# Walkup NMR

*Varian NMR Spectrometer Systems*
*With VNMR 6.1C Software*
*Pub. No. 01-999159-00, Rev. A0800*

VARIAN

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Revision history:
A0800 – Initial release for VNMR 6.1C

Applicability of manual:
Varian NMR spectrometer systems running
VNMR 6.1C software

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# Chapter 1. Introduction to Walkup NMR User Interfaces

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- 1.1 "GLIDE User Interface," this page
- 1.2 "Tcl/dg User Interface," page 8

VNMR provides two walkup NMR user interfaces: *GLIDE* and Tcl/dg. Both interfaces are designed for efficient operation of the spectrometer in open access environments or where only a predefined set of experiments are required and minimal system administrator involvement is needed. Both interfaces are customizable to meet specific needs. As supplied, both interfaces make a wide variety of powerful 1D and 2D NMR experiments available through a graphical user interface. The NMR experiments provided are well suited for analysis and study of small to medium sized molecules typically, but not exclusively, in deuterated organic solvents.

## 1.1 *GLIDE* User Interface

The *GLIDE* user interface (Figure 1) is designed to make setting up, acquiring, processing, and plotting tasks easy. *GLIDE* provides drop down menus for selection of experiments and pop up dialog panels for routine acquisition or for customization of acquisition. For routine use, you do not have to adjust parameters, which optimizes throughput. The *GLIDE* user interface guides you step-by-step with appropriate menus and choices. An online help button is provides access to online instructions.

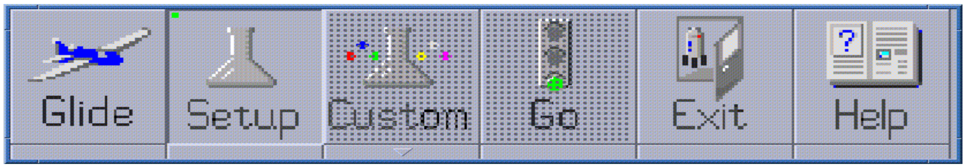


**Figure 1.** *GLIDE* User Interface

*GLIDE* has the following features:

- Customizable icons, buttons, and values.
- Unavailable options are clearly indicated.
- Administrator control of autocalibration access.
- Autocalibration of key probe parameters such as `dmf`, `pw90`, gradients, lock, and `tpwr`.
- Administration tools to predefine available experiments for different groups of users.

The *GLIDE* user interface provides access to most aspects of an experiment. If you need access to parameters and functionality not presented in the *GLIDE* interface, the VNMR menu system, located just below the *GLIDE* window is accessible to the user. If this is still not enough, the *GLIDE* window can be hidden and any VNMR command can be entered in the VNMR input window.

*GLIDE* provides the guidance and opportunity for exploration while always supplying a secure path back through the default buttons in each phase. If the default *GLIDE* buttons do not provide enough adjustment, you can program the buttons for different actions.

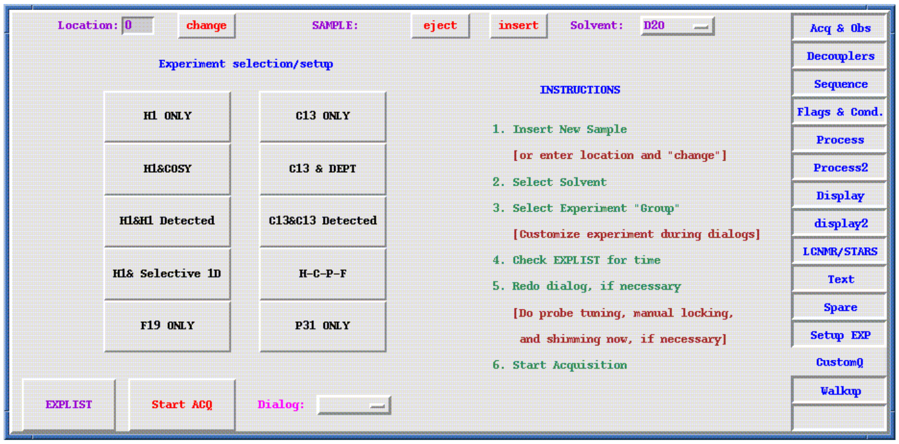
The *GLIDE* interface, operations, calibrations, and customization are covered in the following chapters:

- Chapter 2 "GLIDE Walkup User Interface," page 11
- Chapter 3 "GLIDE Step-by-Step," page 17
- Chapter 4 "GLIDE Calibration," page 47
- Chapter 5 "GLIDE Administrating and Customizing," page 59

## 1.2 Tcl/dg User Interface

VNMR provides three push-button interfaces for selecting and running experiments within the Tcl/dg interface.

**CustomQ** interface, Figure 2, accesses the same experiments available through the *GLIDE* interface and provides access to most aspects of an experiment. Parameters and functionality not presented in the CustomQ interface are accessed through either the VNMR menu system or other Tcl/dg panels.



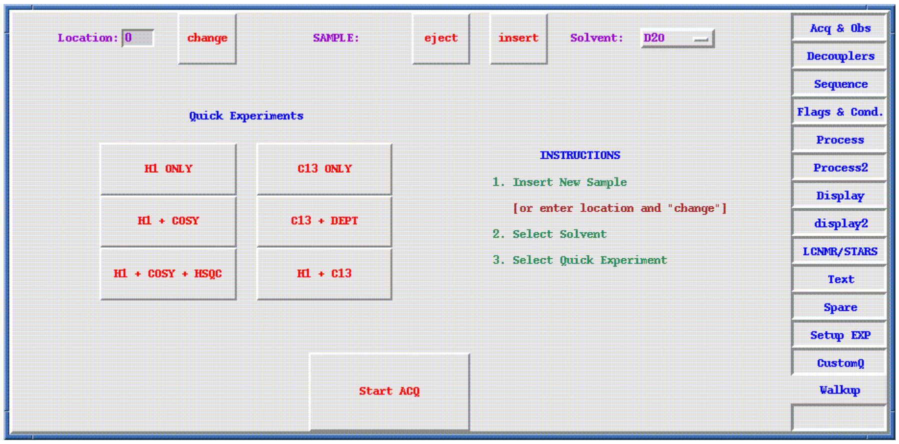
INSTRUCTIONS

1. Insert New Sample
   [or enter location and "change"]
2. Select Solvent
3. Select Experiment "Group"
   [Customize experiment during dialogs]
4. Check EXPLIST for time
5. Redo dialog, if necessary
   [Do probe tuning, manual locking, and shimming now, if necessary]
6. Start Acquisition

**Figure 2.** Tcl/dg CustomQ Interface

**Walkup**, Figure 3, provides one button access to a preset group of experiments which makes set up and acquisition easy. All parameters and plotting options are preset. The experiments are a subset of the experiments available through the CustomQ interface.

**Setup EXP**, Figure 4, accesses all the experiments available through the CustomQ interface as well as several N15 experiments. Setup EXP is designed for the more advanced user and the system administrator. Setup EXP provides access to locally stored probe calibrations.



INSTRUCTIONS

1. Insert New Sample

   [or enter location and "change"]

2. Select Solvent
3. Select Quick Experiment

**Figure 3.** Tcl/dg Walkup Interface

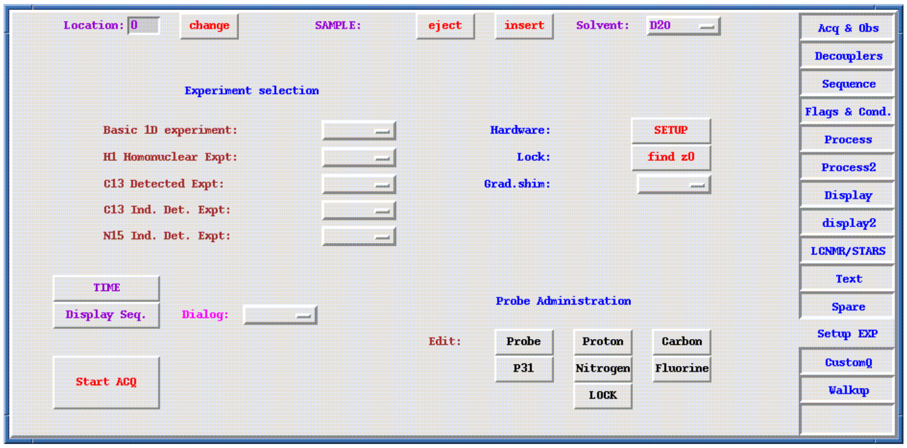


**Figure 4.** Tcl/dg Setup EXP Interface

Each of these interfaces is designed to simplify setting up, acquiring, processing, and plotting tasks easy. Programming and customization of the Tcl/dg window is covered in the *User Programing manual*.

The Tcl/dg interfaces, operations, calibrations, and administration are covered in the following chapters:

- Chapter 6 “Tcl/Tk User Interfaces,” page 85
- Chapter 7 “Tcl/Ttk NMR Interfaces Step-by-Step,” page 91
- Chapter 8 “Tcl/Tk NMR Administration and Calibration,” page 121

# Chapter 2. *GLIDE* Walkup User Interface

Sections in this chapter:

- 2.1 “Standard GLIDE Experiments,” this page
- 2.2 “GLIDE Buttons,” page 12

This chapter provides a general overview of the *GLIDE* user interface and features of the *GLIDE* buttons.

Step-by-step operation, administration, and customization of the *GLIDE* interface are covered in separate chapters (or other manuals), listed below:

- Chapter 3, “GLIDE Step-by-Step,” for instructions on how to run experiments using *GLIDE*.
- Chapter 4, “GLIDE Calibration,” for instructions on calibration.
- Chapter 5, “GLIDE Administrating and Customizing,” for instructions on how to administrate and customize *GLIDE* for local use.
- Chapter 9, “Processing and Plotting Saved Data,” for instructions on how to retrieve, process and plot saved data.
- *Getting Started* for detailed information on spectrometer operations.
- *User Guide: Liquids NMR* for additional information about various experiments.

## 2.1 Standard *GLIDE* Experiments

The *GLIDE* interface provides a large number of powerful 1D and 2D experiments. The experiments and groups of experiments are the following:

- Standard Proton 1D, Carbon 1D, Fluorine 1D, and Phosphorus 1D
- Chained Proton, Carbon, Fluorine, and Phosphorus 1D
- Chained Proton 1D and COSY
- Chained Carbon 1D and DEPT
- Proton 1D with options for chained 2D experiments:
    - COSY
    - gCOSY
    - gDQCOSY
    - TOCSY
    - NOESY
    - ROESY
    - HMQC
    - gHMQC

  - HSQC
  - gHSQC
  - gHMBC or HMBC if gradients are not present
  - HMQCTOXY
  - HSQCTOXY
  - gHMQCTOXY
  - gHSQCTOXY
  - CARBON 1D
- Carbon 1D with options for chained 1D and 2D experiments:
  - APT
  - DEPT
  - HETCOR
  - gHETCOR
  - PROTON 1D
  - COSY
  - gCOSY
- Proton 1D with options for chained selective experiments:
  - TOCSY1D
  - NOESY1D
  - ROESY1D
  - HOMODEC

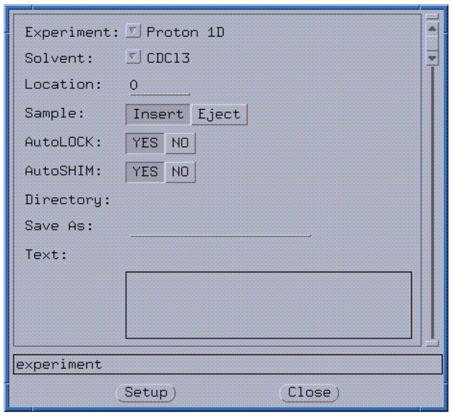
## 2.2 *GLIDE* Buttons

The *GLIDE* interface contains an icon box (labeled Glide) and five buttons: Setup, Custom, Go, Exit, and Help. When *GLIDE* is first activated, the Custom and Go buttons appear shaded to indicate that they are not yet active. Each button is described below.

### Setup Icon

Click the Setup icon on the *GLIDE* interface window to display the Experiment Setup window, shown in Figure 5.

The Experiment Setup window provides two drop-down menus, one for selecting the experiment and another for selecting the solvent. If a sample changer is configured for the instrument, a sample location field is active. Sample Insert and Eject buttons are active for instruments with automated insert/eject/spin. AutoLOCK and AutoSHIM options are selected in this window. The spectrum or spectra will be saved using the file name entered in the Save As field. Additional sample information can be entered in the Text box.



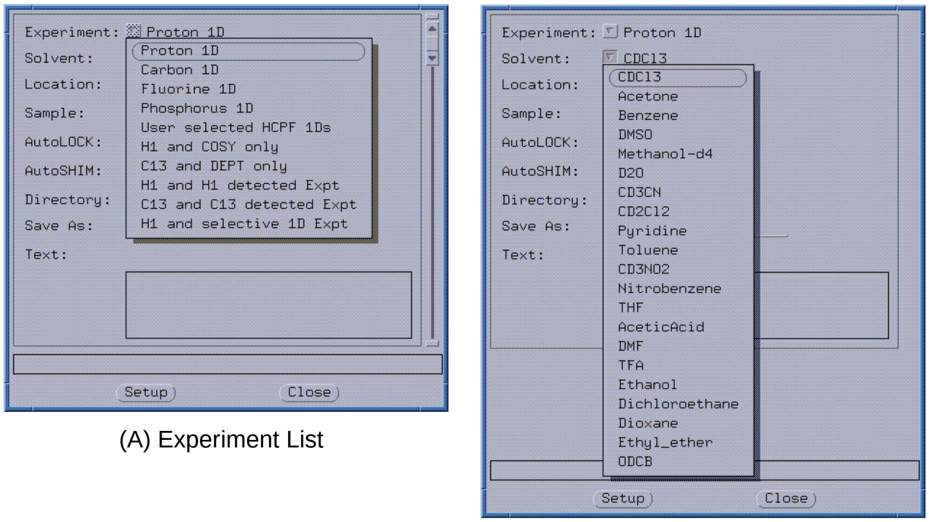
Experiment: Proton 1D
Solvent: CDCl3
Location: 0
Sample: Insert Eject
AutoLOCK: YES NO
AutoSHIM: YES NO
Directory:
Save As:
Text:
experiment

**Figure 5.** *GLIDE* Experiment Setup Window

Click on the Experiment button with the right mouse button to display the *GLIDE* experiment menu. The choices are:

- Proton 1D
- Carbon 1D
- Phosphorus 1D
- Fluorine 1D
- User selected HCPF 1Ds
- H1 and COSY only
- C13 and DEPT only
- H1 and H1 detected Experiments
- C13 and C13 detected Expt
- H1 and selective 1D Exp

Make a choice by clicking the appropriate item with the left mouse button, see Figure 6A. Similarly, to choose a solvent, click on the Solvent button with the right mouse button, see Figure 6A. A list of solvents appears with choices such as CDCl3, Acetone, Benzene, and DMSO. Click on the solvent you are using.



(A) Experiment List

(B) Solvent List

**Figure 6.** *GLIDE* Experiment List (A) and Solvent List (B)

If optional automation hardware is installed, this window also shows Insert and Eject buttons, and if a sample changer is enabled (`traymax` parameter not set to 0), a location for a sample can be entered.

Below these buttons, you can enter a file name and text for the sample. For routine 1D experiments, saving data is optional and will not occur if this field is left blank. For all combination experiments, saving data is required. A default name is generated for the data directory if none is entered in the Save As field. Data is saved in `~vnmrsys/data`.

To close the Experiment Setup window and activate the choices shown, click on the Setup button at the bottom of the window. To leave the values unaltered and close the window, click instead on Close. Click on Close only if you decide not to run any experiment.

When setup is complete, the shading disappears from the Custom and Go buttons.

## Custom Icon

The Custom drop-down menu appears, as in Figure 7, following the initial Experiment Setup and contains three buttons labeled Acquire, Process, and Plot. Each button opens a window with a number of fields and buttons. The choices available in these individual windows is determined by the experiment and nucleus selected during the Setup step.

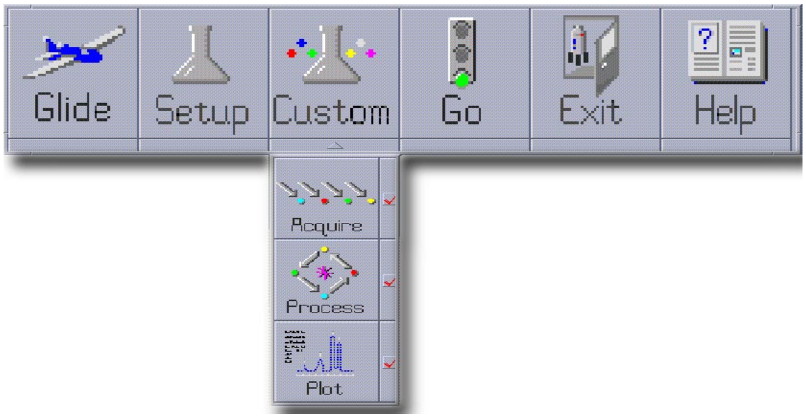


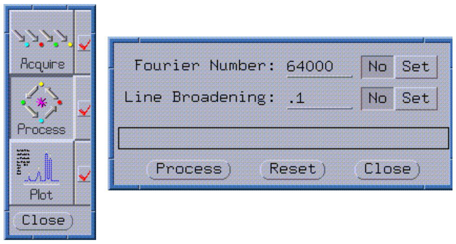
**Figure 7.** Custom Setup Window (*GLIDE*)

The select button next to each button in the Custom menu can be changed from selected to not selected. If selected, that phase of the experiment is executed when the Go button is clicked. If the button is not selected, that phase is not automatically executed, but can be executed after the acquisition is complete. The ability to postpone experiment execution is most often useful for the Plot option, because you have the opportunity to interactively define plot-related values (e.g., integral normalization) before making a plot.

### *Acquire Button*

After setting up an experiment using the Experiment setup window the Custom menu automatically appears below the Custom icon when the basic Experiment Setup process is completed, see Figure 7. The Proton 1D, Carbon 1D, Phosphorus 1D, or Fluorine 1D experiments can be performed immediately, without changing any parameters, because the parameters have default values. Combination experiments, User selected HCPF 1Ds, H1 and COSY only, C13 and DEPT only, H1 and H1 detected Experiments, C13 and C13 detected Expt, or H1 and selective 1D Exp provide additional choices of experiments and experimental conditions. Each choice is presented with a default setting and a selection of optional acquisition parameters. Clicking the Acquire icon presents the user with various acquisition options for customizing the individual 1D experiments or defining options for the combination experiments. Chapter 3, “GLIDE Step-by-Step,” provides details for customizing and defining acquisition options.

### Process Button

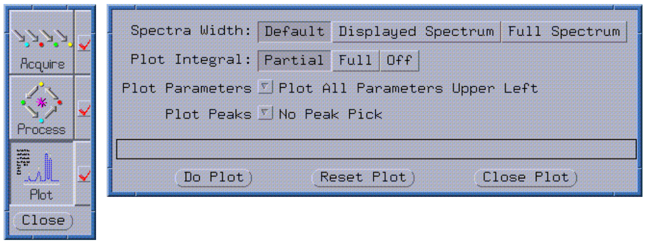


Fourier Number: 64000

Line Broadening: .1

The Process button brings up the process options popup menu. The popup window allows the user to enter values for two key processing parameters, the fourier number and line broadening. The current values of these processing parameters are displayed in the popup window. Either or both values can be change. To change a value, highlight the current value, type in a new value and press the SET button. Pressing the Reset button returns the parameters to their original values. Pressing the Close button saves the new values and exits the window without processing the data. Pressing the Process button exits the window and processes the current data set using the currently displayed values.

### Plot Button



Spectra Width: Default

Plot Integral: Partial

Plot Parameters: Plot All Parameters Upper Left

Plot Peaks: No Peak Pick

The Plot button brings up the plot options popup menu. The popup window allows the user to enter values for plotting the spectrum, spectral width, integral (partial, full, or none), parameters (various options as displayed in the drop down menu), and plotting of peaks (No peak plot and various peak plot options are displayed in the drop down menu). Pressing the Reset Plot button returns the settings to their original values. Pressing the Close Plot button saves the new values and exits the window without plotting the data. Pressing the Do Plot button exits the window and plots the current data set using the currently displayed values.

## Go Icon

The Go button is shaded and inactive until at least the Experiment Setup has been completed. Once the experiment setup and (optional) customization are complete, clicking on the Go button causes *GLIDE* to acquire, process, plot, and save the selected experiment(s). Calibrations stored in the probe file are automatically used by the appropriate macros.

## Exit Icon

Clicking on the Exit button closes the *GLIDE* user interface.

## Help Button and One Line Help

Clicking on the Help button displays a help window with buttons for each of the experiments in the Setup window experiment list. Pressing a button displays a help file in the text window.

Each window contains a help line just above the window control buttons. As you move the cursor across the window, a context sensitive description is displayed in this box.

An example of this one line help is shown here. Although the mouse cursor is not shown in the graphic, it is over the title “Directory”. In the help window the message “Default directory is userdir+’/data’” is displayed indicating that the data will be saved in the directory “data” in the current user directory.

## Popup Window Buttons

The final action in using each window is to click on one of the buttons (Do, Reset, or Close) at the bottom of the window:

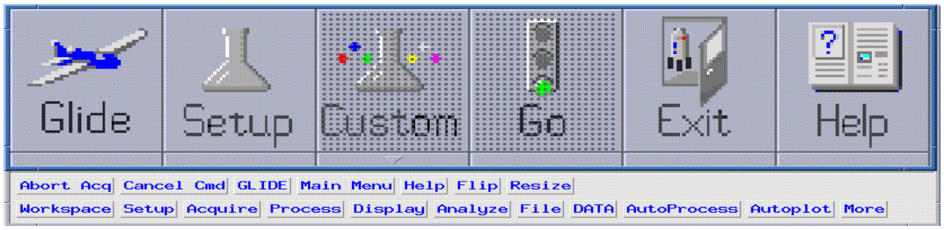
- **Do** does acquisition, processing, or plotting, corresponding to the choices made in the current window. This choice is most often useful for reprocessing or replotting data that has already been acquired.
- **Rese**t changes all the values back to the defaults. Defaults are always the first choices in a list.
- **Close** saves any changes made and closes the window. Choices made in all selected windows will be automatically used after the Go button is clicked to start an acquisition.

# Chapter 3. *GLIDE* Step-by-Step

Sections in this chapter:

## 3.1 Opening and Closing *GLIDE*

When you open the *GLIDE* user interface the menu overlays the top of the VNMR window.



### To Open *GLIDE*

To open the *GLIDE* user interface window, take *one* of the following actions:

- Click on the *GLIDE* button on the Main Menu
  – OR–
- Enter the command `glide` in the VNMR input window

### To Hide / Show *GLIDE*

The *GLIDE* button in the Permanent Main Menu acts as a toggle, allowing the *GLIDE* window to be moved into view or hidden behind other windows.

- To hide the *GLIDE* user interface window from the display but keep the program running, click on the *GLIDE* button in the VNMR Permanent menu. To show the *GLIDE* window, click again on the *GLIDE* button or enter the command `glide`

### To Close *GLIDE*

To close the *GLIDE* program so it no longer is running, take one of the following actions:

- Click on the **Exit** button, or
- Enter the command **`glide('exit')`**.

You might be asked to confirm that you want to exit *GLIDE*. Customizing the file `glide_defaults` (described in Chapter 5 “GLIDE Administrating and Customizing,” page 59) determines whether or not you see the confirmation window.

## 3.2 Proton 1D Spectrum

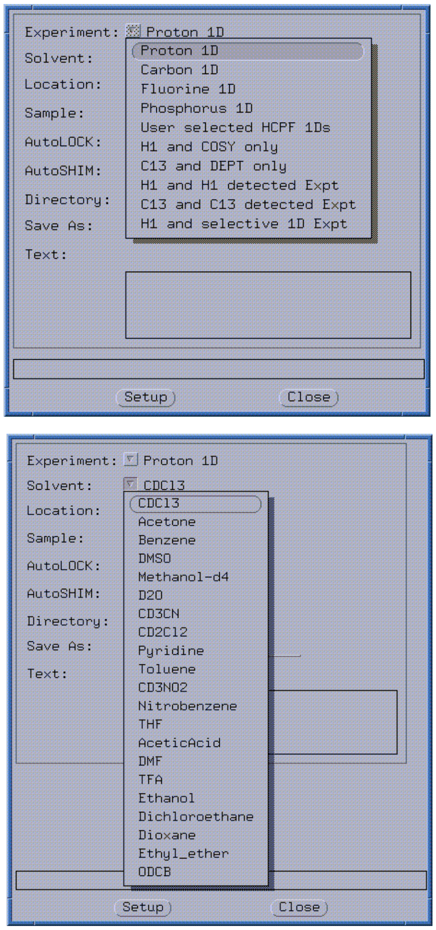
This section describes how to setup, customize, and acquire a proton 1D spectrum.

### *Setup*

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **Proton 1D**, as shown in Figure 8.
4. Right click the **Solvent** drop-down menu and select the appropriate lock solvent, as shown in Figure 8.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

   Standard proton parameters are recalled. Relevant parameters and text are reset according to your needs.

   If you set Autoshim and Autolock to NO, manually lock and shim now.


Experiment: Proton 1D

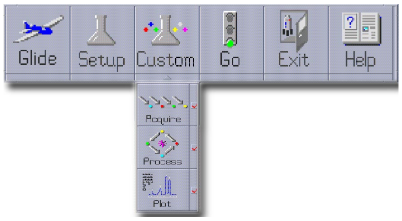
Experiment: Proton 1D
Solvent: CDCl3

**Figure 8.** *GLIDE* Setup for Proton 1D

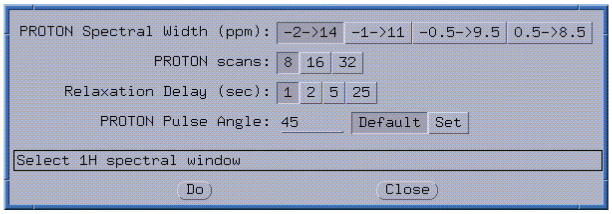
If you prefer to use default settings and not customize, you should skip now to "Acquire," page 20.

## Customize

At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.



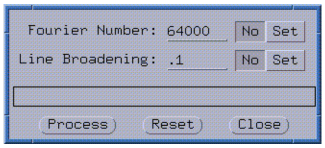
1. Click the **Acquire** button to open the Acquisition Options window.



PROTON Spectral Width (ppm): -2->14 -1->11 -0.5->9.5 0.5->8.5
PROTON scans: 8 16 32
Relaxation Delay (sec): 1 2 5 25
PROTON Pulse Angle: 45 Default Set
Select 1H spectral window

2. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
3. Select the number of proton scans to acquire in the **PROTON scans** field.
4. Select a relaxation delay in the **Relaxation Delay (sec)** field.
5. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.
6. Click on **Close** to save the values you selected and continue on with customizing processing, and plotting options.

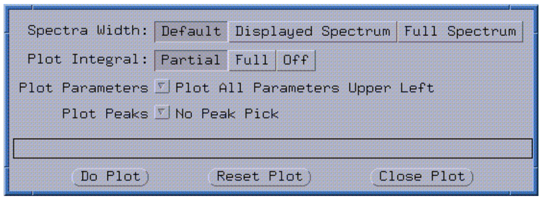
   Click on **Do** if you want to save the values you selected, skip the customizing processing, and plotting options, and immediately start acquisition.
7. Click the **Process** button to open the Process Setup window.
8. Enter a Fourier number in the **Fourier Number** field and click on **Set**, or click on **NO** to use default Fourier number.



Fourier Number: 64000 No Set
Line Broadening: .1 No Set

9. Enter a line broadening factor in the **Line Broadening** field and click on **Set** or click on **NO** to turn off line broadening.
10. Click on **Close** to save the values you selected.

    Do not click on Process unless you clicked on the Do button in step 6 and acquisition has been completed.
11. Click the **Plot** button to open the Plot Setup window.
12. Select Default, Displayed Spectrum, or Full Spectrum in the **Spectral Width** field.
13. Select Partial, Full, or Off in the **Plot Integral** field.



Spectra Width: Default Displayed Spectrum Full Spectrum
Plot Integral: Partial Full Off
Plot Parameters ☐ Plot All Parameters Upper Left
Plot Peaks ☐ No Peak Pick

14. Select how to plot the parameters from the **Plot Parameters** menu.
15. Select a peak-picking option from the **Plot Peaks** menu.
16. Click on **Close Plot** to save the values you selected.

    Do not click on **Do Plot** unless acquisition and processing have been completed.

### Acquire

Click the **Go** button on the *GLIDE* user interface to start acquisition.

The proton spectrum is acquired, processed, plotted, and saved according to the choices you made. The FID is saved with the name `PROTON.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FID is saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## 3.3 Carbon 1D Spectrum

This section describes how to setup, customize, and acquire a carbon 1D spectrum.

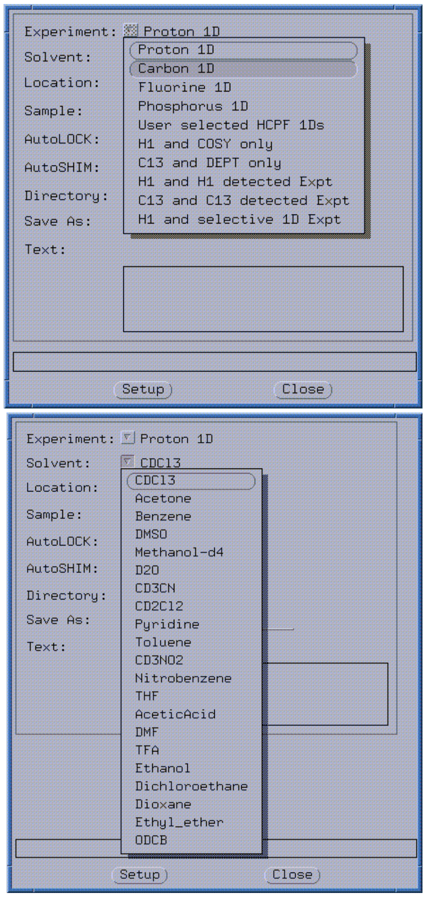


**Figure 9.** *GLIDE* Setup for Carbon 1D

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **Carbon 1D**, as shown in Figure 9.
4. From the **Solvent** menu, select the appropriate lock solvent, as shown in Figure 9.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

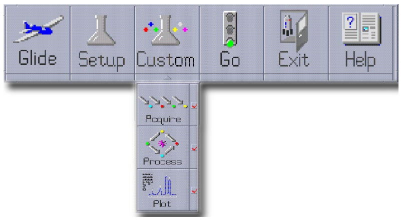
    Standard carbon parameters are recalled. Relevant parameters and text are reset according to your choices.

    If you set Autoshim and Autolock to NO, manually lock and shim now.

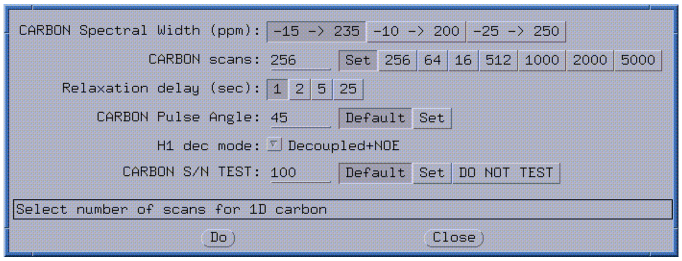
If you prefer to use default settings, and not customize, you should skip now to "Acquire," page 22.

## Customize

At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.

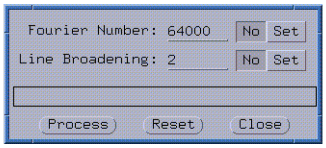


1. Click the **Acquire** button to open the Acquisition Setup window.


CARBON Spectral Width (ppm): -15 -> 235 | -10 -> 200 | -25 -> 250
CARBON scans: 256 | Set | 256 | 64 | 16 | 512 | 1000 | 2000 | 5000
Relaxation delay (sec): 1 | 2 | 5 | 25
CARBON Pulse Angle: 45 | Default | Set
H1 dec mode: Decoupled+NOE
CARBON S/N TEST: 100 | Default | Set | DO NOT TEST
Select number of scans for 1D carbon

2. Select the spectral window in the **CARBON Spectral Width (ppm)** field and the number of scans to acquire or enter a value in the **CARBON scans** field.
3. Select a relaxation delay in the **Relaxation Delay (sec)** field and enter a value for the pulse angle (observe pulse) in the **CARBON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.
4. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
5. Select CARBON S/N TEST option: **Default** (S/N=100), **`Set`** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. The signal to noise is measured on the tallest peak in the spectrum which is often the solvent peak. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.
6. Click on **Close** to save the values you selected and continue on with customizing processing, and plotting options.

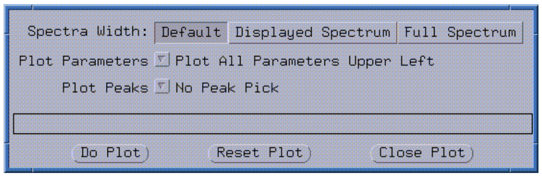
   Click on **Do** if you want to save the values you selected, skip the customizing processing, and plotting options, and immediately start acquisition.


Fourier Number: 64000 | No | Set
Line Broadening: 2 | No | Set

7. Click the **Process** button to open the Process Setup window.
8. Enter a Fourier number in the **Fourier Number** field and click on **Set**, or click on **NO** to use default Fourier number.
9. Enter a line broadening factor in the **Line Broadening** field and click on **Set**, or click on **NO** to turn off line broadening.
10. Click on **Close** to save the values you selected.

Do not click on Process unless you clicked on the Do button in step 6 and acquisition has been completed.

11. Click the **Plot** button to open the Plot Setup window.



Spectra Width: Default | Displayed Spectrum | Full Spectrum

Plot Parameters: Plot All Parameters Upper Left

Plot Peaks: No Peak Pick

12. Select Default, Displayed Spectrum, or Full Spectrum in the **Spectral Width** field.
13. Select how to plot the parameters from the **Plot Parameters** menu.
14. Select a peak-picking option from the **Plot Peaks** menu.
15. Click on **Close Plot** to save the values you selected.

    Do not click on **Do Plot** unless acquisition and processing have been completed.

## Acquire

If you did not start the acquisition in step 6, click the Go button in the *GLIDE* user interface to start acquisition.

The carbon spectrum is acquired, processed, plotted, and saved according to the choices you made.

The FID is saved with the name `CARBON.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FID is saved in the directory `~/vnmrsys/data/`*`filename-date-time.`*

## 3.4 Fluorine 1D Spectrum

This section describes how to setup, customize and acquire a fluorine 1D spectrum.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **Fluorine 1D**, as shown in Figure 10.
4. Right click the **Solvent** drop-down menu and select the appropriate lock solvent, as shown in Figure 10.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

   Standard fluorine parameters are recalled. Relevant parameters and text are reset according to your choices.

   If you set Autoshim and Autolock to NO, manually lock and shim now.

