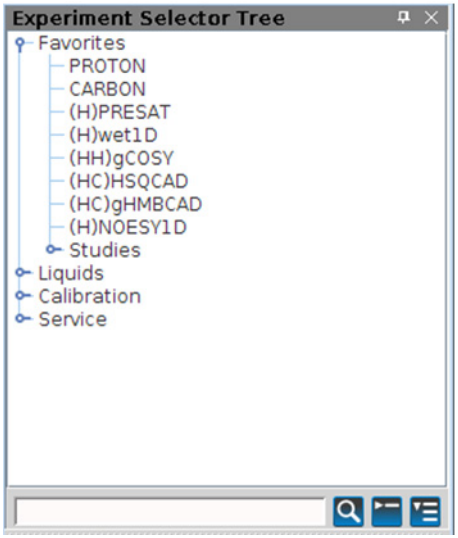

Figure 54 Experiment Selector Tree

Each experiment is added to the Study Queue and displayed as a node.

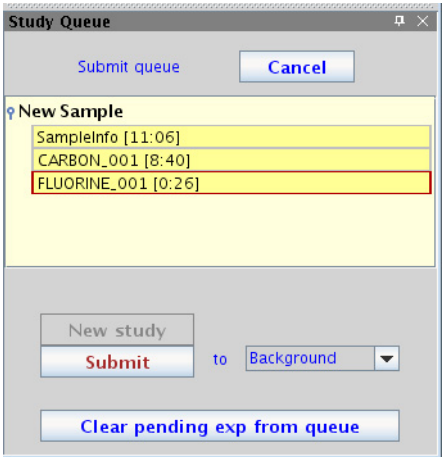

Figure 55 Study Queue

Run a Study Queue

1 Click **Submit** to run the Study Queue.

The Acquisition Status display on the hardware toolbar shows:

- the task being performed
- time left for the task to run
- **Idle** when waiting for a process to complete, or **Inactive** when no process is being run.

The Study Queue experiment nodes appear green if completed, blue if active, and yellow if queued.

NOTE

For systems with a robot sample changer:
The same Study Queue can be submitted to multiple samples by:
changing the sample information, selecting a sample-tray location, and clicking **Submit**.

Using Express Submit with a sample changer

The Express Submit utility uses automation to quickly submit a sample to a specific tray location. To use Express Submit: a sample changer must be present and selected in **Edit > System Settings > System config** and a default experiment which will be added to each new study must be defined in: **Edit > Preferences > Queue** tab.

1 Right-click on the location in the Tray Display that holds the sample and select **Express Submit.**

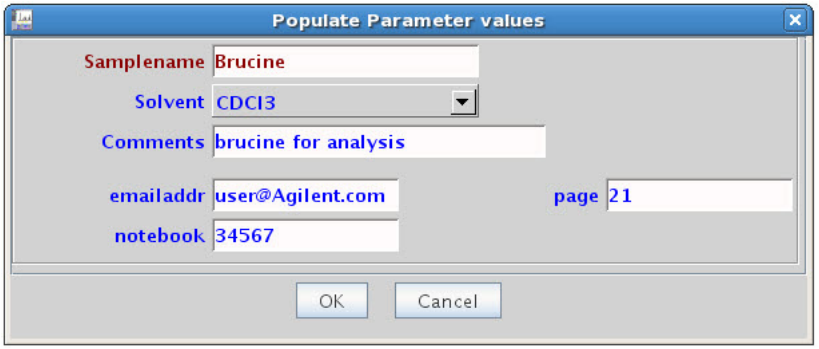

Figure 56 Express submit - populate parameter values

2 In the Express Submit popup, choose the solvent, fill in the required fields (red labels), and fill in any of the optional fields as desired.

3 Click **OK** to submit the default experiment to that location and close the pop-up window.

Stopping an Experiment

There are four ways to stop an experiment:

- Click the **Stop** button.
- Click **Acquisition** in the VnmrJ menu bar, and then select **Abort Acquisition**.
- Click the **Stop** button in the bar at the top of the Parameter Panel (when either the **Start** or the **Acquire** panel is selected).
- Enter `aa` on the command line.

6
Processing Data

Once a spectrum is acquired, there are a wide variety of ways you can view and process the data. This section describes some of the most commonly used processing tasks. See the *Agilent VnmrJ Spectroscopy User Guide* for more detailed information.

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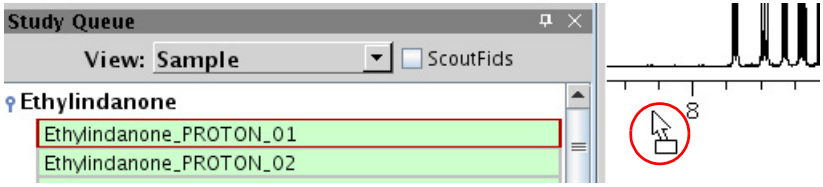
Loading Data from the Study Queue

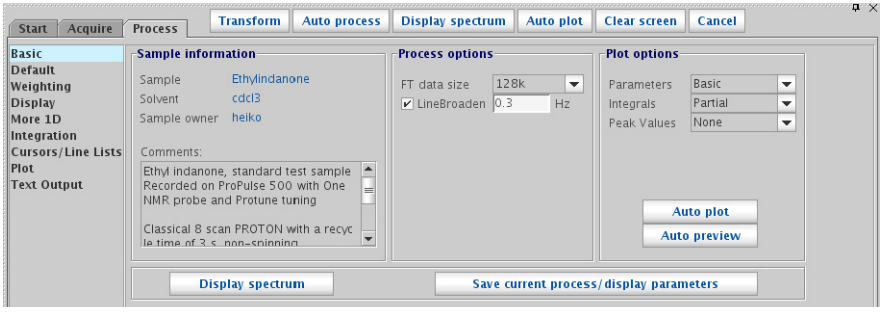
1 Select and drag a completed experiment node to the graphics canvas to automatically process and load the data set.

In the following example, “Ethylindanone_Proton_01” has been selected from the Study Queue and is being dragged to the Graphics Canvas.



2 Click on the **Process** tab to display the data manipulation tools.

Basic processing tools are available on the **Process > Basic** parameter panel.



Retrieving a Data Set

Before you can reprocess a data set, the desired data set must be in the current workspace. For information on changing to a different workspace/experiment/viewport, see the *Agilent VnmrJ Spectroscopy User Guide*.

Use the file browser to open a data set

To retrieve the data: **File> Open**.

The resulting pop-up lets you access the desired data directory.

1 Select the desired file.

2 Click the **Open** button.

The selected data set is loaded into the current workspace.

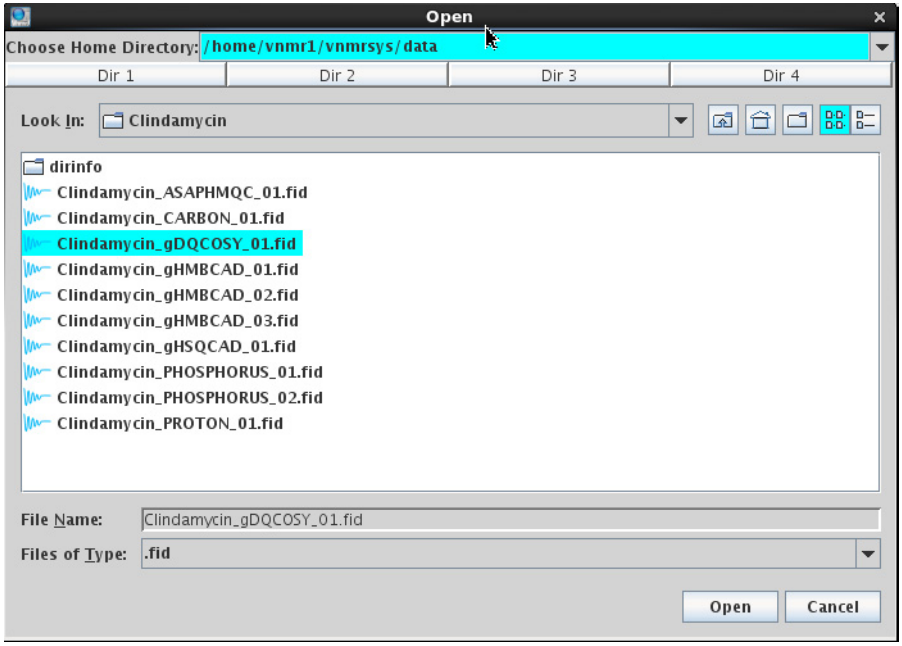


Figure 57 Open dialog box

Use the VJ Locator to search the database

The VJ Locator, Figure 58, is a database browser that provides access to data sets, experiments, shim sets, commands, and so on.

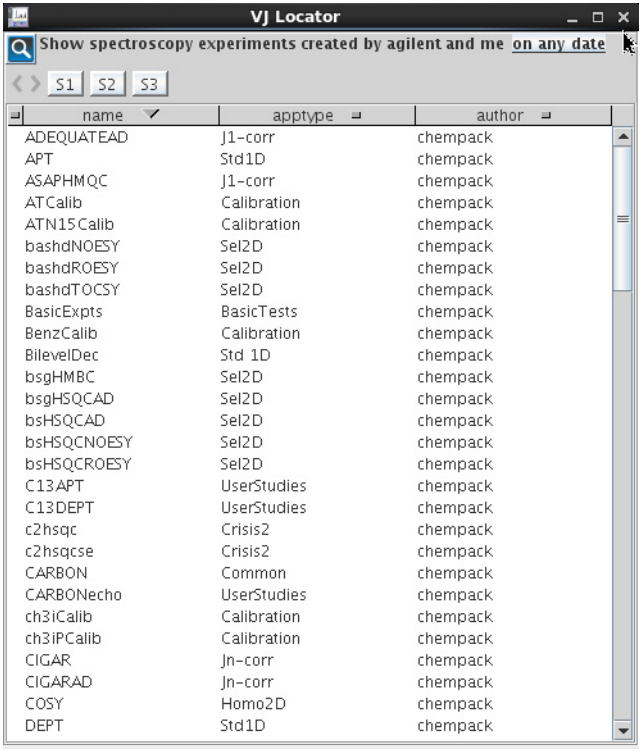


Figure 58 VJ Locator

The Locator provides quick access to information on all or part of the disk environment. The administrator determines the scope of the Locator actions.

Locator menu and controls

The magnifying glass and the current Locator statement are at the top of the VJ Locator window, as shown in Figure 59.

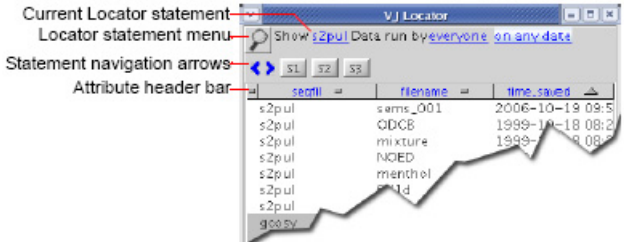


Figure 59 Locator menus and controls

Click the magnifying glass to open a menu of currently available Locator statements. This menu includes both statements provided by Agilent and those customized and saved by the user for searching the database. For more details on using the Locator, see the *Agilent VnmrJ Spectroscopy User Guide*.

Drag and drop items from the locator

To select an item, click the item in the **Locator** list. The selected item can be dragged to the graphics canvas or the Parameter Panel area for an appropriate action. For example, dragging a data set to the graphics canvas retrieves that data set into the current experiment workspace and displays the spectrum. Dragging a workspace to the graphics canvas selects that experiment workspace. Dragging and dropping an item has an action appropriate to the context. Often the same effect can be obtained by double-clicking an object.

Fourier Transform the Data Set

Fourier transform of 1D and 2D data can be performed in a variety of ways. For more information, see Fourier transform of one-dimensional data and Fourier transform of two-dimensional data. For more information on Fourier transform, see the *Agilent VnmrJ Spectroscopy User Guide*.

Fourier transform of one-dimensional data

The data is typically Fourier transformed into a spectrum before analysis. The data is stored as time-domain data. The FT converts it to frequency-domain data. FT can be done using any of the following buttons/ menu:

- The blue-green **Transform** button in the Action Bar
- The **Transform All** button on the upper left of the Process / Default page (it is also on the Process/Weighting page)
- The **Process** button in the middle bottom of the Process / Basic page
- The **Process** menu, which has options for either **Process** or **Display 1D** and **Full Process**

Fourier transform of two-dimensional data

The FT of a 2D dataset can also be done in several equivalent ways:

- The blue-green **Transform** button in the Action Bar
- The **Full 2D Transform** button on the upper left of the Process / Default page (it is also on the Process/Weighting page and the Process/More 2D page)
- The **Process** button in the middle bottom of the Process / Basic page
- The **Process** menu, which has options for Full Process 2D
- The full processing of a 2D spectrum requires a Fourier Transform along two perpendicular directions, called t1 and t2. These two processing steps can be done one at a time if desired. This allows you to customize the processing parameters in each direction (if desired). For more details, see the corresponding Spectroscopy Guide.

Alter Processing Parameters

More information can be extracted from an NMR spectrum if the processing parameters are optimized specifically for that spectrum (optimized in ways which help answer the questions being asked). Examples include changing the parameters that control processes like zero-filling, weighting functions (and apodizations), linear prediction, referencing, or integral reset points. These parameters are typically controlled using the **Process** tab.

Zero-filling

Zero-filling is controlled by the Transform Size controls, which are located on multiple pages, such as Basic, Default, Weighting, and More 1D pages. If the number of points used is larger than the number of points acquired, zero filling is being performed. This helps to better define shapes of the peaks. It is common and advantageous to transform twice as many points as were acquired. The user can transform fewer acquired data points, which allow the FT calculation to be faster, but at the expense of a less well-defined lineshape.

Weighting and apodization

The detailed parameters controlling the weighting functions and functions that are applicable to the FID before the FT, are defined in the Weighting page in the Process tab. There is also a simplified set of controls on the Default page. Typically, weighting functions are used to increase signal-to-noise, at the expense of broader lines. These functions are used to remove truncation wiggles from the spectrum as needed. The "apodization" process is when the weighting functions are used to remove truncation wiggles

Linear prediction

All of the detailed parameters that control linear prediction are located in the **More 1D** page. There is a simplified set of controls on the Default page. The **Auto** buttons set up a default set of conditions for either forward or backward linear prediction. Many of the protocols in the Experiment

Selector set up appropriate parameters for using linear prediction automatically. For more detailed information about controlling linear prediction, see the *Agilent VnmrJ Spectroscopy User Guide*.