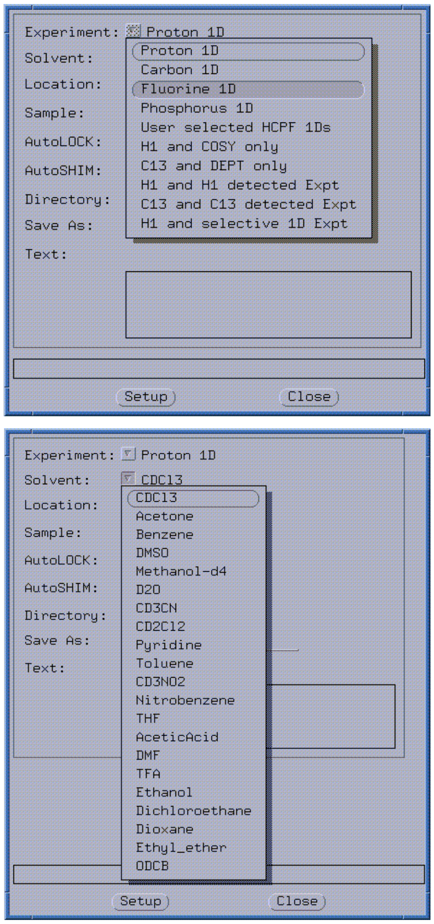
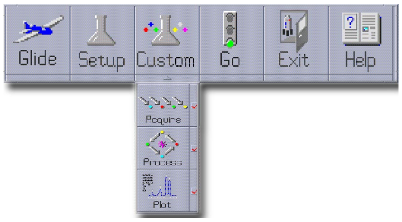


**Figure 10.** *GLIDE* Setup for Fluorine 1D

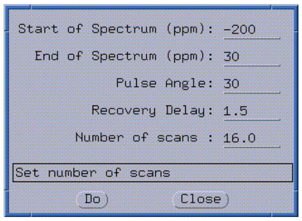
If you prefer to use default settings and not customize, you should skip now to "Acquire," page 24.

### Customize

At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.



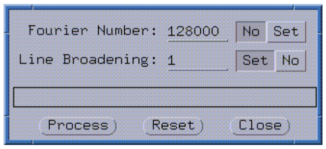
1. Click the **Acquire** button to open the Acquisition Setup window).
2. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window. Enter all values in ppm.



Start of Spectrum (ppm): -200
End of Spectrum (ppm): 30
Pulse Angle: 30
Recovery Delay: 1.5
Number of scans : 16.0
Set number of scans

3. Enter a value for the **pulse angle** or make no entry and accept the default value.
4. Enter a value for the **recovery delay** or make no entry and accept the default value shown.
5. Enter the number of **scans to acquire** or make no entry and accept the default value.
6. Click on **Close** to save the values you selected and continue on with customizing processing, and plotting options.

   Click on **Do** if you want to save the values you selected, skip the customizing processing, and plotting options, and immediately start acquisition.
7. Click the **Process** button to open the Process Setup window.
8. Enter a Fourier number in the **Fourier Number** field and click on **Set**, or click on **NO** to use default Fourier number.

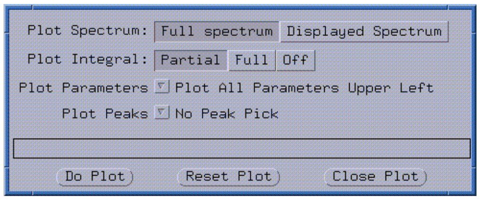


Fourier Number: 128000

Line Broadening: 1

9. Enter a line broadening factor in the **Line Broadening** field and click on **Set**, or click on **NO** to turn off line broadening.
10. Click on **Close** to save the values you selected.

    Do not click on Process unless you clicked on the Do button in step 6 and acquisition has been completed.
11. Click the **Plot** button to open the Plot Setup window.
12. Select Displayed Spectrum or Full Spectrum in the **Spectral Width** field.
13. Select Partial, Full, or Off in the **Plot Integral** field.



Plot Parameters: Plot All Parameters Upper Left

Plot Peaks: No Peak Pick

14. Select how to plot the parameters from the **Plot Parameters** menu.
15. Select a peak-picking option from the **Plot Peaks** menu.
16. Click on **Close Plot** to save the values you selected.

    Do not click on **Do Plot** unless acquisition and processing have been completed.

## Acquire

If you did not start the acquisition in step 6, click the Go button in the *GLIDE* user interface to start acquisition. The fluorine spectrum is acquired, processed, plotted, and saved according to the choices you made.

The FID is saved with the name `FLUORINE.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FID is saved in the directory `~/vnmrsys/data//`*`filename-date-time`*.

## 3.5 Phosphorus 1D Spectrum

This section describes how to setup, customize, and acquire a phosphorus 1D spectrum.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **Phosphorus 1D**, as shown in Figure 11.
4. Right click the **Solvent** drop-down menu and select an appropriate lock solvent, as shown in Figure 11.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

   Standard phosphorus parameters are recalled. Relevant parameters and text are reset according to your choices.

   If you set Autoshim and Autolock to NO, manually lock and shim now.

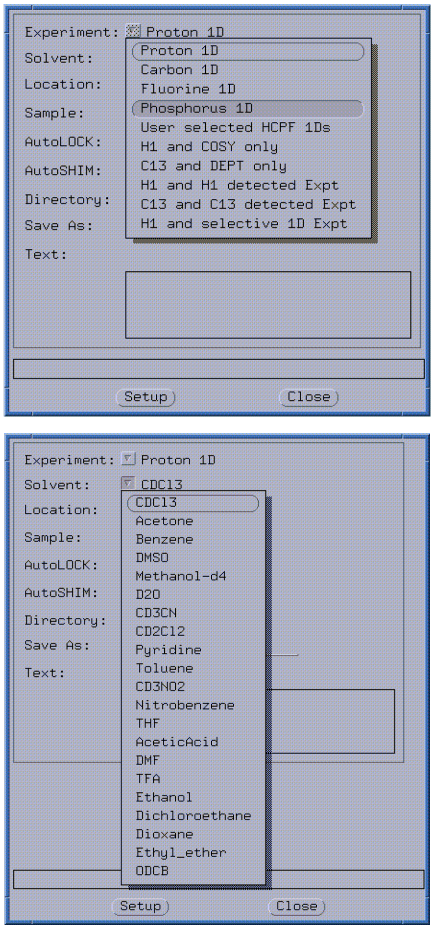
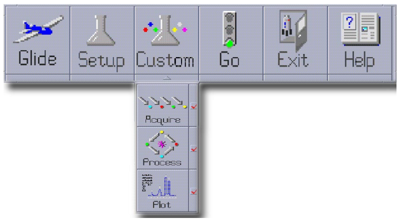


**Figure 11.** *GLIDE* Setup for Phosphorus 1D

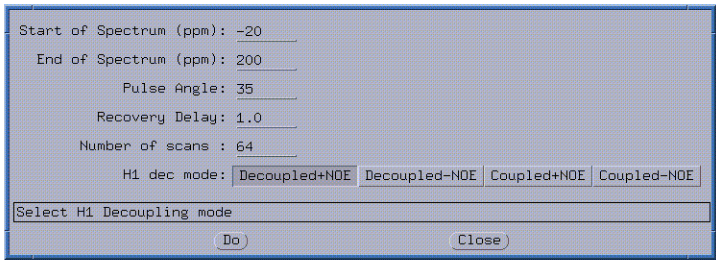
If you prefer to use default settings and not customize, you should skip now to "Acquire," page 26.

### Customize



At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.

1. Click the **Acquire** button to open the Acquisition Setup window (Figure 12).
2. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window. Enter all values in **ppm**.
3. Enter a value for the **pulse angle** and the **recovery delay**.
4. Enter a value for the number of **scans to acquire**.



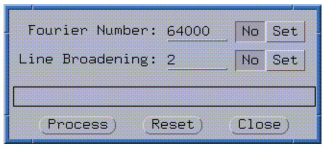
Start of Spectrum (ppm): -20
End of Spectrum (ppm): 200
Pulse Angle: 35
Recovery Delay: 1.0
Number of scans : 64
H1 dec mode: Decoupled+NOE

Select H1 Decoupling mode

**Figure 12.** *GLIDE* Phosphorus 1D Acquisition Options

5. If you make no change a 35-degree pulse angle is selected.
6. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
7. Click on **Close** to save the values you selected and continue on with customizing processing, and plotting options.

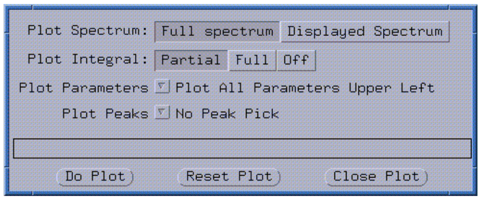
   Click on **Do** if you want to save the values you selected, skip the customizing processing, and plotting options, and immediately start acquisition.
8. Click the **Process** button to open the Process Setup window.
9. Enter a Fourier number in the **Fourier Number** field and click on **Set**, or click on **NO** to use default Fourier number.



Fourier Number: 64000
Line Broadening: 2

10. Enter a line broadening factor in the **Line Broadening** field and click on **Set**, or click on **NO** to turn off line broadening.
11. Click on **Close** to save the values you selected.

    Do not click on Process unless you clicked the Do button in step 7 and acquisition has finished.
12. Click the **Plot** button to open the Plot Setup window.
13. Select Displayed Spectrum or Full Spectrum in the **Spectral Width** field.
14. Select Partial, Full, or Off in the **Plot Integral** field.



Plot Spectrum: Full spectrum
Plot Integral: Partial
Plot Parameters Plot All Parameters Upper Left
Plot Peaks No Peak Pick

15. Select how to plot the parameters from the **Plot Parameters** menu.
16. Select a peak-picking option from the **Plot Peaks** menu.
17. Click on **Close Plot** to save the values you selected.

    Do not click on **Do Plot** unless acquisition and processing have been completed.

### Acquire

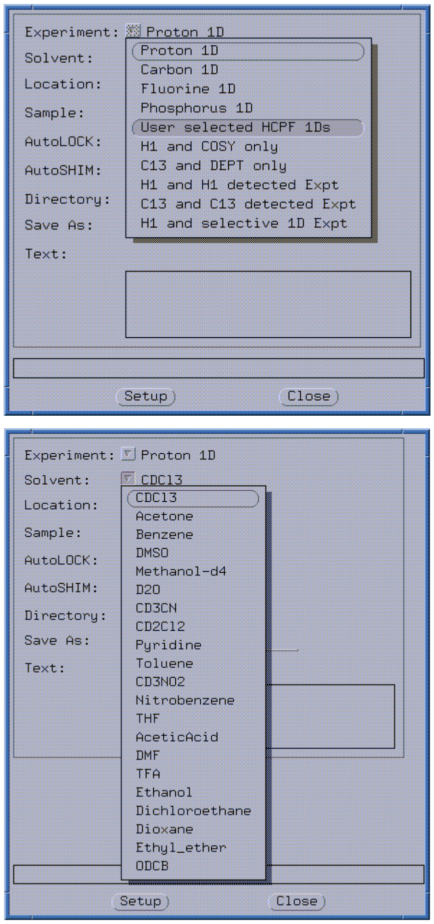
If you did not start the acquisition in step 7, click the Go button in the *GLIDE* user interface to start acquisition.

The phosphorus spectrum is acquired, processed, plotted, and saved according to the choices you made.

The FID is saved with the name `PHOSPHORUS.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FID is saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## 3.6 User-Selected HCPF 1D Spectra

This section describes how to setup, customize, and acquire a selected HCPF 1D spectra.



Experiment: Proton 1D

Solvent: CDCl3

**Figure 13.** *GLIDE* Setup for HCPF 1D

### *Setup*

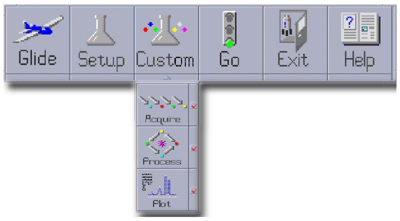
1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **User selected HCPF 1D**, as shown in Figure 13.
4. Right click the **Solvent** drop-down menu and select an appropriate lock solvent, as shown in Figure 13.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. **Enter** a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

   Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices.

   If you set Autoshim and Autolock to NO, manually lock and shim now.

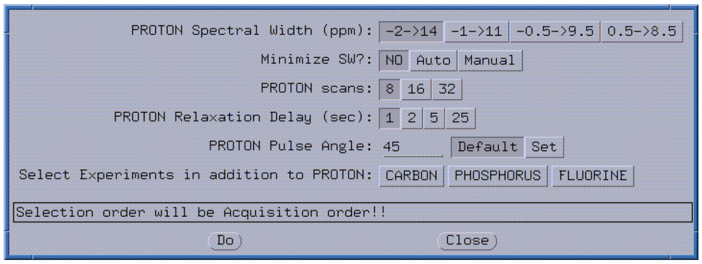
If you prefer to use default settings and not setup to observe a nucleus other than proton or customize the acquisition parameters, click on close and then the GO icon.

## Customize and Acquire



At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.

1. Click the **Acquire** button to open the Acquisition Options window.

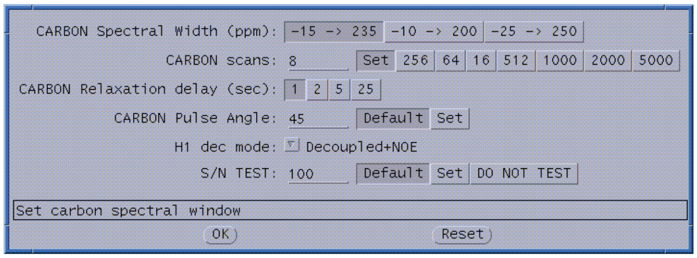


PROTON Spectral Width (ppm): -2->14 | -1->11 | -0.5->9.5 | 0.5->8.5
Minimize SW?: NO | Auto | Manual
PROTON scans: 8 | 16 | 32
PROTON Relaxation Delay (sec): 1 | 2 | 5 | 25
PROTON Pulse Angle: 45 Default | Set
Select Experiments in addition to PROTON: CARBON | PHOSPHORUS | FLUORINE
Selection order will be Acquisition order!!

2. Customize the **proton** acquisition:
    a. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
    b. Select the number of proton scans to acquire in the **PROTON scans** field.
    c. Select a relaxation delay in the **Relaxation Delay (sec)** field.
    d. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.
    e. To acquire only a proton spectrum, click on **Do** or click **Close** and then click on the **Go** button.

   The remaining three nuclei are presented in this order: carbon, phosphorus, and fluorine. You have the option to acquire the 1D spectrum for each nucleus or a combination of nuclei in any desired order. Acquisition always begins with a proton 1D followed by each selected nucleus.

3. Customize the **carbon** acquisition:
    a. Select **CARBON** to open the carbon acquisition options window.



CARBON Spectral Width (ppm): -15 -> 235 | -10 -> 200 | -25 -> 250
CARBON scans: 8 Set | 256 | 64 | 16 | 512 | 1000 | 2000 | 5000
CARBON Relaxation delay (sec): 1 | 2 | 5 | 25
CARBON Pulse Angle: 45 Default | Set
H1 dec mode: Decoupled+NOE
S/N TEST: 100 Default | Set | DO NOT TEST
Set carbon spectral window

    b. Select the spectral window in the **CARBON Spectral Width (ppm)** field.
    c. Select the number of carbon scans to acquire or enter a value in the **CARBON scans** field.
    d. Select a relaxation delay in the **Relaxation Delay (sec)** field.
    e. Enter a value for the pulse angle (observe pulse) in the **CARBON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.

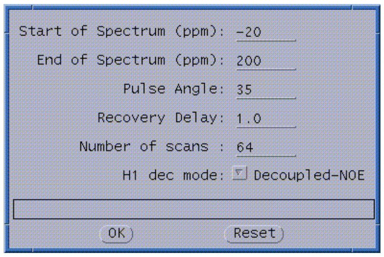
   f. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).

   g. Select CARBON S/N TEST option: **Default** (S/N=100), **Set** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. The signal to noise is measured on the tallest peak in the spectrum which is often the solvent peak. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.

   h. **Click OK** to save the values you selected and return to the HCPF acquisition options window or click on RESET to return the carbon acquisition options to their default values.

4. Add phosphorus or begin acquisition of proton and carbon:
   - To add phosphorus, go to the next step (step 5).
   - To save the values you selected and begin acquisition, click **Do**.
   - To save acquisition parameters but not begin data acquisition until the **Go** button is pressed, click **Close**.

5. Customize the **phosphorus** acquisition:



Start of Spectrum (ppm): -20
End of Spectrum (ppm): 200
Pulse Angle: 35
Recovery Delay: 1.0
Number of scans : 64
H1 dec mode: Decoupled-NOE

   a. Click the **PHOSPHORUS** button in the HCPF acquisition options window.

   b. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window. Enter all values in **ppm**.

   c. Enter a value for the pulse angle (observe pulse) in the **PHOSPHORUS Pulse Angle** field.

   d. Enter a relaxation delay in the **Recovery Delay (sec)** field.

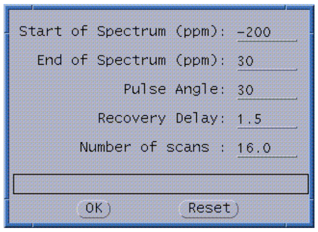
   e. Enter the number of scans to acquire in the **PHOSPHORUS scans** field.

   f. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).

   g. **Click OK** to save the values you selected and return to the HCPF acquisition options window or click on RESET to return the carbon acquisition options to their default values.

6. Add fluorine or begin acquisition of proton, carbon, and phosphorus:
   - To add phosphorus, go to the next step (step 7).
   - To save the values you selected and begin acquisition, click **Do**.
   - To save acquisition parameters but not begin data acquisition until the **Go** button is pressed, click **Close**.

7. Customize the **fluorine** acquisition:
   a. Click the **FLUORINE** button in the HCPF acquisition options window.
   b. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window. Enter all values in **ppm**.
   c. Enter a value for the **pulse angle** or make no entry and accept the default value shown.
   d. Enter a value for the **recovery delay** or make no entry and accept the default value shown.
   e. Enter the number of **scans to acquire** or make no entry and accept the default value shown.
   f. Click **OK** to save the values you selected and return to the HCPF acquisition options window or click on RESET to return the carbon acquisition options to their default values.



Start of Spectrum (ppm): -200
End of Spectrum (ppm): 30
Pulse Angle: 30
Recovery Delay: 1.5
Number of scans : 16.0

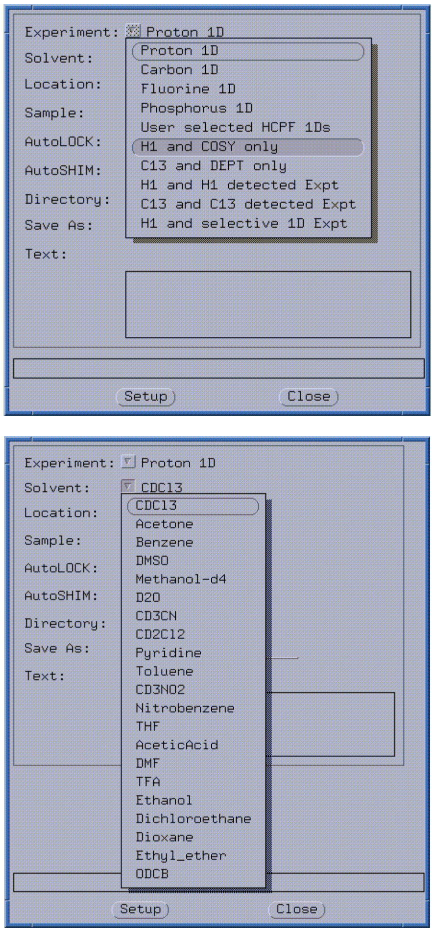
8. Begin the HCPF acquisition:
   - To save the values you selected and begin acquisition, click **Do**.
   - To save acquisition parameters but not begin data acquisition until the **Go** button is pressed, click **Close**.

A proton and each of the selected experiments spectra are acquired, processed, plotted, and saved according to the choices you made.

The FIDs are saved with the names `PROTON.fid, CARBON.fid,` PHOSPHORUS`.fid`, or `FLUORINE.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, theFIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## 3.7 H1 and COSY Experiments

Depending on the type of probe (PFG or non-PFG) and the system, this experiment automatically selects the gCOSY (PFG probe) or COSY (non-PFG probe) experiment.


Experiment: Proton 1D

Solvent: CDCl3

**Figure 14.** *GLIDE* Setup for H1 and COSY

### *Setup*

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **H1 and COSY only**, as shown in Figure 14.
4. Right click the **Solvent** drop-down menu and select an appropriate lock solvent, as shown in Figure 14.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.

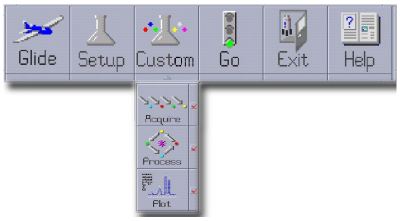
   *Note* that autoshimming and autolocking is done only once prior to the proton 1D acquisition and is turned off before the COSY acquisition.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

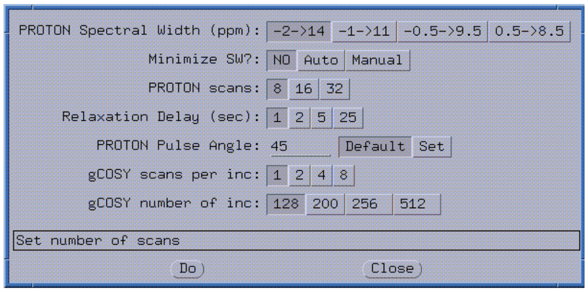
   Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices.

   If you set Autoshim and Autolock to NO, manually lock and shim now.

### *Customize*

At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.





1. Click the **Acquire** button to open the Acquisition Options window.
2. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
3. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 2, **Auto** examines the proton 1D and sets SW, and **Manual** permits the user to set sw after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button. The COSY experiment executes using this SW.
4. Select the number of proton scans to acquire in the **PROTON scans** field.
5. Select a relaxation delay in the **Relaxation Delay (sec)** field.
6. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.
7. Select the number of **scans per increment** to acquire for the COSY experiment.
8. Select the **number of increments** to acquire for the COSY experiment.
9. Click the **Do** button to save the values you selected and start acquisition.

## Acquire

Click the **Go** button in the *GLIDE* user interface to start acquisition.

A proton and COSY (or gCOSY) spectra are acquired, processed, plotted, and saved according to the choices you made.

The FIDs are saved with the names `PROTON.fid` and `COSY.fid` (or `gCOSY.fid`) in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## 3.8 C13 and DEPT Experiments

This section describes how to setup, customize, and acquire a selected C13 and DEPT spectra.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window (Figure 15A).
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **C13 and DEPT only**, as shown in Figure 15.
4. Right click the **Solvent** drop-down menu and select an appropriate lock solvent, as shown in Figure 15.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

   Standard carbon parameters are recalled. Relevant parameters and text are reset according to your choices.

   If you set Autoshim and Autolock to NO, manually lock and shim now.

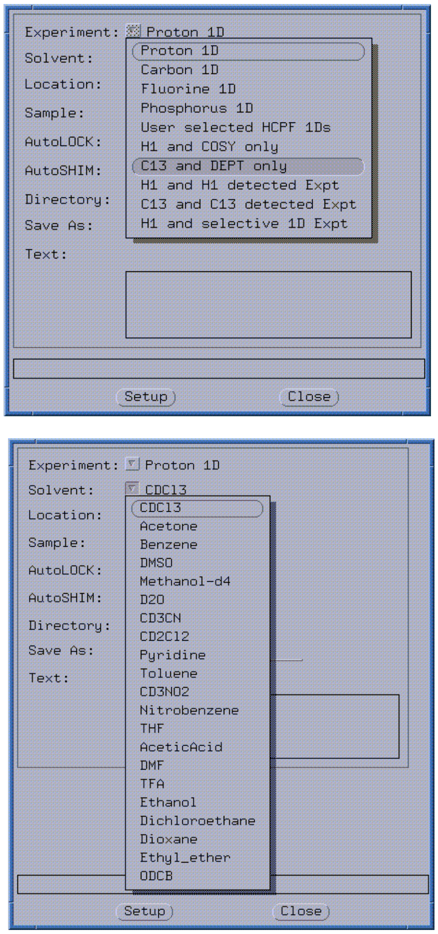
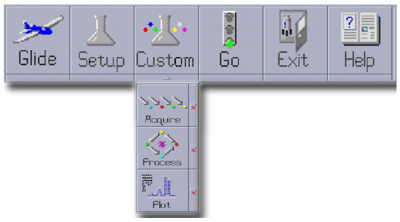


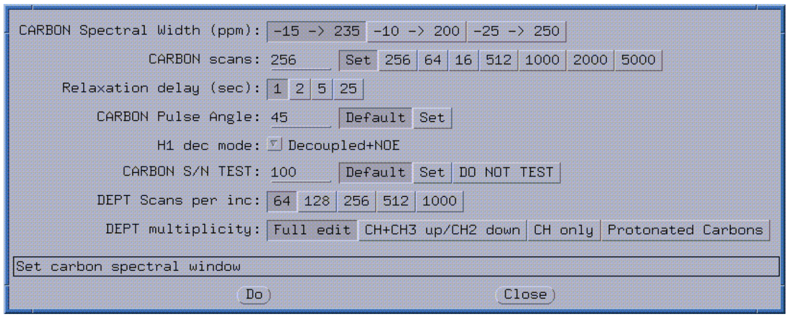
**Figure 15.** *GLIDE* Setup for C13 and DEPT

### Customize

At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.



1. Click the **Acquire** button to open the Acquisition Options window (Figure 16).
2. Select the spectral window in the **CARBON Spectral Width (ppm)** field and the number of scans to acquire or enter a value in the **CARBON scans** field.
3. Select a relaxation delay in the **Relaxation Delay (sec)** field and enter a value for the pulse angle (observe pulse) in the **CARBON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.

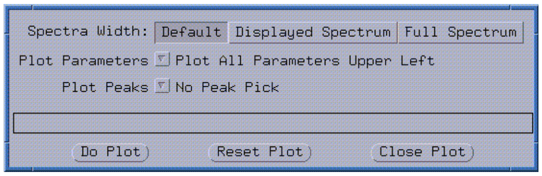


CARBON Spectral Width (ppm): -15 -> 235 | -10 -> 200 | -25 -> 250
CARBON scans: 256 Set | 256 | 64 | 16 | 512 | 1000 | 2000 | 5000
Relaxation delay (sec): 1 | 2 | 5 | 25
CARBON Pulse Angle: 45 Default | Set
H1 dec mode: Decoupled+NOE
CARBON S/N TEST: 100 Default | Set | DO NOT TEST
DEPT Scans per inc: 64 | 128 | 256 | 512 | 1000
DEPT multiplicity: Full edit | CH+CH3 up/CH2 down | CH only | Protonated Carbons
Set carbon spectral window
Do Close

**Figure 16.** *GLIDE* Customize 13C and DEPT Acquisition

4. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
5. Select CARBON S/N TEST option: **Default** (S/N=100), **Set** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. The signal to noise is measured on the tallest peak in the spectrum which is often the solvent peak. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.
6. Select the number of **DEPT Scans per inc:** to acquire for the DEPT experiment.
7. Select a **DEPT multiplicity**:
    a. **Full Edit** produces 4 edited sub-spectra showing: all protonated carbons, CH carbons only, $CH_2$ carbons only, and $CH_3$ carbons only.
    b. **CH and CH3 up/CH2 down** produces an unedited dept 135 experiment.
    c. **CH only** produces and unedited dept 90 experiment.
    d. **Protonated Carbons** produces an unedited spectra containing only protonated carbons.
8. Click the **Do** button to save the values you selected and start acquisition and use the default processing and plotting values (recommended) or click Close to customize the processing and plotting.

    Do not click on Process unless you clicked on the Do button in step 8 and acquisition has been completed.
9. Click the **Plot** button to open the Plot Setup window. The choices apply to the carbon 1D not the DEPT spectra. DEPT spectra are plotted based on the options selected in step 7.



Spectra Width: Default | Displayed Spectrum | Full Spectrum
Plot Parameters: Plot All Parameters Upper Left
Plot Peaks: No Peak Pick
Do Plot Reset Plot Close Plot

10. Select Default, Displayed Spectrum, or Full Spectrum in the **Spectral Width** field.
11. Select how to plot the parameters from the **Plot Parameters** menu.
12. Select a peak-picking option from the **Plot Peaks** menu.

13. Click on **Close Plot** to save the values you selected.

    Do not click on **Do Plot** unless acquisition and processing have been completed.

### Acquire

Click the Go button in the *GLIDE* user interface to start acquisition.

Carbon and DEPT spectra is acquired, processed, plotted, and saved according to the choices you made.

The FIDs are saved with the names `CARBON.fid` and `DEPT.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

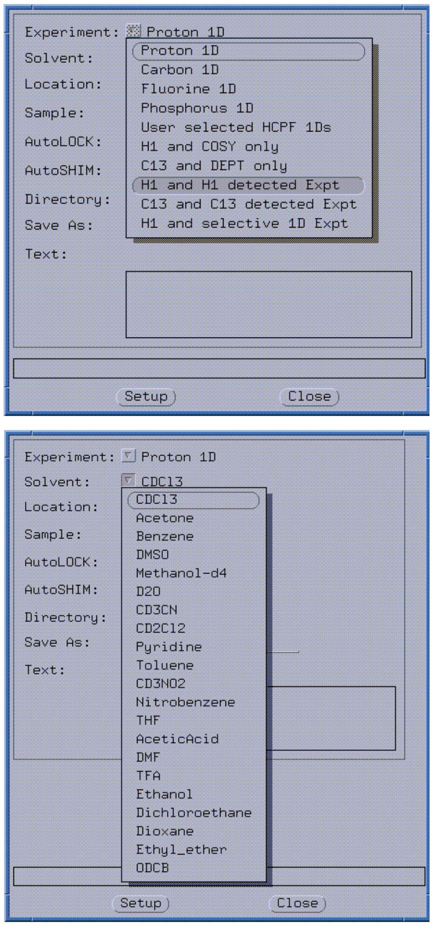
## 3.9 H1 and H1 Detected Experiments

An experiment chain of H1, gCOSY, HMQC, gHMBC, and gHSQCTOXY representing a portion of the available H1 and H1 detected experiments provided with *GLIDE* is described below.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **H1 and H1 detected Exp**, as shown in Figure 17.
4. Right click the **Solvent** drop-down menu and select an appropriate lock solvent, as shown in Figure 17.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.

   *Note* that autoshimming and autolocking is done only once prior to the proton 1D acquisition and then turned off.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.



Experiment: Proton 1D

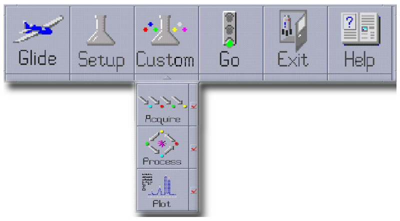
Solvent: CDC13

**Figure 17.** *GLIDE* Setup for H1 and H1 Detected Experiments

Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices.

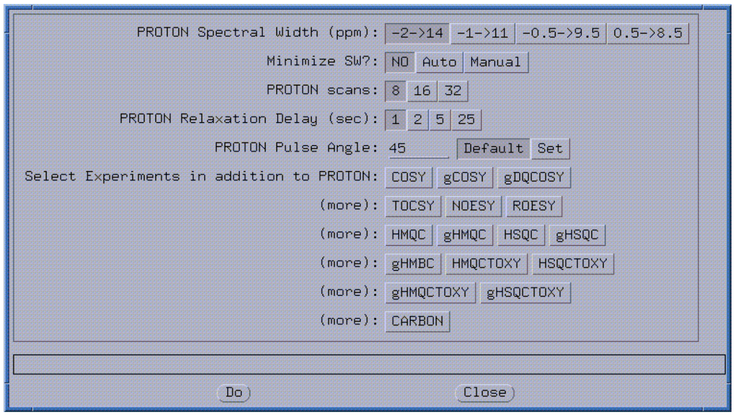
If you set Autoshim and Autolock to **NO**, manually lock and shim now.

## Customize



At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.

- Click the **Acquire** button to open the Acquisition Options window.



PROTON Spectral Width (ppm): -2->14 | -1->11 | -0.5->9.5 | 0.5->8.5

Minimize SW?: NO | Auto | Manual

PROTON scans: 8 | 16 | 32

PROTON Relaxation Delay (sec): 1 | 2 | 5 | 25

PROTON Pulse Angle: 45 | Default | Set

Select Experiments in addition to PROTON: COSY | gCOSY | gDQCOSY

(more): TOCSY | NOESY | ROESY

(more): HMQC | gHMQC | HSQC | gHSQC

(more): gHMBC | HMQCTOXY | HSQCTOXY

(more): gHMQCTOXY | gHSQCTOXY

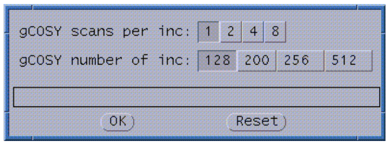
(more): CARBON

## Proton Acquisition

1. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
2. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 1, **Auto** examines the proton 1D and sets SW, and **Manual** permits the user to set sw after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button. The 2D experiment is executed using this SW.
3. Select the number of proton scans to acquire in the **PROTON scans** field.
4. Select a relaxation delay in the **Relaxation Delay (sec)** field.
5. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.

## Acquiring Selected 1H Detected Experiments

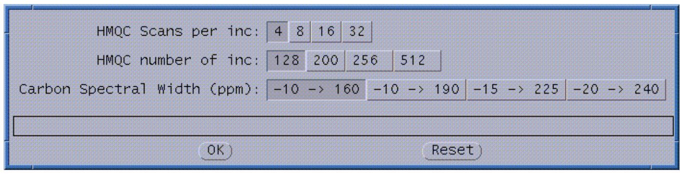
All chained experiments begin with a 1D S2PUL experiment. In this case a proton 1D will be the first experiment. Selected experiments are run, following the 1D experiment, in the order in which they are selected. Each experiment has an associated popup window for customizing the acquisition parameters associated with the experiment. In this example the order of the experiments, following the proton 1D is: gCOSY, HMQC, gHMBC, and gHSQCTOXY.



1. Add **gCOSY** Acquisition to the experiment chain:
   a. Select **gCOSY** and open the gCOSY Acquisition popup window.
   b. Select a value for **gCOSY scans per inc** to acquire from the choices in the popup window.
   c. Select a value for **gCOSY number of inc** to acquire from the choices in the popup window.
   d. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

   gCOSY is added to the experiment chain.

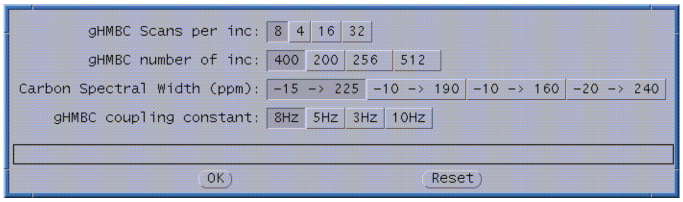
2. Add **HMQC** acquisition to the experiment chain:
   a. Select **HMQC** and open the HMQC Acquisition popup window.



   b. Select a value for **HSQC scans per inc** to acquire from the choices in the popup window.
   c. Select a value for **HSQC number of inc** to acquire from the choices in the popup window.
   d. Select a **Carbon Spectra Width (ppm)** from the choices presented.
   e. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

   HMQC is added to the experiment chain.

3. Add **gHMBC** acquisition to the experiment chain:
   a. Select **gHMBC** and open the gHMQC Acquisition popup window.



   b. Select a value for **gHMBC scans per inc** to acquire from the choices in the popup window.
   c. Select a value for **gHMBC number of inc** to acquire from the choices in the popup window.
   d. Select a **Carbon Spectra Width (ppm)** from the choices presented.

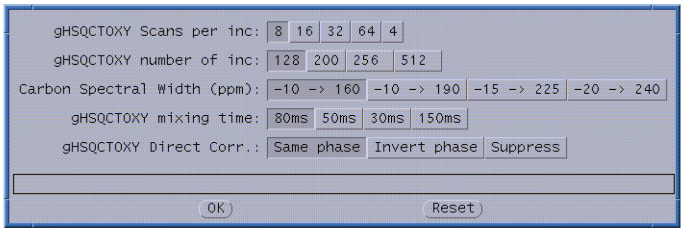
e. Select a **gHMBC coupling constant** from the choices presented.

f. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

gHMBC is added to the experiment chain.

4. Add **gHSQCTOXY** acquisition to the experiment chain:

   a. Select **gHSQCTOXY** and open the gHHSQCTOXY Acquisition popup window.



   b. Select a value for **gHSQCTOXY scans per inc** to acquire from the choices in the popup window.

   c. Select a value for **gHSQCTOXY number of inc** to acquire from the choices in the popup window.

   d. Select a **Carbon Spectra Width (ppm)** from the choices presented or make no choice and accept the default.

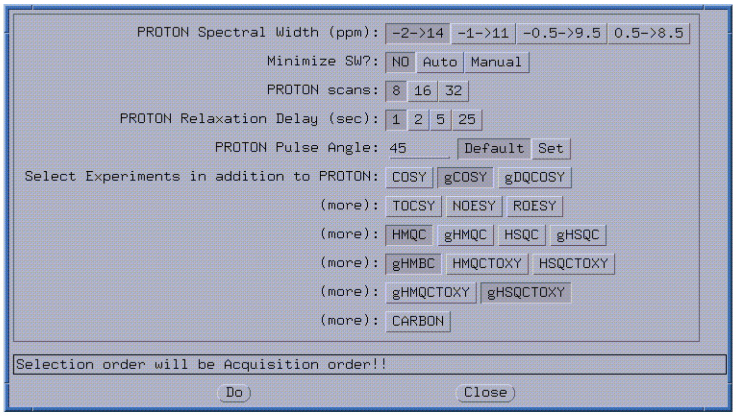
   e. Select a **gHSQCTOXY mixing time** from the choices presented or make no choice and accept the default.

   f. Select a **gHSQCTOXY Direct Corr.** from the choices presented or make no choice and accept the default.

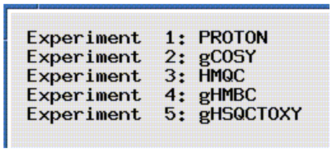
   g. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

gHSQCTOXY is added to the experiment chain.

The Select H1 and H1 Detected Experiments window shows the selected experiments and proton 1D acquisition parameters.



### Verifying the Experiment List



```
Experiment  1: PROTON
Experiment  2: gCOSY
Experiment  3: HMQC
Experiment  4: gHMBC
Experiment  5: gHSQCTOXY
```

The order that you selected experiments in the Acquisition Setup window is the acquisition order which is displayed in the Text panel of the dg screen. To remove a selection from the experiment chain, deselect it by clicking on the button again. For example, clicking the gHSQCTOXY button a second time deselects it and removes any saved parameter customization for gHSQCTOXY.

### Acquire

Click the Do button in the Acquisition Setup window to select you custom options and start acquisition.Spectra is acquired (according to the choices you made and the order of experiment selection), processed, plotted (proton and absolute-value 2Ds only), and saved.

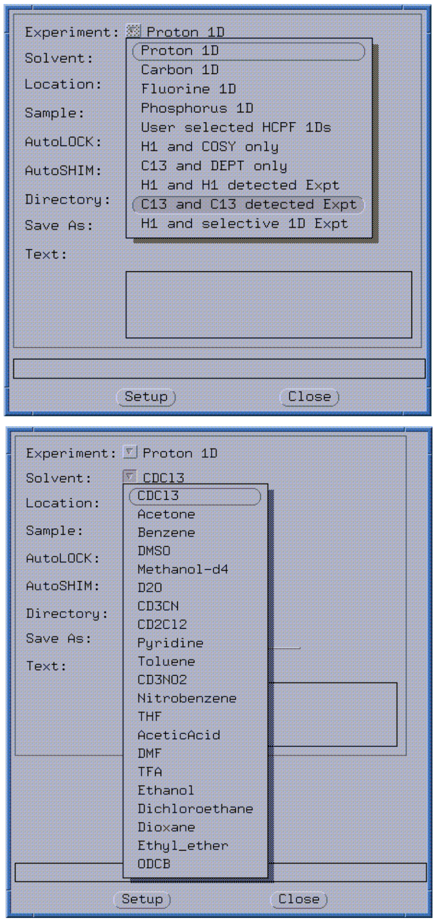
The FIDs are saved with the names `PROTON.fid`, `gCOSY.fid`, `HMQC.fid`, `gHMBC.fid`, and `gHSQCTOXY.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## 3.10 C13 and C13 Detected Experiments

An experiment chain of proton, carbon, APT, DEPT, and gHETCOR representing a portion of the available C13 and C13 detected experiments provided with *GLIDE* is described below.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **C13 and C13 detected Expt**, as shown in Figure 18.
4. Right click the **Solvent** drop-down menu and select an appropriate lock solvent, as shown in Figure 18.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.



Experiment: Proton 1D

Solvent: CDCl3

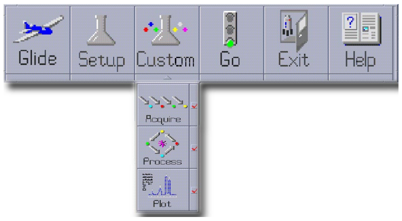
**Figure 18.** *GLIDE* Setup for C13 and C13 Detected Experiments

8. Click on **Setup**.

   Standard carbon parameters are recalled. Relevant parameters and text are reset according to your choices.

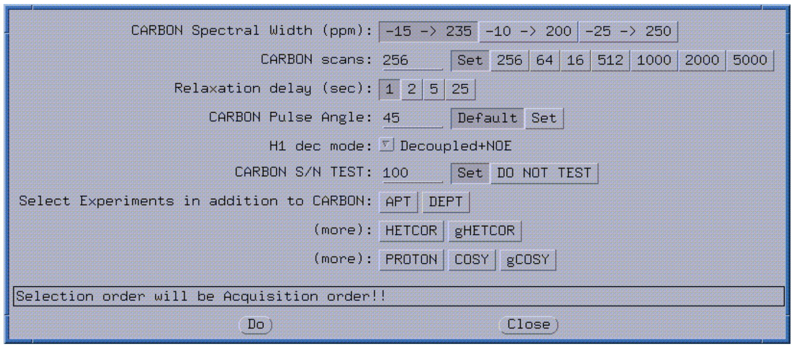
   If you set Autoshim and Autolock to NO, manually lock and shim now.

### Customize



At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.

- Click the **Acquire** button to open the Acquisition Options window.



```
               CARBON Spectral Width (ppm): -15 -> 235 | -10 -> 200 | -25 -> 250
                       CARBON scans: 256      Set | 256 | 64 | 16 | 512 | 1000 | 2000 | 5000
                 Relaxation delay (sec): 1 | 2 | 5 | 25
                  CARBON Pulse Angle: 45      Default | Set
                         H1 dec mode: Decoupled+NOE
                     CARBON S/N TEST: 100     Set | DO NOT TEST
Select Experiments in addition to CARBON: APT | DEPT
                              (more): HETCOR | gHETCOR
                              (more): PROTON | COSY | gCOSY
Selection order will be Acquisition order!!
                 Do                                  Close
```

### Carbon Acquisition

1. Select the spectral window in the **CARBON Spectral Width (ppm)** field and the number of scans to acquire or enter a value in the **CARBON scans** field.

2. Select a relaxation delay in the **Relaxation Delay (sec)** field and enter a value for the pulse angle (observe pulse) in the **CARBON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.

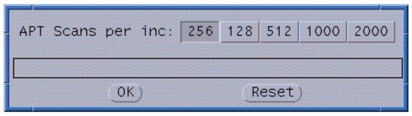
3. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).

4. Select CARBON S/N TEST option: **Default** (S/N=100), **Set** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. The signal to noise is measured on the tallest peak in the spectrum which is often the solvent peak. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.

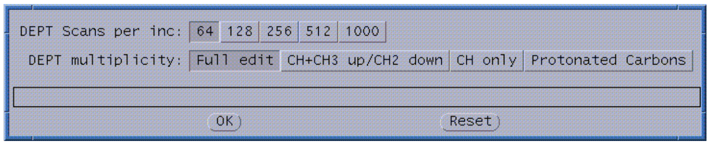
### Acquiring Selected $^{13}$C-Detected Experiments

All chained experiments begin with a 1D S2PUL experiment. If the proton 1D experiment option is selected, it will be the first experiment run regardless of when it is selected. The proton 1D experiment is followed by a carbon S2PUL. Selected experiments are run, following the carbon S2PUL experiment, in the order in which they are selected. Each experiment has an associated popup window for customizing the acquisition parameters associated with the experiment. In this example the order of the experiments, following the carbon 1D is: APT, DEPT, and gHETCOR.

1. Add **APT** acquisition to the experiment chain:
    a. Select **APT** from the Select C13 and C13 Detected Experiments window and the APT Acquisition popup window opens.



    b. Select the number of **APT Scans per inc:** to acquire for the APT experiment.
    c. Click OK to use the values chosen and return to the Select C13 and C13 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select C13 and C13 Detected Experiments window.
2. Add **DEPT** acquisition to the experiment chain:
    a. Select **DEPT** from the Select C13 and C13 Detected Experiments window and the DEPT Acquisition popup window opens.



    b. Select the number of **DEPT Scans per inc:** to acquire for the DEPT experiment.
    c. Select a **DEPT multiplicity**.

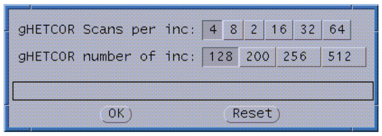
    **Full Edit** produces 4 edited sub-spectra showing: all protonated carbons, CH carbons only, $CH_2$ carbons only, and $CH_3$ carbons only.

    **CH and CH3 up/CH2 down** produces an unedited dept 135 experiment.

    **CH only** produces and unedited dept 90 experiment.

    **Protonated Carbons** produces an unedited spectra containing only protonated carbons.

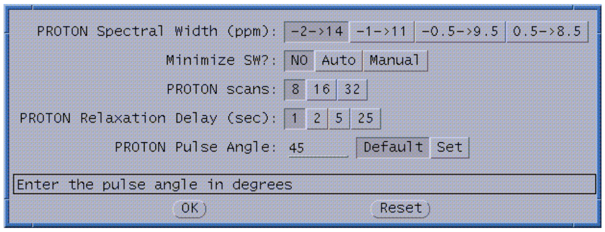
    d. Click OK to use the values chosen and return to the C13 and C13 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select C13 and C13 Detected Experiments window.
3. Add **gHETCOR** acquisition to the experiment chain:
    a. Select **gHETCOR** from the Select C13 and C13 Detected Experiments window and the gHETCOR Acquisition popup window opens.



    b. Select a value for **gHETCOR scans per inc** to acquire from the choices in the popup window.
    c. Select a value for **gHETCOR number of inc** to acquire from the choices in the popup window.

d. Click OK to use the values chosen and return to the C13 and C13 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select C13 and C13 Detected Experiments window.

## Proton Acquisition



PROTON Pulse Angle: 45

Enter the pulse angle in degrees

1. Select **PROTON** from the Select C13 and C13 Detected Experiments window and the PROTON Acquisition popup window opens.

   This will be the first experiment run even though it is your last experiment selection.

2. Select the spectral window in the **PROTON Spectral Width (ppm)** field.

3. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 2, **Auto** examines the proton 1D and sets SW, and **Manual** prompts the user for input after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button. The HETCOR experiment executes using this SW.

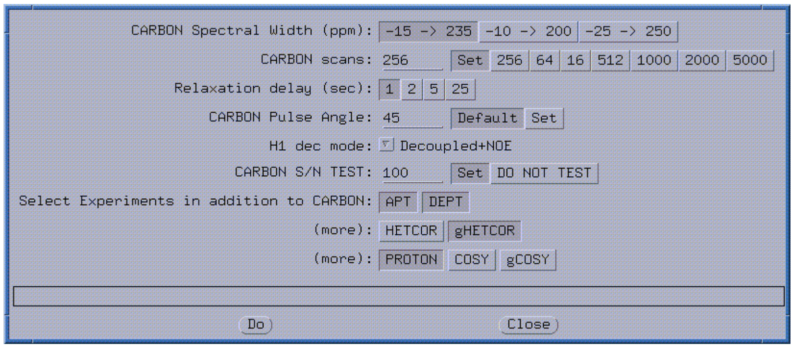
4. Select the number of proton scans to acquire in the **PROTON scans** field.

5. Select a relaxation delay in the **Relaxation Delay (sec)** field.

6. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set.** If you make no change or click on **Default,** a 45-degree pulse angle is selected.

7. Click **OK** to use the values chosen and return to the Select C13 and C13 Detected Experiments window. Click **RESET** to return to the default values and either use the default values or enter different parameters. Click **OK** to close the popup window and return to the Select C13 and C13 Detected Experiments window.

The Select C1 and C13 Detected Experiments window shows the selected experiments and proton 1D acquisition parameters..



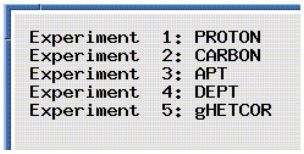
CARBON scans: 256

CARBON Pulse Angle: 45

H1 dec mode: Decoupled+NOE

CARBON S/N TEST: 100

### Verifying the Experiment List



```
Experiment  1: PROTON
Experiment  2: CARBON
Experiment  3: APT
Experiment  4: DEPT
Experiment  5: gHETCOR
```

PROTON (if it is selected) always runs first followed by CARBON and the other experiments in the order that you selected experiments in the Acquisition Setup window is the acquisition order which is displayed in the Text panel of the dg scree.. To remove a selection from the experiment chain, deselect it by clicking on the button again. For example, clicking the DEPT button a second time deselects it and removes any saved parameter customization for DEPT.

### Acquire

Click the **Do** button to start acquisition or click the **Close** button and begin the acquisition with the **Go** button on the *GLIDE* user interface.Spectra is acquired (according to your choices and the order of experiment selection), processed, plotted (1Ds and absolute-value 2Ds only), and saved.

The FIDs are saved with the names PROTON.fid, `CARBON.fid`, `APT.fid`, DEPT.fid and `gHETCOR.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## 3.11 H1 and Selective 1D Experiments

An experiment chain of H1, TOCSY1D, and NOESY1D representing a portion of the available H1 and Selective H1 experiments provided with *GLIDE* is described below.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment Setup window.
2. Eject the sample from the magnet and insert your sample.
3. Right click the **Experiment** drop-down menu and select **H1 and Selective 1D Expt**, as shown in Figure 17.
4. Right click the **Solvent** drop-down menu and select an appropriate lock solvent, as shown in Figure 17.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.

   *Note* that autoshimming and autolocking is done only once prior to the proton 1D acquisition and then turned off.

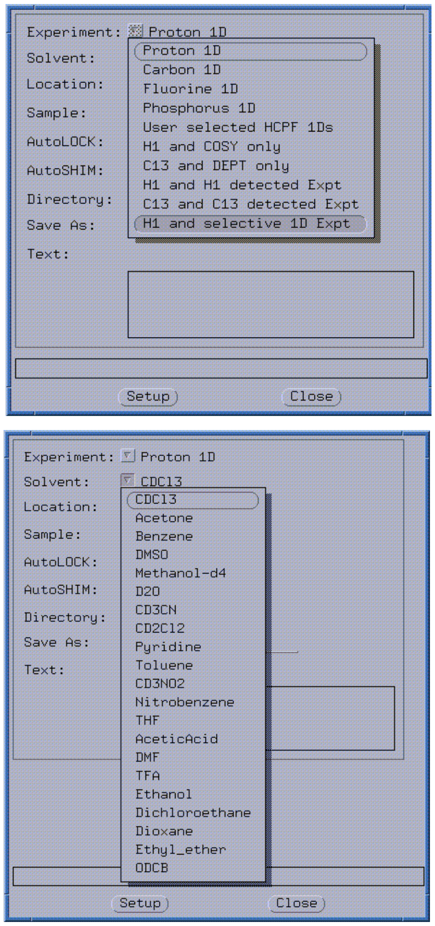


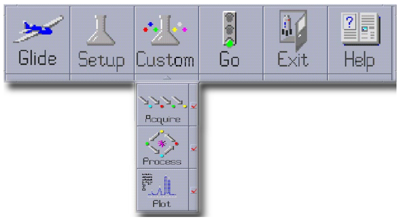
**Figure 19.** *GLIDE* Setup for H1 and Selective 1D Experiments

6. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used.
7. Enter appropriate text in the **Text** box for your sample.
8. Click on **Setup**.

   Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices.

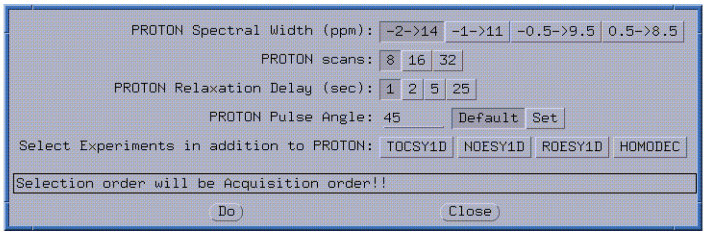
   If you set Autoshim and Autolock to NO, manually lock and shim now.

### Customize



At the end of the setup operation, the Custom button in the *GLIDE* user interface is no longer shaded and the Acquire, Process, and Plot buttons are displayed.

- Click the **Acquire** button to open the Acquisition Options window.



PROTON Spectral Width (ppm): -2->14 -1->11 -0.5->9.5 0.5->8.5

PROTON scans: 8 16 32

PROTON Relaxation Delay (sec): 1 2 5 25

PROTON Pulse Angle: 45 Default Set

Select Experiments in addition to PROTON: TOCSY1D NOESY1D ROESY1D HOMODEC

Selection order will be Acquisition order!!

Do Close

### Proton Acquisition

1. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
2. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 1, **Auto** examines the proton 1D and sets SW, and **Manual** permits the user to set sw after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button. The selective 1D experiment executes using this SW.
3. Select the number of proton scans to acquire in the **PROTON scans** field.
4. Select a relaxation delay in the **Relaxation Delay (sec)** field.
5. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.

### Acquiring Selected 1H Detected Experiments

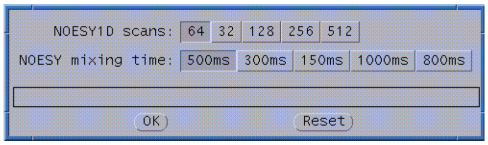
All chained experiments begin with a 1D spectrum, in this case a proton 1D. Selected experiments are run, following the 1D experiment, in the order in which they are selected. Each experiment has an associated popup window for customizing the acquisition parameters associated with the experiment. In this example the order of the experiments, is PROTON 1D, TOCSY1D, and NOSY1D.

1. Adding **TOCSY1D** acquisition to the experiment chain:

a. Select **TOCSY1D** and open the TOCSY1D Acquisition popup window.
b. Select a value for **TOCSY1D scans per inc** to acquire from the choices in the popup window.
c. Select a value for **TOCSY1D mixing time** from the choices in the popup window. If you select **Array** a series of experiments will be run with mixing time arrayed from 10 ms to 100 ms.
d. Click OK to use the values chosen and return to the Select H1 and Selective 1D Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Selective Experiments window.

TOCSY1D is added to the experiment chain.

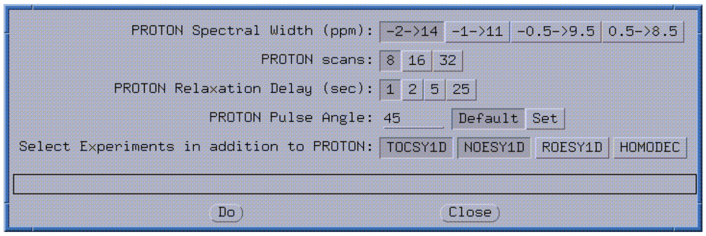
2. Add **NOESY1D** acquisition to the experiment chain:



a. Select **NOESY1D** and open the NOESY1D Acquisition popup window.
b. Select a value for **NOESY1D scans per inc** to acquire from the choices in the popup window.
c. Select a value for **NOESY1D mixing time** from the choices in the popup window.
d. Click OK to use the values chosen and return to the Select H1 and Selective 1D Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Selective Experiments window.

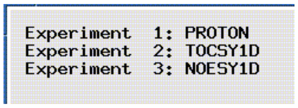
NOESY1D is added to the experiment chain.

The Select H1 and Selective 1D Experiments window shows the selected experiments and proton 1D acquisition parameters..



PROTON Pulse Angle: 45

## Verifying the Experiment List



```
Experiment  1: PROTON
Experiment  2: TOCSY1D
Experiment  3: NOESY1D
```

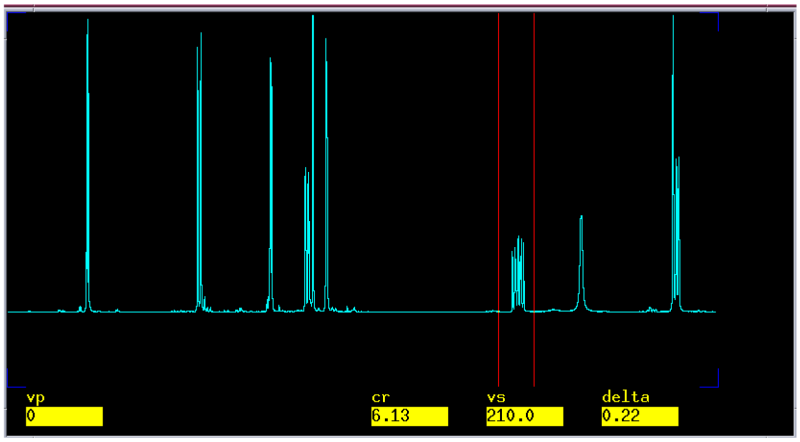
The order that you selected experiments in the Acquisition Setup window is the acquisition order which is displayed in the Text panel of the dg screen.

To remove a selection from the experiment chain, deselect it by clicking on the button again. For example, clicking the TOCSY1D button a second time deselects it and removes any saved parameter customization for TOCSY1D.

## Acquire

1. Click the **Do** button in the Select H1 and Selective 1D Experiments window to start acquisition. A proton spectrum is acquired, processed, plotted and saved.

   TOCSY1D experiment parameters are set up and the proton spectrum displays, similar to Figure 20. Five buttons appear on the second row of the VNMR menu bar, **Cursor, Expand, Select**, **Proceed, Cancel, restart, and Return**.



vp 0

cr 6.13

vs 210.0

delta 0.22

**Figure 20.** *GLIDE* Selection of Peaks for TOCSY1D and NOESY1D

2. Select the peak you want using the left and right mouse buttons by placing two cursors on either side of the peak. Expand the proton spectrum as needed.
3. Click the **Select** button on the menu bar.

   Select additional peaks repeating step 2 and step 3 for a series of TOCSY1D spectra.
4. Click the **Proceed** button to start a series of TOCSY1D acquisitions.

   TOCSY1D spectra are acquired and individually saved. NOESY1D experiment parameters are set up and the proton spectrum is redisplayed to enable peak selection for NOESY1D.
5. Repeat step 2 and step 3 to select peaks and start NOESY1D acquisition.
6. Click the **Proceed** button to start a series of NOESY1D spectra.

   NOESY1D spectra are acquired and individually saved.

All FIDs are saved with the file names `PROTON.fid`, `TOCSY1D_ppm1.fid`, `TOCSY1D_ppm2.fid`, etc., `NOESY1D_ppm3.fid`, `NOESY1D_ppm4.fid`, etc., where `ppm1` to `ppm4` are center of the selected band. The HOMODEC experiment is run as an array of decoupling frequencies and saved as `HOMODEC.fid`.

The FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

# Chapter 4. *GLIDE* Calibration

Sections in this chapter:

## 4.1 Introduction to System Calibration Using *Glide*

Proper calibration of the instrument is essential for experimental success. The *GLIDE* user interface provides the system administrator with a simple method to automatically calibrate the system. Autocalibration options are added to the system administrator list of standard experiments accessible through the *GLIDE* interface. The system administrator can automatically calibrate the system to make sure that its performance is optimum. *GLIDE* Autocalibration options are *not* accessible to other users.

When the autocalibration is run by the user VNMR1, all results are automatically written to the probe file in:
`/vnmr/probes/probe_name or $vnmrsys/probes/`*`probe_name`*

The autocalibration macros first determine power and the 90° pulse width, then write the power and pulse width values into the probe's file.

The autocalibration macros call four parameter sets:

- `stdpar/H1.par` (either the system `/vnmr/stdpar/H1.par` or the user's `vnmrsys/stdpar/H1.par`).
- `/vnmr/tests/gamah2`.
- `/vnmr/tests/P31sn.par`.
- `/vnmr/tests/F19sn.par`.

If the user is not `vnmr1` but is part of the `admin` group, the probe calibration file is locally created in ~`/vnmrsys/probes`. If the user is `vnmr1`, the probe's calibration file is created in `/vnmr/probes`.

Total time for system calibration is about 45 minutes.

## Autocalibration Samples

The samples listed in Table 1 can be used for autocalibration. Not all samples are provided with each system. The required samples for the acceptance test procedure during system installation will include one or more of these six samples.

**Table 1.** AutoCalibration Samples

| *Sample* | *Calibrate Option* | *Part Number* |
|---|---|---|
| 0.1% ethylbenzene in $CDCl_3$ $^{1}$H sensitivity | Proton | 00-968120-70 |
| 40% dioxane in $C_6D_6$ $^{13}$C sensitivity | Carbon | 00-968120-69 |
| 0.485 M triphenylphosphate in $CDC1_3$ $^{31}$P sensitivity | Phosphorus | 00-968120-87 |
| 0.05% trifluorotoluene in benzene–$d_6$ $^{19}$F sensitivity | Fluorine | 00-968120-82 |
| 1% $^{13}$C-enriched methyl iodide, 1% trimethyl phosphite, and 0.2% Cr(AcAc) in Chloroform-d | Proton, Carbon, ID, and Gradients (organic solvents) | 00-968120-96 |
| 0.1% $^{13}$C-enriched methanol with 0.30 mg/ml $GdCl_3$ in 1% $H_2O$/99% $D_2O$<br>(AutoTest Sample) | Proton, Carbon, ID, and Gradients (aqueous solvents) | 00-968120-68 |
| 2 Hz $D_2O$ | LOCK, gmap and Z0 | 01-901855-01 |

## Autocalibration Macros

The following macros improve system automated calibration:

- `AC1S–AC11S` are called by the interactive autocalibration window and determine the $^{1}$H 90° pulse width, $^{13}$C 90° pulse width, decoupler $\gamma H_2$, and 90° pulse width of the decoupler at high power, $^{19}$F 90° pulse width, and $^{31}$P 90° pulse width.
- `AC1S–AC11S` perform automatic calibration on UNITY*INOVA*, *MERCURY*-Series, and *GEMINI 2000* systems. When the macros finish the calibration routines, the current probe file is updated. If the probe is new to the system (i.e., all values in the probe file are zero), then the macros determine system power followed by calibration. If power levels are listed in the current probe file, these values are used, instead of taking time to determine power. The macro `AC1S` determines $^{1}$H pw90, `AC5S` begins $^{13}$C calibration, including decoupler power calibrations. `AC10S` performs $^{19}$F calibration, and `AC11S` performs $^{31}$P calibration.
- `ACreport` is called by the autocalibration macros `AC1S-AC11S` to print a copy of the probe file after calibration is completed.
- `ACbackup` is called by the autocalibration macros `AC1S-AC11S` to back up the probe file before beginning a new autocalibration run. This macro is not usually called by the user.

## Setting up Probe Calibration Files

Before you calibrate a probe for the first time, enter the following command:

- To make a probe file available to all system users enter **`addprobe(`*`probename`*`,'system')`**.
- To create a new probe entry in the current user directory, enter **`addprobe(`*`probename`*`)`**, where *probename* is a name of your choice (e.g., `addprobe('idpfg')`).

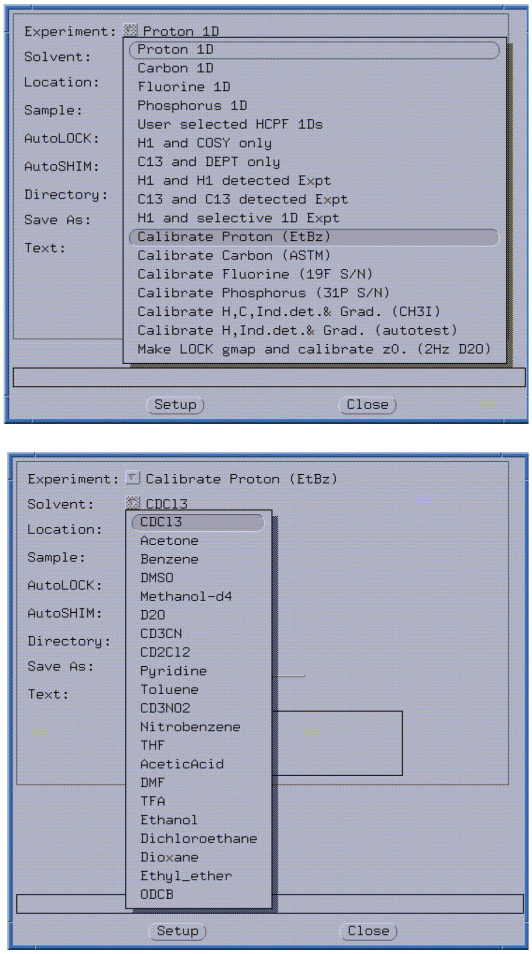
## 4.2 Calibrate Proton

This section describes how to calibrate proton.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment and Calibration Setup.
2. Eject the sample from the magnet and insert the 0.1% ethylbenzene in $CDCl_3$ $^1H$ sensitivity sample. Tune the probe if needed.
3. Right click the **Experiment** drop-down menu and select **Calibrate Proton (EtBz)**, as shown in Figure 21.
4. Right click the **Solvent** drop-down menu and select **CDCl3** as shown in Figure 21.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Click on **Setup**.

   Standard proton parameters are recalled and the sample confirmation window appears.



Experiment: Proton 1D

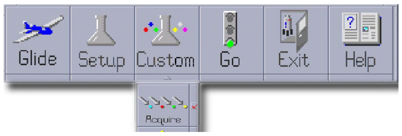
Experiment: Calibrate Proton (EtBz)

Solvent: CDCl3

**Figure 21.** *GLIDE* Calibrate Proton

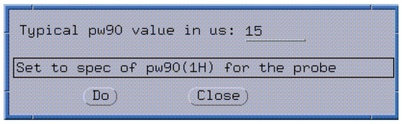
7. Click the **Confirm** button if the correct sample is inserted in the magnet. Click **Cancel** if the wrong sample is inserted and to end the calibration routine and begin again. If you set Autoshim and Autolock to **NO**, manually lock and shim now.

### Customize and Acquire



The Custom button is no longer shaded and the Acquire button appears after the Confirm button is selected at the end of the setup operation.

1. Click the **Acquire** button to open the Acquisition Setup window



Typical pw90 value in us: 15

2. Enter the max **pw90** value that your probe and spectrometer typically achieve. The value is usually the H1 pulse specification for your probe.
3. Click the **Do** button to start the calibration routine.

   At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

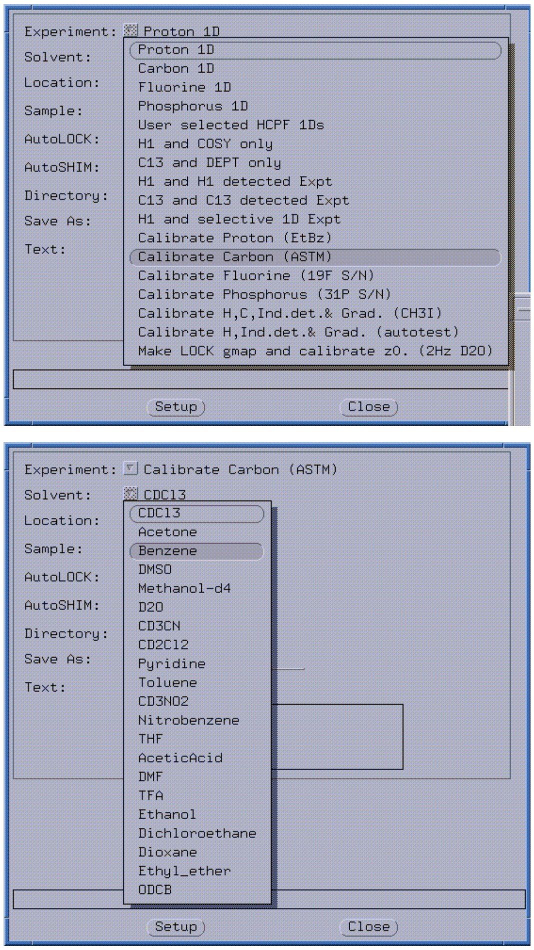
## 4.3 Calibrate Carbon

This section describes how to calibrate carbon.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment and Calibration Setup window.
2. Eject the sample from the magnet and insert the 40% dioxane in $C_6D_6$ $^{13}$C sensitivity sample. Tune the probe if needed.
3. Right click the **Experiment** drop-down menu and select **Calibrate Carbon (ASTM)**, as shown in Figure 22.
4. Right click the **Solvent** drop-down menu and select **Benzene** as shown in Figure 22.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Click on **Setup**.

   Standard carbon parameters are recalled and the sample confirmation window appears.


Experiment: Proton 1D

Experiment: Calibrate Carbon (ASTM)

Solvent: CDCl3

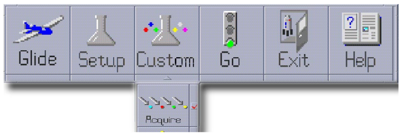
**Figure 22.** *GLIDE* Calibrate Carbon

7. Click the **Confirm** button if the correct sample is inserted in the magnet. Click **Cancel** if the wrong sample is inserted and to end the calibration routine and begin again.

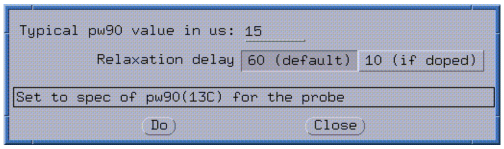
   If you set Autoshim and Autolock to **NO** in step 6, this would be the time to perform a manual lock and shim.

### Customize and Acquire

The Custom button is no longer shaded and the Acquire button appears after the Confirm button is selected at the end of the setup operation.



1. Click the **Acquire** button to open the Acquisition Setup window.
2. Enter the max **pw90** value that your probe and spectrometer typically achieve. The value is usually the $^{13}$C pulse specification for your probe.


Typical pw90 value in us: 15

Set to spec of pw90(13C) for the probe

3. Select a **Relaxation delay**. Choose **60 (default)** for the undoped signal to noise sample (P/N 00-968120-69) or choose **10 (if doped)** for a doped sample (not supplied).
4. Click the **Do** button to start the calibration routine.

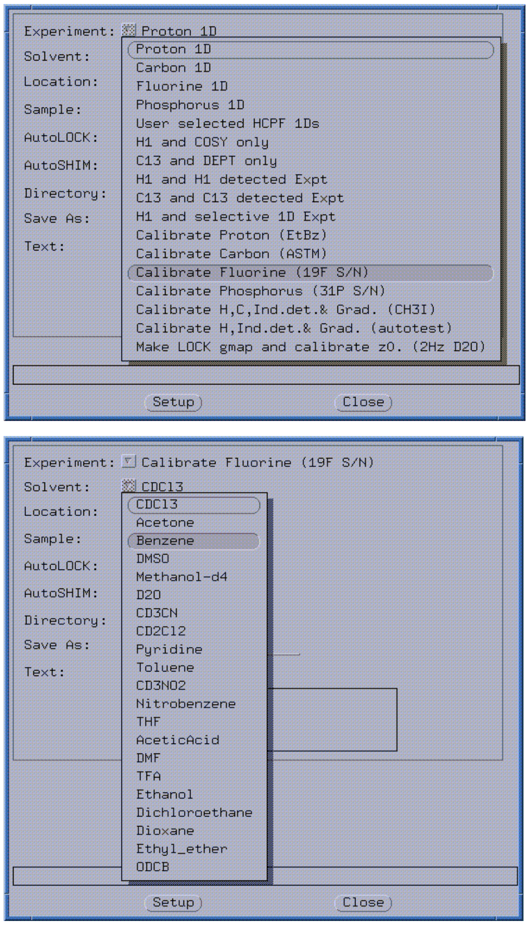
   At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

## 4.4 Calibrate Fluorine

This section describes how to calibrate fluorine.