Referencing

Automatic processing uses a routine to provide default referencing for the spectrum. To alter the referencing, use the controls located in either the Default or the Display pages. Referencing By Solvent or By TMS automatically analyzes the spectrum. Referencing the spectrum to a certain cursor position requires the user to place the cursor at the desired location in the spectrum and type in the desired numerical value for that position in the Reference cursor to entry box.

Integration

Integral regions are automatically set up for Proton spectra during automated processing. Further manipulations of the integral can be made by using the controls in the Integration page on the Process tab, or in the graphical toolbar, see Interact with the spectrum using the graphical toolbar.

Phasing

Proper spectral phasing is automatically set up for all spectra during automated processing. Further manipulations of the phasing can be made using the graphical toolbar.

Interacting with the Spectrum Using the Graphical Toolbar

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. For details on specific toolbars, see

"Common graphics display toolbar controls" on page 19

"1D display spectrum toolbar controls" on page 20

"nD display toolbar controls" on page 21

"Display FID toolbar controls" on page 23

"Annotation toolbar controls" on page 24

Integration and graphics controls

The graphics controls for displaying, and plotting integrals is located on the "1D display spectrum toolbar controls" on page 20.

Aligning and Stacking Spectra

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

- All selected viewports need to use a common scale.
- Data in the viewports may have different nuclei, different spectral widths, or different spectral regions. The common scale is determined based on data in all selected viewports and determines whether 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 has the same axis (H1, C13 etc).
- Stacking is enabled when data in all viewports have the same axis/axes.

For details on aligning and stacking spectra, see the *Agilent VnmrJ Spectroscopy Users Guide*.

Displaying and Plotting Integrals

The graphical controls for displaying and plotting integrals are located on the Display 1D Spectrum toolbar (Figure 60). For step-by-step instructions, see the *Agilent VnmrJ Spectroscopy User Guide*.

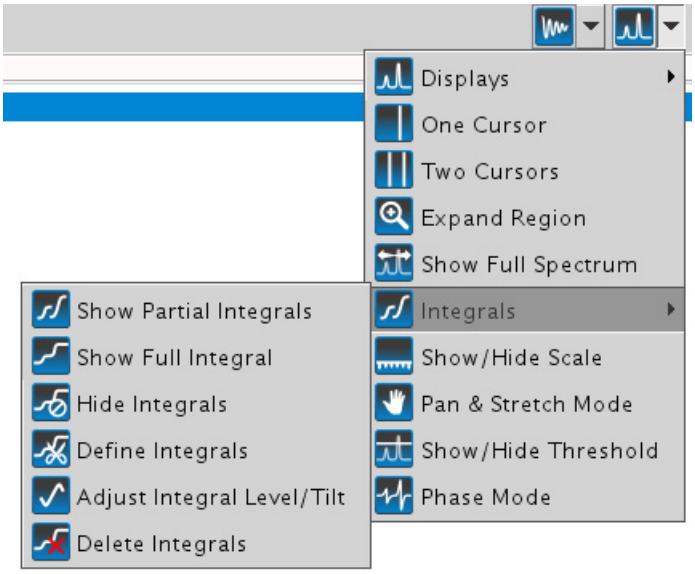


Figure 60 Controls for displaying and plotting integrals

Baseline Correction

Most operations performed on spectra assume a "good" baseline. Line lists, integrations, resolution measurements, 2D volume integrations, and so on measure intensities from "zero" and do not perform any baseline adjustments. Perform a baseline correction operation before performing further data reduction if the baseline in your spectrum is not "good." Two types of baseline corrections are provided, linear and non-linear, and are available using the buttons on the **Display** page of the **Process** tab.

Working with Viewports

All VnmrJ graphics are displayed in frames. The viewport has a default frame that occupies the entire viewport graphics area. An inset frame initially shares the same workspace and data as the original frame and is configured in the same way as the default frame. Insets are configured and modified using the Frame vertical panel. (See "Frame vertical panel" on page 41.) For more information on creating and changing inset frames, see the *Agilent VnmrJ Spectroscopy User Guide*.

Using Viewports Controls

Use the Viewport vertical panel to control the appearance of data in the viewports. See “Viewport vertical panel” on page 45. The viewport controls are present if there are two or more viewports.

Show and hide viewports

The selected viewports are arranged on the graphics canvas based on the layout selection. See “Set viewport layout” on page 171.

1. In the Viewport vertical panel, select the check box next to each viewport to show on the graphics canvas.
2. Clear the check box next to a view port to hide the viewport.
3. Point the cursor to the box next to the viewport label and hold down the left mouse button to temporarily hide a viewport.
4. Release the 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.

Make a viewport active

1. In the Viewport vertical panel, click 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.

Add a label to the viewport

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

1 In the Viewport vertical panel, click inside a viewport 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.

A new label is now associated with this viewport.

Set viewport layout

In the Viewport vertical panel, select a layout icon to arrange the view ports on the graphics canvas. Click the **Overlay Viewports** to stack viewports on top of one another. The overlay layout is useful for placing high resolution 1D spectra on the appropriate 2D axes.

Table 43 Viewport layout

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

Synchronize cursors and axes

Use the following controls in the Viewport vertical panel to synchronize cursors and axes.

Table 44 Cursors and axis

Check box	Description
Sync cursor	Select this check box to link and synchronize the cursors and crosshairs in multiple viewports.
Sync Axis	Select this check box to link and synchronize axes in multiple viewports. Axis is synchronized to the current active viewport.

Set crosshair, fields, and axis display options

Use the following controls in the Viewport vertical panel to turn on or off crosshair, fields, and axes.

Table 45 Crosshair, fields, axis display

Check Box	Description
Show crosshair	Displays cross hair and chemical shift(s) of the cursor position when mouse is moved over the spectrum. This is 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 required while in the cursor mode.
Show fields	Select this check 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	Select this check box to show the axis or remove the check to hide the axis.

Assign colors to spectra by viewport

Use the Viewport vertical panel to assign colors to spectra displayed in viewports.

Table 46 Assigning Colors to Spectra

Check box	Description
Color by viewport	Select this check box to display the spectral data using colors assigned by the viewport, see Figure 13. Default color assignment: • Spectra are displayed using a different color for each viewport if the box is checked. • The spectra are 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.

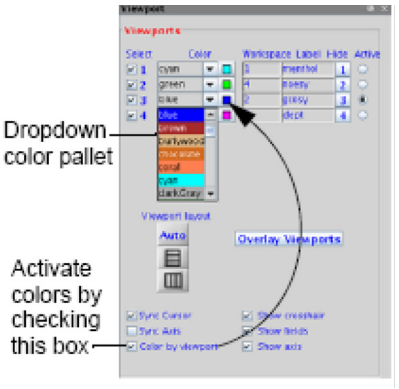


Figure 61 Setting Spectra Colors by Viewport

Using viewports as a spectral interpretation tool

The **Viewports** tool displays and presents data and provides a powerful interface to interpret spectral data. A collection of NMR data sets acquired on a given sample are typically more informative when considered together and simultaneously. Information presented in a 1D data set is often complimentary to that provided by a homonuclear or heteronuclear 2D data set. Many 2D data sets are closely linked from an interpretational point of view. Viewports provide powerful options for interrogating spectral data.

Overlaying homonuclear data sets

When interpreting homonuclear data, concurrently consider COSY or scalar coupling interactions (that is, through-bond) with NOESY or dipolar coupling interactions (that is, through-space).

For example, Figure 62 shows the graphics window with COSY and NOESY data sets in Viewports 1 and 2, respectively, collected on the ethylindanone standard sample. The **Overlay** and **Align Spectra** buttons have been used to provide a composite display. By selecting the **Show Crosshair** check box, a yellow cursor line, or crosshair, is displayed simultaneously in each window. The crosshairs are linked, allowing responses from one data set to be immediately interpreted with respect to the other. This display clearly differentiates those responses observed in the NOESY spectrum that are derived from long-range relaxation from the vicinal and geminal responses.

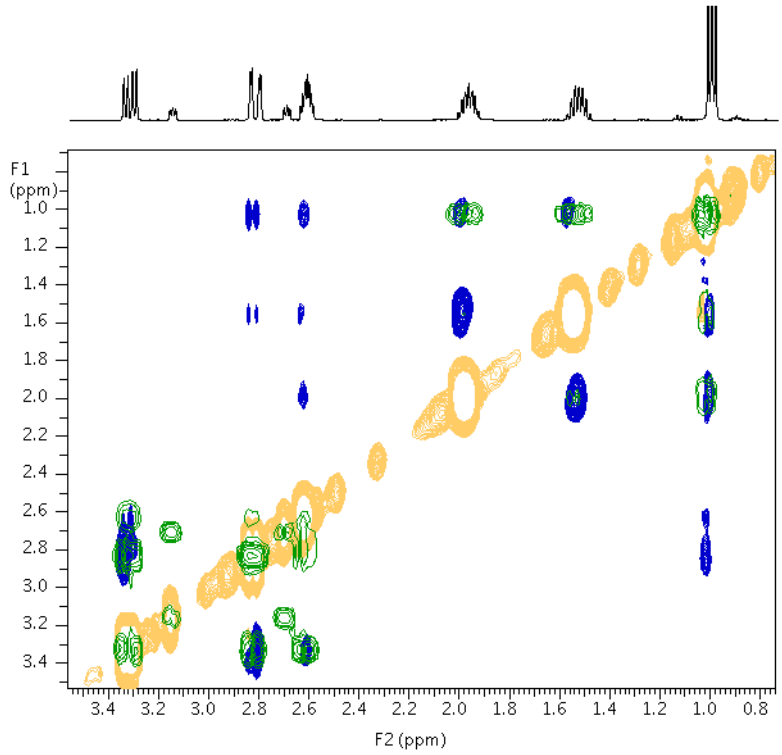


Figure 62 Overlaid COSY and NOESY spectra of ethylindanone

COSY responses are shown in green, while the phase-sensitive NOESY data are displayed in blue and yellow.

Cross referencing heteronuclear data sets

Many heteronuclear data sets provide complimentary insights into molecular structure. As shown in Figure 63 on page 175, a Viewports overlay of HSQC and HMBC data allows visualization of both 1-bond and long-range coupling in a single, easy-to-interpret arrangement. This type of display is very valuable when spectra become congested, and allows unambiguous assignment of long-range responses to 1-bond J_{CH} spin pairs.

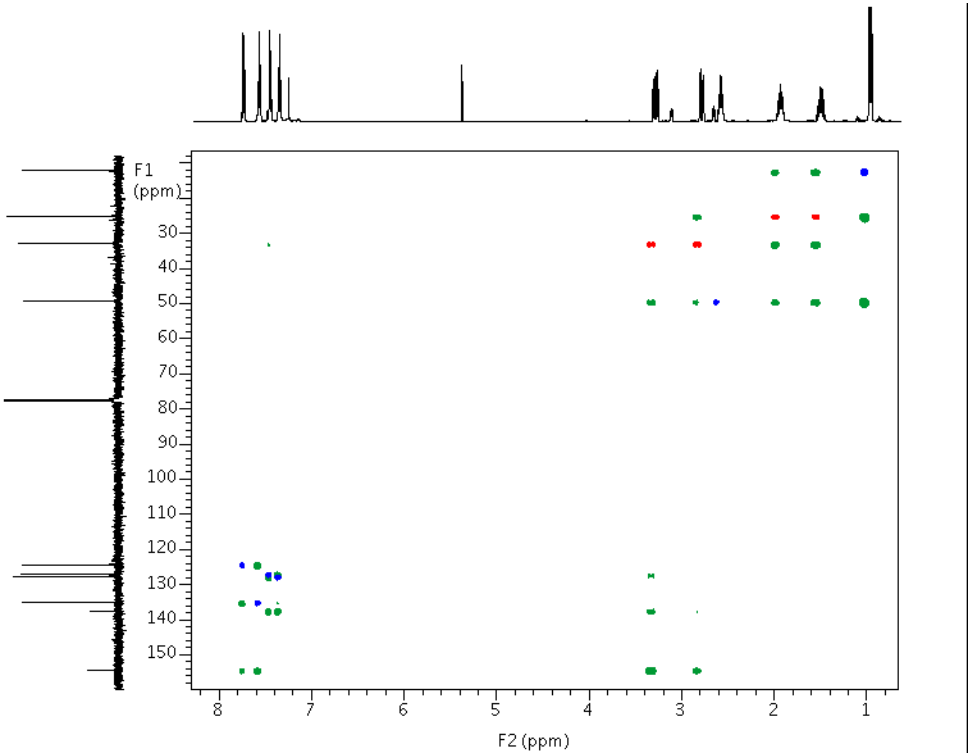


Figure 63 Overlaid HSQC and HMBC spectra of ethylindanone

HMBC responses are shown in green, while the phase-sensitive multiplicity-edited HSQC data are displayed in blue (odd number of protons) and red (even number of protons).

Save Current Process or Display Parameters

In the **Default** page of the **Process** tab, there is a button labeled **Save Current Process/Display Parameters**. Click this button to save a parameter set in the dataset with all the current processing and display information, in a manner that is suitable for GLP requirements. This action stores parameters such as phasing, integral regions (resets points and isadj), and the display information that would be stored by the `s1` and `r1` commands (described above). (It does not store information about referencing, symmetrization, baseline correction, or drift correction.) The next time any **Process** button is clicked, the last-stored set of display parameters will be used to display the resulting spectrum.