### *Setup*

1. Click on the *GLIDE* **Setup** button to display the Experiment and Calibration Setup window.
2. Eject the sample from the magnet and insert the 0.05% trifluorotoluene in benzene-d$_6$ $^{19}$F sensitivity sample. Tune the probe if needed.
3. Right click the **Experiment** drop-down menu and select **Calibrate Fluorine (F19 S/N)**, as shown in Figure 23.
4. Right click the **Solvent** drop-down menu and select **Benzene**, as shown in Figure 23.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.


Experiment: Proton 1D

Experiment: Calibrate Fluorine (19F S/N)

Solvent: CDCl3

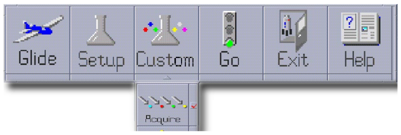
**Figure 23.** *GLIDE* Calibrate Fluorine

6. Click on **Setup**.

   Standard fluorine parameters are recalled and the sample confirmation window appears.
7. Click the **Confirm** button if the correct sample is inserted in the magnet. Click **Cancel** if the wrong sample is inserted and to end the calibration routine and begin again.

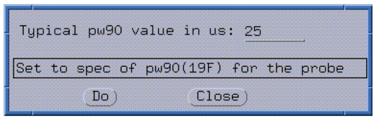
   If you set Autoshim and Autolock to **NO**, manually lock and shim now.

### Customize and Acquire



The Custom button is no longer shaded and the Acquire button appears after the Confirm button is selected at the end of the setup operation.

1. Click the **Acquire** button to open the Acquisition Setup window.
2. Enter the max **pw90** value that your probe and spectrometer typically achieve. The value is usually the $^{19}$F pulse specification for your probe.



Typical pw90 value in us: 25

Set to spec of pw90(19F) for the probe

3. Click the **Do** button to start the calibration routine.

   At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

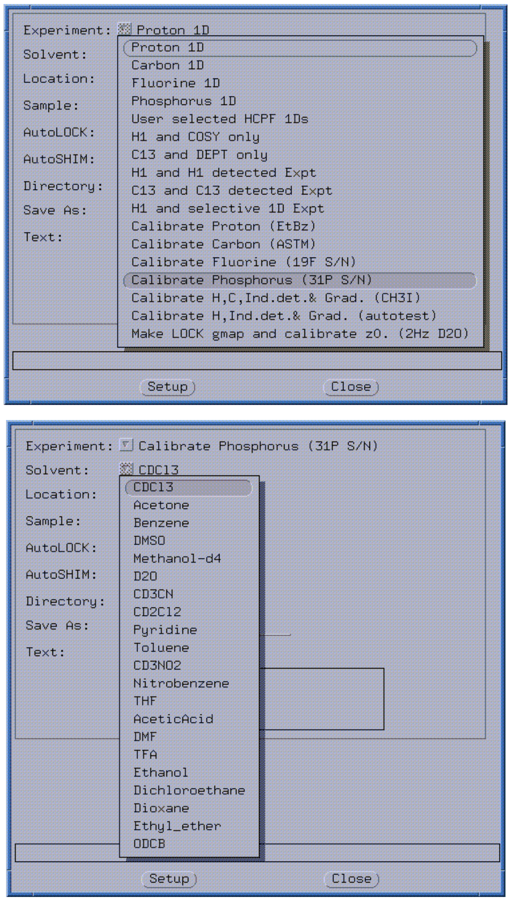
## 4.5 Calibrate Phosphorus

This section describes how to calibrate phosphorus.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment and Calibration Setup window.
2. Eject the sample from the magnet and insert the 0.485 M triphenylphosphate in $CDC1_3$ $^{31}$P sensitivity sample. Tune the probe if needed.
3. Right click the **Experiment** drop-down menu and select **Calibrate Phosphorus (31P S/N)**, as shown in Figure 24.
4. Right click the **Solvent** drop-down menu and select **CDCl3** as shown in Figure 24.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Click on **Setup**.

   Standard proton parameters are recalled and the sample confirmation window appears.



Experiment: Proton 1D

Experiment: Calibrate Phosphorus (31P S/N)

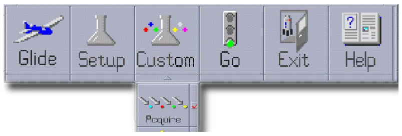
Solvent: CDC13

**Figure 24.** *GLIDE* Calibrate Phosphorus

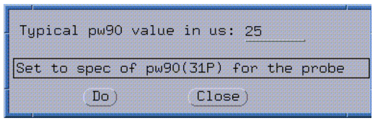
7. Click the **Confirm** button if the correct sample is inserted in the magnet. Click **Cancel** if the wrong sample is inserted and to end the calibration routine and begin again.

   If you set Autoshim and Autolock to **NO**, manually lock and shim now.

### Customize and Acquire



The Custom button is no longer shaded and the Acquire button appears after the Confirm button is selected at the end of the setup operation.


Typical pw90 value in us: 25

Set to spec of pw90(31P) for the probe

1. Click the **Acquire** button to open the Acquisition Setup window.
2. Enter the max **pw90** value that your probe and spectrometer typically achieve. The value is usually the $^{31}$P pulse specification for your probe.
3. Click the **Do** button to start the calibration routine.

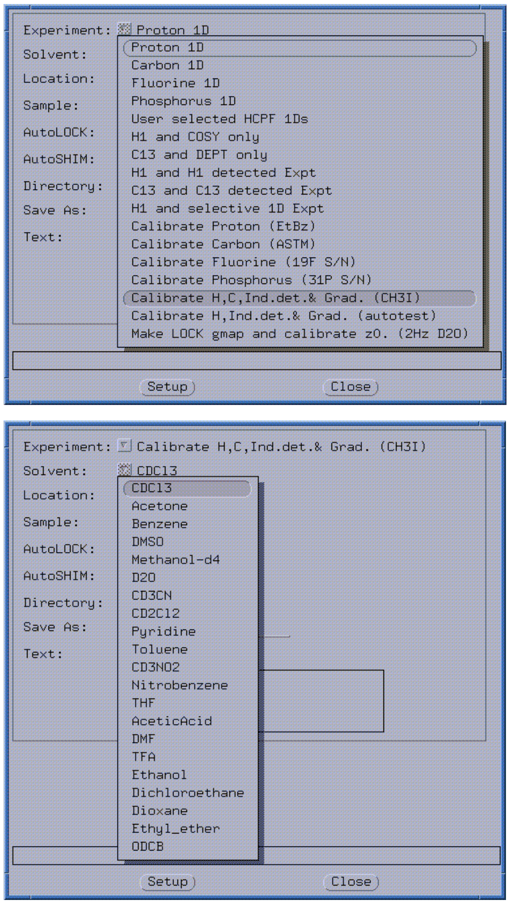
   At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

## 4.6 Calibrate H, C, Ind. Det., and Gradients ($CH_3I$)

This procedure calibrates H1 and C13 observe, H1 and C13 decouple (pulses as well as $\gamma H_2$), and gradients using the Indirect Detection I sample (C1$_3$ enriched $CH_3I$ in $CDCl_3$). Specific calibration routines can be selected in the customization menu.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment and Calibration Setup window.
2. Eject the sample from the magnet and insert the 1% $^{13}$C-enriched methyl iodide, 1% trimethyl phosphite, and 0.2% Cr(AcAc) in Chloroform-d sample. Tune the probe if needed.
3. Right click the **Experiment** drop-down menu and select **Calibrate H, C, Ind. det. & Grad. (CH3I)**, as shown in Figure 25.
4. Right click the **Solvent** drop-down menu and select **CDCl3** as shown in Figure 25.


Experiment: Proton 1D

Experiment: Calibrate H,C,Ind.det.& Grad. (CH3I)

Solvent: CDCl3

**Figure 25.** *GLIDE* Calibrate Using $CH_3I$

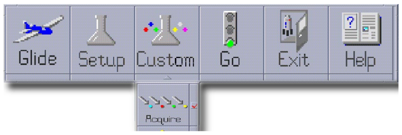
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Click on **Setup**.

   Standard proton parameters are recalled and the sample confirmation window appears.
7. Click the **Confirm** button if the correct sample is inserted in the magnet. Click **Cancel** if the wrong sample is inserted and to end the calibration routine and begin again.

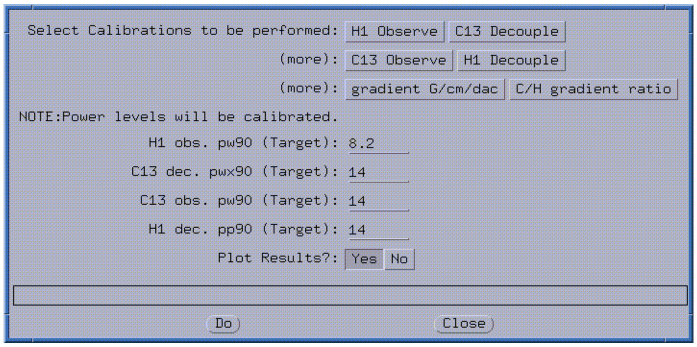
   If you set Autoshim and Autolock to **NO**, manually lock and shim now.

## Customize and Acquire

The Custom button is no longer shaded and the Acquire button appears after the Confirm button is selected at the end of the setup operation.



1. Click the **Acquire** button to open the Acquisition Setup window.



Select Calibrations to be performed: H1 Observe C13 Decouple
(more): C13 Observe H1 Decouple
(more): gradient G/cm/dac C/H gradient ratio
NOTE:Power levels will be calibrated.
H1 obs. pw90 (Target): 8.2
C13 dec. pwx90 (Target): 14
C13 obs. pw90 (Target): 14
H1 dec. pp90 (Target): 14
Plot Results?: Yes No

2. Enter the **$^1$H obs pw90, $^{13}$C obs pw90, $^1$H dec pp90,** and **$^{13}$C dec pwx90** values that your probe and spectrometer typically achieve or use the values for the probe's specifications.
3. Select the **H1 Observe, C13 Decouple, C13 Observe**, and **H1 Decouple** calibration options. If the probe is equipped with gradients, also select **gradient G/cm/dac** and **C/H gradient ratio** options. These are typical calibration for autoswitchable, indirect detection, and triple resonance probes.
4. Click the **Do** button to start the calibration routine.

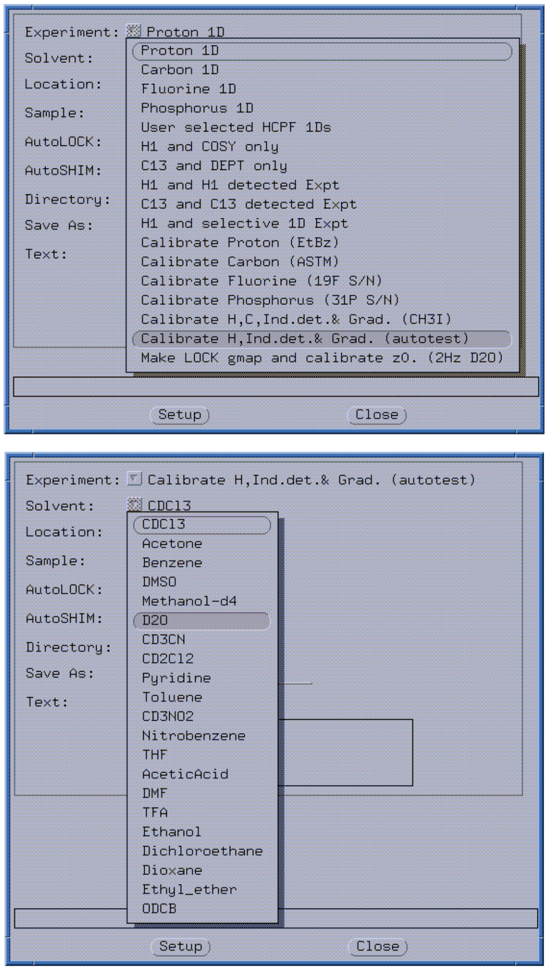
   At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file. If the gradient calibration options are selected, the gradient calibrations are written into the probe calibration file.

## 4.7 Calibrate H, Ind. Det., and Gradients ($CH_3OH$)

This procedure calibrates H1, C13 decouple (pulse as well as $\gamma H_2$), and gradients using the AutoTest sample (C13 enriched $CH_3OH$ in doped $D_2O$). You can select specific calibration routines in the customization menu.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment and Calibration Setup window.
2. Eject the sample from the magnet and insert the AutoTest sample. Tune the probe if needed.
3. Right click the **Experiment** drop-down menu and select **Calibrate H, C, Ind. det. & Grad. (CH3OH)**, as shown in Figure 26.
4. Right click the **Solvent** drop-down menu and select **D2O** as shown in Figure 26.
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.


Experiment: Proton 1D

Experiment: Calibrate H,Ind.det.& Grad. (autotest)

Solvent: CDC13

**Figure 26.** *GLIDE* Calibrate Using $CH_3OH$

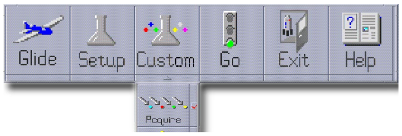
6. Click on **Setup**.

   Standard proton parameters are recalled and the sample confirmation window appears.

7. Click the **Confirm** button if the correct sample is inserted in the magnet. Click **Cancel** if the wrong sample is inserted and to end the calibration routine and begin again.

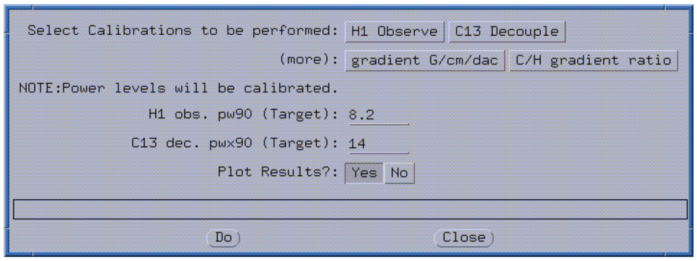
   If you set Autoshim and Autolock to **NO**, manually lock and shim now.

### Customize and Acquire



The Custom button is no longer shaded and the Acquire button appears after the Confirm button is selected at the end of the setup operation.

1. Click the **Acquire** button to open the Acquisition Setup window.



Select Calibrations to be performed: H1 Observe C13 Decouple

(more): gradient G/cm/dac C/H gradient ratio

NOTE:Power levels will be calibrated.

H1 obs. pw90 (Target): 8.2

C13 dec. pwx90 (Target): 14

Plot Results?: Yes No

2. Enter the $^{1}$**H obs pw90** and $^{13}$**C dec pwx90** values that your probe and spectrometer typically achieve or use the values for the probe's specifications.
3. Select the **H1 Observe**, and **C13 Decouple** calibration options. If the probe is equipped with gradients, also select **gradient G/cm/dac** and **C/H gradient ratio** options. These are typical calibration for AutoSwitchable, indirect detection, and triple resonance probes.
4. Click the **Do** button to start the calibration routine.

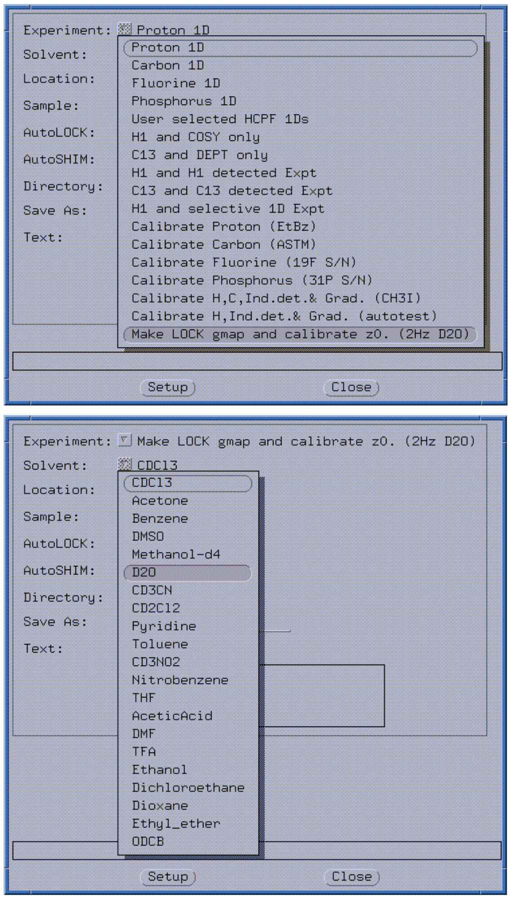
   At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file. If the gradient calibration options are selected, the gradient calibrations are written into the probe calibration file.

## 4.8 Calibrate Z0 and Make LOCK gmap

This procedure calibrates Z0 and makes a gradient map for gradient shimming for systems with gradients and gradient probes.

### Setup

1. Click on the *GLIDE* **Setup** button to display the Experiment and Calibration Setup window (Figure 27A).
2. Eject the sample from the magnet and insert the 2-Hz $D_2O$ sample. Tune the probe if needed.
3. Right click the **Experiment** drop-down menu and select **Make Lock gmap and calibrate Z0 "(2 Hz D2O)**, as shown in Figure 27.
4. Right click the **Solvent** drop-down menu and select **D2O** as shown in Figure 27.
5. Set **Autoshim** and **Autolock** to **NO**
6. Click on **Setup**.



Experiment: Proton 1D

Experiment: Make LOCK gmap and calibrate z0. (2Hz D2O)

Solvent: CDCl3

**Figure 27.** *GLIDE* Calibrate LOCK

Standard proton parameters are recalled and the sample confirmation window appears.

7. The message **“Set z0 exactly on-resonance before starting acquisition”** is displayed in the vnmr window. See *Getting Started* for more information on setting the lock. Open the lock display and set the lock as directed.

### Customize and Acquire

1. Click on the **GO** icon to calibration. There are no customization option.
2. When the calibration finishes, it updates the probe calibration file.

# Chapter 5. *GLIDE* Administrating and Customizing

Sections in this chapter:

*GLIDE* Administration

*GLIDE* Customization

This chapter covers the administration of the *GLIDE* environment and user privileges and how to customize *GLIDE* for local or global use.Almost everything about the *GLIDE* interface can be modified by the user. This includes the parameters for each individual experiment, the titles shown on windows, and even the text on each button.

## 5.1 Administration

The probe calibration files must be maintained in order for GLIDE to work properly. Following are general guidelines for required calibrations. The calibration routines are only accessible by vnmr1 and users added to the *GLIDE* admin group. All members of the *GLIDE* admin group can access the local user directory probe calibration files but only vnmr1 can access the global probe calibration file.

1. To make a probe file available to all system users enter **`addprobe(`*`probename`*`,'system')`**.
2. To create a new probe entry in the current user directory, enter **`addprobe(`*`probename`*`)`**, where *probename* is a name of your choice (e.g., `addprobe('idpfg')`).
3. Refer to previous appropriate sections for calibration procedures.

Almost everything about the *GLIDE* interface can be modified by the user. This includes the parameters for each individual experiment, the titles shown on windows, and even the text on each button.

## 5.2 Administrative Customization and Key *GLIDE* Files

*GLIDE* can be customized by defining groups of users and then defining the environment, experiments, and solvents for each group. The *GLIDE* administration tool `gadm` simplifies the process.

If the customization is for a single user, the files are kept in the `$vnmruser/glide` directory. If the changes are for all users, the files should be stored in the directory `$vnmrsystem/glide`.

### Defining Groups of Users

As many groups as needed can be created. Defining different groups of users is accomplished by editing the `group` file in the `adm` subdirectory. The following example shows how a `group` file might appear if there are three groups (`applab`, `RD`, and `marketing`.

```
applab:              krish, george, paul, steve
RD:                  dan, frits, greg, phil, hung, chin
marketing:           jan, evan, lisa, laima
```

**Listing 1.** `/vnmr/glide/adm/group` file

When a particular user logs in and runs *GLIDE*, that user can be assigned a specific experiments list, a solvents list, and a Store Data window, depending on the group to which that user has been assigned.

### Defining the Environment for Each Group

Each group listed in the `group` file requires a file describing the functions of the group. This environment file is created automatically by the *GLIDE* Administration tool when a new group is created. This file and related files can also be created by using the `vi` text editor and modeling the new file after the corresponding standard file. In the example Listing 1, these files would be named `applab.env`, `RD.env`, and `marketing.env`. If a user does not belong to any group, the file `public.env` is used.

Provided in the software is the file `public.env` (see Listing 2) that shows how `env` files are laid out:

```
experiment_list:  std_exp_unity
solvent_list:     std_solvents
archive_def:      /tmp
custom:           On
disk_archive:     On
```

**Listing 2.** `/vnmr/glide/adm/public.env` file

The first two entries, `experiment_list` and `solvent_list`, specify the files defining the experiments and solvents for the group. Each group could have its own files with names such as `exp_applab` and `solv_applab` for the `applab` group in the example above.

The `custom` entry can be set to `On` or `Off` (the letters are not case-sensitive). If set to `On`, the group can adjust the parameters of the experiment; if set to `Off`, the group can view the parameters, but any changes are ignored, and the default values are used.

Finally, the last entry, `disk_archive`, sets whether saving of data is allowed or disallowed. If set to `Off`, no saving of data is allowed and the Store button is not displayed in the Custom window for all users in this group. If set to `On`, the method of saving data can be selected by specifying a file name.

A typical example of a customized `.env` file is the file `applab.env` shown in Listing 3.

```
experiment_list:  exp_applab
solvent_list:     solv_applab
archive_def:
custom:           On
disk_archive:     On
```

**Listing 3.** Example of a Custom .env file; `applab.env`

Note that if users create their own `glide.env` file in `$vnmruser/glide/adm`, that `glide.env` file overwrites the group's environment file. However, the entry for `disk_archive` in `$vnmruser/glide/adm/glide.env` is ignored, and the entry in `$vnmrsystem/glide/adm` for that user is applied instead.

This way, the VNMR administrator has control over disk use. If users create their own local `glide.env` in `$vnmruser/glide/adm`, they must also have an `experiment_list` and `solvent_list` in `$vnmruser/glide.adm`, and vice versa.

## Defining Experiments and Solvents for Each Group

Individualized experiment and solvent lists can be created for individual groups of users. For example, a group of users that will only need to run 1D proton, carbon, fluorine, and phosphorus experiments that have samples that are dissolved in either CDCl3 or acetone-d6 need only these experiments and solvents as choices. The system administrator can prepare a customized experiment list and solvent list for this group and create group of users called, for example, **`group1`.** As you follow through the balance of this section on Administrative Customization, all the files necessary to create a new group with a customized environment in which only a 1D proton, carbon, fluorine, or phosphorus experiment is available will be set up.

### *Defining an Experiment List*

The experiments available to a group are defined by entries in the `experiment_list` file which and is located in `$vnmrsystem/glide/adm` or `$vnmruser/glide/adm` directory. In the `experiment_list` file, each experiment is defined by a group three lines:

| ***Line*** | ***Required Label*** | ***Entry*** |
|---|---|---|
| 1 | `macro:` | "`macro name`" |
| 2 | `label:` | "`Button Label`" |
| 3 | `directory:` | "`directory containing the macro`" |

*Note:* `$vnmrsystem` is a variable created in UNIX that stores the path to the vnmr files. Typically these files are located in `/export/home/vnmr`. `$vnmruser` is another variable created in UNIX, in this case it is the path to the current user's vnmrsys directory. Typically this is located in `/export/home/<user>/vnmrsys`.

For example, the first four experiments: Proton 1D, Carbon 1D, Fluorine 1D, and Phosphorus 1D, in the standard experiment list (see Listing 4) are defined by the first four groups of three lines in the `$vnmrsystem/glide/adm/std_experiments` file:

```
macro: "AuH"
label: "Proton 1D"
directory: ""

macro: "AuC"
label: "Carbon 1D"
directory: ""

macro: "AuF"
label: "Fluorine 1D"
directory: ""

macro: "AuP"
label: "Phosphorus 1D"
directory: ""
```

**Listing 4.** Partial Listing of `$vnmrsystem/glide/adm/std_experiments` file

The macro, AuH in the example above, sets up the proton 1D experiment. When the OK button is clicked in the Setup window, this macro and several others are executed by VNMR. The Custom icon is active and an Acquisition Button appears.User selected acquisition parameters are loaded later when the **Do** button in the acquisition panel or the **Go** icon is pressed. If no customization of the acquisition is required and the **Go** icon is pressed, preset default parameters are loaded and acquisition begins.

The text in the `label` field is the text that will appear in the Experiment menu of the Setup window.

The directory field in this example does not have an entry. When the macro is called the local maclib directory will be checked first and then the system directory. This is a typical entry for the `directory` field.

Creating a customized experiment list using the *GLIDE* Administration interface is explained in the section "Setting Up An Experiment List Using," page 67. A customized experiment list can also be created using `vi` or other text editor. The customized experiment list for the new user group, **`group1`**, is created by copying the first four entries in the `std_experiment` file into a file called **`group1_exps_list`**. The **`group1`** users now have custom experiment list containing only these experiments.

The macros that call the standard experiments available to all users, the experiment's *GLIDE* button label, and short descriptions of the macros are listed in Table 2

**Table 2.** Standard Experiments

| *Macro* | *Experiment Menu Label* | *Description of Macro** |
|---|---|---|
| AuH | Proton 1D | Standard 1D experiment |
| AuC | Carbon 1D | Standard 1D experiment |
| AuF | Fluorine 1D | Standard 1D experiment |
| AuP | Phosphorus 1D | Standard 1D experiment |
| AuH4nuc | User selected HCPF 1Ds | Chained Proton, Carbon, Fluorine, and Phosphorus 1D experiments |
| AuHCOSY | H1 and COSY only | Chained Proton 1D and COSY |
| AuCDEPT | C13 and DEPT only | Chained Carbon 1D and DEPT |
| AuHexp | H1 and H1 detected Expt | Proton 1D with options for chained 2D experiments: COSY, gCOSY, gDQCOSY, TOCSY, NOESY, ROESY, HMQC, gHMQC, HSQC, gHSQC, gHMBC, HMBC, HMQCTOXY, HSQCTOXY, gHMQCTOXY, gHSQCTOXY, and CARBON 1D |
| AuCexp | C13 and C13 detected Expt | Carbon 1D with options for chained 1D and 2D experiments: APT, DEPT, HETCOR, gHETCOR, PROTON 1D, COSY, and gCOSY |
| AuHsel | H1 and selective 1D Expt | Proton 1D with options for chained selective experiments: TOCSY1D, NOESY1D, ROESY1D, and HOMODEC. |

*Gradient experiments are only available if a gradient equipped probe is installed and the console is equipped with the gradient option.

Additional macros are accessible to vnmr1 and users in the adm group for system and probe calibrations. These calibration macros are listed in Table 3 and added to the list of standard experiments in Table 2. The administrator's experiment list is in `$vnmrsystem/glide/adm/admin_experiments`.

**Table 3.** Calibration Macros

| *Macro* | *Experiment Menu Label* | *Calibrate*** |
|---|---|---|
| AC1S | Calibrate Proton (EtBz) | $^{1}$H pw90 |
| AC5S | Calibrate Carbon (ASTM) | $^{13}$C pw90 and 13C pwx90 |
| AC10S | Calibrate Fluorine (19F S/N) | $^{19}$F pw90 |
| AC11S | Calibrate Phosphorus (31P S/N) | $^{31}$P pw90 |
| AuCALch3i1* | Calibrate H,C,Ind.det.& Grad. (CH3I) | $^{1}$H pw90, $^{1}$H pp90, $^{13}$C pw90, $^{13}$C pwx90, gradient G/cm/dac, and C/H gradient ratio |
| AuCALch3oh1* | Calibrate H,Ind.det.& Grad. (autotest) | $^{1}$H pw90, $^{13}$C pwx90, gradient G/cm/dac, and C/H gradient ratio |
| Augmapz0 | Make LOCK gmap and calibrate z0 (2Hz D2O) | Lock and make gmap |

* Gradient experiments are only available if a gradient equipped probe is installed and the console is equipped with the gradient option.

**The calibration samples and part numbers are listed in Table 1 on page 48.

### Defining a Solvent List

Similarly, the file for the `solvent_list` entry, in `$vnmrsystem/glide/adm` or `$vnmruser/glide/adm`, contains two lines for each solvent:

```
macro: "CDCl3"
label: "CDCl3"

macro: "acetone"
label: "Acetone"
```

The macros are used to set up the experiment, and the labels are shown in the Solvent menu of the Setup window. For instance, if Proton 1D and Chloroform are selected, the command `AuH('CDCl3')` is entered in the macro. Of course, the macro `AuH` must exist in `maclib` and CDCl3 must exist in `$vnmrsystem/solvents`. When OK is clicked, the definition files in the directory `exp/`are loaded into *GLIDE*.

A custom solvent list can be created to match the requirements of the experiments in **`group1_exps_list`** by copying these two entries into a new file called **`group1_solvent_list`** in `$vnmrsystem/glide/adm` or `$vnmruser/glide/adm`.

## 5.3 Administrative Customization with *GLIDE* Administration Tool

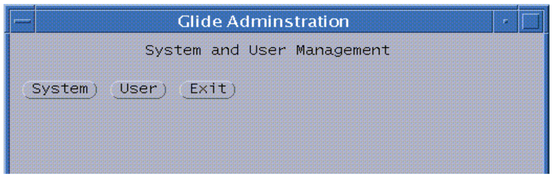
This is a graphic interface for the management of user groups, experiment lists, and the *GLIDE* environment. You must be logged in as vnmr1 to use the GLIDE Administration Tool.

### Starting the Glide Administration Tool

1. Type `gadm` on the VNMR command line or from UNIX window type:

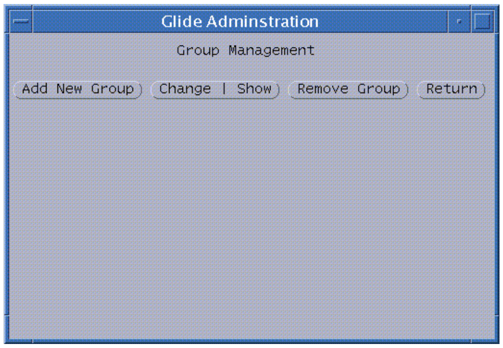
   ```
   vnmr1> gadm
   ```

   To Start the *GLIDE* administration tool.

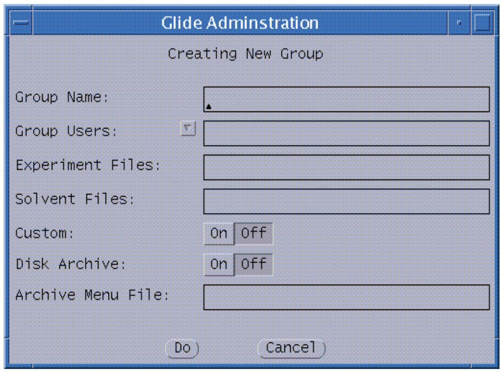


2. The main *GLIDE* Administration window has three buttons, **System, User,** and **Exit**. Select the *System* button to access **Group, Experiment**, and **Solvent** management windows. Select *User* to access local user *GLIDE* environment files. The local user *GLIDE* environment file have the same structure and function as their global counter parts but are located in `$vnmruser/glide/adm`.

## Setting Up Groups



Glide Group Management Window



Glide Create New Group Window

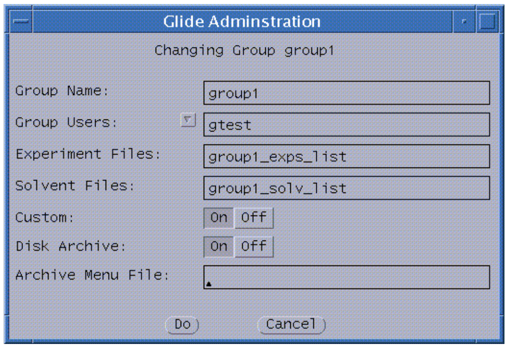
**Figure 28.** Add New Group Window

1. Click the **System** button in the Glide Administration Main Window. The System Management window appears.

   All definition files, list files and group lists that are created in this window will be written in `$vnmrsystem/glide/adm`. Clicking on the **User** causes these files to be written to `vnmruser/glide/adm`. Use this option to create various *GLIDE* user groups within a single VNMR (and UNIX) user login.

2. Click the **Group** button in the System Management window and the Group Management window, Figure 28, appears.
3. Click **Add New Group** in the Group Management window and the Creating New Groups window, Figure 28, appears.
4. Enter the new group name in the **Group Name** field. For this example, enter group1.
5. **GLIDE Enter** the name or names of the users to be included in the group in the **Group Users** field. Right mouse button on the Group Users menu button and a drop down list of all users in the local hosts file. If the computer is on a network with a name server all names on the network are displayed. Click on the user to select and add the user to the Group Users field.
6. Enter the name of the experiment list file in the **Experiment Files** field. For this example enter *group1_exps_list*.
7. Enter the name of the solvent list file in the **Solvent File** field. For this example enter *group1_solvent_list*.
8. Leave the **Archive Menu File** field empty.
9. Click the **Custom** to **On** if you want the group to be able to customize their experiments (otherwise the Custom Setup icon remains inactive at all times).
10. Click the **Disk Archive** to **On** if you want this group to be able to save their data (otherwise, the Store Data button in the Custom Setup window is always inactive).

The completed form is shown in Figure 29.



Changing Group group1

Group Name: group1
Group Users: gtest
Experiment Files: group1_exps_list
Solvent Files: group1_solv_list
Custom: [✓ On] Off
Disk Archive: [✓ On] Off
Archive Menu File:

**Figure 29.** *GLIDE* Completed Create New Group Window

11. Click on **Do**.

    File `group1.env` is created in `$vnmrsystem/glide/adm` and the users are listed in the file `$vnmrsystem/glide/adm/group` as part of `group1`. The listing for `group1.env` is shown in Figure 5A and the listing for the group file is shown in Figure 5B.

```
experiment_list: group1_exps_list
solvent_list:    group1_solv_list
archive_def:
custom:          On
disk_archive:    On
```

(A)`$vnmrsystem/glide/adm/group1.env`

```
admin:          vnmr1
public:
group1:         paul dan mike daina
```

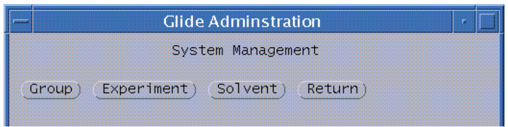
(B)`$vnmrsystem/glide/adm/group`

**Listing 5.** Sample Files Created by *GLIDE* Group Management Tool

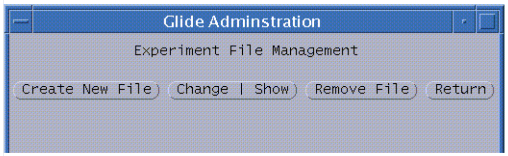
## Setting Up An Experiment List Using

1. If the *GLIDE* Administration window is running begin at step2. If the *GLIDE* Administration window is not running see "Starting the Glide Administration Tool" on page 64.
2. If you have just finished adding a new group go to step 3.

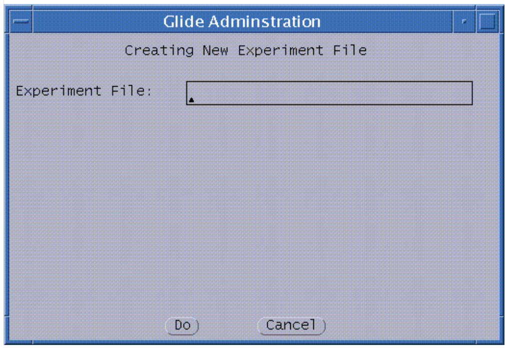
   If you has just opened the *GLIDE* Administration window the main window appears, click on **System**. Go to step 4.
3. Click on **Return** in the Group Management window (Figure 28A) to return to the System Management Window (Figure 30A).
4. Click on **Experiment** in the System Management Window (Figure 30A).
5. Click on **Create New File** (Figure 30B) in the Experiment File Management Window.
6. Enter the file name used in step 6 on page 65, *group1_exps_list*, in the **Experiment File** field of the Creating New Experiment File window (Figure 30C). Click on **Do**.
7. Enter the macro and Label for each entry in group1's experiments list in the **Creating Experiment File** widow (Figure 30D). For our example, enter the following macro and label pairs by clicking the **New** button between each pair: AuH and Proton 1D, AuC and Carbon 1D, AuF and Fluorine 1D, and AuP and Phosphorus 1D. Click on **Do.**
8. Click on **Yes** in the Confirmation window (Figure 30E).
9. If you are not going to make and further additions click on **Return ->Return->Exit**. If you are going to add a custom solvent list, continue with "Setting Up A Solvent List Using" on page 68.