7
Plotting Data

Agilent Technologies

Plotting Data Saved as a Study

1 In the Parameter Panel, click **Process > Plot** to display the plotting tools.

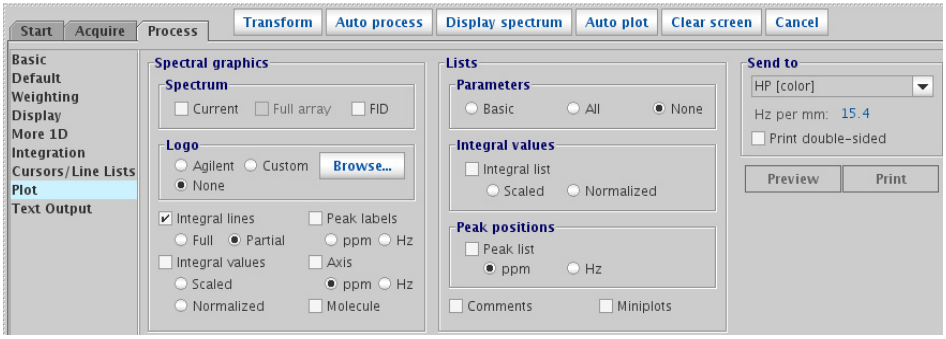


Figure 64 1D plot setup in the Plot page of the Process tab

These preferences, once set, are retained for a given spectrum. By default, most of these options are turned off the first time that the Plot panel is accessed for a given spectrum, so it will usually be necessary to turn several options on, especially the Spectrum **Current** check box, which toggles whether or not the plot includes a graph of the spectrum.

Auto plotting tools are also available on the **Process > Basic** parameter panel.

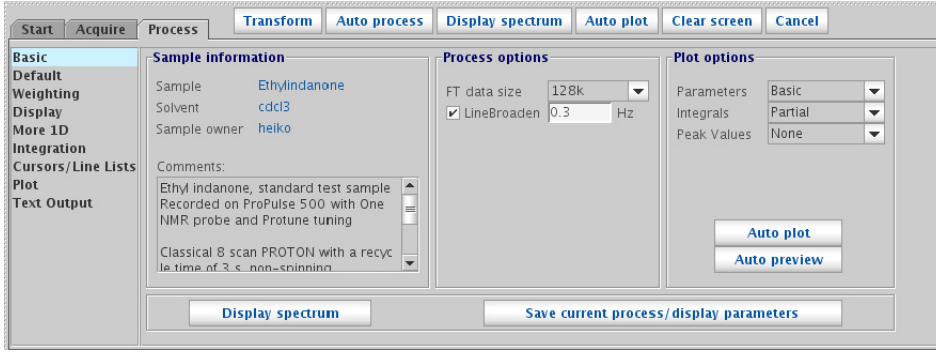


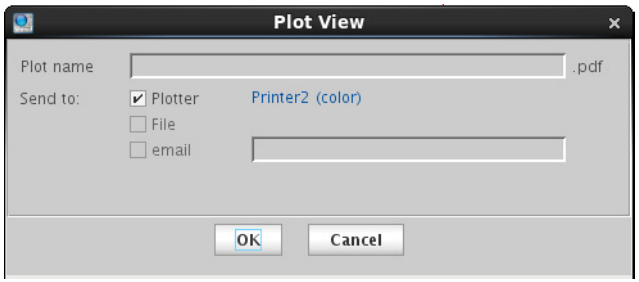
Figure 65 Plot options in the Basic page of the Process tab

2 Use the Graphics Toolbar to adjust the displayed spectrum.

Hovering the mouse over the icons displays tool tips.

3 Click **Auto Preview** to render a duplicate of the displayed spectrum in Adobe Reader.

The **Plot View** dialog box appears.



a Review the formatted plot and readjust as needed.

4 Select one or more check boxes on the **Plot View** dialog box to print, save as a PDF file, or email the plot.

5 Click **OK**.

Saving and Printing a Graphics File

After processing, the 1D or 2D spectrum is displayed in the graphics canvas so that the scale, expansion, and threshold can be adjusted.

To print the spectrum:

1 Click **File** from the menu.

2 Select **Print Screen**.

The pop-up in Figure 66 appears.

3 Select the **name** of the printer to print to it.

4 Select the print area, either **Viewports** or **VnmrJ Window**. Viewport will capture the contents of the Viewport, while VnmrJ Window will capture the entire VnmrJ window.

5 Choose the **number of copies** to print.

6 Click the **Print** or the **Preview** button.

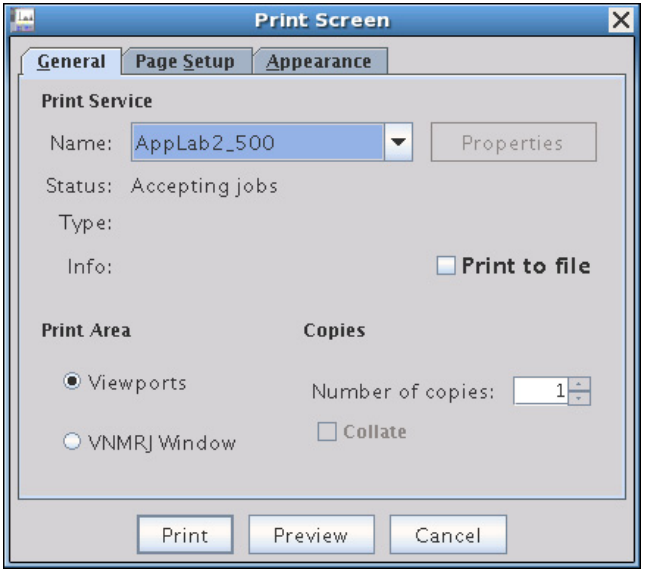


Figure 66 General tab of the Print Screen pop-up

Plotting the Data

Plotting is based around the concept of a plot file. Setting up and submitting a plot can be done from the vertical and horizontal panels and from the command line. The **Plot** parameter page is accessed from the **Process** tab after the spectrum or FID is displayed. Items selected on the **Plot** parameter page (Figure 67 and Figure 68) are added to a temporary plot file. The Preview button opens the plot in Adobe Reader where you can preview it, then save or send it to a printer or email. The **Print** button submits the plot file to the selected printer.

For details on plotting data, see the *Agilent VnmrJ Spectroscopy User Guide*.

Plot options for 1D data

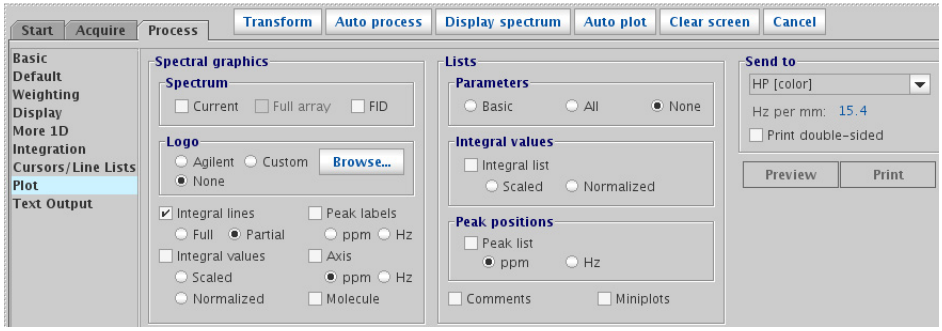


Figure 67 The Plot parameter page for a 1D data set

Table 47 Options in the 1D Plot panel

Item	Description
Spectral graphics	
Spectrum	Select how to display the spectrum on the plot: Current, Region, Full array, FID

Table 47 Options in the 1D Plot panel (continued)

Item	Description
Logo	Select to include a logo on the plot: Agilent, None, or Custom (If Custom, click Browse and then find and select the logo file to use.)
Additional graphics options	
Integral lines	Select to include full or partial lines on plot
Integral values	Select to include scaled or normalized integral values on plot
Axis	Select to display axis on plot in ppm or Hz
Peak labels	Select to display peak labels on plot in ppm or Hz
Molecule	Select if molecule is displayed on graphics canvas to include it in the plot
Lists	
Parameters	Select level of detail to include for parameters list: Basic, All, or None
Integral values	Select **Integral list** to display integral values, then select Scaled or Normalized
Peak positions	Select **Peak list** to include list of peak frequencies in lists, then select units of ppm or Hz
Comments	Select to include comments in lists
Miniplots	Select to include miniplots in lists
Send to	In the drop-down menu, select the printer to use.
Print double-sided	If the selected printer has the ability to print double-sided, select this option to enable double-sided printing for the plot.
Preview	Opens the plot in Adobe Reader with currently selected options, along with the Plot View pop-up where you can select to save the file, print it, or email it.
Print	Sends the plot with currently selected options to the selected printer.

Plot options for 2D data

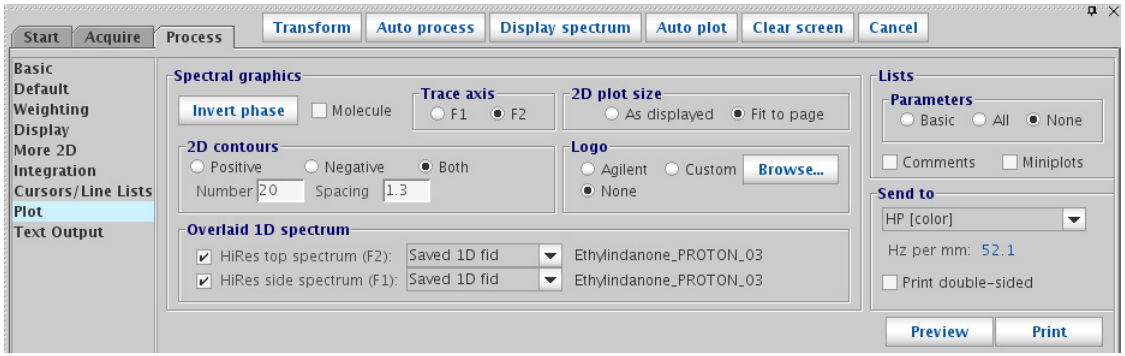


Figure 68 The Plot parameter page for a 2D data set

Table 48 Options in the Plot parameter page for a 2D data set

Item	Description
Spectral graphics	
Invert phase	Click to invert phase
Molecule	Select if molecule is displayed on graphics canvas to include it in the plot
Trace axis	Select **F1** or **F2**
2D plot size	Select **As displayed** or **Fit to page**
2D contours	Select to include Positive, Negative, or Both Enter **Number** of contours to display Enter the **Spacing** for the contours
Logo	Select to include a logo on the plot: Agilent, None, or Custom (If Custom, click Browse and then find and select the logo file to use.)

Table 48 Options in the Plot parameter page for a 2D data set (continued)

Item	Description
Overlaid 1D spectrum	Select to include 1D spectrum at the top and side of the 2D plot. HiRes top spectrum (F2) HiRes side spectrum (F1) For each, select Saved 1D fid, Projection, or Other workspace.
Lists	
Parameters	Select level of detail to include for parameters list: Basic, All, or None
Comments	Select to include comments in lists
Miniplots	Select to include miniplots in lists
Send to	In the drop-down menu, select the printer to use.
Print double-sided	If the selected printer has the ability to print double-sided, select this option to enable double-sided printing for the plot.
Preview	Opens the plot in Adobe Reader with currently selected options, along with the Plot View pop-up where you can select to save the file, print it, or email it.
Print	Sends the plot with currently selected options to the selected printer.

Changing Color Themes

Printer and Plotter color output is defined using the **Styles and Themes** window, **Plot** option. which provides access to the display colors and the VnmrJ interface colors. You access the **Styles and Themes** window using **Edit > Display Options**. There, you can set colors and save the color "theme" to a file. Once you save a color theme file, you can import and use it at a later time. Setting the styles and themes options are described in detail in the *Agilent VnmrJ Spectroscopy User Guide*.

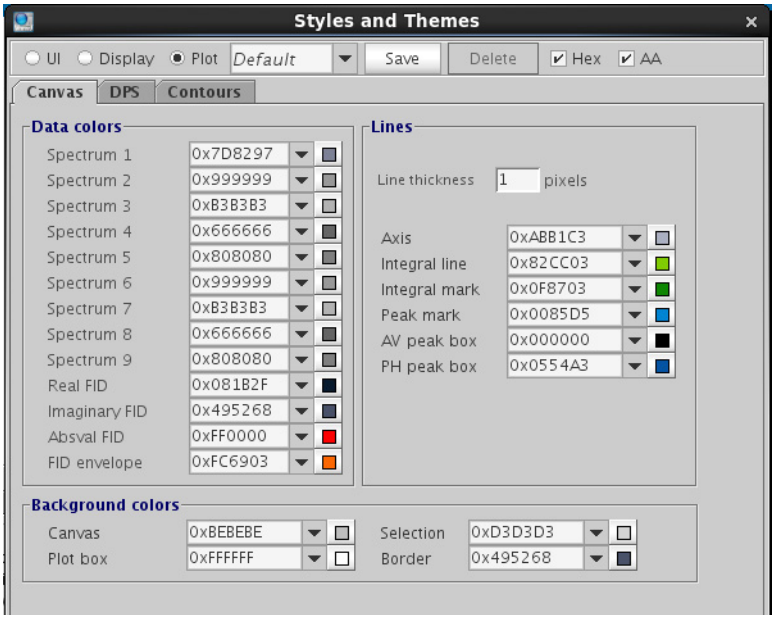


Figure 69 Styles and Themes window

Pasting Text into a Text Editor or Other Application

Text output that appears in the **Integration**, **Cursors/Line Lists/Text Output** parameter pages can be pasted into a text editor to be saved or used elsewhere.

1. Highlight the text to be pasted by clicking the left mouse button and dragging the mouse to the end of the desired text.
2. Release the mouse button at the end of the desired text. The selected text is highlighted indicating what has been selected.
3. Start the text editor or application and place the mouse cursor on the active document.
4. Click the middle mouse button to paste the highlighted text into the text editor.