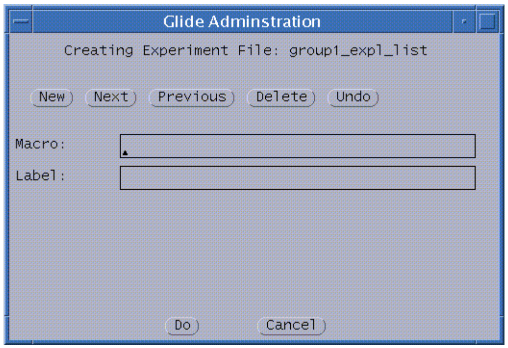
(A) *GLIDE* System Management Window



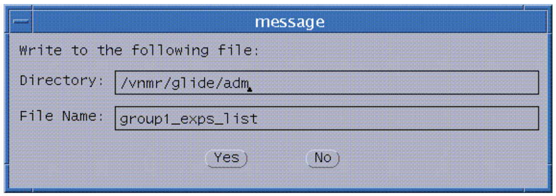
(B) *GLIDE* Experiment Management Window



(C) *GLIDE* Create New Experiment File Window



(D) *GLIDE* Add Macro and Label to Experiment List



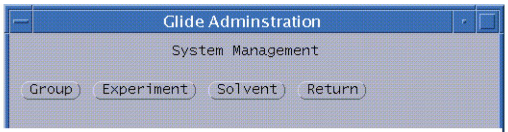
Directory: /vnmr/glide/adm

File Name: group1_exps_list

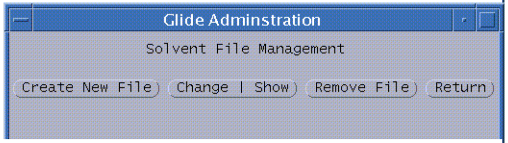
(E) *GLIDE* Confirm Experiment List File Name

**Figure 30.** Add Experiment List Windows

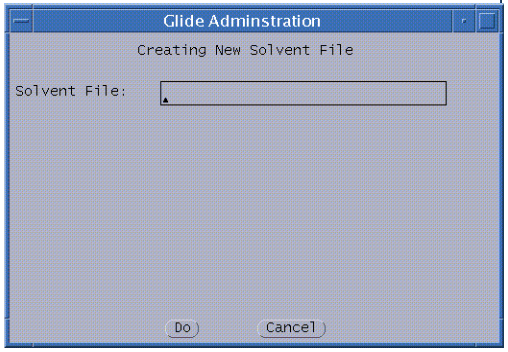
## Setting Up A Solvent List Using



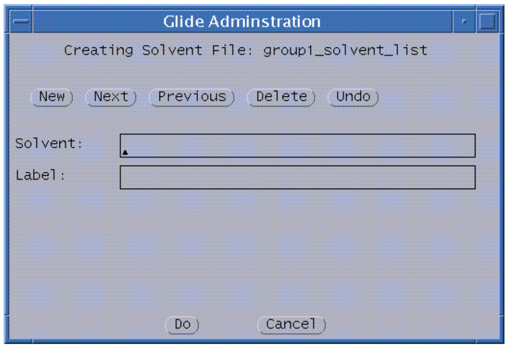
(A) *GLIDE* System Management Window



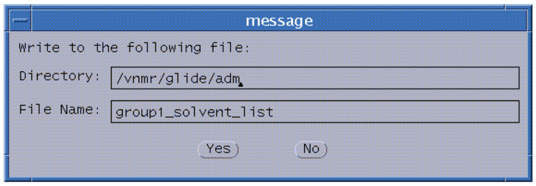
(B) *GLIDE* Solvent Management Window



(C) *GLIDE* Create New Solvent File Window



(D) *GLIDE* Add Solvent and Label to Solvent List



Write to the following file:

Directory: /vnmr/glide/adm

File Name: group1_solvent_list

(E) *GLIDE* Confirm Solvent List File Name

**Figure 31.** Add Solvent List Windows

1. If the *GLIDE* Administration window is running begin at step2. If the *GLIDE* Administration window is not running see “Starting the Glide Administration Tool” on page 64.

2. If you have just finished adding a new group go to step 3.

   If you has just opened the *GLIDE* Administration window the main window appears, click on **System**.

3. Click on **Return** in the Group Management window (Figure 31A) to return to the System Management Window (Figure 30A).

4. Click on **Solvent** in the System Management Window (Figure 31A).

5. Click on **Create New File** (Figure 31B) in the Solvent File Management Window.

6. Enter the file name used in step 7 on page 65, *group1_solvent_list*, in the **Solvent File** field of the Creating New Experiment File window (Figure 31C). Click **Do**.

7. Enter the macros and Labels for the experiments list of group1 in the **Creating Solvent File** widow (Figure 31D).

   For our example, enter the following macro and label pairs by clicking the **New** button between each pair: CDCl3 and Deutero Chloroform, and acetone and Acetone D6. The solvent’s name and case must be the same as its entry in the file `$vnmruser/solvent`. Solvent based shim files are case sensitive and the wrong or no shim file could be retrieved if solvent name in the custom solvent file list is not entered correctly.Click on **Do.**

8. Click on **Yes** in the Confirmation window (Figure 31E).

9. If you are not going to make and further additions click on **Return ->Return->Exit**.

## 5.4 *GLIDE* Directory Structure

All information is stored in the `glide` and `dialoglib` directories and their subdirectories. When the *GLIDE* program searches for its input, it first searches the user's directories in `$vnmruser/glide` and `$vnmruser/dialoglib`, and then the system directories `$vnmrsystem/glide` and `$vnmrsystem/dialoglib`. There are four subdirectories in the default layout provided with the software:

- `adm` subdirectory contains files for defining groups of users. Each group can have its own environment, defining a experiment list and a solvent list, customization can be allowed or disallowed, and archive capabilities can be set.
- `def` subdirectory contains definitions for popup windows.
- `exp` subdirectory contains further subdirectories, one for each experiment named in the list of standard experiments. Within each experiment subdirectory are files that describe which parameters can be adjusted for a particular experiment. Defining acquisition, processing, and plotting are the files called `acquire.def`, `process.def`, and `plot.def`, respectively.
- `dialoglib` subdirectory contains further subdirectories for each of the experiments that can be run in *GLIDE*, e.g., CARBON, COSY, etc. Each subdirectory contains the files `acquire.def`, `process.def`, and `plot.def`, which contain default parameter values and choices for an experiment. `dialoglib` is similar to the `glide/exp` directory, except that the experiments covered in `dialoglib` do not directly appear in the Experiment Setup experiment selection menu.
- `templates` subdirectory contains the `glide_defaults` file and template files for each icon displayed on the buttons in *GLIDE* (e.g., `Acquire.icon`). The `glide_defaults` file defines default values for the program. Listing 6 contains the complete text of the current default version. By replacing, adding, or deleting entries in this file, users can customize the look and feel of *GLIDE*.

**Listing 6.** Listing of `glide_defaults` File

```
# main buttons: Glide, Help, Recall, Expsolv, Custom, Go
# the order of the buttons will be the same order as their apperance

*Glide*Glide*icon:           Glide.icon
*Glide*Expsolv*icon:         Expsolv.icon
*Glide*Custom*icon:          Custom.icon
*Glide*Go*icon:              Go.icon
#*Glide*Recall*icon:         Recall.icon
*Glide*Exit*icon:            Exit.icon
*Glide*Help*icon:            Help.icon

# the resizeable can be yes or no
# the orientation can be horizontal or vertical

#*Glide*resizeable:          no
*Glide*orientation:          horizontal

# buttons under the Custom: Acquire, Process, Plot, Archive

*Custom*Acquire*icon:            Acquire.icon
*Custom*Process*icon:            Process.icon
*Custom*Plot*icon:               Plot.icon
*Custom*Archive*icon:            Archive.icon

#*Custom*resizeable:         no
*Custom*icon*orientation:    vertical

# action:  EXIT, CUSTOM, ARCHIVE, GO, DEF, VNMREXEC, MENU
# each button can have one and only one type of action.
#  EXIT will popup a window to confirm exit.
#  CUSTOM will popup a row of button for acquire, process, plot, and
# archive.
#  GO will do all selected jobs in CUSTOM.
#  DEF will popup a window which contents is defined in the file xx.def
#   for example,
#   *Glide*Mybutton*icon:    mybutton.icon
#   *Glide*Mybutton*action:  DEF
#   *Glide*Mybutton*def:     my.def
#   There will be a button using the pixmap in the file mybutton.icon,
#   and when this button was clicked it will popup a subwindow that
#   contains whatever defined in the file my.def.
#  ARCHIVE is the same as DEF, except its appearance is based on the
#   flag of archive.
```

**Listing 6.** Listing of `glide_defaults` File (continued)

```
#  VNMREXEC will send command, which defined in the exec, to Vnmr.
#   for example,
#   *Glide*Mybutton*action:  VNMREXEC
#   *Glide*Mybutton*exec:    dg
#   When this button was clicked it will send command 'dg' to Vnmr.
#  MENU will popup a window which contains a row of buttons.
#

*Glide*Exit*action:          VNMREXEC
*Glide*Exit*exec:            glide('exit') write('line3','Glide
                               exit')
*Glide*Help*action:          DEF
*Glide*Help*def:             help.def
*Glide*Recall*action:        DEF
*Glide*Recall*def:           recall.def
*Glide*Expsolv*action:       DEF
*Glide*Expsolv*def:          expsolv.def
*Glide*Custom*action:        CUSTOM
*Glide*Go*action:            GO

# alignment can be left, right, or none
*Glide*Expsolv*label*alignment: left

# name will be used as alias
*Glide*Expsolv*name:         Expsolv
*Glide*Custom*name:          Custom
*Glide*Go*name:              Go

# openAction: the actions will be executed when open the subwindow.
# closeAction: the actions will be executed when close the subwindow.

*Glide*Expsolv*openAction:  MASK(Custom) MASK(Go)
#*Glide*Expsolv*closeAction: UNMASK(Custom) UNMASK(Go) OPEN(Custom)

# updown:  yes, no
# updown is used to display an updown button under icon, which will
# popup or popdown its subwindow

*Glide*Custom*updown:        yes

*Custom*Acquire*action:      ACQUIRE
*Custom*Acquire*def:         acquire.def
*Custom*Process*action:      DEF
*Custom*Process*def:         process.def
*Custom*Plot*action:         DEF
*Custom*Plot*def:            plot.def
*Custom*Archive*action:      ARCHIVE
*Custom*Archive*def:         archive.def

# call:  the function or macro will be executed after each task was
# done

*Glide*Go*goAcquire:         glideau
*Glide*Go*noAcquire:         glidewexp
*Custom*Acquire*call:        glideau
```

**Listing 6.** Listing of `glide_defaults` File (continued)

```
*Custom*Process*call:       process
*Custom*Plot*call:          plot
*Custom*Archive*call:       archive($where)

*Custom*label*alignment:    right
*Custom*visibleLines:       9
*Custom*Process*visibleLines:  12

# Each window can have a row of buttons. Each button has attributes of
# label, exec, and help.
# The exec of button are: VNMREXEC, DO, RESET, CLOSE, MASK, UNMASK,
# OPEN, SHOW.
#  VNMREXEC: will send command to Vnmr.
#    *Glide*Process*button*4*exec: VNMREXEC(ft)
#    When this button was clicked it will send command 'ft' to Vnmr.
#  DO: will have Vnmr to do the all things in the specified window.
#  RESET: reset the contents of pecified window to the default values.
#  CLOSE: close window.
#  MASK: deactivate button.
#  UNMASK: activate button.
#  OPEN:  open window.
#  SHOW:  open subwindow.
# help: the text will be displayed in the footer.
#

*Glide*Recall*button*1*label:   Retrieve
*Glide*Recall*button*1*exec:    DO CLOSE UNMASK(Custom) UNMASK(Go)
*Glide*Recall*button*1*help:    Retrieve file
*Glide*Recall*button*2*label:   Close
*Glide*Recall*button*2*exec:    CLOSE
*Glide*Recall*button*2*help:    Close this window

*Glide*Expsolv*button*1*label:  Setup
*Glide*Expsolv*button*1*exec:   DO CLOSE
*Glide*Expsolv*button*1*help:   Setup experiment
*Glide*Expsolv*button*2*label:  Close
*Glide*Expsolv*button*2*exec:   CLOSE
*Glide*Expsolv*button*2*help:   Close this window

*Glide*Help*button*1*label:  Close
*Glide*Help*button*1*exec:   CLOSE
*Glide*Help*button*1*help:   Close this window
*Help*visiblelines:         25

*Custom*Acquire*button*1*label:  Do
*Custom*Acquire*button*1*exec:   DO CLOSE CLOSE(Custom)
*Custom*Acquire*button*1*help:   Vnmr will do acquire now
#*Custom*Acquire*button*2*label: Reset
#*Custom*Acquire*button*2*exec:  RESET
#*Custom*Acquire*button*2*help:  Reset to the defaults
*Custom*Acquire*button*3*label:  Close
*Custom*Acquire*button*3*exec:   CLOSE
*Custom*Acquire*button*3*help:   Close this window

*Custom*Process*button*1*label: Process
*Custom*Process*button*1*exec:  DO CLOSE CLOSE(Custom)
*Custom*Process*button*1*help:  Vnmr will do these selections ...
```

**Listing 6.** Listing of `glide_defaults` File (continued)

```
*Custom*Process*button*2*label: Reset
*Custom*Process*button*2*exec:  RESET
*Custom*Process*button*2*help:  Reset selections
*Custom*Process*button*3*label: Close
*Custom*Process*button*3*exec:  CLOSE
*Custom*Process*button*3*help:  Close  window

*Custom*Plot*button*1*label: Do Plot
*Custom*Plot*button*1*exec:  DO CLOSE CLOSE(Custom)
*Custom*Plot*button*1*help:  Vnmr will do plot now
*Custom*Plot*button*2*label: Reset Plot
*Custom*Plot*button*2*exec:  RESET
*Custom*Plot*button*2*help:  Reset these selections
*Custom*Plot*button*3*label: Close Plot
*Custom*Plot*button*3*exec:  CLOSE
*Custom*Plot*button*3*help:  Close  window

*Custom*Archive*button*1*label: Do
*Custom*Archive*button*1*exec:  DO
*Custom*Archive*button*1*help:  Vnmr will do archive now
*Custom*Archive*button*2*label: Reset
*Custom*Archive*button*2*exec:  RESET
*Custom*Archive*button*2*help:  Reset selections
*Custom*Archive*button*3*label: Close
*Custom*Archive*button*3*exec:  CLOSE
*Custom*Archive*button*3*help:  Close  window

# the following are the attributes for Confirmer window

*Glide*Confirm*title:       Notice
*Glide*Confirm*Yes*label:   Yes
*Glide*Confirm*Ok*label:    Ok
*Glide*Confirm*No*label:    No
*Glide*Confirm*exit*message:   Do you want to exit from glide?

#*Glide*Main*geometry:          468x72-0+0
*Glide*Custom*geometry:         +10+200
*Glide*Expsolv*geometry:        +300+200
*Glide*Help*geometry:           +300+200
*Glide*Acquire*geometry:        +250+200
*Glide*Process*geometry:        +250+200
*Glide*Plot*geometry:           +250+200
*Glide*Archive*geometry:        +250+200
*Glide*Recall*geometry:         +10+200
*Glide*Confirm*geometry:        +500+300

*Glide*Recall*title:         Recall Setup
*Glide*Expsolv*title:        Experiment Setup
*Glide*Help*title:           Manual Help
*Glide*Custom*title:         Custom Setup
*Custom*Acquire*title:       Acquire Setup
*Custom*Process*title:       Process Setup
*Custom*Plot*title:          Plot Setup
*Custom*Archive*title:       Archive Setup

*Glide*font:                  9x15
*Glide*Confirm*font:          courb24
```

## 5.5 Customizing *GLIDE* Look and Feel

The look and feel of the *GLIDE* program is easily customized by editing the contents of the `glide_defaults` file, which is located in `$vnmrsystems/glide/templates` or `$vnmruser/glide/templates`. Listing 6 contains the default version of this file. Most of *GLIDE* can be customized, including button icons, fonts, text, and actions.

### Modifying Button Icons

Icons are in the 48×48×PM format. Although any colors can be used, we recommend that you use only the standard set provided by the icon editor. The icon for a button can be changed from an existing button or created from scratch. If you want to change an icon, take the following steps.

1. Copy the icon you want to modify from `$vnmrsystem/glide/templates` to your own `$vnmruser/glide/templates` directory. For example, if you want to modify Go.icon, enter the following `cp` command to copy the `Go.icon` file (type the command on a single line without the backslash):

   ```
   > cp $vnmrsystem/glide/templates/Go.icon \
               $vnmruser/glide/templates/Go.icon
   ```

2. Open the UNIX CDE tool `dticon` and modify the icon:

   ```
   > /usr/dt/bin/dticon
   ```

   or select the icon editor from the CDE desktop applications.

   If you start from scratch with `dticonedit`, you must select XPM as the format and 48 × 48 as the size. Make sure you save the new icon in the directory `$vnmruser/glide/templates`.

3. Save the icon. If you save the icon using the same file name as in the default directory, skip the next two steps and continue at step 6.

   If you do not use the default file name, you must perform steps 4, 5, and 6.

4. If you haven't already done so, copy the file `glide_defaults` from the default directory `$vnmrsystem/glide/templates` to your own `$vnmruser/glide/templates`. Use the `cp` command as follows (type the command on a single line without the backslash):

   ```
   > cp $vnmrsystem/glide/templates/glide_defaults \
           $vnmruser/glide/templates/glide_defaults
   ```

5. Using a text editor, modify the `glide_defaults` file so that the name of the icon you changed is listed in the second column. For example, if you changed the Go icon (`Go.icon` file) and stored it as `Mygo.icon`, change `glide_defaults` as follows:

   ```
   *Glide*Go*icon:      Go.icon
   ```

   to

   ```
   *Glide*Go*icon:      Mygo.icon
   ```

   If you changed another icon, look for the corresponding line. If the original line does not exist, add the new line as a separate line anywhere in `glide_defaults`. Most names are fairly self-explanatory.

   Be sure you include the colon in the line as shown.

6. Exit *GLIDE* by clicking on the Exit button, then restart *GLIDE* by clicking on the *GLIDE* button in the Permanent menu. Check that the new icon is now used.

After you restart *GLIDE*, if the word custom appears where the new icon should be, *GLIDE* could not find the file you specified in `glide_defaults`. Most likely you typed the wrong file name or did not store the new icon in `$vnmruser/glide/templates`.

Additional changes are possible by editing the `glide_defaults` file. Refer to the comments in the default version of the file (Listing 6) for more information.

## Changing the Font and Text

By default, *GLIDE* uses the 9×15 font. If you want to change the font, follow these steps:

1. If you haven't already done so, copy the file `glide_defaults` from the default directory `$vnmrsystem/glide/templates` to your own `$vnmruser/glide/templates` Use the `cp` command as follows (type the command on a single line without the backslash):

   ```
   > cp $vnmrsystem/glide/templates/glide_defaults \
         $vnmruser/glide/templates/glide_defaults
   ```

2. Using a text editor, modify the line for the font in the `glide_defaults` file. For example, to change to the 7 × 14 font, change the second column from

   ```
   *Glide*font:   9x15
   ```

   to

   ```
   *Glide*font:   7x14
   ```

   Be sure you include the colon in the line as shown.

3. Exit *GLIDE* by clicking on the Exit button, then restart *GLIDE* by clicking on the GLIDE button in the Permanent menu. Check that the new font is now used.

The text associated with the font (`*Title`, `*label`, `*message`, etc.) can be changed similarly. Remember that the first column must remain unchanged (exactly as shown in Listing 6), but the second column can be any text. This enables *GLIDE* to be translated into any language.

## Additional Icon Options

Some additional options are available through `glide_defaults`:

`*resizable:    yes or no`

Sets whether the *GLIDE* icons can or cannot be resized. Default is yes.

`*orientation:  horizontal or vertical`

Sets whether the icons are laid out horizontal or vertical. Default is horizontal.

`*updown:       yes or no`

Sets whether the *GLIDE* icons will or will not have an up/down button under it. The effect of an up/down button is the same as clicking the icon, but its use is sometimes more obvious. Default is no.

`*name:         string`

Used as an alias. Can also be used as an argument to *GLIDE* internal functions such as MASK and OPEN.

`*openAction:`
`*closeAction:`

Sets actions to perform when an icon opens or closes a window. The window is normally defined with a `.def` file.

`*goAcquire:`
`*noAcquire:`

Sets action associated only with the Go icon. This action is performed before any other.
`*goAcquire` is executed when Acquire is selected in the Custom window.
`*noAcquire` is executed when Acquire is not selected in the Custom window.

`*help:`

Specifies message on a window displayed when the cursor is at rest over the icon.

## Setting the Actions of the Icon Buttons

Each icon button in the main interface (such as Exit, Help, Go, and user-defined button names) can have the following attributes to define the action of the button:

| | | |
|---|---|---|
| `action:` | One (and only one) of the following internal *GLIDE* actions:. | |
| | CUSTOM: | Pops up the row of buttons for acquire, process, plot, and archive. This action is normally only associated with the Custom button. |
| | GO: | Does all jobs as selected in the Custom window. This action is normally only associated with the Go button. |
| | DEF: | Pops up a window with contents defined in a_.def file.<br>The .def file is named in the corresponding *def. |
| | ARCHIVE: | Same as DEF, except the button is only active if the archive flag in the .env file is set to Yes. |
| | ACQUIRE: | Same as DEF, except the results of the window actions are executed by the GO function before any other window commands, such as Process and Plot. Normally, there is only one ACQUIRE action within *GLIDE*, and it is inside the Custom window, associated with the Acquire Setup window. |
| | MENU: | Pops up a window that contains a row of buttons. |
| | VNMREXEC: | Sends a command to VNMR. The command string is defined by a corresponding *exec |
| `exec:` | Defines the VNMR command for the VNMREXEC action. | |
| `def:` | Defines the name of the .def file for DEF, ACQUIRE, or ARCHIVE. | |
| `name:` | Specifies an alias for the corresponding icon. | |

The following examples show how these terms are used in the default version of the `glide_defaults` file:

```
*Glide*Exit*action:   VNMREXEC
*Glide*Exit*exec:     glide('exit') write('line3','Glide
*Glide*Expsolv*actio  exit')
n:                    DEF
*Glide*Expsolv*def:   expsolv.def
```

The following example shows how the action of a new button (`Mybutton`) is being defined. It will use the icon defined by the user in the file `mybutton.icon`. When the new button is clicked, it will popup a subwindow that contains whatever is defined by the user in the file `my.def`:

```
*Glide*Mybutton*icon:     mybutton.icon
*GLIDE*Mybutton*action    DEF
*Glide*Mybutton*def:      my.def
```

The following example adds an icon button (`Myicon.icon`) in the *GLIDE* window. This button is an up/down button that shows two icons (`Myicon2.icon` and

`Myicon3.icon`). Each of these two icons pops up a window defined by `myicon2.def` and `myicon3.def`:

```
*Glide*Myicon*icon:          Myicon.icon
*Myicon*updown:              yes
*Myidon*action:              MENU
*Myicon*Myicon2*icon:        Myicon2.icon
*Myicon*Myicon3*icon:        Myicon3.icon
*Myicon*Myicon2*action:      DEF
*Myicon*Myicon3*action:      DEF
*Myicon*Myicon3*def:         Myicon2.def
*Myicon*Myicon3*def:         Myicon3.def
```

Refer to Listing 6 for more information.

## Setting the Actions of the Popup Window Buttons

Each popup window in *GLIDE* has a row of buttons, such as the Do, Default, and Close buttons in the Acquire, Process, and Plot Setup windows. Additionally, each popup window may have buttons as part of `choice_button`, `menus`, and `check_button`. These buttons are defined in the file `glide_defaults` and can be customized:

`exec:` One or more of the following internal *GLIDE* actions:

| | |
|---|---|
| `CLOSE` | Close the window itself |
| `CLOSE(icon_name)` | Close window or menu associated with icon_name. |
| `OPEN` | Open window or menu of icon clicked. |
| `OPEN(icon_name)` | Open window or menu associated with icon_name. |
| `SHOW` | Open up/down window of icon clicked. |
| SHOW(icon_name) | Open up/down window associated with icon_name. |
| RESET | Reset (default) contents of this window. |
| RESET(icon_name) | Reset (default) contents of the window associated with icon_name. |
| MASK | Deactivate window. |
| MASK(icon_name) | Deactivate window associated with icon_name. |
| UNMASK | Activate window. |
| UNMASK(icon_name) | Activate window associated with icon_name. |
| DO | Generate output and send it to VNMR. A macro is created, executed by VNMR, and deleted. |
| DO(icon_name) | Same as DO, except for window associated with icon_name. |
| SAVE | Generate output and save it to a file. The name of the file is specified by the second argument of the dialog command. |
| SAVE(icon_name) | Same as SAVE, except for window associated with icon_name. |
| VNMREXEC(command) | Send command string to VNMR. |

| | | |
|---|---|---|
| | SETVAL(item,value) | Sets the value of item to value. This is used in the .def file only. (The use of id is discussed later).<br>SETVAL(input<(id)>,xxx)<br>SETVAL(menu<(id)>,1 to n)<br>SETVAL(choice<(id)>,1 to n)<br>SETVAL(check_button<(id)>, \ 0 or 1)<br>SETVAL(value<(id)>,xxx) |
| `help:` | Help text displayed when the cursor is over the button. | |

The following examples show the use of button attributes:

```
*Glide*Process*button*1*labe  Process
l:                            DO
*Glide*Process*button*1*exec  "VNMR will process this
:                             selections"
*Glide*Process*button*1*help  VNMREXEC(ft)
:                             Ft
*Glide*Process*button*2*labe  "VNMR will execute ft right now"
l:
*Glide*Process*button*2*exec
:
*Glide*Process*button*2*help
:
```

Displayed in the Process window are two buttons: `Process` and `Ft`. When `Process` is clicked, a macro `eou_process` is created that contains all selections made, and VNMR executes this macro right away. When `Ft` is clicked, VNMR executes `ft` only. If the attribute `exec` is empty or missing, VNMR does not execute. See Listing 6 for more examples of defining *GLIDE* buttons.

### Changing the *GLIDE* Help Page

If you change the look and feel of *GLIDE*, remember that the help page displayed by entering `man('glide')` refers to items by certain names. You should also modify the help page by editing the file `$vnmrsystem/manual/glide`.

## 5.6 Creating Popup Window Definition Files for *GLIDE*

Experiments can be fully customized through experiment definition files. This section describes these files and shows how to create and use them.

All popup windows in *GLIDE* and for dialog boxes are defined with `.def` files. Icons and `.def` files can be created for *GLIDE* buttons, buttons in the Custom window, or buttons in an up/down menu.

The location of the `.def` files follows these rules:

1. The `.def` files specified in the `glide_defaults` file are stored in either `$vnmruser/glide/def` or `$vnmrsystem/glide/def`.
2. For experiments named directly in the Experiment Setup selection menu, such as the 1D experiments for each nucleus, the `.def` files to appear in the Custom window are

in either `$vnmruser/glide/exp/exp_name` or `$vnmrsystem/glide/exp/exp_name`. `exp_name` must correspond to the name of the macro used in the Experiment list. The exception to this rule is the file `archive.def`, which is only in `$vnmrsystem/glide/def` but is added for all experiments to the Custom window.

3. For experiments such as APT or COSY that are selected and set up within the Custom Acquire menu, the `.def` files are in either `$vnmruser/dialoglib/EXP_NAME` or `$vnmrsystem/dialoglib/EXP_NAME`. The spelling of `EXP_NAME` must be the same as the entry in the experiment selection menu. The experiment setup macro itself (in `maclib`) must also have the same name with matching uppercase/lowercase characters (the convention is that all uppercase names are used).
4. If an absolute path is given for the `.def` file, the file can be stored anywhere.

Most of the `.def` files are created for a new experiment. Icons are already defined for acquire, process, and plot with their corresponding `.def` files, called `acquire.def`, `process.def`, and `plot.def`, respectively. If the `.def` file cannot be found, the icon is not displayed. For example, the directory structure for the “Proton 1D” experiment is

```
$vnmrsystem/glide/exp/AuH/acquire.def
$vnmrsystem/glide/exp/AuH/process.def
$vnmrsystem/glide/exp/AuH/plot.def
```

The icons for these `.def` files will appear in the Custom window. None of the `.def` files are necessary to make an experiment. If omitted, no customization is possible.

For experiments setup using the Custom Acquire menu selection, the `.def` files are located in the directory .../`dialoglib/EXP_NAME`. The file `acquire.def` is read when the corresponding experiment is chosen, and immediately defines a new popup window that allows you to set acquisition parameter values for that experiment. The `process.def` and `plot.def` files are stored with the FID and recalled when the data is loaded for processing. When the data is loaded, you can customize processing and plotting by modifying the `process.def` and `plot.def` files, which define the Custom Process and Custom Plot menus (as well as default processing and plotting).

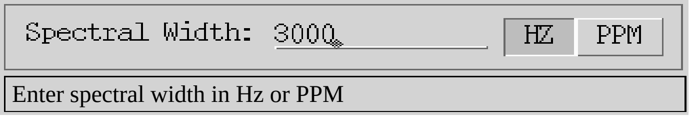
As an example, the following procedure adds a double-quantum-filtered COSY experiment (DQFCOSY) to the list of proton-detected experiments (accessible by choosing “H1 and H1 detected Experiments” in the Experiment Setup experiment selection menu).

1. Add DQFCOSY to the file `exp/AuHexp/acquire.def`; add it to the experiment selection menus towards the end of the file.
2. Create a new subdirectory called `$vnmruser/dialoglib/DQFCOSY.def` that includes the files `acquire.def`, `process.def`, and `plot.def`. Each of these files contains fields for parameters–such as relaxation delay (`d1`), `ni`, and `nt` in `acquire.def` or processing parameters such as linear prediction or `fn` in `process.def`–that you are allowed to change.

Within the `.def` files are entries describing one parameter-change-line. Each entry is enclosed in braces{ }. For example,

```
{
label:            Spectral Width
input:            3000
choice:           "Hz" "PPM"
choice_value:     "" "p"
output:           "sw=$input$choice_value"
remark:           "Enter spectral width in Hz or PPM"
show:             (sw<2000) and (np>3200)
}
```

would appear as



Spectral Width: 3000

Enter spectral width in Hz or PPM

Note that each entry between braces consists of several lines. Each line contains a label, a colon, and one or more values. Possible labels and their values are the following:

| | |
|---|---|
| `label:` | String that serves as the label for the item being defined. |
| `input:` | Default numerical or string value for the item. |
| `choice:` | Series of string values to appear on radio buttons. The first value is the default. |
| `choice_value:` | String values to be used as $choice_value in output when the radio buttons are selected. The number of strings for choice_value must equal the number of values for choice. |
| cols: | Number of columns for item. Sets the line length of input. |
| rows: | Number of rows for item. Sets the number of lines of input. |
| `menu:` | Series of string values to appear on a menu. The first value is the default. |
| abbreviate_menu: | Same as menu, except the selected menu item is not shown, and only the menu button is shown |
| `menu_value:` | String values to be used as $menu_value in output when choices in the menu are selected. The number of strings for menu_value must equal the number of values for menu. |
| value(id): | Same as menu_value, choice_value, or input, when used. If id is missing, this line is ignored. id is any number assigned to an item to distinguish it from other similar items. For example, if you tried to create two choice buttons but did not assign id to each button, only one button would be created. |
| exec: | Sets *GLIDE* action. If no id is specified, the action applies to every button, menu, and choice. |
| text: | Displays the text. |
| button: | Button displayed in the bottom row of a window. By default, Do, Default, and Close are displayed. |
| check_button: | Multiple selection row of buttons. |
| check_set_exec: | Sets *GLIDE* actions for check_button when set or selected. If no id is specified, the action applies to every check_button. |
| `output:` | String to be inserted in a macro executed by VNMR. The string can contain characters, $input, $choice_value, and $menu_value. |

| | |
|---|---|
| `rtoutput:` | String to be sent to VNMR immediately (in real time). The string can contain characters, $input, $choice_value, and $menu_value. |
| `help:`<br>`remark:` | String, up to 40 characters long, to be displayed on the bottom of the window when the cursor is over the entry, as user help. |
| `show:` | Sets a MAGICAL if condition as to whether or not to display this item. This condition is checked when the .def files are read in; that is, when the Recall button or Setup button is clicked. |

By making several entries in each file, an experiment can be completely defined. If more entries are defined than fit in the window a scrollbar is automatically generated.

## 5.7 Example: Adding VT Control to the Experiment List

You can customize as much as you wish the list of choices in the Experiment and Solvent popup menus. As an example, the following steps add an experiment called “1D proton with VT” to the list of experiments.

1. If you haven’t already done so, copy the default experiments list for your system from the directory `$vnmrsystem/glide/adm` to your own `$vnmruser/glide/adm`. Use the `cp` command as follows (type the command on a single line without the backslash)—on *MERCURY-VX*, *MERCURY*, and *GEMINI 2000* systems, enter:

```
> cp $vnmrsystem/glide/adm/std_exp_gem \
       $vnmruser/glide/adm/my_std_exp
```

   On systems other than *MERCURY-VX*, *MERCURY*, and *GEMINI 2000*, enter:

```
> cp $vnmrsystem/glide/adm/std_exp_unity \
       $vnmruser/glide/adm/my_std_exp
```

2. Start the *GLIDE* administration tool:

```
> gadm
```

   The opening window appears with three buttons: System, User, and Exit.

3. In the window, click on User | Do | Experiment | Change | Show.

   A new window appears with a single field labeled Experiment File.

4. Type in the new file name you want to give the experiment list:

```
Experiment File:   my_std_exp
```

   Then click on Do.

   Another window appears with fields labeled Macro and Label for the first entry in the file `my_std_exp`.

5. Click on Next until an empty entry is shown (or click on New), then type in a new macro name and label. For our example, enter the following:

```
Macro:   H1_VT
Label:   1D proton with VT
```

   Be sure to remember the macro name you enter because it will be the name of the macro used to set up the experiment and will also be the name of the directory that hold the `.def` files that define the experiment (see below). Therefore, the macro name must be a valid VNMR and UNIX name. The label will be the text shown in the experiment list.

Beside adding an experiment using this window, notice you can replace an old experiment with the new one by erasing an entry and typing the new experiment in its place. You can also delete unneeded experiment here.

6. Click on Do and when the confirmation message appears click on Yes.

   The list is now created. Next we need to tell *GLIDE* that we want to use this list.

7. Click on **Return** > **Preference**.

   The window that appears has three fields, labeled Experiment files, Solvent files, and Archive Menu file.

8. Because we are changing the experiment list only, we change only the experiment file entry, as follows:

   ```
   Experiment files:   my_std_exp
   ```

   We leave the other two entries alone. If we had instead changed the solvents list, we would of course modify that entry, or both entries if both were changed.

9. Click on **Do** and, when the confirmation message appears, click on **Yes**.

10. Exit `gadm` by clicking on **Return** > **Exit**.

11. Exit *GLIDE* by clicking on the **Exit** button, then restart *GLIDE* by clicking on the **GLIDE** button in the Permanent menu. Check that the new experiment appears in the list of experiments.

The next section shows how to create customization definition files for this experiment.

## Creating New Customization Definition Files

In the example above, the experiment H1_VT was added to the experiments list. Now we need to create customization definition files for the experiment. These files, which have the `.def` extension, define the parameters that can be adjusted in the Custom Setup window. The easiest way to proceed is to copy the `.def` files from an existing experiment and modify the files as needed.