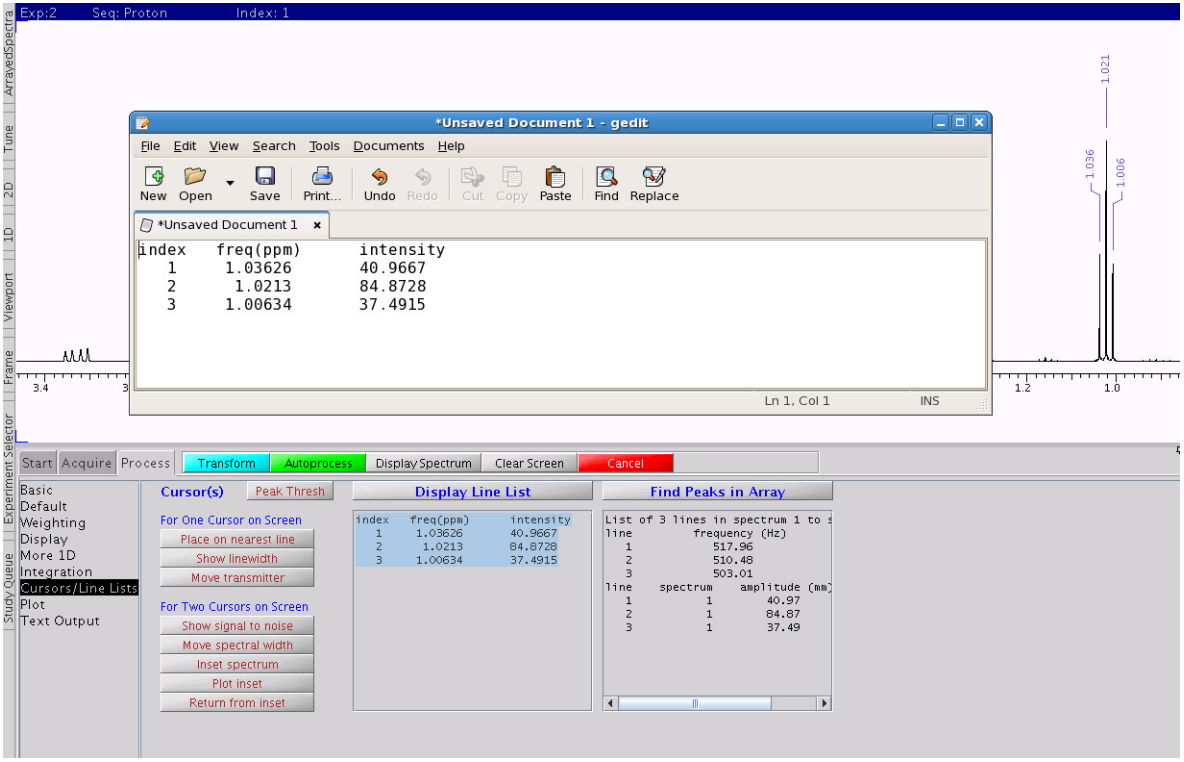


Figure 70 Contents of the Display Line List text box copied into the Linux gedit text editor.

8 Customizing VnmrJ Actions

VnmrJ has incorporated tools that allow each user account to be customized to suit the individual user tastes. There are 6 tools that can be used to create new buttons in the Experiment Selector, each generating a distinct button. These tools are located in the **Tools > Study Clones** menu. This section describes how to use these tools to customize the Experiment Selector.

Clone a New Study

This tool allows the user to create a new study based on those protocols already present in the Experiment Selector. Studies created using this tool will inherit any subsequent changes made to those protocols. For instance, if a Study Clone is made that includes the CARBON protocol, any subsequent changes made to the behavior of the CARBON protocol will be reflected in the Study Clone, also.

This tool is commonly used to create a composite study of multiple experiments. It is also very useful when a user wants to create a customized copy of an existing protocol without changing the original protocol (that is, a new "**Q_PROTON**" button with a very long relaxation delay, or an "**overnight_CARBON**" button that is parameterized to run all night).

Selecting this tool places the software into Submit Mode and opens an empty study in the Study Queue. The user can then populate this study with any experiment(s) from the Experiment Selector and customize each node in the queue as desired (double click on the node to open it in the current workspace, make any changes, and click the green **Save** button on the parameter panel toolbar). Once the study is configured as desired, click the yellow **Save Study** button on the bottom of the **Study Queue** window. This will open the **Save Study Queue** popup.

In the **Save Study Queue** popup window:

1. Select the **Allow Customization** check box if you wish to allow users to customize the nodes in this study on a per-sample basis. Deselecting the check box will lock the study so that users can make no changes.
2. Select the **Include Sample Tags** check box to write the current sampletags into the new study clone.
3. Choose where the new study will be saved from the **Applications Directory** drop-down menu.
4. Choose the tab in the **Experiment Selector** where the new button will appear by selecting an existing tab from the drop-down menu, or select **New Tabname** from the list and fill in the tabname field to create a new tab.
5. Fill in the Study Name field with the name of the study. This is the name that will appear on the new button. This name can not be the name of a macro currently in the search tree.

6 Click **Save/Update** to create the new button.

The Experiment Selector will now be updated to reflect the addition of the new study. Clicking this button will build the saved study in the study queue or in the current experiment, as appropriate.

Clone Current Study

This tool is identical to Clone New Study (“Clone a New Study” on page 190), except that it acts on the study currently present in the Study Queue. This allows the user to clone a completed study or to create a study clone while entering a study to be run on a sample.

Clone Current Experiment

This tool is typically used when the user wishes to clone the experiment in the current workspace. In contrast to Study Clones ("Clone a New Study" on page 190 and "Clone Current Study" on page 192), the **Clone Experiment** tool creates a new parameter file that is read in directly when the new button is selected. This truly yields an exact duplicate of the parameter set in curpar that can be used in a study queue. This tool is commonly used when it is desired to collect exactly the same data set on a large number of samples.

Before selecting this tool, configure the experiment in the current workspace as desired. Then select **Tools> Study Clones> Clone Current Experiment**. The **Clone Experiment** popup is opened.

1. Select the **Allow Customization** check box if you wish to allow users to customize the parameters in this experiment on a per-sample basis. Deselecting the check box will lock the experiment so that the users can make no changes.
2. Select the **Include Sample Tags** check box write the current sampletags into the new experiment clone.
3. Choose where the new experiment will be saved from the **Applications Directory** drop-down menu.
4. Choose the tab in the **Experiment Selector** where the new button will appear by selecting an existing tab from the drop-down menu, or select **New Tabname** from the list and fill in the tabname field to create a new tab.
5. Fill in the **Study Name** field with the name of the study. This is the name that will appear on the new button. This name can not be the name of a macro currently in the search tree.
6. Click **Save/Update** to create the new button.

Clone Location Queue

This tool allows the user to create a study clone from a location queue in the sample tray display.

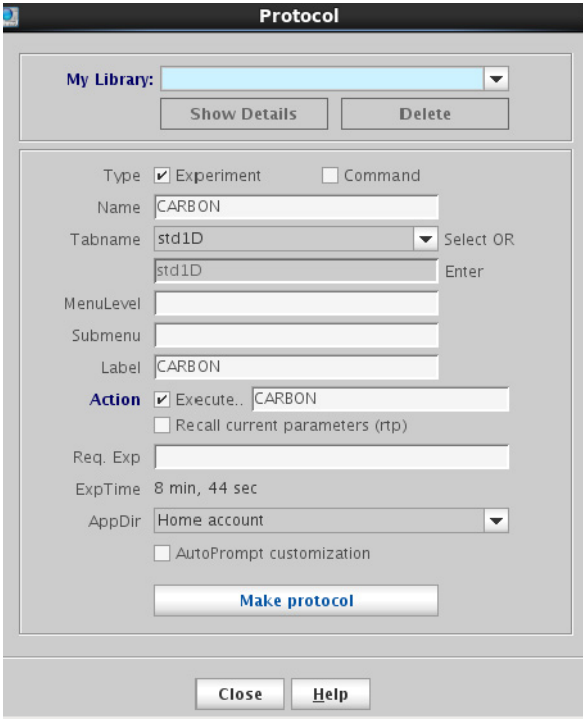
First, select a location in the sample tray (that already has a study queue assigned to it) by clicking on that location. Then select **Tools > Study Clones > Clone Location Queue**. This will open the **Save Study Queue** popup.

In the **Save Study Queue** popup window:

1. Select the **Allow Customization** check box if you wish to allow users to customize the nodes in this study on a per-sample basis. Deselecting the check box will lock the study so that the users can make no changes.
2. Select the **Include Sample Tags** check box write the current sampletags into the new study clone.
3. Choose where the new Study will be saved from the **Applications Directory** drop-down menu.
4. Choose the tab in the **Experiment Selector** where the new button will appear by selecting an existing tab from the drop-down menu, or select **New Tabname** from the list and fill in the tabname field to create a new tab.
5. Fill in the **Study Name** field with the name of the study. This is the name that will appear on the new button. This name can not be the name of a macro currently in the search tree.
6. Click **Save/Update** to create the new button.

Command and Protocol Buttons

This tool serves two purposes. Creating a Command Protocol allows the user to execute a VNMRJ command or macro at run time as part of a Study Queue. This function does not collect data but returns to the next item in the study upon completion. The Experiment Protocol function is used to generate an experiment button in the Experiment Selector (that is, it generates the appropriate XML file) to call a pre-existing set-up macro for loading a pulse sequence and parameter file. In other words, this tool can be used to import pre-VJ3 experiments and their associated files into the current system.



To create a Command Protocol:

1. Select **Tools > Study Clones > Command and Protocol Buttons** to open the **Protocol** popup.
2. Confirm that the **Command** check box is selected.
3. Fill in the name to be used for the protocol.
4. Choose the tab in the **Experiment Selector** where the new protocol will appear by selecting an existing tab from the drop-down menu, or select **New Tabname** from the list and fill in the tabname field to create a new tab.
5. Confirm that the **Execute** check box is selected
6. Fill in the field with the name of the macro to be run in the protocol.
7. Choose where the new protocol will be saved from the **App Dir** drop-down menu.
8. Click **Make Protocol**.
9. The new Command Protocol will now appear in the Experiment Selector.

To create an Experiment Protocol:

1. First, execute the set-up macro for the desired experiment in the current workspace and parameterize the experiment as desired.
2. Select **Tools > Study Clones > Command and Protocol Buttons** to open the **Protocol** popup.
3. Confirm that the **Experiment** check box is selected.
4. Fill in the name to be used for the protocol.
5. Choose the tab in the **Experiment Selector** where the new protocol will appear by selecting an existing tab from the drop-down menu, or select **New Tabname** from the list and fill in the tabname field to create a new tab.
6. Choose the **Recall** current parameters check box to use the parameters in curpar as the basis for loading the new experiment, or choose the **Execute** check box and fill in the name of a set-up macro to parameterize the new experiment.

7 Fill in the **Req Exp** field with a rational starting experiment(s) as desired.

   a Leaving this field blank will cause the new protocol to load from the default set-up macro (based on the value of tn) when used in the Study Queue, or it will load on top of the parameters in the current workspace when used in Review mode.

   b By filling in this field, the new protocol will check for the presence of the specified experiments and operate on the last such parameter set that exists in the sample queue, or it will add the required experiment to the queue if one doesn't already exist. This is the default behavior for the protocols supplied with the system and is the recommended action.

8 Choose where the new protocol will be saved from the **App Dir** drop-down menu.

9 Click **Make Protocol**.

The new protocol will now appear in the Experiment Selector. Assuming that the **Required Experiments** field was populated appropriately, the protocol will behave as do all the standard system protocols. Adding the new protocol to a Study Queue will preserve the sample tags and locked parameters (that is, `sw`, `pw`, solvent suppression parameters, etc.) from the last valid starting data set in that queue, and the node can be customized as desired.

Edit Parlib

This tool is used to create a complete protocol, including a set-up macro, parlib entry, XML file, etc., for inclusion in the Experiment Selector. This tool is intended to be used only when the starting point is a VJ3 system protocol.

The **Edit Parlib** tool is commonly used to add a new protocol for acquisition of data on a nucleus different than those supplied in the standard Experiment Selector interface (i.e., ^{29}Si, ^{17}O, ^{23}Na, etc.).

After configuring the parameters in the current workspace appropriately:

1. Select **Tools > Study Clones > Edit Parlib** to open the **Edit Parlib** popup.
2. Fill in the name to be used for the protocol.
3. Choose the tab in the **Experiment Selector** where the new protocol will appear by selecting an existing tab from the drop-down menu, or select **New Tabname** from the list and fill in the tabname field to create a new tab.
4. Populate the **Lock Parameters** field with those parameters whose values should be retained by subsequent experiments.
5. Fill in the **By default, start with** field with any protocol that must be executed before the new one being created.
6. Fill in the **User Customization** field with any customization that should be performed at set-up time.
7. Click **Save/Update**.
8. The new protocol will appear in the **Experiment Selector**.

9 Customer Training

This chapter describes the familiarization training provided by the Agilent installation engineer at time of installation. This training is intended to be a general overview of the instrument, basic maintenance requirements, software features, data acquisition and storage, file maintenance, and other routine tasks. Comprehensive training classes are offered at various Agilent Applications Laboratories around the world. Call your sales representative or contact the Agilent Technologies NMR systems office nearest you for class offerings, schedules and cost.

Training

The installation engineer is providing this training as a service to the customer to use the spectrometer. The engineer may not be able to answer detailed questions beyond the scope of this training. There is no expectation that the installer can provide all of the training needs for the customer. Training is most effective if the end user performs all the tasks.

This training covers only basic operation of a solution-state NMR spectrometer – it does not cover the operation of spectrometers doing bio-NMR (samples in H2O), solids, or imaging applications. This training is for a maximum duration of one day, and for a maximum attendance of one customer for each training session. To obtain more complete training, or to train a larger group of people at your customer's facility, please suggest that the customers attend one of Agilent's applications lab training classes, arrange an on-site training visit, call the Agilent Technical Assistance Center (TAC) or your local salesperson, or refer to the appropriate manual.

Previous Experience with Agilent NMR Software

If customers are already familiar with certain topics, they may choose to skip the topics. Customers may have no knowledge of how this version of software has changed since their last experience with a previous version of VnmrJ software.

Documentation

Give an overview of the documentation. Explain where to start looking for information and where to get help.

- *QuickStart Guide* – start all new users here.
- *VnmrJ 4 Administration Guide* – start all new system administrators here. This provides quick start information and detailed explanations.
- *VnmrJ 4 Familiarization Guide* - gives an overview of the VnmrJ 4 software and how to use it to acquire data. Also provides descriptions of the User Interface.
- *Spectroscopy User Guide* – a more advanced manual for experienced users, or for those performing more advanced experiments.
- *Command and Parameter Reference Manual (CPR)* – a favorite reference manual, which contains details on every command, macro, and parameter.
- *User Programming Manual* – (Optional, advanced) the primary manual for details about writing new pulse sequences, creating shapes, or modifying parameter characteristics. Any activity that might be called "programming" is documented here.
- Additional manuals (Probe manuals, accessories) – these are general reference material.

Show the customer how to get the documentation.

- Various hard-copy manuals are shipped with the spectrometer.
- Purchase hard copies.
- Visit the Agilent Spinsights site, http://www.spinsights.net. A password is required.
- Access the online documentation using VnmrJ 4 Help, using **Help > Manuals**.
- The installation DVD downloads documentation located on the VnmrJ 4 interface.

Sample Requirements

1. Review with the end user the contents of the *Quick Start Guide*, including sections on how to prepare and load a sample.
2. Point out the depth gauge, show how to use it, and how to document the number to which it is currently set. (The customer should document this number in a logbook.)

Introduction to VnmrJ 4 Operation

Instruct the customer to follow all the steps in the *Quick Start Guide* to acquire a spectrum. This allows customers to acquire the first spectrum (acquire, process, plot, and save – all automatically).

Do this by preferably using the sealed "2-Ethyl Indanone" sample (provided with the system; part number 0190185503).

Overview of the VnmrJ 4 Interface

Give an overview of the layout of the VnmrJ 4 display, using the following list. Point out the location and simple use of:

- The **Main Menu** (for example, shows the location of **File > Open**, **Edit > System Settings**, and **Tools > Probe Tuning**)
- The **Vertical Panels** (show the Protocols, Frame, and Viewport tabs)
- The **Graphics Window** (this is where the spectral data always appears)
- The **Graphics Toolbar** (shows that it can be moved and docked elsewhere)
- The **Parameter panels** (shows how to navigate between the Start, Acquire, and Process tabs, and their various panels)
- The **Action Toolbar** (shows how to use the Show Time button on the Acquire tab, and the Transform button on the Process tab)
- The **Hardware Toolbar** (point out the following: Trash Can, Real-Time Monitors, Probe Selection, Acquisition Status, and Error-Message Display. (Optional) up-arrow acqstatus display)
- The **Command Line** (optional, show how to type `pwd` to print the working directory, or `ls` to list files)

Basic (Automated) VnmrJ 4 Operation

Give the customer more insight into the operation of VnmrJ 4 by doing the following:

1 Acquire data “In the Study Queue” – by using the **Submit** button and the **StudyQ**.

   a Acquire a queue composed of a ^{1}H 1D (PROTON), a ^{13}C 1D (CARBON), APT, gCOSY, and gHSQCAD (typically on 2-ethylindanone in CDCl3).

   b Fill out the **Start > Sample Info page** (specifically Sample Name, Solvent, Comment, tune, autolock, autoshim).

   c Show the customer how to customize parameters for a node (within the StudyQ, prior to acquisition). Use the **Acquire > Acquisition** page to customize various parameters (that is, `nt`, `d1`, `gain`).

NOTE The data is saved automatically when using the StudyQ, using the filename templates within Edit / Preferences / Templates.

   d Acquire enough data to be sure to use the **New Study**, **Submit**, and **Continue Study** buttons.

2 Acquire data “Without the Study Queue” (in “manual mode”) – by using the **Acquire** button.

   a Show the customer how to save data in this mode by using **File > AutoSave**.

3 Show the customer how to bring old data back into the StudyQ (**File > Open**).

4 Show the customer how to reprocess data in the StudyQ (for example, use the **Transform** button in the action bar of the **Process** tab)

5 Show the customer how to replot data in the StudyQ (use the **Process > Plot** page, **File > Print Screen**, or optionally the command line)

6 Customize the protocols by adding a new button:

   a Clone a study (using **Tools > Study Clones > Clone Current Study**)

Review where the documentation for these tasks is located within the manuals.

Detailed (Manual) VnmrJ 4 Operation

Teach the end user detailed software operation by doing each of the following:

1. Demonstrate the use of the features in the Main Menu (such as, **File > Open**, **Acquisition > Abort Acquisition**, **Tools > Probe tuning,** and so forth).
2. Demonstrate the use of the icons in the System Toolbar (such as, **Cancel Command**, **Stop Acquisition**). Point out the "Floating Tool Tips" that tell you what the icon will do, even without pushing it, and the use of context-sensitive help.
3. Demonstrate use of **File > Open** and **File > Save As** pop-up windows to open and save data, respectively.

   These windows can each be in different locations within the directory structure.

   These windows only show the files determined by "Files of Type". They may not show all the files in each directory unless configured to do so with the "Files of Type" menu.
4. Demonstrate the Action bar buttons (that is, **Acquire**, **Show Time**, and **Autoprocess**).
5. Demonstrate use of the command line, and adjusting the size of the error window.
   a. Type `pwd` and `ls`, then show how the text output goes to the **Process > Text** window.
   b. Adjust the size of the error window – and then hide the command line completely – by dragging the window size.
6. (Optional) Teach the use of multiple experiments (cexp (3), jexp3, mf (2,3), and so forth).
7. (Optional) Teach the end user closing and pinning windows, and how to use the View menu to open closed windows. Demonstrate pinning and closing on the graphical tool bar, the parameter panels page, the hardware toolbar on the bottom, and a vertical panel. Show how to redisplay closed windows by using the View menu.
8. Show how to use the depth gauge (and the knurled locking knob).

9 Insert and Eject

a from the buttons on the panels.

b from the switch on the upper barrel.

c from the command line (by typing `eject` and `insert`, or `e` and `i`. This is optional.

NOTE You cannot eject with one method and then insert using another method. This may confuse the hardware.

10 Teach the end user "semi-manual" locking (push the **Find z0** button).

Teach the end user manual locking (adjust Z0, lock power, and lock gain).

An ideal target lock level is 80%, so the lock gain should be adjusted to achieve this. Point out that users should generally note at which value they set the lock level (to ensure that it is normal for a given lock power, lock gain, and solvent, and to verify after time that the lock level did not decay too much during long-term acquisitions).

11 Teach the end user "semi-manual" shimming (by using the **Gradient Shimming** button on the **Start > Lock** page).

12 Teach the end user manual shimming (show use of the **Start > Shim** page).

13 Adjust lock phase (on the **Start > Lock** and **Start > Shim** pages) while monitoring the lock level.

(Explain that this should be done only when the system is well shimmed, and ideally on a standard sample that has a sharp lock -- like the lineshape sample. The lock phase should be documented in the system logbook. The optimal lock phase value can change by 90 degree steps whenever the console is power cycled.)

14 Save shims:

a To the local user account (the default, saves the shims in `~/vnmrsys/shims`).

b (Optional) To the system account (`/vnmr/shims`).

15 Load shims:

- **a** From the combination of the probe file and the preferences option.
- **b** From the Shim page (Note that this may require the use of a terminal window or the Locator to find the exact filename.)
- **c** By dragging and dropping from the **Tools > Browser** window.
- **d** (Optional) By dragging and dropping from the **Tools > Locator** window.
- **e** By using the **Open** button in the **File > Open** window (you need to select "**shim**" via the display menu to see the files).

16 Select a probe file, and learn how to determine if a given probe file is either a "System" or a "User" probe file. Learn how to determine if a given probe file is a "Probe ID" file or not. Show how ProbeID is turned on-and-off by using the configuration page and the check boxes in the probe pop-up window.

17 Show the customer how to review the contents of a probe file (that is, check the Edit box, review the tabs for different nuclei).

18 Show the customer how to set the Temperature (use the **Spin > Temp** page).

19 Show the customer how to set the spin rate (use the **Spin > Temp** page).

We suggest you also select (mark) the check box for "Control spinner from this panel only".

20 Tuning:

- **a** If ProTune is installed, show how to manually use ProTune (by using **Tools > Probe Tuning > Auto Tune Probe**). Tune a nucleus.
- **b** Show the customer how to use mtune to view (monitor) the quality of tuning (by using **Tools > Probe Tuning > Manually Tune Probe**).
- **c** Using mtune, demonstrate tuning by using the knobs on the bottom of the probe if they are accessible (no ProTune), or by using the knobs on the ProTune box.
- **d** (Optional) Show the customer how to tune using the Tune box on the tether.
  [To do so, set the `rf` on channel 1 to H1 and channel 2 to C13, then adjust the controls on the tether box (channels = 1 or 2, gain = 8) and tune to the resulting display].

21 Show the customer how to use the graphical toolbar:

a On a 1D spectrum, demonstrate expanding, contracting, integral on/off, threshold, and phasing.
Ensure that every end user spends time learning how to phase manually. This is a difficult concept to master if you have never used it before, and it is impossible to teach over the phone, so we need at least one user at each site to have mastered how to phase manually. The next most confusing (but not difficult) task is integration. See the optional topic below.

b On a 2D spectrum, demonstrate expanding, vertical-scale adjustment, panning, trace, and rotate.

22 (Optional) Teach setting up the integral.
For beginning users, this is easier to teach by using the **Process > Integration** page.
This task can also be done using the graphical toolbar.

23 Show the customer how to plot "manually" (when not using the StudyQ for automation):

a By using the buttons on the parameter panels.

b (Optional) By entering pl `pscale page` on the command line

24 (Optional) Show the customer how to setup gradient shimming and make a new map (that is, explain how to use **Tools > Standard Calibration Experiments > Set up Gradient shimming**). Detailed directions on how to do this are in the *Gradient Shimming* chapter of the *Spectroscopy Guide*. Contrast this with gradient shimming via the **Lock > Gradient Shim** button, which requires no user interaction.

25 (Optional) Show the customer how to setup arrays and then clear them (demonstrate a `pw` array).

26 (Optional) Show the customer how to use the Arrayed Spectra vertical panel to process and display arrayed data.

27 (Optional) Show the customer how to set up Quantification.

Linux Training

1. Provide the end user with written copies of the usernames and passwords for root, vnmr1, and any other user accounts, as were set up by the installer.
2. Show the customer how to login a user account.
3. Show the customer how to logout of a user account.

   Let the users login to each account so they know each password works.
4. Show the customer how to start VnmrJ 4 (click on the icon on the desktop, or enter `vnmrj` in a terminal window)
5. Show how to exit VnmrJ 4 (**File > Exit VnmrJ 4**).

   Explain that this should be done before a user logs out of the user account (if possible). Do this by using **File > Exit** in the Main menu, or entering "`exit`".
6. Show the customer how to start VnmrJ 4 Adm (which requires vnmr1 permission) (click on the icon on the desktop, or enter `vnmrj adm` in a terminal window)
7. Show the customer how to reboot the host computer:
   a. From the Linux menu
   b. (Optional) From a terminal window, enter `su`, enter the root password, enter `reboot`
8. Show the customer how to reboot the communication with the console: `su acqproc`, reset the master, `su acqproc`, load shims.

   (Discuss that "resetting the master" is optional here.)
   (Run `/vnmr/bin/makesuacqproc` if needed.)
9. (Optional) Show the customer how to set up a printer in Linux.
10. (Optional) Show the customer how to read the manual pages in a terminal window (that is >man ls), or call up the Help documentation in Linux.
11. (Optional) Show the customer how to use >ps –ef, then >kill (>kill -3 pid). (This requires root permission.)
12. (Optional) Show the customer how to tar up (data) directories into a single tar file:

    `tar cvf filename.tar` filename – this copies filename into filename.tar.

`tar xvf filename.tar` – this extracts the contents of filename.tar.

13 (Optional) Discuss how to obtain and load patches to VnmrJ 4.

VnmrJ 4 Administration

Provide training in VnmrJ 4 Administration:

1. Make a new user. (New User, [enter **User Login** and **Interface Type**], Save)
   a. Explain that there are three interface types: Spectroscopy, Imaging, LC-NMR/MS. Use Spectroscopy for liquids and solids NMR.
   b. Explain how making a new user may not allow that user to access existing local files in another user account [probe file, gshimlib, shapelib, and so forth].
2. (Optional) Make a new Operator in a User Account.
3. (Optional) Show the customer how to "Switch Operators" in VnmrJ 4.
4. (Optional) Show the customer how to set the default operator password.
5. Delete a user account by highlighting the username, right-click, delete.
6. Update a user account (**Configure > Users > Update users**).
7. Show the customer how to set up a Printer in VnmrJ 4.
8. (Optional) Show the customer how to use VnmrJ 4 Accounting.
9. (Optional, if installed) Show the customer how to turn Probe ID on-and-off, and use the probe popup in both modes.

VnmrJ 4 Administration - Quick Start

Review all the topics in the Admin Quick Start chapter of the *VnmrJ 4 Administration Guide*.

1. Show the customer how to use **Edit > Preferences** (User Preferences).
2. Review the contents of every tab.
   a. **Templates tab:** Show the customer how to modify the automation directory and file-saving parameters.
   b. **Queue tab:** Show the customer how to modify the defaults for autolocking, autoshimming, and protune.
3. Show the customer how to use **Edit > System Settings**
   a. Show the customer how to turn on/off "automatic processing upon drag-and-drop".
   b. Show the customer how to turn on/off WYSIWYG.
   Explain what this does, and that it may influence how much of the graphics screen is used to display data.
   c. Show the customer how to turn on the PFG usage for each new user (which is the same as `pfgon='nny'`).
4. Show the customer how to select a printer and plotter for each new VnmrJ 4 user (**File > Printers**).
5. Show the customer how to use **Edit > System Settings > System Config** pop-up window. (Explain that this is only accessible to the vnmr1 user.)
6. (Optional) Show the customer how to use "`appdirs`" (**Edit > Applications**; this is needed for Biopack, and so forth).
7. Show the customer how to change a password:
   a. In VnmrJ 4 (**Tools > Change Password**)
   b. (Optional) In VnmrJ_Adm
   c. (Optional) In Linux (>passwd username)
8. Explain how the Experiment Protocol buttons read the calibrations stored in the Probe File. (When you push the **Proton** button, you read in a proton parameter set, and update it to account for the values stored in the probe file. So if the probe file is not set properly, the calibrations – and hence the data – will not be proper). The probe file is now required for proper operation on VnmrJ 4

9 Show the customer how to do a probe-file calibration.

   a Demonstrate it on an existing probe file (that is, using the Doped D2O sample). Also rerun the methyl iodide calibration if time allows.

   b Explain that the “target values” in some of the calibrations come from the probe specification sheets (which may not be readily available to the end user when they want them).

   c (Optional) Add and then remove a nucleus from the probe file by using the button on the probe popup.

10 (Optional) Show the customer how to change the probe file’s default shimmap (`Probelkmap` in the probe file). Explain that this exact file is what is used during automated acquisition (even if another map is set in the gradient shimming parameter panels [`gmapsys`]).