1. Because our example is a 1D proton experiment, start by copying $^1$H `.def` files from `$vnmrsystem/glide/exp/h1` to your directory `$vnmruser/glide/exp/H1_VT`. The directory `H1_VT` is used because that is the name of the macro specified in the experiments list. Note the use of the “-r” option because we recursively want to copy a directory:

   ```
   >cp -r $vnmrsystem/glide/exp/h1  \
            $vnmruser/glide/exp/H1_VT
   ```

2. List the files in H1_VT:

   ```
   > cd $vnmruser/glide/exp/H1_VT
   > lf
   acquire.def     process.def     plot.def
   ```

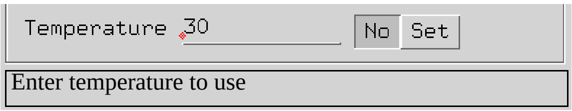
   These three `.def` files determine which parameters can be adjusted for this experiment. Note that there is no file `archive.def`, because archiving privileges are set only by the VNMR system administrator.

3. Use a text editor add the following entry to the file `acquire.def`:

   ```
   {
      label: Temperature
      input: 30
      choice: “No” “Set”
   ```

```
   choice_value: ”’n’” “$input”
   output: temp=$choice_value”
   remark: Enter temperature to use
   show: (vttype<>0)
}
```

Notice that the entry is enclosed between braces “`{ }`” and consists of several lines. Each line has a label, a colon, followed by one or more values. The label must be exactly as shown—any typos and the line is ignored. A complete list of labels is given earlier in this chapter. This entry produces this graphic (note that No is selected because that is the first value following the choice label):



Temperature 30

Enter temperature to use

4. Save the file and exit the editor.

   We leave the `process.def` and the `plot.def` files unchanged. Notice that if the `process.def` and the `plot.def` files did not exist in the `H1_VT` directory, the Process Setup and Plot Setup icon are not active in the Custom Setup window.

The next section considers writing a macro to set up this experiment.

## Creating a Setup Macro

*GLIDE* now has the ability to set the temperature for a proton 1D experiment. But a macro is still needed to set up the experiment. This macro is called when, after an experiment and solvent is selected, the Setup button is clicked in the Experiment Setup window.

1. As with the `.def` files, it is easiest to start by copying and modifying an existing macro for an experiment similar to the new experiment. The closest macro to the new experiment is the `h1` macro. In fact, because all we added to the existing 1D proton experiment was the ability to change an existing parameter, we do not have to change `h1`, but we must call it `H1_VT` (of course we could also create a macro `H1_VT` that just calls `h1`):

   ```
   > cp $vnmrsystem/maclib/h1 $vnmruser/maclib/H1_VT
   ```

2. Processing and plotting is done with the standard proton 1D macros and need no further work.

We are now ready to run this experiment from *GLIDE*.

## 5.8 Further Considerations in Customizing *GLIDE*

A few things should be remembered when programming for *GLIDE*. As described in the examples above, the macro name in the experiment list must be the same as the name of the setup macro as well as the same as the name of the directory that holds the `.def` files. The experiment description is located in `$vnmrsystem/glide/exp` or in `$vnmruser/glide/exp`. The names must be VNMR and UNIX compliant. They are also case sensitive; for example, `h1` and `H1` are not the same.

We didn't modify the `h1` macro, just copied it to `H1_VT`, because we allowed for customizing of an already existing parameter (all parameter sets from Varian have the `temp` parameter). If we used a parameter unique to the experiment, we would have to create the parameter in the setup macro, the same as always.

What happens if the Go button is pushed?

1. *GLIDE* creates a macro, called `eou_go` that contains all the lines defined by the "output:" lines in the `acquire.def` file. At the end of `eou_go`, the value defined by `*Glide*Go*goAcquire*` in `glide_defaults` is added. By default, this value is `glideau`.
2. In the same manner, the macros `eou_process_go`, `eou_plot_go`, and `eou_archive_go` are created. Each get their lines from the corresponding `.def` file and one line is added from `glide_defaults`. By default, this is `process` for `eou_process_go`, `plot` for `eou_plot_go`, and `archive($where)` for `eou_archive_go`. These macros are stored in the current experiment and are erased as soon as they are executed.
3. After *GLIDE* creates these macros, it sends the macro `eou_go` to VNMR. VNMR sets the parameters as prescribed by `eou_go` and executes `glideau`. `glideau` resets the `wexp` parameter to be `glidewexp` (unless the experiment is a chained experiment such as H-C-APT, then it removes the first in the chain) and executes an `au`.
4. When the experiment is completed, `glidewexp` is executed. `glidewexp` first executes `eou_process_go`, which sets the processing parameters and executes the macro `process`. Next, `glidewexp` executes `eou_plot_go`, which sets the plotting parameters and executes the macro `plot`. Finally, `glidewexp` executes `eou_archive_go,` which sets archiving parameters (usually none) and executes `archive($where)`. (`$where` is set by the VNMR system administrator when it creates the different groups and assigns archiving privileges.)
5. Ultimately the macros `process` and `plot` are executed. These macros process and plot all experiments; decisions on how to process and plot are based on the observe nucleus parameter `tn` for 1D, and whether certain parameter such as `ni` exists for 2D.

Refer to the manual *VNMR Command and Parameter Reference* for more information on `plot` and `process`.

# Chapter 6. Tcl/Tk User Interfaces

Sections in this chapter:

There are three Tcl/Tk user interfaces supplied with VNMR 6.1C. Each interface provides the user with push button access to an extensive list of standard experiments. Through the **Setup EXP** window, an individual experiment can be set up and fully customized. Automated multiple experiment acquisition is set up using the **Custom Q** window. Predefined groups of experiments can be setup and run automatically as a series of experiments with no additional user intervention. Menu driven customization of acquisition and plotting parameters is an integral part of the **Custom Q** interface. The **Walkup** window provides one button operation for quick data acquisition and plotting.

This chapter covers the functions of the buttons in each of the user interfaces and the experiments available through each interface.

Chapter 7, “Tcl/Ttk NMR Interfaces Step-by-Step,” covers step-by-step operation and data acquisition.

## 6.1 Experiments Available Through Each Tcl/Tk Interface

Table 4 lists the experiments available for each Tcl/Tk interface.

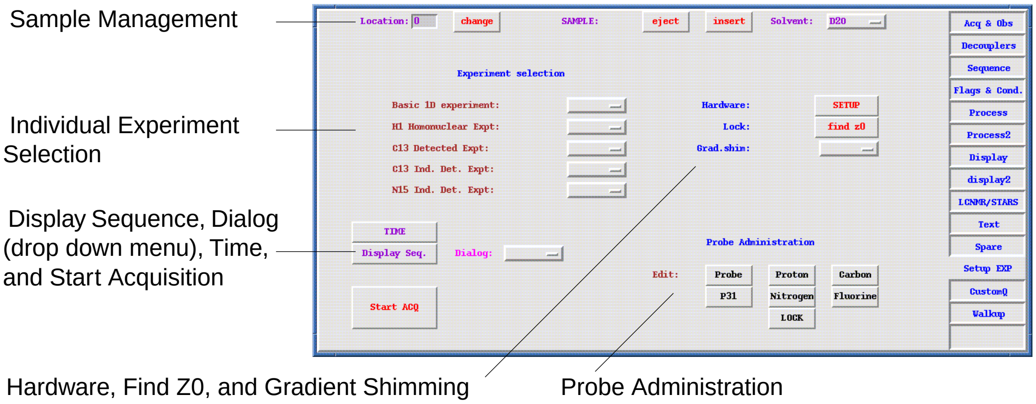
**Table 4.** Available Experiments in Each Tcl/Tk Interface

| ***Experiment**** | ***Setup EXP*** | ***CustomQ*** | ***Walkup*** |
|---|---|---|---|
| Proton 1D | ✔ | ✔ | ✔ |
| Carbon 1D | ✔ | ✔ | ✔ |
| Fluorine 1D | ✔ | ✔ | |
| Phosphorus 1D | ✔ | ✔ | |
| Chained Proton, Carbon, Fluorine, and Phosphorus 1D experiments | | ✔ | |
| Chained Proton 1D and COSY | | ✔ | ✔ |
| Chained Carbon 1D and DEPT | | ✔ | ✔ |
| Proton 1D with chained proton detected 2D experiment options | | ✔ | ✔ |
| gCOSY / COSY | ✔ | ✔ | ✔ |
| gDQCOSY | ✔ | ✔ | |
| gHMQC / HMQC | ✔ | ✔ | |
| gTOCSY / TOCSY | ✔ | ✔ | |
| gNOESY / NOESY | ✔ | ✔ | |
| gROESY / ROESY | ✔ | ✔ | |
| gHSQC / HSQC | ✔ | ✔ | ✔ |
| gHMBC / HMBC | ✔ | ✔ | |
| gHMQCTOXY / HMQCTOXY | ✔ | ✔ | |
| gHSQCTOXY / HSQCTOXY | ✔ | ✔ | |
| CARBON 1D | | ✔ | ✔ |
| Carbon 1D with chained 1D and $^{13}$C detected 2D experiments options | | ✔ | ✔ |
| APT | ✔ | ✔ | |
| DEPT | ✔ | ✔ | ✔ |
| gHETCOR / HETCOR | ✔ | ✔ | |
| PROTON 1D | | ✔ | |
| gCOSY / COSY | | ✔ | |
| Proton 1D with options for chained selective experiments | | ✔ | |
| gTOCSY1D | ✔ | ✔ | |
| gNOESY1D | ✔ | ✔ | |
| gROESY1D | ✔ | ✔ | |
| HOMODEC | ✔ | ✔ | |
| Nitrogen indirect detection experiments | ✔ | | |
| gHMQC / HMQC | ✔ | | |
| gHSQC / HSQC | ✔ | | |
| gHMBC / HMBC | ✔ | | |
| gHMQCTOXY / HMQCTOXY | ✔ | | |
| gHSQCTOXY / HSQCTOXY | ✔ | | |

*Experiments requiring gradients are indicated by the prefix ’g’ (e.g. gCOSY) and are only available if a gradient equipped probe is installed, the console is equipped with the gradients, and the gradient field in the probe file is set to’y’.

## 6.2 Setup EXP Window

The **Setup EXP** panel in the Tcl/dg window provides access to the experiments listed in Table 4 in the Setup EXP column. Open the Setup EXP window, shown in Figure 32, by clicking the **Setup EXP** button in the Tcl/dg window.


Location: 0

Solvent: D20

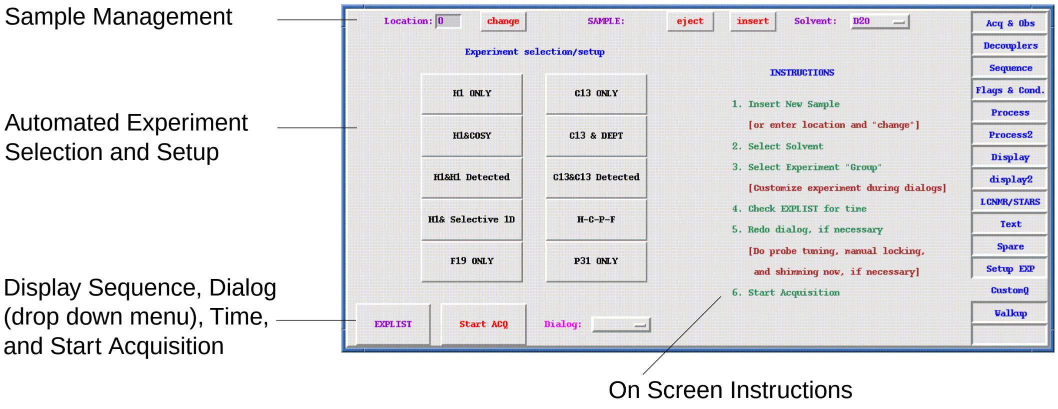
**Figure 32.** Setup EXP Window

The **Setup EXP** window is divided into five major areas:

- **Sample Management** menus and buttons. These buttons facilitate changing the sample and setting the lock solvent. If the system is equipped with a sample changer the location of the sample is entered in the *Location window* and the change button used to change the sample. *Eject* and *Insert* buttons are provided for systems that do not have a sample changer. The appropriate lock solvent is selected from the list of lock solvents available in the drop down *Solvent* menu.
- **Individual Experiment Selection** menus. Use these menus to set up one experiment at a time. For example selecting HMQC from these menus converts the parameter set in the current experiment to HMQC. Parameters can be adjusted before starting the acquisition. The data is collected and processed. Plotting of data and saving of the FIDs are done manually. For step-by-step instruction, refer to Tcl/Ttk NMR Interfaces Step-by-Step on page 91.
- **Display Sequence**, **Dialog (drop down menu)**, **Time**, and **Start Acquisition** buttons. These buttons are basic tools for displaying a pulse sequence, interactively adjusting acquisition, display and plotting parameters, calculating time (only for individual experiment), and starting acquisition.
- **Hardware, Find Z0, and Gradient Shimming** buttons and menus. The *SETUP* button sets up the hardware, *find z0* starts the autolocking routine, and *Grad. shim* is a drop down menu of gradient shimming options. Gradient shimming is an integral part of *Setup EXP* operation. When the acquisition is started using the **Start Acquisition** button, the requirements for gradient shimming are automatically explored and the necessary files are found, gradient shimming is done before acquisition. See Tcl/Tk NMR Administration and Calibration on page 121.
- **Probe Administration** buttons and menus. Use these buttons and menus for probe administration, which is a key requirement for successful operation. Probes files can be calibrated automatically using the Autocalibration menus or manually edited. See Administration of Probe Calibration Files on page 121 for details on the probe administration files and Autocalibration.

## 6.3 CustomQ Window

The *CustomQ* interface panel in the Tcl/dg window provides access to the experiments listed in Table 4 in the CustomQ column. Open the *CustomQ* window, shown in Figure 33, by clicking the **CustomQ** button in the Tcl/dg window.



INSTRUCTIONS

1. Insert New Sample
   [or enter location and "change"]
2. Select Solvent
3. Select Experiment "Group"
   [Customize experiment during dialogs]
4. Check EXPLIST for time
5. Redo dialog, if necessary
   [Do probe tuning, manual locking, and shimming now, if necessary]
6. Start Acquisition

Sample Management

Automated Experiment Selection and Setup

Display Sequence, Dialog (drop down menu), Time, and Start Acquisition

On Screen Instructions

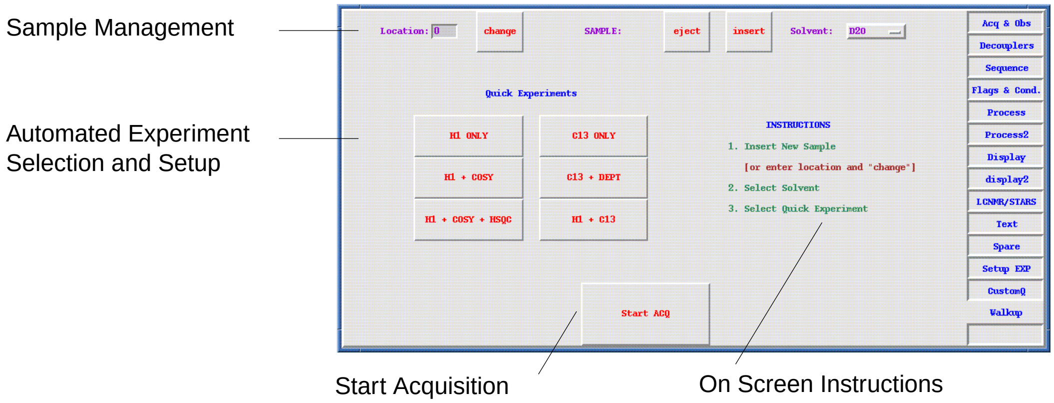
**Figure 33.** CustomQ Window

The **CustomQ** window is divided into four major areas:

- **Sample Management** menus and buttons. These buttons facilitate changing the sample and setting the lock solvent. If the system is equipped with a sample changer the location of the sample is entered in the *Location window* and the change button used to change the sample. *Eject* and *Insert* buttons are provided for systems that do not have a sample changer. The appropriate lock solvent is selected from the list of lock solvents available in the drop down *Solvent* menu.
- **Automated Experiment Selection and Setup** buttons. Use these buttons to set up and run either predefined or a custom chain of experiments on the sample. In these selections, experiments are acquired, processed, plotted and saved automatically. You have access to the collected FID for reprocessing and replotting. For step-by-step instructions, refer to Tcl/Ttk NMR Interfaces Step-by-Step on page 91.
- **EXPLIST**, **Start Acquisition**, and **Dialog (drop down menu)** buttons. These buttons are basic tools for displaying the list of experiments that have been selected, interactively adjusting acquisition, display and plotting parameters, and starting acquisition.
- **On Screen Instructions** provide step-by-step basic instructions for operation using the **CustomQ** window.

## 6.4 Walkup Window

The Walkup interface provides one button access to a preset group of experiments which makes set up and acquisition easy. The experiments are listed in Table 4 in the Walkup Column. Experiments are accessed from the *Walkup* window in the Tcl/dg window. Open the *Walkup* window, shown in Figure 34, by clicking the **Walkup** button in the Tcl/dg window.



INSTRUCTIONS

1. Insert New Sample

   [or enter location and "change"]

2. Select Solvent

3. Select Quick Experiment

**Figure 34.** Walkup Window

The *Walkup* window is divided into three major areas:

- **Sample Management** menus and buttons. These buttons facilitate changing the sample and setting the lock solvent. If the system is equipped with a sample changer the location of the sample is entered in the *Location window* and the change button used to change the sample. *Eject* and *Insert* buttons are provided for systems that do not have a sample changer. The appropriate lock solvent is selected from the list of lock solvents available in the drop down *Solvent* menu.
- **Automated Experiment Selection and Setup** buttons. Use these buttons to set up and run predefined experiments on the sample. Experiments are acquired, processed, plotted automatically. For step-by-step instructions, refer to Tcl/Ttk NMR Interfaces Step-by-Step on page 91.
- **Start Acquisition** button.
- **On Screen Instructions** provide step-by-step basic instructions for operation using the **Walkup** window.

# Chapter 7. Tcl/Ttk NMR Interfaces Step-by-Step

Sections in this chapter:

- 7.1 "Setup EXP Window Experiments," this page
- 7.2 "CustomQ Window Experiments," page 94
- 7.3 "Walkup Window," page 120

This chapter gives step-by-step instructions for performing automated and individual walkup NMR experiments using the Tool Command Language/Display Group (Tcl/dg) interface.

The general procedure for walkup NMR is to open the Setup EXP window (described in the next section):

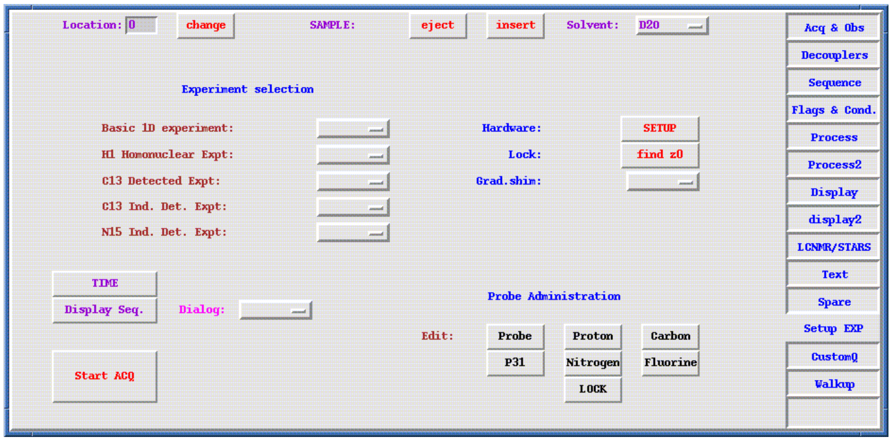
- select a solvent
- insert the sample
- select a experiment from a list in the window

Once an experiment is selected, a window appears for setting up, customizing, and running the experiment.

## 7.1 Setup EXP Window Experiments

Perform the following steps to set up an individual experiment:

1. Click the **Setup EXP** button in the right side of the Tcl/dg window. The Setup EXP window shown in Figure 35 is displayed. Do the following steps to set up and customize the experiment.



Location: 0

Solvent: D20

**Figure 35.** Setup EXP Window

2. Select the solvent in the sample management region of the window (Figure 35) by holding down the left mouse button on the solvent menu (Figure 36) and choosing the appropriate solvent from the solvent menu list.
3. Eject the current sample from the magnet and insert the new sample.

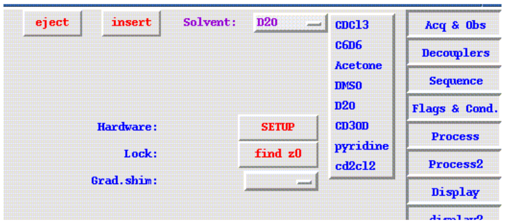


**Figure 36.** Setup EXP - Changing Samples

4. Click on the **Eject** and **Insert** buttons (Figure 36) in the sample management region of the **Setup EXP window** (Figure 35) **or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.
5. Lock and shim the sample.
6. Click on the *find z0* button (Figure 37) to AutoLock or manually establish lock.
7. Select a gradient shim method from the drop down Gradient Shim menu. Gradient shimming will take place when the start acquisition button is pressed.

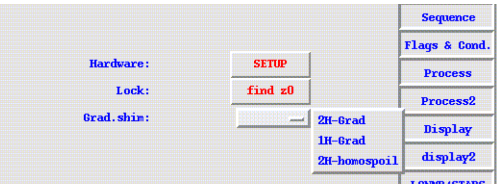
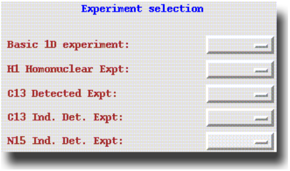
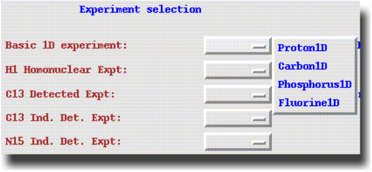


**Figure 37.** Setup EXP - Setup, Find Z0 and shim

8. Select the experiment you want to perform from the **Experiment selection** menus by holding down the left mouse button on the appropriate menu and selecting the “required” experiment from the menu list.



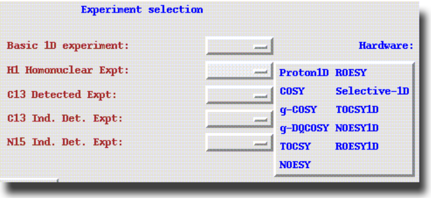
- Click on the **Basic 1D Experiments** button to run a basic 1D proton, carbon, phosphorus, or fluorine experiment. Select an experiment from the list.



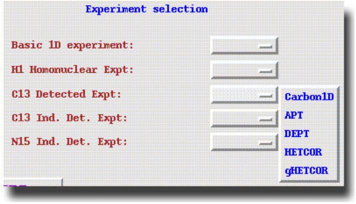
For proton1D and carbon1D experiments, standard parameters are selected from `stdpar/H1.par` and `stdpar/C13.par` files. For all other experiments, the current parameter set is modified. For example selecting HMQC converts the parameter set in the current experiment to do HMQC.

- Click the **H1 Homonuclear Expt** button to run proton detected 2D experiments. Select an experiment from the list.

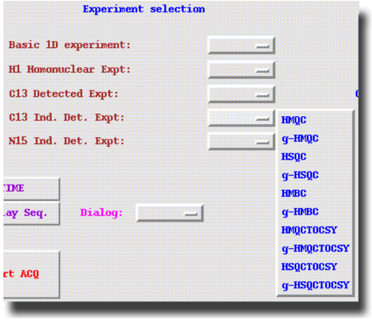
  For selective 1D experiments (such as tocsy1D or NOESY1D), a “processed” proton spectrum is required in the current experiment.



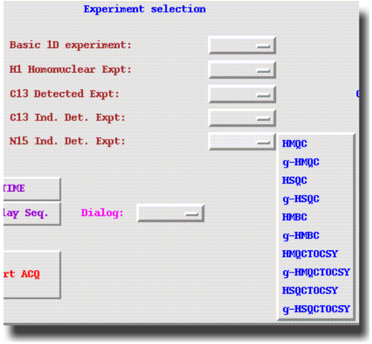
- Click the **C13 Detected Expt** button to run carbon and carbon detected 1D and 2D experiments. Select an experiment from the list.



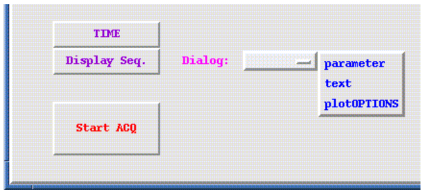
- Click the **C13 Ind. Det. Expt** button to run carbon indirect detection experiments. Select an experiment from the list.



- Click the **N15 Ind. Det. Expt.** button to run nitrogen indirect detection experiments. Select an experiment from the list.



9. After selecting an experiment, you can modify any parameters manually before starting the acquisition. Alternatively, you can use the **Do Parameter Dialog** button to open a dialog box. A customization window similar to those in Automated Experiment setup appears.



10. Start the acquisition by clicking the **start Acquisition** button. The acquired data is automatically processed at the end of the acquisition.

## 7.2 CustomQ Window Experiments

Selections listed below provide step-by-step instructions.

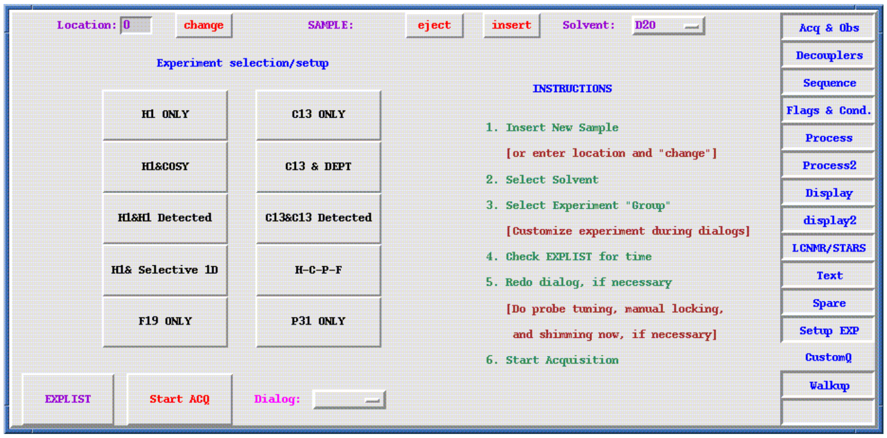
1. Begin with:
   - “Setting Up an Automated Experiment,” this page
2. Continue with one of the following experiments or experiment groups:
   - “Proton 1D Spectrum,” page 95
   - “Carbon 1D Spectrum,” page 97
   - “Phosphorus 1D Spectrum,” page 100
   - “User Cued HCPF 1Ds,” page 101
   - “H1 and COSY Experiments,” page 105
   - “C13 and DEPT Experiment,” page 107
   - “H1 and H1 Detected Experiments,” page 108
   - “C13 and C13 Detected Experiments,” page 112
   - “H1 and Selective 1D Experiments,” page 116

You access the same experiments through *CustomQ* interface in the Tcl/dg window and the *GLIDE* interface. The *CustomQ* interface provides menus and popup windows for easy experiment set up and acquisition.

### Setting Up an Automated Experiment

Perform the following steps to set up an experiment:

1. Click the **CustomQ** button in the left side of the Tcl/dg window to display it.



Location: 0

SAMPLE:

Solvent: D2O

Experiment selection/setup

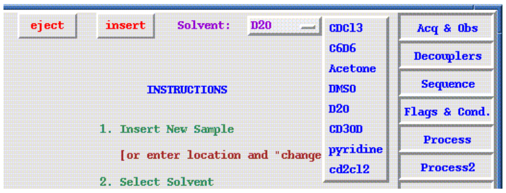
INSTRUCTIONS

1. Insert New Sample
   [or enter location and "change"]
2. Select Solvent
3. Select Experiment "Group"
   [Customize experiment during dialogs]
4. Check EXPLIST for time
5. Redo dialog, if necessary
   [Do probe tuning, manual locking,
   and shimming now, if necessary]
6. Start Acquisition

Dialog:

**Figure 38.** CustomQ Window

1. Eject the current sample from the magnet and insert the new sample.
2. **Click** on the **Eject** and **Insert** buttons (Figure 38) in the sample management region of the **CustomQ window** (Figure 39) **or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.



INSTRUCTIONS

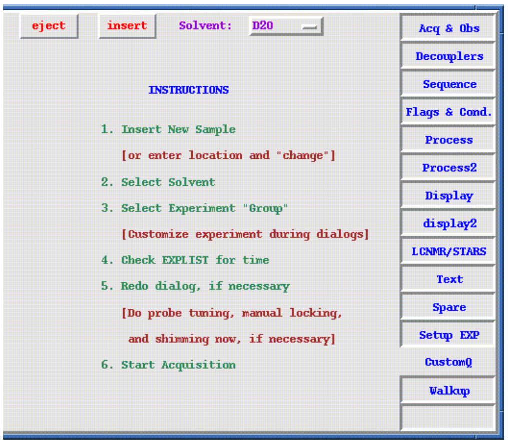
1. Insert New Sample

[or enter location and "change

2. Select Solvent

**Figure 39.** CustomQ - Changing Samples

3. Select the solvent in the sample management region of the window (Figure 38) by holding down the left mouse button on the solvent menu (Figure 39) and choosing the appropriate solvent from the solvent menu list.
4. **On screen** instructions (Figure 40) are provided to assist the user in setting up the automated experiment list.
5. Choose the experiment you want to perform by clicking on the button in the *Automated Experiment Selection and Setup* region of the **CustomQ** window.



INSTRUCTIONS

1. Insert New Sample

[or enter location and "change"]

2. Select Solvent

3. Select Experiment "Group"

[Customize experiment during dialogs]

4. Check EXPLIST for time

5. Redo dialog, if necessary

[Do probe tuning, manual locking,

and shimming now, if necessary]

6. Start Acquisition

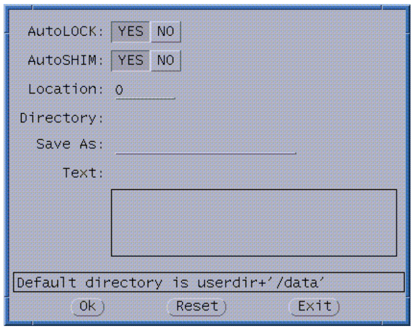
**Figure 40.** CustomQ - On Screen Instructions

## Proton 1D Spectrum

### *Setting Up and Customizing the Experiment*

1. Follow the directions in "Setting Up an Automated Experiment" on page 94 and select the **H1 Only** experiment from the **Experiment selection/setup** buttons.

   The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.



AutoLOCK: YES NO

AutoSHIM: YES NO

Location: 0

Directory:

Save As:

Text:

Default directory is userdir+'/data'

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
4. Enter appropriate text in the **Text** box for your sample.

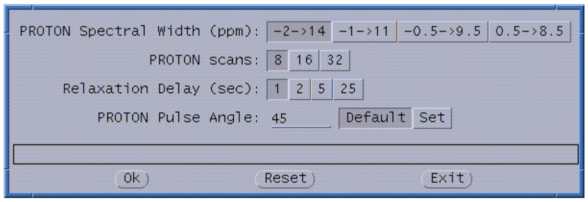


**Figure 41.** CustomQ Proton 1D Acquisition Options

5. Click on **OK**, then **Exit**. The window shown in Figure 41 opens.
6. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
7. Select the number of proton scans to acquire in the **PROTON scans** field.
8. Select a relaxation delay in the **Relaxation Delay (sec)** field.
9. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.
10. Click on **OK** and click on **Exit**.

    Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices. The **Text** panel displays the experiment that will be run.
11. Click on the **CustomQ** tab.
12. Click on the **Dialog** button in the *Display Sequence, Dialog (drop down menu), Time, and Start* region and select **plotOPTIONS** from the drop down menu.to start the customize the plot window. Skip this step to use the default plotting options.

13. Select Displayed Spectrum or Full Spectrum in the **Spectral Width** field.
14. Select Partial, Full, or Off in the **Plot Integral** field.
15. Select how to plot the parameters from the **Plot Parameters** menu.
16. Select a peak-picking option from the **Plot Peaks** menu.
17. Click on **OK** to save the values you selected or click **Reset** to return to the default conditions.
18. Click **Exit** to close the window.
19. If you set the **Autoshim** and **Autolock** options to **NO** in step 2, now is the time to manually lock and shim your sample. Tune the probe if needed.

## Acquiring the Spectrum

Click the **Start ACQ** button in the **CustomQ** window.

- The proton spectrum is acquired, plotted, and saved according to your choices.
- The FID is saved with the name PROTON.fid in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FID is saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

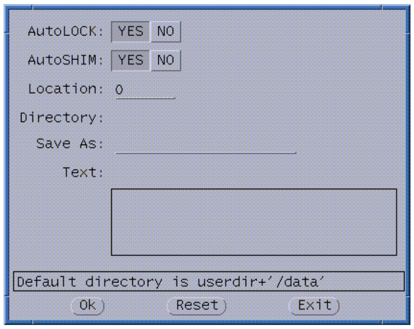
## Carbon 1D Spectrum

### *Setting Up and Customizing the Experiment*

1. Follow the directions in “Setting Up an Automated Experiment” on page 94 and select the **C13 Only** experiment from the **Experiment selection/setup** buttons.

   The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.

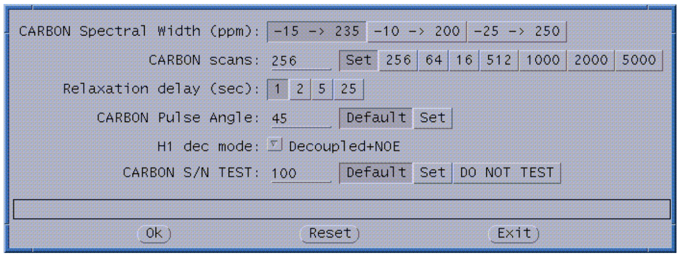
2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.



Location: 0

Default directory is userdir+'/data'

4. Enter appropriate text in the **Text** box for your sample.
5. Click on **OK**, then **Exit**. The window shown in Figure 42 opens.



CARBON scans: 256

CARBON Pulse Angle: 45

H1 dec mode: Decoupled+NOE

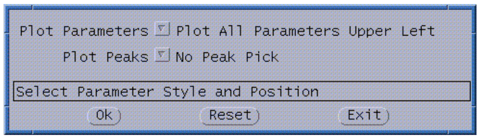
CARBON S/N TEST: 100

**Figure 42.** CustomQ Carbon 1D Acquisition Options

6. Select the spectral window in the **CARBON Spectral Width (ppm)** field and the number of scans to acquire or enter a value in the **CARBON scans** field.
7. Select a relaxation delay in the **Relaxation Delay (sec)** field and enter a value for the pulse angle (observe pulse) in the **`CARBON Pulse Angle`** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.
8. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
9. Select CARBON S/N TEST option: **Default** (S/N=100), **Set** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. The signal to noise is measured on the tallest peak in the spectrum which is often the solvent peak. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.
10. Click on **OK** and click on **Exit**.

Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices. The **Text** panel displays the experiment that will be run.

11. Click on the **CustomQ** tab.
12. Click on the **Dialog** button in the *Display Sequence, Dialog (drop down menu), Time, and Start* region and select **plotOPTIONS** from the drop down menu.to start the customize the plot window. Skip this step to use the default plotting options.



Plot Parameters: Plot All Parameters Upper Left

Plot Peaks: No Peak Pick

Select Parameter Style and Position

13. .Select how to plot the parameters from the **Plot Parameters** menu.
14. Select a peak-picking option from the **Plot Peaks** menu.
15. Click on **OK** to save the values you selected or click **Reset** to return to the default conditions.
16. Click **Exit** to close the window.
17. If you set the **Autoshim** and **Autolock** options to **NO** in step 2, now is the time to manually lock and shim your sample. Tune the probe if needed.