11 (Optional) Show the customer how to start and stop the cold probe (if appropriate) using the Cryo vertical panel

12 Document the following into a logbook:

   a The console serial number (Show the customer where it is)

   b Write down `lockfreq` (in the System Configuration panel, see the section below)

   c The air-flow and air-pressure values on both the pneumatics box and on “the wall” (at the regulator at the source of the gas to the room)

   d The current value of the lock phase

   e The value that the depth gauge screw is set to

13 Save a copy of shims into `/vnmr/shims`

   a By using the command line (`svs('/vnmr/shims/shimname')`)

   b By using the VnmrJ 4 GUI on the Start > Lock page (type in the whole path name: `/vnmr/shims/shimname`)

   c By using the terminal window

14 Show the customer how to calibrate Protune.

Hardware Overview

1. Point out the console, the RF front end, the Pneumatics box, the probe (Optional: ProTune, the robotics, cold-probe units, pfg cable (which moves top-to-bottom sometimes), FTS, Remote Status Unit, Tune Box (on the tether, and so forth).
   a. Show the customer where the console serial number is located (inside the front door).
2. Review **Edit > System Settings** (as vnmr1) as needed to explain hardware options.
   a. Write down lockfreq.
   b. Take a screenshot of the config pop-up window and save it in vnmr1's home directory as a backup. (use the Linux menu **Applications > Accessories > Take Screenshot**).
3. Show the customer the customer where the extra probes (in their boxes) are located (if appropriate).
4. Show the customer how to place a red plastic cap on the probe when it is not in use, especially when it is in the probe case. Explain that this is important to keep debris out of the probe, especially static-prone particles of probe-case foam.
5. Show the customer how to power cycle the console after a power interruption.
   a. Point out and explain the use of the blue-green button on VNMRS.
   b. There are also power switches on the RF Front End unit, the Protune unit, the PFG amp, the console's power supplies, and so forth.
6. Show the customer where the "master reset button" is located in the console (again).
7. (Optional) Demonstrate probe installation and operation:
   a. Show the customer how to install the probe.
   b. Show the customer how to reposition the probe (that is, push the probe up, push the upper barrel down, tighten the clamp).
   c. Show the customer how the manually tune the probe, if automated probe tuning is not present.
8. The arrows on the directional couplers point away from the probe and towards the filters and console.

9 (Optional) Explain the meanings of the console lights and the lights on the pneumatic box.

10 (Optional) Explain how to use the FTS unit.

11 Train the customer on magnet safety and cryogen fill techniques:

- Warning signs posted
- Cryogenics handling and safety
- Magnet filling
- Flow meters and Cryogen meters
- Homogeneity disturbances

Customer Support Information

1. Provide the contact details to be used when help is needed.

   Contact Center: 1-800-227-9770, option 3, option 7.

   a. Show the customer where to find the console serial number (which will be needed when you call TAC).

   b. Show the customer how to use Help > About VnmrJ to find the software version and patch level.

2. Show the customer the Agilent Web site (http://www.chem.agilent.com/en-us/ContactUS/Pages/ContactUs.aspx), especially the “User Pages”.

   a. The user needs to register to use the “User Pages” (to get the username and password).

   b. (Optional) Register the user right now.

3. Show the customer how to get to the Agilent Web site for NMR help.

   a. Through a regular Web browser (www.chem.agilent.com > Instruments & Systems > Nuclear Magnetic Resonance).

   b. Through the online help within the VnmrJ 4 user interface, by selecting **Help > Spinsights Community Help Site**.

Lock Frequency (lockfreq)

Magnets lose a small amount of their current over time. The magnet “drift” means that the frequency needed to lock the deuterium signals will decrease slowly with time. This means that the Z0 value for any given solvent will slowly decrease with time. Eventually the system “lockfreq” will need to be reset to compensate. This needs to be done when the Z0 value runs out of range, making it impossible to establish lock. This will typically be observed first on CDCl3 and C6D6. When the drift happens, which may take six months to two years, contact Agilent service for detailed instructions on how you can “reset your lockfreq due to magnet drift”.

Administrative Chores

1. Show the customer where the NMR data from installation is stored (for example, S/N, lineshape, and so forth).
2. Obtain sign-off on the installation.

10 Automated Data Collection and Spectra Interpretation

This chapter contains a basic walkthrough of collecting and analyzing NMR data using the automated tools in VnmrJ.

Agilent Technologies

Automated Data Acquisition

The automated data acquisition procedures outline several 1D and 2D experiments using the ethylindanone sample.

These experiments demonstrate the capabilities of the spectrometer, the correct calibration of the instrument, and validate the correct functioning of the instrument. If a sample changer is present, submit acquisitions to background.

The following is part of the training session. How to:

- Set up and use the VnmrJ interface
- Use the Experiment Panel to select the application type, Std1D, Hetero 2D, and Homo 2D experiments
- Set up 1D, 2D, gradient (if appropriate hardware is installed) and non gradient protocols. Click the experimental protocols for proton and carbon 1D, homonuclear 2D, and heteronuclear 2D experiments from the list of protocols.
- Create, run, save data, and plot the results obtained from the composite protocol

These experiments can be run using either the Account Owner or Operator interface.

Refer to the *Agilent VnmrJ Administration Guide* for instructions on setting the user interface (both the administrator and operator) and for working with the VnmrJ interface.

Sample for Automated Data Acquisition

Sample	Sample size	Part number
2% 2-ethyl-1-indanone in chloroform-*d*	5 mm	01-901855-03

Login to VnmrJ

1 Log in using the operating system VnmrJ Account Owner.

2 Select the account owner from the **Operator** menu, enter the password, and click **OK**.

3 Select **Automation > Automation Run > New Automation Run**.

4 Make sure that the printer/plotter is set up, `pfgon` is set properly, and shim map has been copied into `/vnmr/shimmaps`.

Setting up the study and lock solvent

1 Insert the indanone sample (01-901855-03).

2 Click **New Study** in the Study Queue.

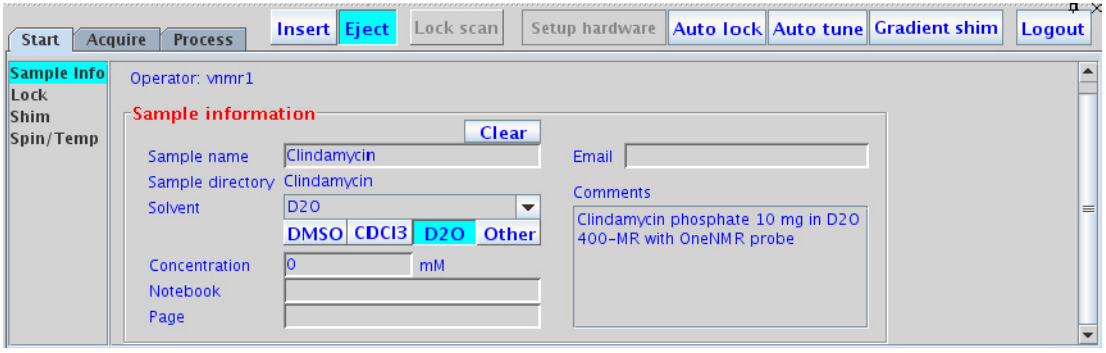


Figure 71 The Sample info page

3 Click the **Start** tab, then in the **Sample info** page enter the **Sample name**: `2-ethyl-1-indanone`

4 Select **chloroform** from the **Solvent** menu.

5 Confirm that the following items are selected:

- **Autoplot**
- **Shim**

6 Confirm that **Lock?** is set to **Yes (alock <>n)**.

Do not click **Email when study complete** or **Email when fid complete**.

Building a Study

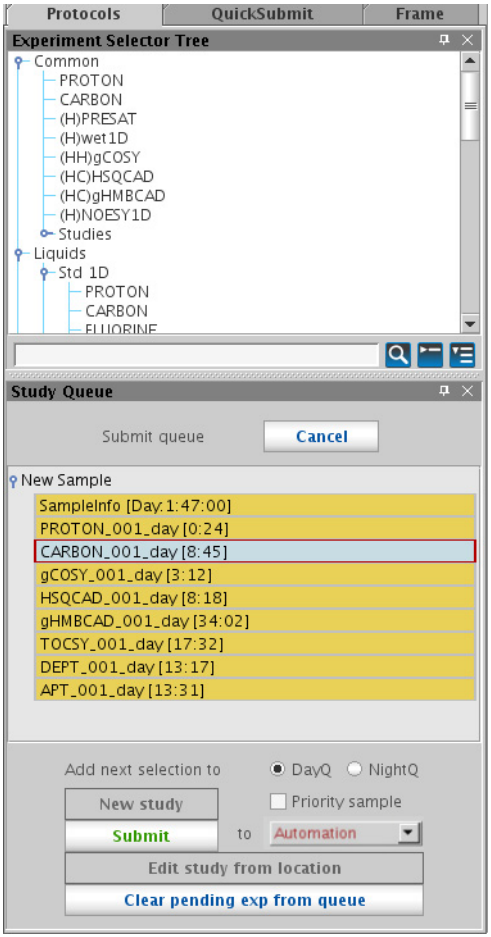


Figure 72 Protocols tab showing Experiment Selector Tree and Study Queue

Common tab

In the Experiment Selector tree, select **Common**, Figure 72, and double-click the following experimental protocols in the following order:

1 **PROTON**

2 **CARBON**

3 **(HH)gCOSY**

4 **(HC)HSQCAD**

5 **(HC)gHMBCAD**

Under **Liquids**, click **(HH)Homo2D** and select

6 **TOCSY**

then click **Std1D**, and select:

7 **DEPT**

8 **APT**

Customizing the parameters and starting data acquisition

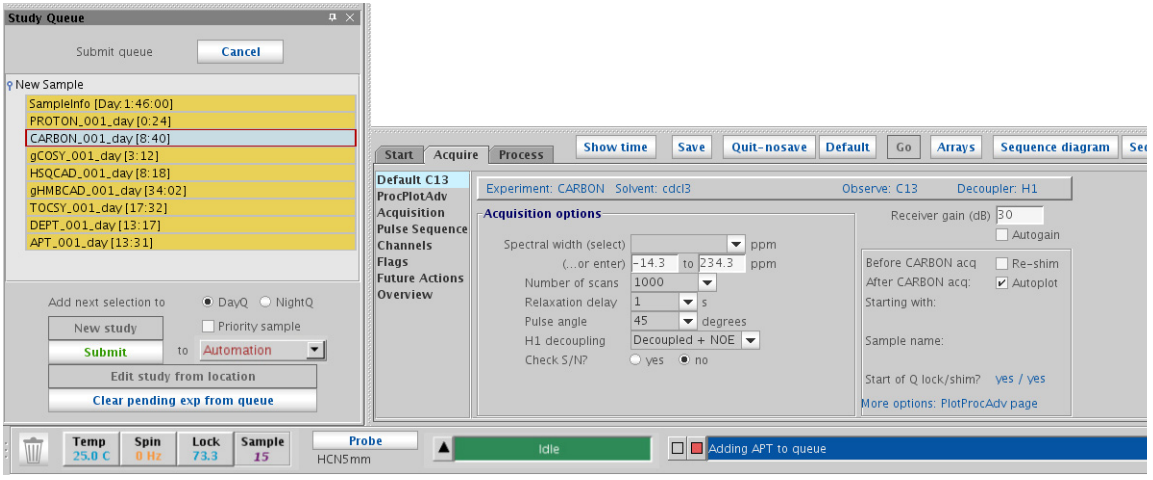


Figure 73 Customized carbon

The **Study Queue** contains the protocols in the order each one was selected and should look similar to the study queue shown in Figure 73.

1 Double-click on the CARBON protocol time to retrieve the parameters.

2 Click the **Acquire** tab.

3 Select the **Defaults C13** page (if more than one page is available).

4 Select **1000** from the **Number of Scans** menu.

Starting data acquisition using a study

1 Select **Background** from the **Study Queue-Submit to** pulldown menu.

2 Click **Submit**.

- All the protocols are locked automatically.
- Acquisition starts.

Interpreting the Indanone Spectra

In this section, the data obtained from the automated probe calibration and 2% 2-ethyl-1-indanone sample are interpreted.

Calibration – When is it Necessary

The spectrometer must first be calibrated before acquiring spectra of a sample if:

- A new probe is installed.
- The original calibration used a sample in an organic solvent and the new sample has changed from an organic solvent to an aqueous solvent or aqueous solvent with a high salt concentration.
- The current probe calibrations have not been verified recently.

Interpretation of the Calibration Data

The first of the spectra, shown in Figure 74, is a ^{1}H observe with $CDCl_3$ as the lock solvent. This data is saved as `H1ref`. This spectrum contains three $^{13}CH_3I$ resonances centered at about 2.2 ppm. The center resonance is from the protons attached to carbon-12 and the two outer resonances are from the protons attached to ^{13}C. The other resonances in the sample are from trimethylphosphite that has reacted with the methyl iodide.

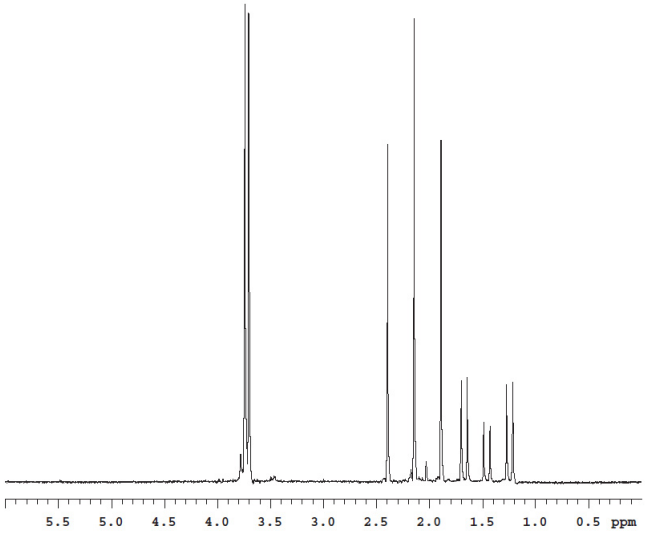


Figure 74 ^{1}H Sprectrum of ^{13}C-Methyl Iodide

All trimethylphosphite has reacted to form a phosponate ester $(CH_3)P(=O)(OCH_3)_2$. This phosponate ester has a doublet at about 1.5 ppm, methyl group attached directly to ^{31}P and a triplet of doublets centered around 4 ppm that arise from ^{13}C (outer pair of doublets) and 12C inner doublet of the methyl ester. The analysis of this sample is fully discussed in an article by Paul Keifer in *Magnetic Moments* (Keifer, P.A., *Magnetic Moments*, **1996**, 8 (#2), 18–20). The reaction results in a sample is partially enriched to give approximately 60% abundance of ^{13}C in methyl iodide. The natural abundance of ^{13}C is 1.1% so this level of enrichment is more then adequate for the purposes of calibration.

The spectrum, shown in Figure 75, is an array of increasing ^{1}H pulse widths based on the ^{1}H pulse you specified in the Acquire window. If you did not enter a value for the pulse width it is set to the default targets `pw90` is set to 15 ìs and `tpwr` of 51.

The observe transmitter power is set to the value you specified and reduce by 3 for the first test. If the resulting pw90 is shorter then the value you specified (or the default, if you did not specify a pw90 target) the next test is started. If the pw90 is longer then the target, the observe power is increased. Two attempts are made. If the calibration fails to achieve a pw90 that is less than the specified pw90 the AutoCalibration exits. If either attempt yields a pw90 that is less then the specified value the AutoCalibration routine adjusts the observe power the remaining tests are aborted. If the pw90 is less then the specified value, the AutoCalibration then adjusts the power until the measured pw90 is no greater then the specified value but not more then 0.5 µs less than this value.The spectra from a successful calibration are saved as H1pw90.

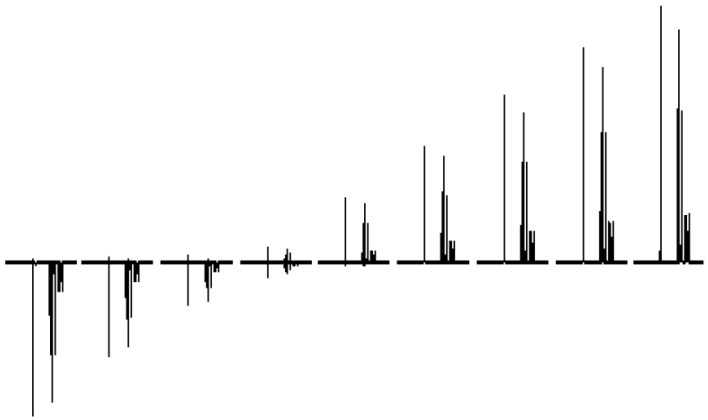


Figure 75 ^{1}H pw Array

The carbon pwx90 calibration is the next experiment. The pulse sequence changes from s2pul to PWXCAL. The specification for the carbon pw90 and tpwr are used as the target values. If no values were specified, the default values of 15 µs at power, in this case pwxlvl, of 51 are used as the target values. Just as with the proton pw90 calibration, the AutoCalibration makes two attempts to achieve the specification and exits

the AutoCalibration if the target specification is not reached after the second attempt. The data from the `PWXCAL` are saved as `C13pwx` and shown in Figure 76.

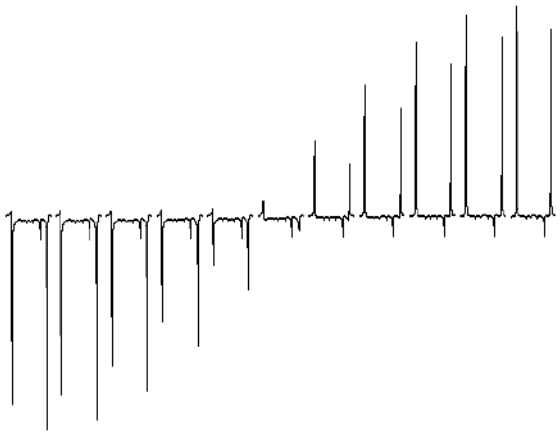


Figure 76 ^{13}C pwx Array

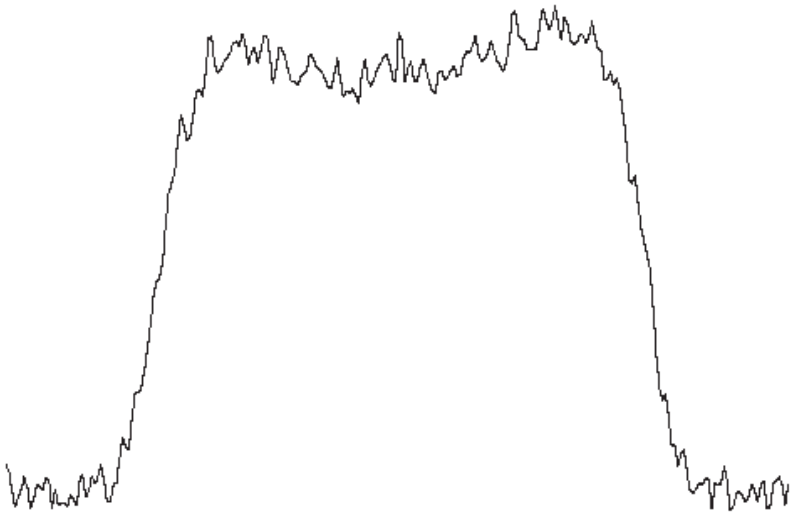


Figure 77 Gradient profile

The next two experiments are run only if you have gradients. The first experiment calibrates the Z-gradient strength, produces the profile shown in Figure 77, and stores this information in the parameter gcal.

The next experiment calculates the ratios of the gradients to be used in various $^{1}H\{^{13}C\}$ indirect detection experiments and stores this information in the parameter `Cgrad` (for only ^{13}C), Figure 78.

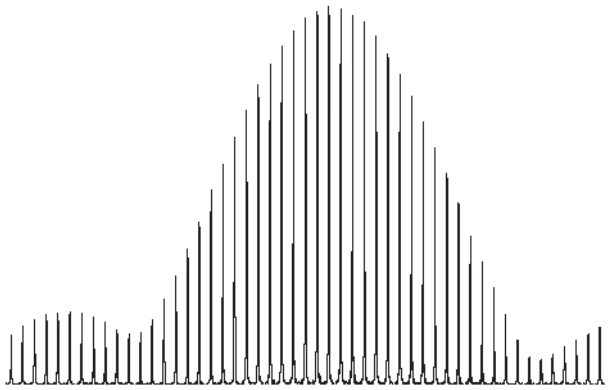


Figure 78 Gradient calibrations

The next calibration is carbon observe pulse width and the pulse sequence is changed to `s2pul` for direct observation of the carbon. The calibration will follow the same pattern as the calibration of the proton `pw90` and the carbon `pwx90` using default values for target values if no target specification is given. A reference carbon spectrum is obtained first. The full reference spectrum contains three sets of resonances, at the far right (approximately –22 ppm) is the ^{13}C resonance from methyl iodide, the doublet at 10 ppm is from the ^{13}C resonance from the phosponate methylester, and the 1:1:1 triplet (far left) at 78 ppm is the ^{13}C resonance of chloroform-d, $^{2}HCCl_3$. The carbon `pw90` calibration is analogous to the proton calibration. The reference carbon spectrum, shown in Figure 79, is saved as `C13ref`.

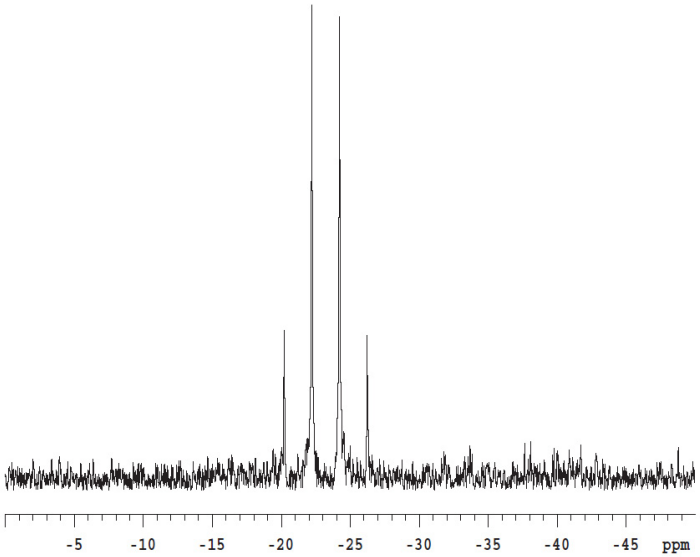


Figure 79 Proton coupled 13C spectrum of 13C-Methyl Iodide

The carbon observe `pw90` is determined using a pw array, see Figure 80, and saved as `C13pw90`.

The final calibration is of the proton decoupler. The first calibration step determines the value of γH_2 at a decoupler power of 40 (the default value).

This measurement is made using continuous wave, `cw`, decoupling. The pulse sequence is the same as in the previous experiment, carbon observe with proton decoupling, except `pw` is now set to a fixed value, decoupler modulation mode; `dmm` is set to 'c', decoupler mode `dm`; is set to 'yyy', and the decoupler offset; `dof` is arrayed to produce the spectra shown in Figure 16.

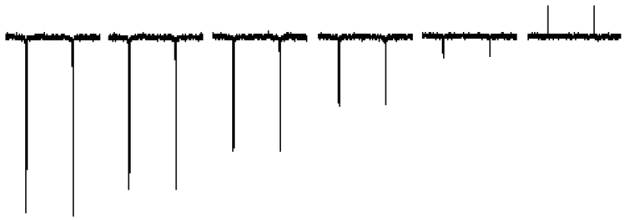


Figure 80 13C Observe pw array of proton coupled spectra3

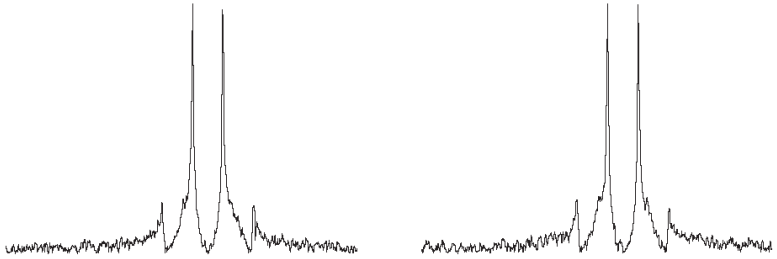


Figure 81 Proton decoupler dof array

The first estimate of the proton decouple `pw90` is made from these spectra. Using the relationship between the pulse width and the decoupler field strength, $\gamma H2$, shown in the equation below, the decoupler `pw90` is determined.

$$\gamma H2 = \frac{1}{4(pw90)} \qquad pw90 = \frac{1}{4(\gamma H2)}$$

The sequence is now set to `ppcal` and the proton decoupler 90° pulse, `pp`, is determined. These spectra, shown in Figure 82 are saved as `Hdec_dept`.

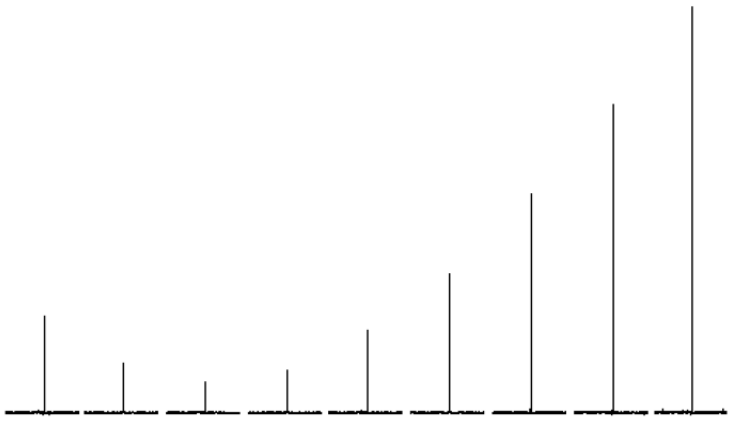


Figure 82 Calibration of the decoupler 90° pulse width

These parameters and calibrations are used to setup WALTZ decoupling. This completes the calibrations. During the calibration procedure, spectra and the array values are plotted to provide a permanent record of the calibrations.

Interpretation of 2-Ethyl-1-Indanone Spectra

The proton NMR shows several distinct features. First, there are some impurities in the sample. These impurities, shown in Figure 83, are at the 2% level and some crosspeaks will show up in the 2D. The very large triplet for the methyl group has ^{13}C satellites at `J=125 Hz`. The singlet at 7.24 ppm is the residual $CHCl_3$ in the $CDCl_3$ solvent.

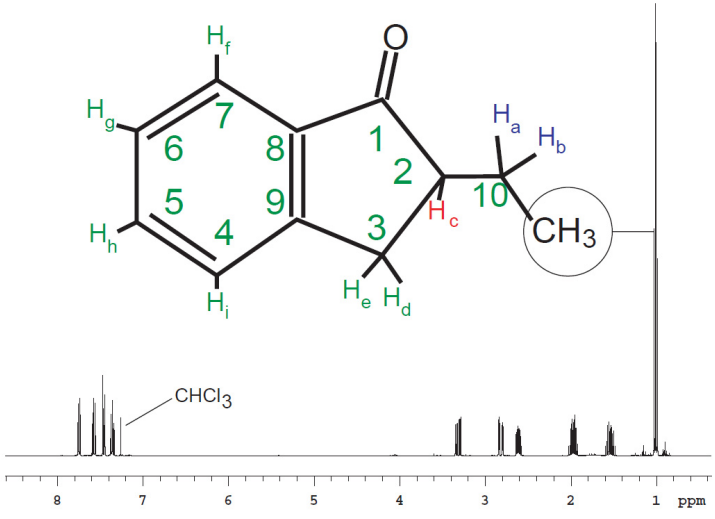


Figure 83 Proton spectrum of 2-Ethyl-1-Indanone

The protons are assigned in the two expansions. The assignments are based upon the 2D data for the compound. The protons of the two CH_2 groups in the molecule, shown in Figure 84, are magnetically nonequivalent and show up as individual multiplets. The signals at 1.9 ppm and 1.55 ppm belong to protons on carbon 10. The two double doublets at 2.8 ppm and 3.26 ppm belong to protons on carbon 3. A complex multiplet at 2.6 ppm is the single proton on carbon 2.