### *Acquiring the Spectrum*

Click the **Start ACQ** button in the **CustomQ** window.

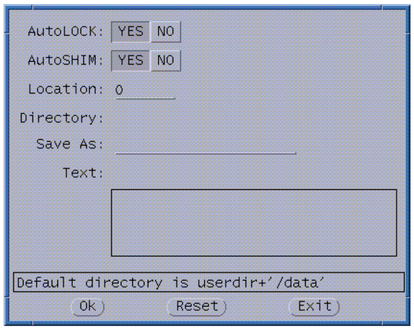
- The Carbon spectrum is acquired, plotted, and saved according to your choices.
- The FID is saved with the name CARBON.fid in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FID is saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## Fluorine 1D Spectrum

### *Setting Up and Customizing the Experiment*

1. Follow the directions in “Setting Up an Automated Experiment” on page 94 and select the **F19 Only** experiment from the **Experiment selection/setup** buttons.

   The AutoLOCK-AutoSHIM window shown in opens. Do the following steps to set up and customize the experiment.



AutoLOCK: YES NO

AutoSHIM: YES NO

Location: 0

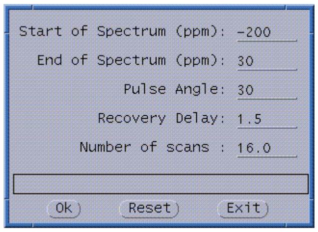
Directory:

Save As:

Text:

Default directory is userdir+'/data'

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
4. Enter appropriate text in the **Text** box for your sample.



Start of Spectrum (ppm): -200
End of Spectrum (ppm): 30
Pulse Angle: 30
Recovery Delay: 1.5
Number of scans : 16.0

**Figure 43.** CustomQ Fluorine 1D Acquisition Options

5. Click on **OK**, then **Exit**. The window shown in Figure 43 opens.
6. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window. Enter all values in **ppm**.
7. Enter a value for the **pulse angle**.
8. Enter a value for the **recovery delay**.
9. Enter the number of **scans to acquire**.
10. Click on **OK** to save the values you selected or click **Reset** to return to the default conditions.
11. Click on **Exit**.

    Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices. The **Text** panel displays the experiment that will be run.
12. Click on the **CustomQ** tab.
13. Click on the **Dialog** button in the *Display Sequence, Dialog (drop down menu), Time, and Start* region and select **plotOPTIONS** from the drop down menu.to start the customize the plot window. Skip this step to use the default plotting options.

Spectra Width: Displayed Spectrum Default
Plot Integral: Partial Full Off
Plot Parameters Plot All Parameters Upper Left
Plot Peaks No Peak Pick
Select Parameter Style and Position

14. Select Displayed Spectrum or Full Spectrum in the **Spectral Width** field.
15. Select Partial, Full, or Off in the **Plot Integral** field.
16. Select how to plot the parameters from the **Plot Parameters** menu.
17. Select a peak-picking option from the **Plot Peaks** menu.
18. Click on **OK** to save the values you selected or click **Reset** to return to the default conditions.
19. Click **Exit** to close the window.
20. If you set the **Autoshim** and **Autolock** options to **NO** in step 2, now is the time to manually lock and shim your sample. Tune the probe if needed.

## Acquiring the Spectrum

Click the **Start ACQ** button in the **CustomQ** window.

- The Fluorine spectrum is acquired, plotted, and saved according to your choices.
- The FID is saved with the name `FLUORINE.fid` in the directory `~/vnmrsys/data/`*`filename-date`*`.` If this directory already exists, the FID is saved in the directory `~/vnmrsys/data/`*`filename-date-time.`*

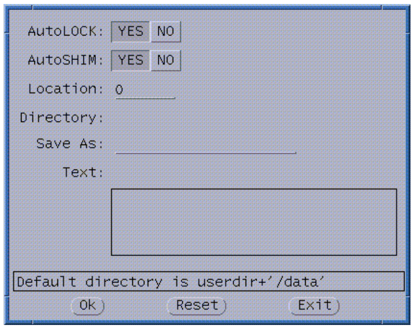
## Phosphorus 1D Spectrum

### Setting Up and Customizing the Experiment

1. Follow the directions in "Setting Up an Automated Experiment" on page 94 and select the **C13 Only** experiment from the **Experiment selection/setup** buttons.

   The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.


AutoLOCK: YES NO
AutoSHIM: YES NO
Location: 0
Directory:
Save As:
Text:
Default directory is userdir+'/data'

4. Enter appropriate text in the **Text** box for your sample.
5. Click on **OK**, then **Exit**. The window shown in Figure 44 opens.

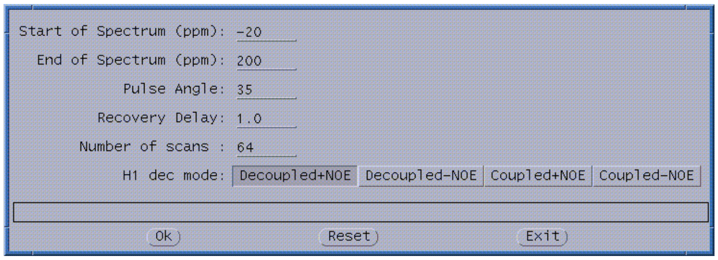

Start of Spectrum (ppm): -20
End of Spectrum (ppm): 200
Pulse Angle: 35
Recovery Delay: 1.0
Number of scans : 64
H1 dec mode: Decoupled+NOE Decoupled-NOE Coupled+NOE Coupled-NOE

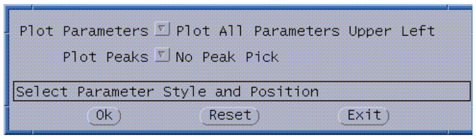
**Figure 44.** CustomQ Phosphorus 1D Acquisition Options

6. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window. Enter all values in **ppm**.
7. Enter a value for the **pulse angle**.
8. Enter a value for the **recovery delay**.
9. Enter the number of **scans to acquire**.
10. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
11. Click on **OK** to save the values you selected or click **Reset** to return to the default conditions.
12. Click on **Exit**.

    Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices. The **Text** panel displays the experiment that will be run.

13. Click on the **CustomQ** tab.

14. Click on the **Dialog** button in the *Display Sequence, Dialog (drop down menu), Time, and Start* region and select **plotOPTIONS** from the drop down menu.to start the customize the plot window. Skip this step to use the default plotting options.



Plot Parameters: Plot All Parameters Upper Left

Plot Peaks: No Peak Pick

Select Parameter Style and Position

15. Select Displayed Spectrum or Full Spectrum in the **Spectral Width** field.
16. Select how to plot the parameters from the **Plot Parameters** menu.
17. Select a peak-picking option from the **Plot Peaks** menu.
18. Click on **OK** to save the values you selected or click **Reset** to return to the default conditions.
19. Click **Exit** to close the window.
20. If you set the **Autoshim** and **Autolock** options to **NO** in step 2, now is the time to manually lock and shim your sample. Tune the probe if needed.

### *Acquiring the Spectrum*

Click the **Start ACQ** button in the **CustomQ** window.

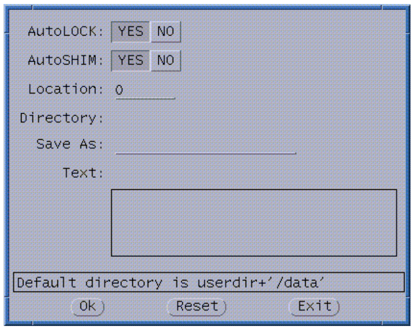
- The Phosphorus spectrum is acquired, plotted, and saved according to your choices.
- The FID is saved with the name `PHOSPHORUS.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FID is saved in the directory `~/vnmrsys/data//`*`filename-date-time`*.

## User Cued HCPF 1Ds

### *Setting Up and Customizing the Experiment*

1. Follow the directions in "Setting Up an Automated Experiment" on page 94 and select the **C13 Only** experiment from the **Experiment selection/setup** buttons.

   The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.



AutoLOCK: YES NO

AutoSHIM: YES NO

Location: 0

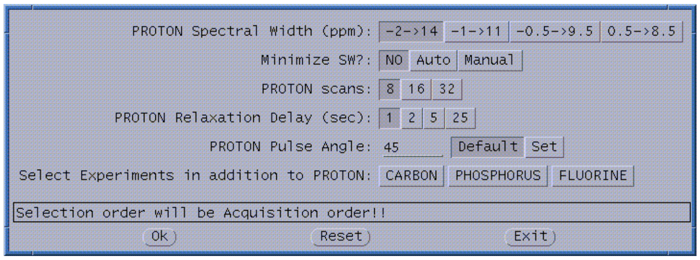
Directory:

Save As:

Text:

Default directory is userdir+'/data'

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
4. Enter appropriate text in the **Text** box for your sample.
5. Click on **OK**, then **Exit**. The window shown in Figure 45 opens.



PROTON Pulse Angle: 45

Selection order will be Acquisition order!!

**Figure 45.** CustomQ HCPF 1D Acquisition Options

## Proton Acquisition

1. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
2. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 1, **Auto** examines the proton 1D and sets SW, and **Manual** prompts the user for input after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button.
3. Select the number of proton scans to acquire in the **PROTON scans** field.
4. Select a relaxation delay in the **Relaxation Delay (sec)** field.
5. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on `Set` or click on **Default** to select a 45-degree pulse angle.

The remaining three nuclei are presented in this order: **CARBON, PHOSPHORUS,** and **FLUORINE**. The user has the option to acquire the 1D spectrum for each nucleus or combination of nuclei in any desired order. Acquisition will always begin with a **proton 1D** followed by the each nucleus in the order of its selection.

- Acquire the proton 1D spectra by doing the following:

a. Click on **OK** and **click Exit.** The experiment list is displayed in the Tcl/dg Text window.

b. Click on the **CustomQ** tab.

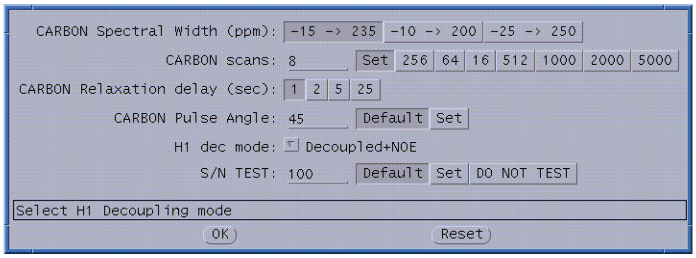
c. Click on the **Dialog** box and select plotting options.

d. Click the **Start ACQ** button to begin acquisition.

- Add another nucleus to the experiment list.

## Carbon Acquisition

1. Select **CARBON** to set bring up the carbon acquisition options window.



CARBON scans: 8

CARBON Pulse Angle: 45

H1 dec mode: Decoupled+NOE

S/N TEST: 100

Select H1 Decoupling mode

2. Select the spectral window in the **CARBON Spectral Width (ppm)** field.
3. Select the number of carbon scans to acquire or enter a value in the **CARBON scans** field.
4. Select a relaxation delay in the **Relaxation Delay (sec)** field.
5. Enter a value for the pulse angle (observe pulse) in the **CARBON Pulse Angle** field.
6. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
7. Select CARBON S/N TEST option: **Default** (S/N=100), **Set** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. The signal to noise is measured on the tallest peak in the spectrum which is often the solvent peak. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.
8. At this point you can do one of the following:
    - Click on **OK** if you want to save the values you selected and return to the *CustomQ HCPF 1D Acquisition Options* window.
    - Click **Reset** to return to the default settings and either accept the defaults by clicking **OK** or select new parameters and then clicking **OK** and return to the *CustomQ HCPF 1D Acquisition Options window.*
9. From the *CustomQ HCPF 1D Acquisition Options* window you can do one of the following:
    - Acquire the 1D spectra of the nuclei selected to this point by doing the following:

      a. Click on **OK** and click **Exit.** The experiment list is displayed in the Tcl/dg Text window.

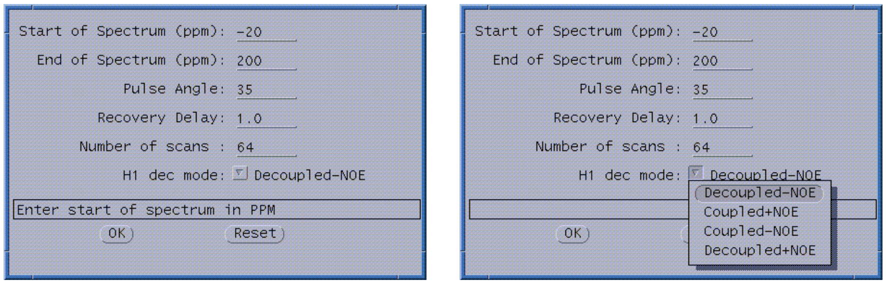
      b. Click on the **CustomQ** tab.

      c. Click on the **Dialog** box and select plotting options.

      d. Click the **Start ACQ** button to begin acquisition.
    - Add another nucleus to the experiment list.

### Phosphorus Acquisition

1. Click on **Phosphorus** in the *CustomQ HCPF 1D Acquisition Options* window. The window shown in Figure 46A opens.
2. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window (Figure 46A). Enter all values in **ppm**.
3. Enter a value for the **pulse angle**, **recovery delay**, and **scans to acquire** (Figure 46A).
4. Click on the decoupler mode button (Figure 46A) and, from the drop down menu (Figure 46B), select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal



Start of Spectrum (ppm): -20
End of Spectrum (ppm): 200
Pulse Angle: 35
Recovery Delay: 1.0
Number of scans : 64
H1 dec mode: Decoupled-NOE
Enter start of spectrum in PPM

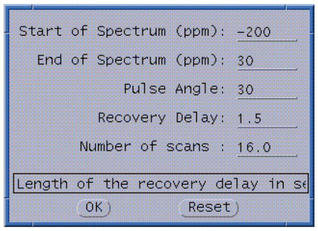
(A) (B)

**Figure 46.** CustomQ Phosphorus 1D Acquisition Options

decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).

5. At this point you can do one of the following:
   - Click on **OK** if you want to save the values you selected and return to the *CustomQ HCPF 1D Acquisition Options* window.
   - Click **Reset** to return to the default settings and either accept the defaults by clicking **OK** or select new parameters and then clicking **OK** and return to the *CustomQ HCPF 1D Acquisition Options* window.
6. From the *CustomQ HCPF 1D Acquisition Options* window you can do one of the following:
   - Acquire the 1D spectra of the nuclei selected to this point by doing the following:
     a. Click on **OK** and click **Exit.** The experiment list is displayed in the Tcl/dg Text window.
     b. Click on the **CustomQ** tab.
     c. Click on the **Dialog** box and select plotting options.
     d. Click the **Start ACQ** button to begin acquisition.
   - Add another nucleus to the experiment list.

## Fluorine Acquisition



Start of Spectrum (ppm): -200
End of Spectrum (ppm): 30
Pulse Angle: 30
Recovery Delay: 1.5
Number of scans : 16.0
Length of the recovery delay in s

**Figure 47.** CustomQ Fluorine 1D Acquisition Options

1. Click on **Fluorine** in the *CustomQ HCPF 1D Acquisition Options* window. The window shown in Figure 47 opens.
2. Enter a start of spectrum value in the **Start of Spectrum** field and an end of spectrum in the **End of Spectrum** field to set the spectral window. Enter all values in **ppm**.
3. Enter a value for the **pulse angle**.
4. Enter a value for the **recovery delay**.
5. Enter the number of **scans to acquire**.
6. At this point you can do one of the following:
   - Click on **OK** if you want to save the values you selected and return to the *CustomQ HCPF 1D Acquisition Options window.*

  - Click **Reset** to return to the default settings and either accept the defaults by clicking **OK** or select new parameters and then clicking **OK** and return to the *CustomQ HCPF 1D Acquisition Options window.*

7. From the *CustomQ HCPF 1D Acquisition Options* window you can do one of the following:
   - Acquire the 1D spectra of the nuclei selected to this point by doing the following:

   a. Click on **OK** and click **Exit.** The experiment list is displayed in the Tcl/dg Text window.

   b. Click on the **CustomQ** tab.

   c. Click on the **Dialog** box and select plotting options.

   d. Click the **Start ACQ** button to begin acquisition.

   - Add another nucleus to the experiment list.

When you have finished selecting the nuclei and related acquisition parameters, the spectra will be acquired in order of their selection beginning with a proton 1D spectrum.

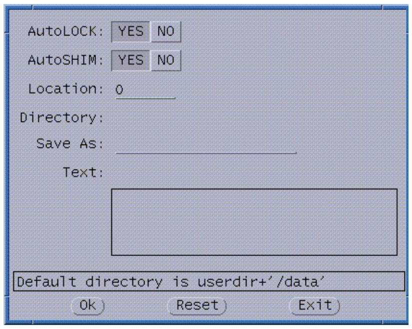
## H1 and COSY Experiments

Depending on the type of probe (PFG or non-PFG) and the system, this experiment automatically selects the gCOSY (PFG probe) or COSY (nonPFG probe) experiment.

### *Setting Up and Customizing the Experiment*

1. Follow the directions in “Setting Up an Automated Experiment” on page 94 and select the **H1&COSY** experiment from the **Experiment selection/setup** buttons.

   The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.

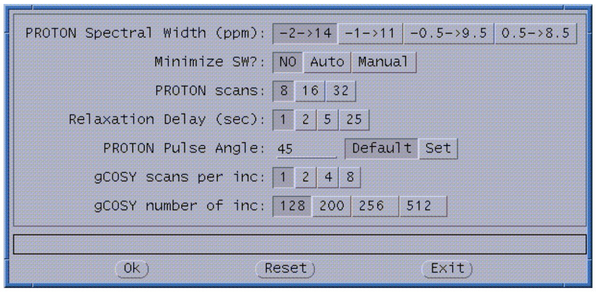


AutoLOCK: YES NO
AutoSHIM: YES NO
Location: 0
Directory:
Save As:
Text:
Default directory is userdir+'/data'

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.

3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.

4. Enter appropriate text in the **Text** box for your sample.



PROTON Spectral Width (ppm): -2->14 -1->11 -0.5->9.5 0.5->8.5

Minimize SW?: NO Auto Manual

PROTON scans: 8 16 32

Relaxation Delay (sec): 1 2 5 25

PROTON Pulse Angle: 45 Default Set

gCOSY scans per inc: 1 2 4 8

gCOSY number of inc: 128 200 256 512

**Figure 48.** CustomQ $^1$H and $^1$H Cosy Acquisition Options

5. Click on **OK** and click on **Exit**. The window shown in Figure 48 opens.
6. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
7. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 6, **Auto** examines the proton 1D and sets SW, and **Manual** prompts the user for input after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button. The COSY experiment executes using this SW.
8. Select the number of proton scans to acquire in the **PROTON scans** field.
9. Select a relaxation delay in the **Relaxation Delay (sec)** field.
10. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.
11. Select the number of scans per increment to acquire for the COSY experiment.
12. Select the number of increments to acquire for the COSY experiment.
13. Click the **OK** button to save the values you selected or click **Reset** to return to the default settings.
14. Click on **OK** and **click Exit**

    The experiment list is displayed in the Tcl/dg Text window.

    Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices. The **Text** panel displays the experiment that will be run.
15. If you set the **Autoshim** and **Autolock** options to **NO**, now is the time to manually lock and shim your sample. Tune the probe if needed.

## Acquiring the Spectrum

1. Click on the **CustomQ** tab.
2. Click on the **Dialog** box and select plotting options.
3. Click the **Start ACQ** button in the Tcl/dg CustomQ window.

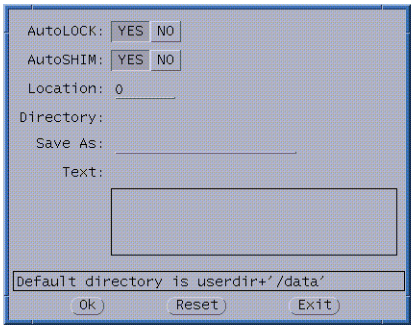
- The proton and COSY spectra are acquired and saved according to your choices.
- The proton data is processed and plotted using the default choices in the `stdpar/H1.par` file. The COSY data is processed and a full spectrum is plotted.
- The FID is saved with the name `PROTON.fid` and `COSY.fid` (or `gCOSY.fid` for gradient probe) in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## C13 and DEPT Experiment

### *Setting Up and Customizing the Experiment*

1. Follow the directions in "Setting Up an Automated Experiment" on page 94 and select the **C13 & DEPT** experiment from the **Experiment selection/setup** buttons.

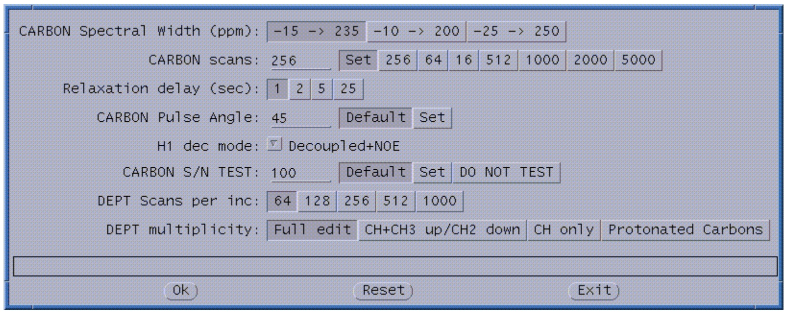
   The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.



Location: 0

Default directory is userdir+'/data'

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
4. Enter appropriate text in the **Text** box for your sample.
5. Click on **OK** and click on **Exit**. The window shown in Figure 49 opens.



CARBON scans: 256

CARBON Pulse Angle: 45

H1 dec mode: Decoupled+NOE

CARBON S/N TEST: 100

**Figure 49.** CustomQ $^{13}$C and DEPT Acquisition Options

6. Select the spectral window in the **CARBON Spectral Width (ppm)** field and the number of scans to acquire or enter a value in the **CARBON scans** field.
7. Select a relaxation delay in the **Relaxation Delay (sec)** field and enter a value for the pulse angle (observe pulse) in the **CARBON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.
8. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
9. Select CARBON S/N TEST option: **Default** (S/N=100), **Set** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. The signal to noise is measured on the tallest peak in the spectrum which is often the solvent peak. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.

10. Select the number of **DEPT Scans per inc:** to acquire for the DEPT experiment.
11. Select a **DEPT multiplicity**.
    a. **Full Edit** produces 4 edited sub-spectra showing: all protonated carbons, CH carbons only, $CH_2$ carbons only, and $CH_3$ carbons only.
    b. **CH and CH3 up/CH2 down** produces an unedited dept 135 experiment.
    c. **CH only** produces and unedited dept 90 experiment.
    d. **Protonated Carbons** produces an unedited spectra containing only protonated carbons.
12. Click the **OK** button to save the values you selected or click **Reset** to return to the default settings.
13. Click on **OK** and click **Exit**

    The experiment list is displayed in the Tcl/dg Text window.

    Standard proton parameters are recalled. Relevant parameters and text are reset according to your choices. The **Text** panel displays the experiment that will be run.
14. If you set the **Autoshim** and **Autolock** options to **NO**, now is the time to manually lock and shim your sample. Tune the probe if needed.

### *Acquiring the Spectrum*

1. Click on the **CustomQ** tab.
2. Click on the **Dialog** box and select plotting options.
3. Click the **Start ACQ** button in the Tcl/dg CustomQ window.

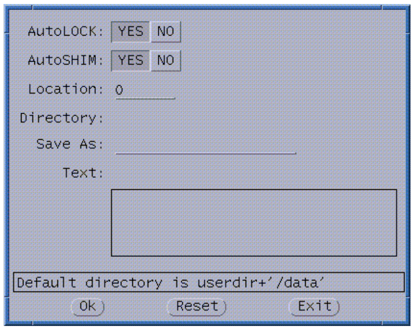
- The carbon and DEPT spectra are acquired and saved according to your choices.
- The carbon data is processed and plotted using the default choices in the `stdpar/C13.par` file. The DEPT data is processed and full spectra is plotted.
- The FID is saved with the name CARBON.fid and DEPT. in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time.`*

## H1 and H1 Detected Experiments

An experiment chain of H1, gCOSY, HMQC, gHMBC, and gHSQCTOXY representing a portion of the available H1 and H1 detected experiments accessible through the CustomQ interface is described below.

### *Setting Up and Customizing the Experiment*

1. Follow the directions in "Setting Up an Automated Experiment" on page 94 and select the **H1&H1 Detected** experiment from the **Experiment selection/setup** buttons.

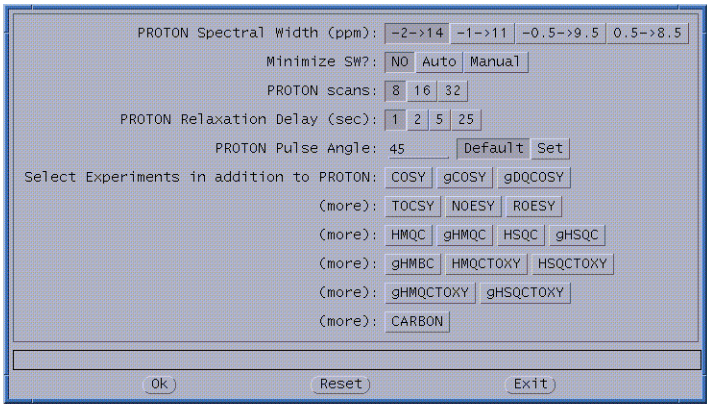


Location: 0

Default directory is userdir+'/data'

The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
4. Enter appropriate text in the **Text** box for your sample.
5. Click on **OK** and click on **Exit**. The window shown in Figure 50 opens.



PROTON Pulse Angle: 45

**Figure 50.** CustomQ $^1$H and $^1$H Detected Experiments Selection Window

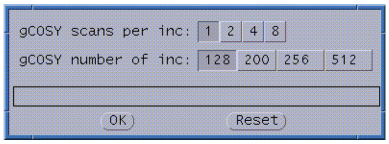
## Proton Acquisition

1. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
2. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 1, **Auto** examines the proton 1D and sets SW, and **Manual** prompts the user for input after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button.
3. Select the number of proton scans to acquire in the **PROTON scans** field.
4. Select a relaxation delay in the **Relaxation Delay (sec)** field.
5. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.

## Acquisition of Selected 1H Detected Experiments

All chained experiments begin with a 1D spectrum, in this case a proton 1D. Selected experiments are run, following the 1D experiment, in the order in which they are selected. Each experiment has an associated popup window for customizing the acquisition parameters associated with the experiment. In this example the order of the experiments, following the proton 1D is: gCOSY, HMQC, gHMBC, and gHSQCTOXY.

*gCOSY Acquisition*

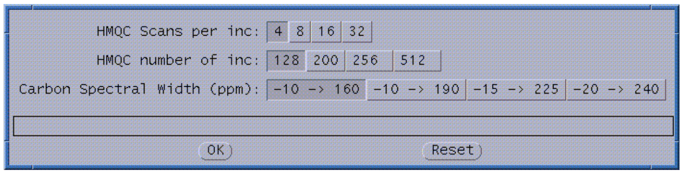


1. Select **gCOSY** and open the gCOSY Acquisition popup window.
2. Select a value for **gCOSY scans per inc** to acquire from the choices in the popup window.
3. Select a value for **gCOSY number of inc** to acquire from the choices in the popup window.
4. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

   gCOSY is added to the experiment chain.

*HMQC Acquisition*

1. Select **HMQC** and open the HMQC Acquisition popup window.

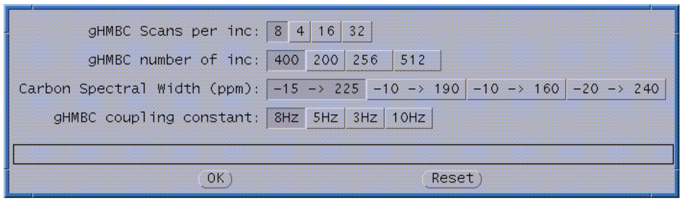


2. Select a value for **HMQC scans per inc** to acquire from the choices in the popup window.
3. Select a value for **HMQC number of inc** to acquire from the choices in the popup window.
4. Select a **Carbon Spectra Width (ppm)** from the choices presented.
5. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

   HSQC is added to the experiment chain.

*gHMBC Acquisition*

1. Select **gHMBC** and open the gHMQC Acquisition popup window.



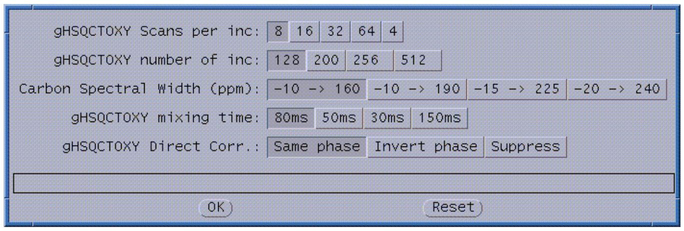
2. Select a value for **gHMBC scans per inc** to acquire from the choices in the popup window.

3. Select a value for **gHMBC number of inc** to acquire from the choices in the popup window.
4. Select a **Carbon Spectra Width (ppm)** from the choices presented.
5. Select a **gHMBC coupling constant** from the choices presented.
6. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

   gHMBC is added to the experiment chain.

*gHSQCTOXY Acquisition*

1. Select **gHSQCTOXY** and open the gHHSQCTOXY Acquisition popup window.



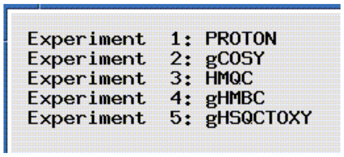
```
    gHSQCTOXY Scans per inc: 8 | 16 | 32 | 64 | 4
    gHSQCTOXY number of inc: 128 | 200 | 256 | 512
Carbon Spectral Width (ppm): -10 -> 160 | -10 -> 190 | -15 -> 225 | -20 -> 240
     gHSQCTOXY mixing time: 80ms | 50ms | 30ms | 150ms
    gHSQCTOXY Direct Corr.: Same phase | Invert phase | Suppress
```

2. Select a value for **gHSQCTOXY scans per inc** to acquire from the choices in the popup window.
3. Select a value for **gHSQCTOXY number of inc** to acquire from the choices in the popup window.
4. Select a **Carbon Spectra Width (ppm)** from the choices presented.
5. Select a **gHSQCTOXY mixing time** from the choices presented.
6. Select a **gHSQCTOXY Direct Corr.** from the choices presented.
7. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and H1 Detected Experiments window.

   gHSQCTOXY is added to the experiment chain.

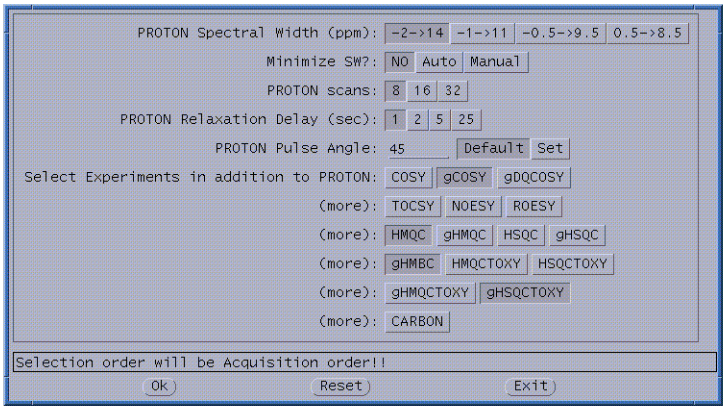
The Select H1 and H1 Detected Experiments window shows the selected experiments and proton 1D acquisition parameters, see Figure 51..

## Verifying the Experiment List



```
Experiment  1: PROTON
Experiment  2: gCOSY
Experiment  3: HMQC
Experiment  4: gHMBC
Experiment  5: gHSQCTOXY
```

The order that you selected experiments in the Acquisition Setup window is the acquisition order which is displayed in the Text panel of the dg screen. To remove a selection from the experiment chain, deselect it by clicking on the button again. For example, clicking the gHSQCTOXY button a second time deselects it and removes any saved parameter customization for gHSQCTOXY.



PROTON Pulse Angle: 45

Selection order will be Acquisition order!!

**Figure 51.** CustomQ Selected H1 and H1 Detected Experiments

1. Click the **OK** button to save the values you selected or click **Reset** to return to the default settings.
2. Click on **OK** and **click Exit**

   The experiment list is displayed in the Tcl/dg Text window.

   Standard proton parameters are recalled, and relevant parameters and text are reset according to your choices.
3. If you set the **Autoshim** and **Autolock** options to **NO**, now is the time to manually lock and shim your sample. Tune the probe if needed.

### *Acquiring the Spectrum*

1. Click on the **CustomQ** tab.
2. Click on the **Dialog** box and select plotting options.
3. Click the **Start ACQ** button in the Tcl/dg CustomQ window.
4. Click the **Start Acquisition** button in the Tcl/dg CustomQ window.

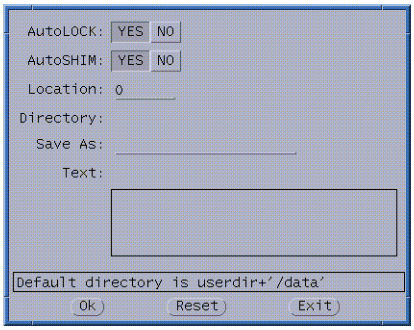
- Spectra are acquired, processed, plotted and saved.
- The FIDs are saved with the names `PROTON.fid`, `gCOSY.fid`, `HMQC.fid`, `gHMBC.fid`, and `HSQCTOXY.fid` in the directory `~/vnmrsys/data`*`/filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time`*.

## C13 and C13 Detected Experiments

An experiment chain of proton, carbon, APT, DEPT, and gHETCOR representing a portion of the available C13 and C13 detected experiments accessible through the CustomQ interface is described below.

### *Setting Up and Customizing the Experiment*

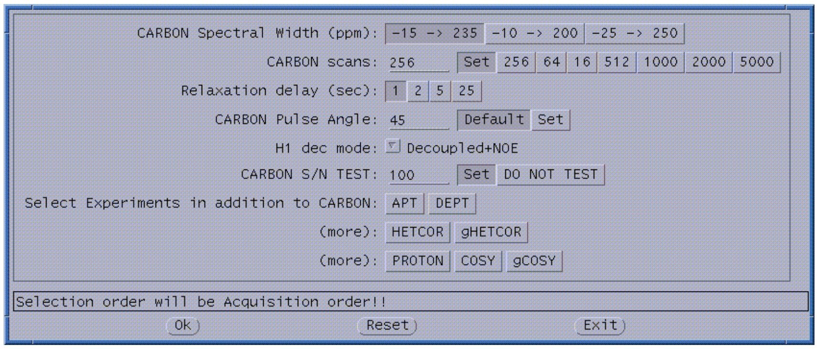
1. Follow the directions in "Setting Up an Automated Experiment" on page 94 and select the **H1&H1 Detected** experiment from the **Experiment selection/setup** buttons.



AutoLOCK: YES NO
AutoSHIM: YES NO
Location: 0
Directory:
Save As:
Text:
Default directory is userdir+'/data'

The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
4. Enter appropriate text in the **Text** box for your sample.
5. Click on **OK** and click on **Exit**. The window shown in Figure 52 opens.



CARBON Spectral Width (ppm): -15 -> 235 | -10 -> 200 | -25 -> 250
CARBON scans: 256 | Set | 256 | 64 | 16 | 512 | 1000 | 2000 | 5000
Relaxation delay (sec): 1 | 2 | 5 | 25
CARBON Pulse Angle: 45 | Default | Set
H1 dec mode: Decoupled+NOE
CARBON S/N TEST: 100 | Set | DO NOT TEST
Select Experiments in addition to CARBON: APT | DEPT
(more): HETCOR | gHETCOR
(more): PROTON | COSY | gCOSY
Selection order will be Acquisition order!!