The protons of the aromatic ring, shown in Figure 85, are assigned based on the gHMBC and gCOSY data. Some minor impurities can be seen as well as the residual $CHCl_3$ signal.

If the sample is shimmed very well there may be some truncation artifact on the $CHCl_3$ signal.

The gradient COSY shows cross peaks describing the coupling pathways. Some smaller cross peaks are also present in the spectrum which actually arise from the impurities shown in Figure 86. An example of this is the cross peak at 3.5 ppm.

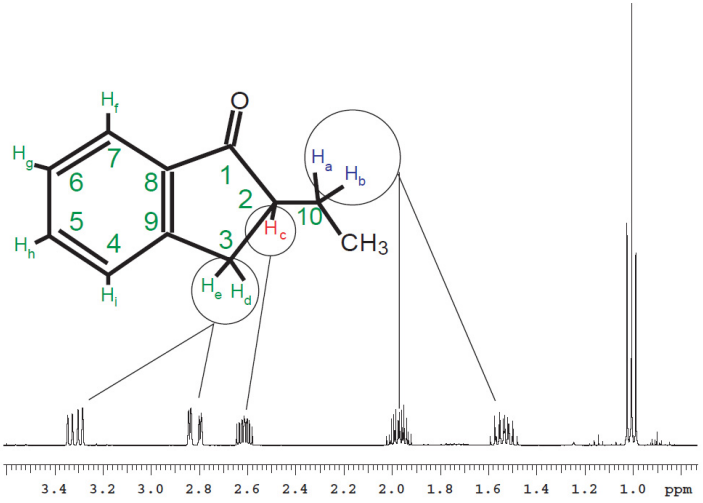


Figure 84 Aliphatic region of the 2-Ethyl-1-Indanone spectrum

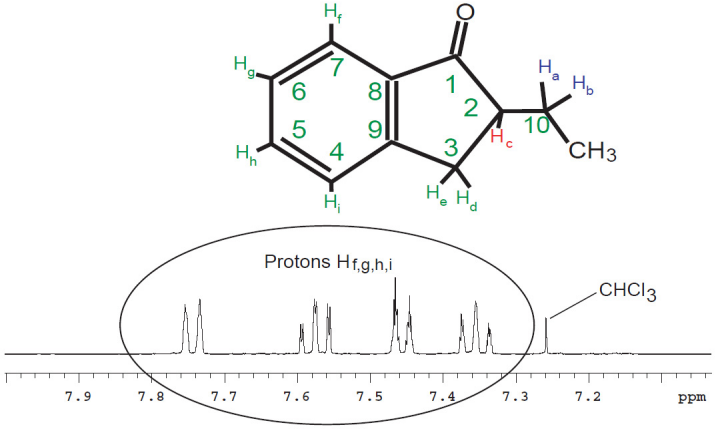


Figure 85 Aromatic region of the 2-Ethyl-1-Indanone spectrum

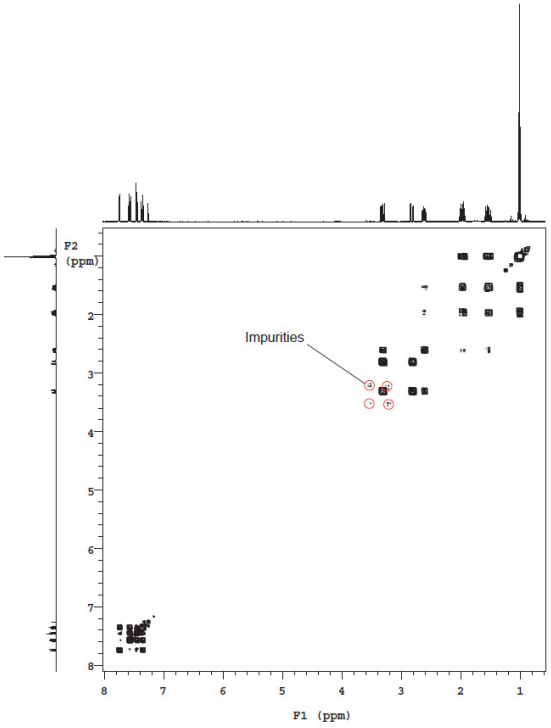


Figure 86 Gradient COSY of 2-Ethyl-1-Indanone

The methyl triplet in Figure 87 shows cross peaks to the H10 protons. The H10 and H2 protons cross peaks multiplicity shows them to be weakly coupled (the J value is small).

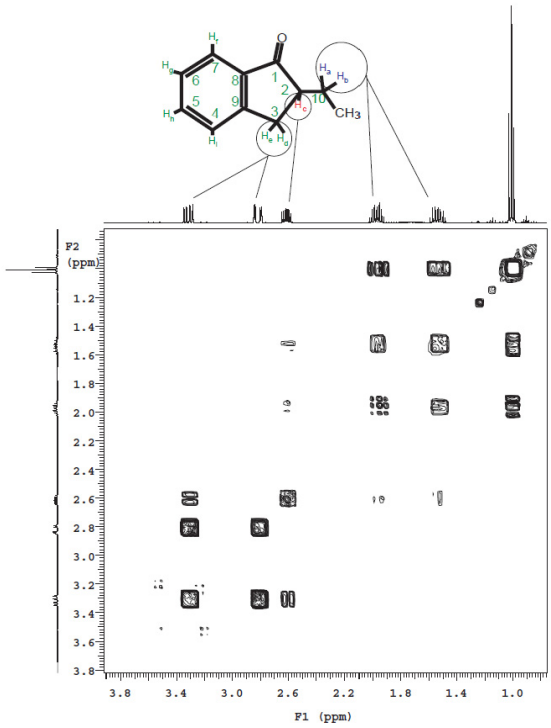


Figure 87 Gradient COSY (gCOSY) of aliphatic region of 2-Ethyl-1-Indanone

Assignment of the aliphatic region, begins with H7, the most deshielded proton, Figure 88. From H7 direct connectivity is apparent to H6. The rest of the assignment is H6 to H5 (the other triplet) and then to H4. The assignment of H7 to the signal at 7.72 ppm is confirmed by the gHMBC data.

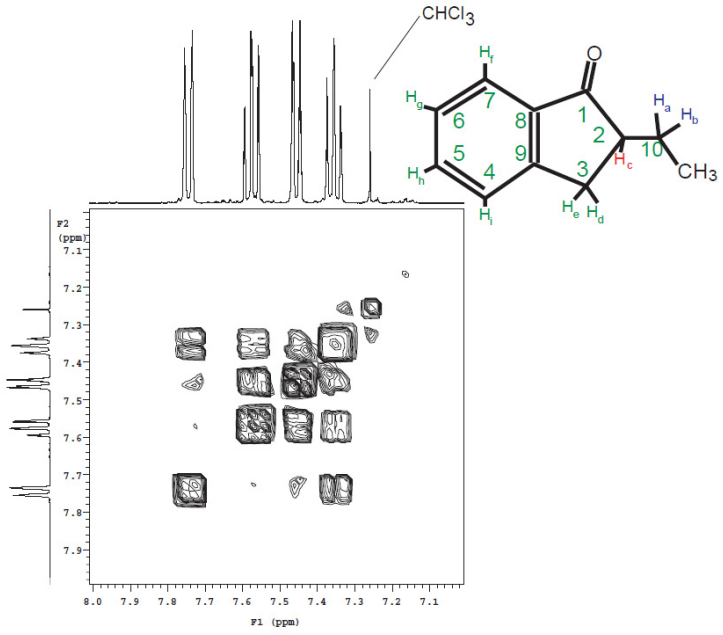


Figure 88 Gradient COSY (gCOSY) of the aromatic region of 2-Ethyl-1-Indanone

TOCSY is a phase sensitive experiment. The cross peaks are narrower than in the COSY giving higher “resolution”. Correlations among all protons in a spin system are observed in the TOCSY spectrum, see Figure 89. The critical parameter is mix. In this case mix is 0.08 seconds which is sufficient to show correlations throughout the entire spin system. Shorter mix times will reveal fewer correlations.

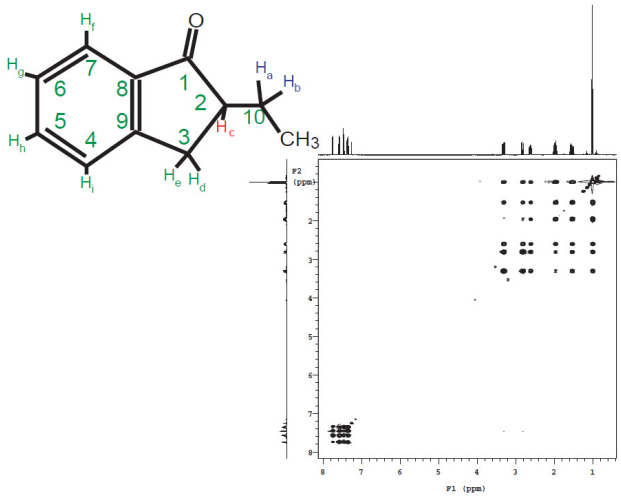


Figure 89 TOCSY of 2-Ethyl-1-Indanone shows correlations among all protons

The expansion shows the completely defined spin system starting with the CH_3 group and ending with protons on C10, Figure 90. A total of 5 crosspeaks are seen in the row.

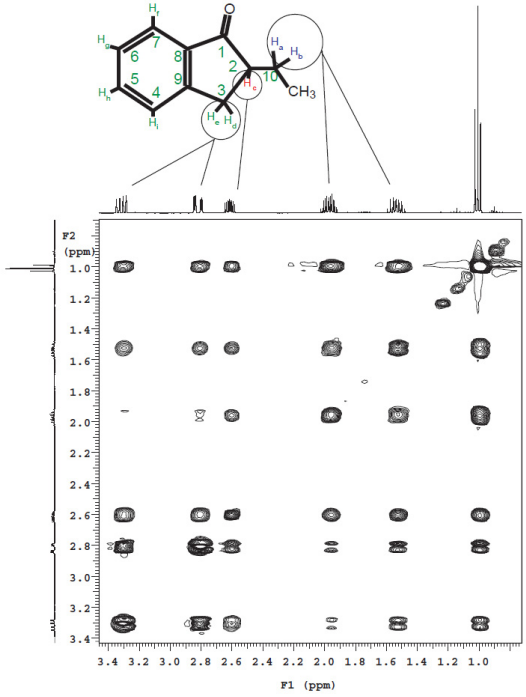


Figure 90 TOCSY of 2-Ethyl-1-Indanone shows correlations among all protons

The indanone sample does not have any significant NOE crosspeaks, Figure 91

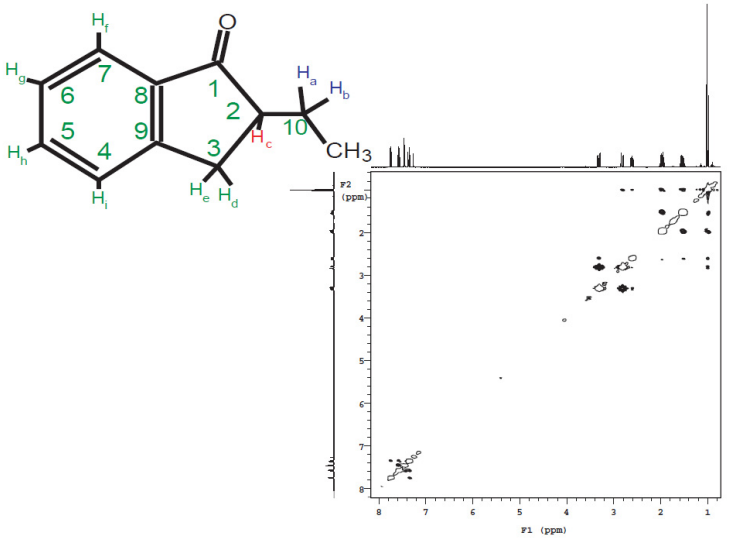


Figure 91 NOESY spectrum of 2-Ethyl-1-Indanone

The main area of interest in this spectrum is to note that the diagonal will be negative and the NOESY crosspeaks will be positive. Crosspeaks which appear to have both positive and negative components are actually not NOE correlations but coupling artifacts.

In the gHSQC (and HSQC) experiment, see Figure 92 the protons correlate with the carbons to which they are attached. The detected nucleus is ^{1}H and this results in a higher signal-to-noise then the ^{13}C detected hetcor experiment. When compared to the HMQC experiment, the HSQC experiment has the advantage that the ^{1}H – ^{1}H homonuclear coupling do not evolve. As a result the resolution in the 2D plane is higher in the HSQC experiment. The higher resolution has the added advantage of improving the signal-to-noise. The version of the HSQC experiment supplied with NMR spectrometer systems has the added benefit that it will distinguish –CH, $–CH_2$, and $–CH_3$ groups. In this case phase is indicated by whether the crosspeak is filled in with multiple contours (above the plane) or is a single contour (below the plane).

By contrast to the gHSQC experiment, the gHMBC (and HMBC) experiment shows long range (mostly 2 and 3 bond) ^{1}H – ^{13}C correlations. This shows connectivity between the non - protonated carbonyl and the protons on C-2.

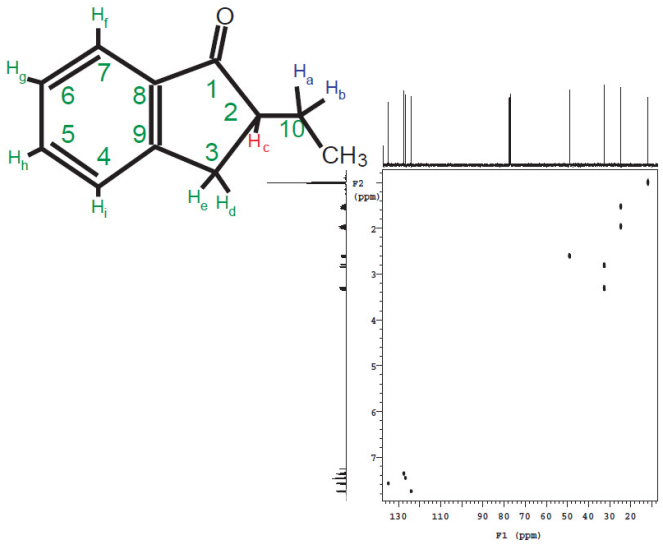


Figure 92 HSQC spectrum of 2-Ethyl-1-Indanone

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