**Figure 52.** CustomQ Selected C13 and C13 Detected Experiments Window

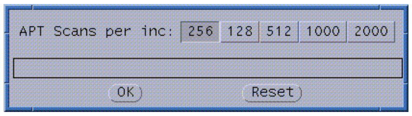
## Carbon Acquisition

1. Select the spectral window in the **CARBON Spectral Width (ppm)** field and the number of scans to acquire or enter a value in the **CARBON scans** field.
2. Select a relaxation delay in the **Relaxation Delay (sec)** field and enter a value for the pulse angle (observe pulse) in the **CARBON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.
3. Select a decoupler mode. Click on the **H1 dec mode** menu button and left click on the decoupler mode. The choices are: Decoupled+NOE (normal decoupled spectrum with NOE), Decoupled-NOE (decoupled spectrum with no NOE - used for integration), Coupled+NOE (coupled spectrum with NOE), and Coupled-NOE (coupled spectrum with no NOE).
4. Select a CARBON S/N TEST option: **Default** (S/N=100), **Set** (user entered value in test field), or **DO NOT TEST**. If either the Default or Set option is selected, the acquisition continues until the signal to noise tests matches the value in the test field or the number of carbon scans are reached, which ever comes first. If the DO NOT TEST options is selected, acquisition continues until the number of carbon scans set in the CARBON scans field are acquired.

## Acquisition of Selected 13C Detected Experiments

All chained experiments begin with a 1D S2PUL experiment. If the proton 1D experiment option is selected, it will be the first experiment run regardless of when it is selected. The proton 1D experiment is followed by a carbon S2PUL. Selected experiments are run, following the carbon S2PUL experiment, in the order in which they are selected. Each experiment has an associated popup window for customizing the acquisition parameters associated with the experiment. In this example the order of the experiments, following the carbon 1D is: APT, DEPT, and gHETCOR.

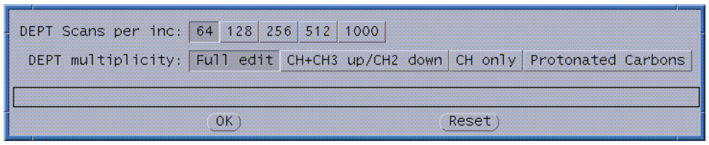
### *APT Acquisition*



1. Select **APT** from the Select C13 and C13 Detected Experiments window and the APT Acquisition popup window opens.
2. Select the number of **APT Scans per inc:** to acquire for the APT experiment.
3. Click OK to use the values chosen and return to the Select C13 and C13 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select C13 and C13 Detected Experiments window.

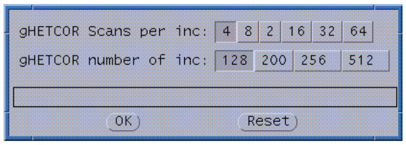
### *DEPT Acquisition*

1. Select **DEPT** from the Select C13 and C13 Detected Experiments window and the DEPT Acquisition popup window opens.



2. Select the number of **DEPT Scans per inc:** to acquire for the DEPT experiment.
3. Select a **DEPT multiplicity**.
4. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select C13 and C13 Detected Experiments window.

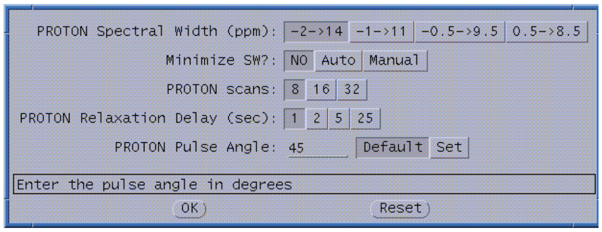
### *gHETCOR Acquisition*



1. Select **gHETCOR** from the Select C13 and C13 Detected Experiments window and the gHETCOR Acquisition popup window opens.
2. Select a value for **gHETCOR scans per inc** to acquire from the choices in the popup window.
3. Select a value for **gHETCOR number of inc** to acquire from the choices in the popup window.
4. Click OK to use the values chosen and return to the Select C13 and C13 Detected Experiments window. Click RESET to return to the default values and either use the

default values or enter different parameters. Click OK to close the popup window and return to the Select C13 and C13 Detected Experiments window.

*Proton Acquisition*

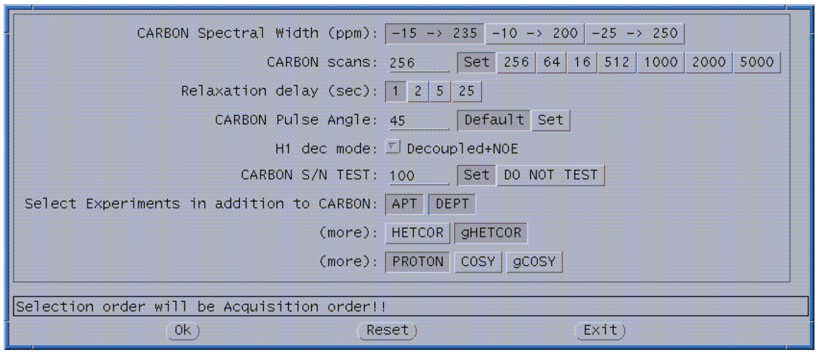


PROTON Pulse Angle: 45

Enter the pulse angle in degrees

1. Select **PROTON** from the Select C13 and C13 Detected Experiments window and the DEPT Acquisition popup window opens.
2. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
3. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 2, **Auto** examines the proton 1D and sets SW, and **Manual** prompts the user for input after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button. The HETCOR experiment executes using this SW.
4. Select the number of proton scans to acquire in the **`PROTON scans`** field.
5. Select a relaxation delay in the **Relaxation Delay (sec)** field.
6. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.
7. Click **OK** to use the values chosen and return to the Select **H1 and H1 Detected Experiments** window. Click **RESET** to return to the default values and either use the default values or enter different parameters. Click **OK** to close the popup window and return to the Select **C13 and C13 Detected Experiments** window.

The Select **C1 and C13 Detected Experiments** window shows the selected experiments and proton 1D acquisition parameters..



CARBON scans: 256

CARBON Pulse Angle: 45

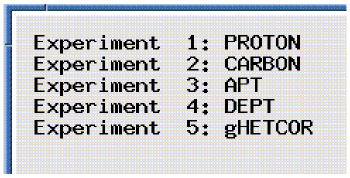
H1 dec mode: Decoupled+NOE

CARBON S/N TEST: 100

Selection order will be Acquisition order!!

### Verifying the Experiment List

PROTON always runs first followed by CARBON and the other experiments in the order that you selected experiments in the Acquisition Setup window is the acquisition order which is displayed in the Text panel of the dg screen. To remove a selection from the experiment chain, deselect it by clicking on the button again. For example, clicking the DEPT button a second time deselects it and removes any saved parameter customization for DEPT.



```
Experiment  1: PROTON
Experiment  2: CARBON
Experiment  3: APT
Experiment  4: DEPT
Experiment  5: gHETCOR
```

1. Click the **OK** button to save the values you selected or click **Reset** to return to the default settings.
2. Click on **OK** and click **Exit**

   The experiment list is displayed in the Tcl/dg Text window.

   Standard proton parameters are recalled.

   Relevant parameters and text are reset according to your choices.
3. If you set the **Autoshim** and **Autolock** options to **NO**, now is the time to manually lock and shim your sample. Tune the probe if needed.

### Acquiring the Spectrum

1. Click on the **CustomQ** tab.
2. Click on the **Dialog** box and select plotting options.
3. Click the **Start ACQ** button in the Tcl/dg CustomQ window.
4. Click the **Start Acquisition** button in the Tcl/dg CustomQ window.

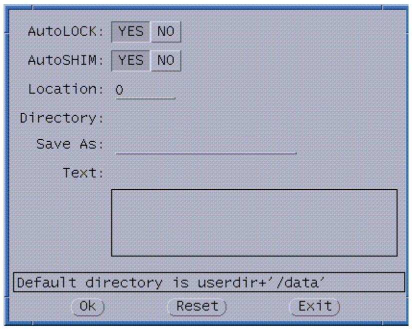
- Spectra are acquired, processed, plotted and saved.
- The FIDs are saved with the names `PROTON.fid`, `CARBON.fid`, `APT.fid`, and `HETCOR.fid` in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data`*`/filename-date-time`*.

## H1 and Selective 1D Experiments

An experiment chain of H1, TOCSY1D, and NOESY1D representing a portion of the available H1 and Selective H1 experiments accessible through the CustomQ interface is described below.

### Setting Up and Customizing the Experiment

1. Follow the directions in "Setting Up an Automated Experiment" on page 94 and select the **H1& Selective 1D** experiment from the **Experiment selection/setup** buttons.

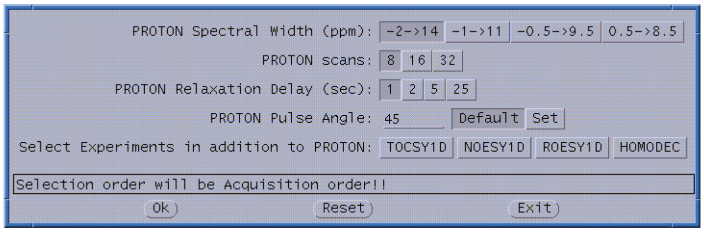


AutoLOCK: YES NO
AutoSHIM: YES NO
Location: 0
Directory:
Save As:
Text:

Default directory is userdir+'/data'

The AutoLOCK-AutoSHIM window opens. Do the following steps to set up and customize the experiment.

2. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to manually lock and shim your sample.
3. Enter a name for the directory, in the **Save As** field, to save the FID after the experiment is completed. If no file name is entered, the login name is used as the name.
4. Enter appropriate text in the **Text** box for your sample.
5. Click on **OK** and click on **Exit**. The window shown in Figure 53 opens.



PROTON Spectral Width (ppm): -2->14 -1->11 -0.5->9.5 0.5->8.5
PROTON scans: 8 16 32
PROTON Relaxation Delay (sec): 1 2 5 25
PROTON Pulse Angle: 45 Default Set
Select Experiments in addition to PROTON: TOCSY1D NOESY1D ROESY1D HOMODEC

Selection order will be Acquisition order!!

**Figure 53.** CustomQ H1 and Selective 1D Experiments Window

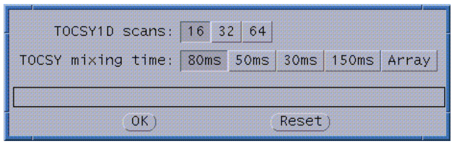
## *Proton Acquisition*

1. Select the spectral window in the **PROTON Spectral Width (ppm)** field.
2. Select an option for “Minimize SW?” **NO** uses the proton spectral width selected in step 1, **Auto** examines the proton 1D and sets SW, and **Manual** prompts the user for input after the 1D spectra has been acquired. If you select **Manual**, the proton spectrum is acquired and a **SetSW** button appears on the second row of the VNMR menu bar. Using the mouse, place the cursors on either side of proton spectrum that is displayed and press the **SetSW** button. The selective 1D experiment executes using this SW.
3. Select the number of proton scans to acquire in the **PROTON scans** field.
4. Select a relaxation delay in the **Relaxation Delay (sec)** field.
5. Enter a value for the pulse angle (observe pulse) in the **PROTON Pulse Angle** field and click on **Set** or click on **Default** to select a 45-degree pulse angle.

## *Acquisition of Selected 1H Selective Experiments*

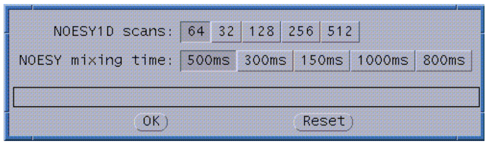
All chained experiments begin with a 1D spectrum, in this case a proton 1D. Selected experiments are run, following the 1D experiment, in the order in which they are selected. Each experiment has an associated popup window for customizing the acquisition parameters associated with the experiment. In this example the order of the experiments, is PROTON 1D, TOCSY1D, and NOSY1D.

*TOCSY1D Acquisition*



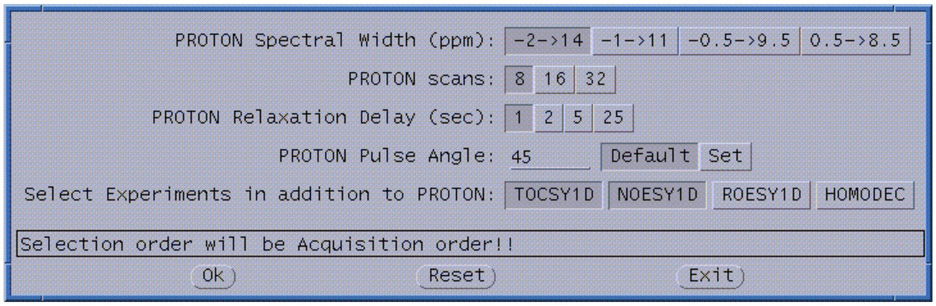
1. Select **TOCSY1D** and open the TOCSY1D Acquisition popup window.
2. Select a value for **TOCSY1D scans per inc** to acquire from the choices in the popup window.
3. Select a value for **TOCSY1D mixing time** from the choices in the popup window.
4. Click OK to use the values chosen and return to the Select H1 and Selective 1D Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and Selective 1D Experiments window.
5. TOCSY1D is added to the experiment chain.

*NOESY1D Acquisition*



1. Select **NOESY1D** and open the NOESY1D Acquisition popup window.
2. Select a value for **NOESY1D scans per inc** to acquire from the choices in the popup window.
3. Select a value for **NOESY1D mixing time** from the choices in the popup window.
4. Click OK to use the values chosen and return to the Select H1 and H1 Detected Experiments window. Click RESET to return to the default values and either use the default values or enter different parameters. Click OK to close the popup window and return to the Select H1 and Selective 1D Experiments window.
5. NOESY1D is added to the experiment chain.

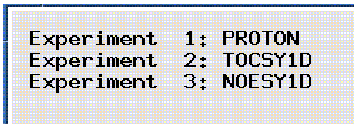
The Select H1 and H1 Selective Experiments window shows the selected experiments and proton 1D acquisition parameters..



Selection order will be Acquisition order!!

## Verifying the Experiment List

The order that you selected experiments in the Acquisition Setup window is the acquisition order which is displayed in the Text panel of the dg screen.



```
Experiment  1: PROTON
Experiment  2: TOCSY1D
Experiment  3: NOESY1D
```

To remove a selection from the experiment chain, deselect it by clicking on the button again. For example, clicking the TOCSY1D button a second time deselects it and removes any saved parameter customization for TOCSY1D.

1. Click the **OK** button to save the values you selected or click **Reset** to return to the default settings.
2. Click on **OK** and click **Exit**

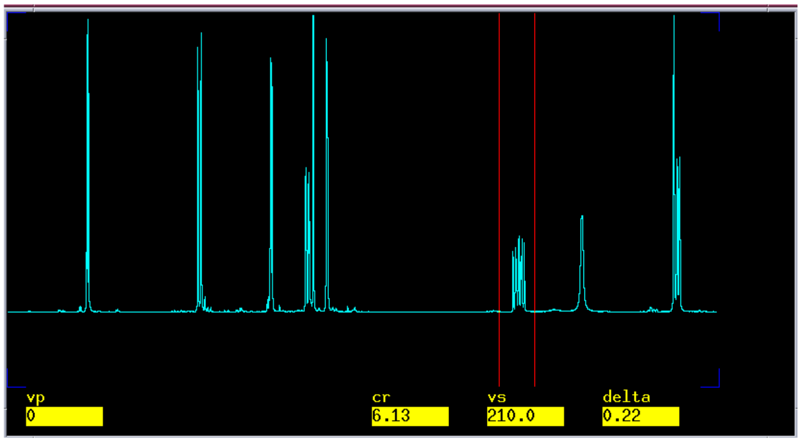
   The experiment list is displayed in the Tcl/dg Text window.

   Standard proton parameters are recalled, and relevant parameters and text are reset according to your choices.
3. If you set the **Autoshim** and **Autolock** options to **NO**, now is the time to manually lock and shim your sample. Tune the probe if needed.

### Acquiring the Spectrum

1. Click on the CustomQ tab.
2. Click on the **Dialog** box and select plotting options.
3. Click the **Start ACQ** button in the Tcl/dg CustomQ window.
4. Click the **Start Acquisition** button in the Tcl/dg CustomQ window.

TOCSY1D experiment parameters are set up and the proton spectrum is displayed (Figure 54). Five buttons appear on the second row of the VNMR menu bar, **Cursor, Expand, Select**, **Proceed, Cancel, restart, and Return**.



vp 0

cr 6.13

vs 210.0

delta 0.22

**Figure 54.** CustomQ Selection of Peaks for TOCSY1D and NOESY1D

5. Select the peak you want using the left and right mouse buttons by placing two cursors on either side of the peak. Expand the proton spectrum as needed.
6. Click the **Select** button on the menu bar.

   Select additional peaks repeating step 5 and step 6 for a series of TOCSY1D spectra.
7. Click the **Proceed** button to start a series of TOCSY1D acquisitions.

   TOCSY1D spectra are acquired and individually saved. NOESY1D experiment parameters are set up and the proton spectrum is redisplayed to enable peak selection for NOESY1D.
8. Repeat step 6 and step 7 to select peaks and start NOESY1D acquisition.
9. Click the **Proceed** button to start a series of NOESY1D spectra.

   NOESY1D spectra are acquired and individually saved.

All FIDs are saved with the file names `PROTON.fid`, `TOCSY1D_ppm1.fid`, `TOCSY1D_ppm2.fid`, etc., `NOESY1D_ppm3.fid`, `NOESY1D_ppm4.fid`, etc., where `ppm1` to `ppm4` are center of the selected band. The HOMODEC experiment is run as an array of decoupling frequencies and saved as `HOMODEC.fid`.

The FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date`*. If this directory already exists, the FIDs are saved in the directory `~/vnmrsys/data/`*`filename-date-time.`*

## 7.3 Walkup Window

### *Acquiring the Spectrum*

1. Click on the **Walkup** tab in the Tcl/dg window to display the *Walkup interface*.
2. **Change** the sample and insert a new sample. Use the **Sample Management** menus and buttons. Click the **Eject** and **Insert** buttons to eject a sample and insert the new sample. If the system is equipped with a sample changer, enter the location of the sample in the **Location window** and click the **change** button.
3. **Select** the appropriate lock solvent from the list of lock solvents available in the drop down **Solvent** menu.
4. **Automated Experiment Selection and Setup** buttons - all parameters are preset.
5. **Start Acquisition** button.
6. Spectra are acquired and plotted automatically.

# *Chapter 8.* Tcl/Tk NMR Administration and Calibration

Sections in this chapter:

- 8.1 “Administration of Probe Calibration Files,” this page
- 8.2 “System Calibrations Using the Calibrate Macro,” page 124
- 8.3 “Manually Editing the Probe File,” page 135

## 8.1 Administration of Probe Calibration Files

The probes file needs to be maintained in order for walkup NMR to properly work. This section contains general guidelines for required calibrations.

**Setup EXP**, **CustomQ**, and **Walkup** NMR require maintaining calibrations for each probe. Beginning with VNMR 5.3B, the calibration results for each probe are stored in a file and retrieved by the setup macros (HMQC, HMBC, COSY, etc.) as needed. Therefore, only one generic parameter set is required for each nucleus (`stdpar`) or experiment (`parlib`), and the probe-specific parameter values are retrieved from the calibration files, which are located in a directory specific to a given probe. These probe-specific directories are all subdirectories of a directory called `probes`, either `/vnmr/probes` or `userdir+/probes`, with the usual distinction between all-user and individual access. In general, it is better to use the `/vnmr/probes` directory.

Autocalibration procedures (described in “System Calibrations Using the Calibrate Macro” on page 124), by default, edit the “local” probe file. To store the probe file in the system directory (`/vnmr/probes`), you must log in as `vnmr1`, and copy the probe directory from the “local” directory to the system.

The `probe` directory contains subdirectories, one for each probe. The names of those subdirectories identify the probe, and the VNMR parameter `probe` (a global variable) must be set to match the name of one of these subdirectories. For example, you might have a 4-nucleus probe and a PFG indirect detection probe. Likely subdirectories would be `../probes/4nuc` and `./probes/pfgid`. Correspondingly, you would set the parameter `probe` to `4nuc` or `pfgid`, depending on which probe was in the magnet. Each subdirectory contains a plain text file, with the same name as the subdirectory itself, e.g., `../probes/4nuc/4nuc`; it is this text file that contains the actual calibrations for different nuclei. Table 5 shows an example of a probe file.

**Table 5.** Example Probe Calibration File

| *Probe:* | *Parameters* |
|---|---|
| Probegradient | y |
| Probegcal | 0.00221 |

**Table 5.** Example Probe Calibration File (continued)

| | |
|---|---|
| Probelkmap | asw_lk_01Oct1998 |
| ProbeH1map | n |
| Probedate | 01-Oct-1998 |
| *H1* | *Parameters* |
| H1pw90 | 9.8 |
| H1tpwr | 57 |
| H1dmf | 10101 |
| H1dpwr | 36 |
| H1pp | 13.6 |
| H1pplvl | 54 |
| H1tpwr_cf | 1.2000 |
| H1dmm | w |
| H1dseq | waltz16 |
| H1dres | 90 |
| H1date | 24-Sep-1998 |
| *F19* | *Parameters* |
| F19pw90 | 00 |
| F19tpwr | 00 |
| F19dmf | 00 |
| F19dpwr | 00 |
| F19pp | 00 |
| F19pplvl | 00 |
| F19tpwr_cf | 1 |
| F19dmm | w |
| F19dseq | waltz16 |
| F19dres | 90 |
| F19date | 00-00-0000 |
| *C13* | *Parameters* |
| C13pw90 | 9.4 |
| C13tpwr | 56 |
| C13dmf | 17094 |
| C13dpwr | 34 |
| C13pwx | 9.7 |
| C13pwxlvl | 54 |
| C13pwxlvl_cf | 1.0000 |
| C13gHratio | 3.98533 |
| C13dmm | p |
| C13dseq | W40_asw |
| C13dres | 9 |
| C13dpwr2 | 0 |

**Table 5.** Example Probe Calibration File (continued)

| | |
|---|---|
| C13dmf2 | 0 |
| C13pwx2 | 0 |
| C13pwx2lvl | 0 |
| C13pwx2lvl_cf | 1 |
| C13dmm2 | g |
| C13dseq2 | garp1 |
| C13dres2 | 1 |
| C13date | 24-Sep-1998 |
| *N15* | *Parameters* |
| N15pw90 | 00 |
| N15tpwr | 00 |
| N15dmf | 00 |
| N15dpwr | 00 |
| N15pwx | 00 |
| N15pwxlvl | 00 |
| N15pwxlvl_cf | 1 |
| N15gHratio | 10.0 |
| N15dmm | g |
| N15dseq | garp1 |
| N15dres | 1 |
| N15dpwr2 | 0 |
| N15dmf2 | 0 |
| N15pwx2 | 0 |
| N15pwx2lvl | 0 |
| N15pwx2lvl_cf | 1 |
| N15dmm2 | g |
| N15dseq2 | garp1 |
| N15dres2 | 1 |
| N15date | 00-00-0000 |
| *P31* | *Parameters* |
| P31pw90 | 00 |
| P31tpwr | 00 |
| P31dmf | 00 |
| P31dpwr | 00 |
| P31pwx | 00 |
| P31pwxlvl | 00 |
| P31pwxlvl_cf | 1 |
| P31gHratio | 2.47 |
| P31dmm | g |
| P31dseq | garp1 |
| P31dres | 1 |
| P31dpwr2 | 0 |

**Table 5.** Example Probe Calibration File (continued)

| | |
|---|---|
| P31dmf2 | 0 |
| P31pwx2 | 0 |
| P31pwx2lvl | 0 |
| P31pwx2lvl_cf | 1 |
| P31dmm2 | g |
| P31dseq2 | garp1 |
| P31dres2 | 1 |
| P31date | 00-00-0000 |

A variety of macros are associated with the probe file maintenance and use. See the *VNMR Command and Parameter Reference* for the macros listed in Table 6.

**Table 6.** Probe File Related Macros

| | |
|---|---|
| `addnucleus` | Add new nucleus to existing probe file |
| `addparam` | Add parameters to current probe file |
| `addprobe` | Create new probe directory and probe file |
| `setparams` | Receive parameter from probe file |
| `setdecpars` | Set decoupler parameter values from probe file |
| `setdec2pars` | Set decoupler 2 parameter values from probe file |
| `setparams` | Write parameter to current probe file |
| `updateprobe` | Update probe file |

## 8.2 System Calibrations Using the Calibrate Macro

Probe calibrations can be done either using autocalibration routines or by manually editing the probe file. See the following sections for details:

- "Samples Required" on page 124
- "Calibrate Lock" on page 127
- "Calibrate Proton" on page 127
- "Calibrate Carbon" on page 128
- "Calibrate Fluorine" on page 129
- "Calibrate Phosphorus" on page 130
- "Calibrate H, C, Ind. Det., and Gradients (CH3I)" on page 132
- "Calibrate H, Ind. Det., and Gradients (CH3OH)" on page 133
- "Manually Editing the Probe File" on page 135

### Samples Required

The six samples listed in Table 7 can be used for autocalibration. Not all samples are provided with each system. The required samples for the acceptance test procedure during system installation will include one or more of these six samples.

**Table 7.** AutoCalibration Samples

| *Sample* | *Calibrate Option* | *Part Number* |
|---|---|---|
| 0.1% ethylbenzene in $CDCl_3$ $^1H$ sensitivity | Proton | 00-968120-70 |
| 40% dioxane in $C_6D_6$ $^{13}C$ sensitivity | Carbon | 00-968120-69 |
| 0.485 M triphenylphosphate in $CDC1_3$ $^{31}P$ sensitivity | Phosphorus | 00-968120-87 |
| 0.05% trifluorotoluene in benzene–$d_6$ $^{19}F$ sensitivity | Fluorine | 00-968120-82 |
| 1% $^{13}C$-enriched methyl iodide, 1% trimethyl phosphite, and 0.2% Cr(AcAc) in Chloroform-d | Proton, Carbon, ID, and Gradients (organic solvents) | 00-968120-96 |
| 0.1% $^{13}C$-enriched methanol with 0.30 mg/ml $GdCl_3$ in 1% $H_2O$/99% $D_2O$<br>(AutoTest Sample) | Proton, Carbon, ID, and Gradients (aqueous solvents) | 00-968120-68 |
| 2 Hz $D_2O$ | LOCK, gmap and Z0 | 01-901855-01 |

When the autocalibration is run by the user VNMR1, all results are automatically written to the probe file in `/vnmr/probes/`*`probe_name`* or `$vnmrsys/probes/`*`probe_name`*.

The autocalibration macros first determine power and the 90° pulse width, then write the power and pulse width values into the probe's file.

The autocalibration macros call four parameter sets:

- `stdpar/H1.par` (either the system `/vnmr/stdpar/H1.par` or the user's `vnmrsys/stdpar/H1.par`).
- `/vnmr/tests/gamah2`.
- `/vnmr/tests/P31sn.par`.
- `/vnmr/tests/F19sn.par`.

If the user is not `vnmr1` but is part of the admin group, the probe's calibration file is locally created in `~/vnmrsys/probes`. If the user is `vnmr1`, the probe's calibration file is created in `/vnmr/probes`.

## Autocalibration Macros

The following macros improve system automated calibration:

- `AC1S–AC11S` are called by the interactive autocalibration window and determine the $^1H$ 90° pulse width, $^{13}C$ 90° pulse width, decoupler $\gamma H_2$, and 90° pulse width of the decoupler at high power, $^{19}F$ 90° pulse width, and $^{31}P$ 90° pulse width.
- `AC1S–AC11S` perform automatic calibration on UNITY*INOVA*, *MERCURY*-Series, and *GEMINI 2000* systems. When the macros finish the calibration routines, the current probe file is updated. If the probe is new to the system (i.e., all values in the probe file are zero), then the macros determine system power followed by calibration. If power levels are listed in the current probe file, these values are used, instead of taking time to determine power. The macro `AC1S` determines $^1H$ pw90, `AC5S` begins $^{13}C$ calibration, including decoupler power calibrations. `AC10S` performs $^{19}F$ calibration, and `AC11S` performs $^{31}P$ calibration.
- `ACreport` is called by the autocalibration macros `AC1S-AC11S` to print a copy of the probe file after calibration is completed.

- `ACbackup` is called by the autocalibration macros `AC1S-AC11S` to back up the probe file before beginning a new autocalibration run. This macro is not usually called by the user.

## Performing an Autocalibration

Before you calibrate a probe for the first time, type the following command:

1. To make a probe file available to all system users enter **`addprobe(`*`probename`*`,'system').`**
2. To create a new probe entry in the current user directory, enter **`addprobe(`*`probename`*`)`**, where *`probename`* is a name of your choice (e.g., `addprobe('idpfg')`).

`addprobe` is a macro that is run during VNMR installation and makes a probe file available only to an individual system user.

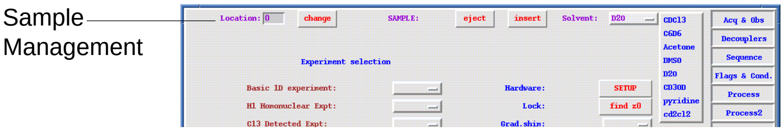
`addprobe(`*`probe_name`*`,'system')`creates a system-level probe directory (typically `/vnmr/probes`; users need write permission to this directory) and makes a probe file available to all users on the system.

Total time for system calibration is about 45 minutes.

## Calibrate LOCK gmap and z0

This procedure calibrates the lock and gradients using the 2 Hz doped $D_2O$ sample. Both the lock and gradients must be calibrated for the autoshim and autolock procedures to function efficiently.

1. Click the **Setup EXP** button in the right side of the Tcl/dg window.
2. **Eject** the current sample from the magnet and **insert** the *2 Hz Doped D2O sample*. Click on the **Eject** and **Insert** buttons (Figure 55) in the sample management region of the **Setup EXP window or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.
3. Select the solvent by holding down the left mouse button on the solvent menu (Figure 55) and choosing the appropriate solvent from the solvent menu list.

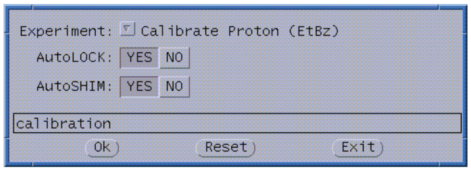

Location: 0

Solvent: D2O

**Figure 55.** Setup EXP - Changing Calibration Samples

4. Select **D2O** from the **Solvent menu** in the *Sample Management* region of the Setup EXP panel**.**

5. Open the acqi window by pressing the **acqi button** on the VNMR menu. Lock onto the D2O resonance. The lock must be set on-resonance.
6. Adjust Z0 as necessary.
7. Adjust Lock Gain and Lock Power and set the lock level at 80%.
8. Exit acqi.
9. Type calibrate on the vnmr command line to display the interactive autocalibration menu (Figure 56A)
10. Set **Autoshim** and **Autolock** to **NO.**
11. Select the **Lock** calibration routine, from the **Autocalibration** menu (Figure 56B), by holding down the left mouse button on the **Autocalibration** menu and selecting **“LOCK:gmap and z0 (2Hz D2O)”** from the menu list.



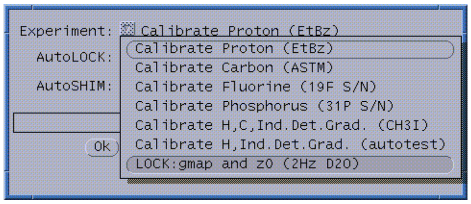
Experiment: Calibrate Proton (EtBz)

AutoLOCK: YES NO

AutoSHIM: YES NO

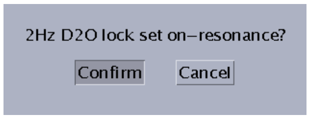
calibration

(A) Calibration Main Window



Experiment: Calibrate Proton (EtBz)

(B) Select “LOCK:gmap and z0 (2Hz D2O)”



2Hz D2O lock set on–resonance?

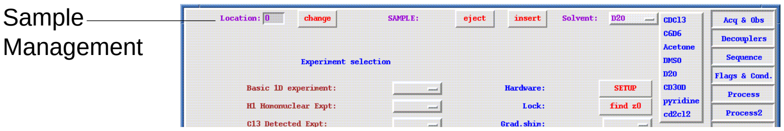
(C) Confirm 2Hz $D_2O$ Lock Set On-resonanc

**Figure 56.** Calibrate Lock

12. Click on **OK** to continue with the lock calibration (or click **Reset** to return to the default value).
13. Click the **Confirm** button (Figure 56C). If the current sample is not the correct sample, click **Cancel**.
14. Click on the **Setup EXP** button.
15. Click on the **Start ACQ** button to begin the calibration.

## Calibrate Proton

1. Click the **Setup EXP** button in the right side of the Tcl/dg window.
2. **Eject** the current sample from the magnet and **insert** the *$^1$H sensitivity sample*. Click on the **Eject** and **Insert** buttons (Figure 57) in the sample management region of the **Setup EXP window or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.
3. Select the solvent by holding down the left mouse button on the solvent menu (Figure 57) and choosing the appropriate solvent from the solvent menu list.



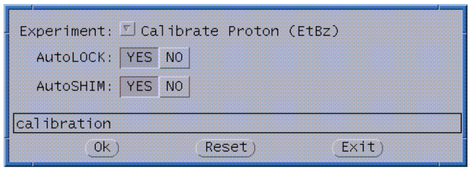
Location: 0

Solvent: D20

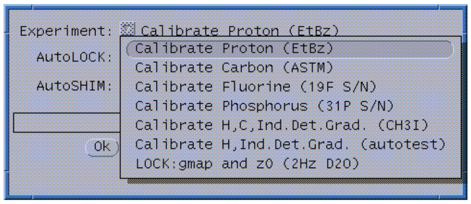
**Figure 57.** Setup EXP - Changing Calibration Samples

4. Type calibrate on the vnmr command line to display the interactive autocalibration menu (Figure 58A).

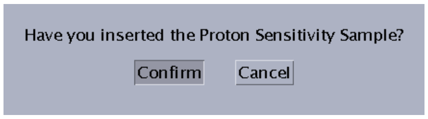
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Select the $^1$H calibration routine from the **Autocalibration** menu (Figure 58B) by holding down the left mouse button on the **Autocalibration** menu and selecting **"Calibrate Proton (EtBz)"** from the menu list. The sample confirmation window opens.
7. Click the **Confirm** button Figure 58C. If the current sample is not the correct sample, click **Cancel**.
8. In the target calibration window (Figure 58D), **Enter** a target pw90 value. The value is usually the $^1$H pulse specification for your probe.
9. Click on **OK** to accept the value shown or the value you entered or click **Reset** to return to the default value.


Experiment: Calibrate Proton (EtBz)
AutoLOCK: YES NO
AutoSHIM: YES NO
calibration

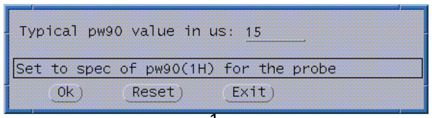
(A) Calibration Main Window


Experiment: Calibrate Proton (EtBz)

(B) Select "Calibrate Proton (EtBz)"


Have you inserted the Proton Sensitivity Sample?

(C) Confirm EtBz sample is inserted


Typical pw90 value in us: 15
Set to spec of pw90(1H) for the probe

(D) Enter Target $^1$H pw90 value

**Figure 58.** Calibrate Proton.

10. Click on **Exit**. Proton sensitivity parameters are recalled.
11. If you set the **Autoshim** and **Autolock** options to **NO** in step 5, manually lock and shim your sample now. Tune the probe if needed.
12. Click on the **Setup EXP** button. Click on the **Start ACQ** button to begin the calibration.

At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

## Calibrate Carbon

1. Click the **Setup EXP** button in the right side of the Tcl/dg window.
2. **Eject** the current sample from the magnet and **insert** the $^{13}$*C ASTM sensitivity sample*. Click on the **Eject** and **Insert** buttons (Figure 59) in the sample management region of the **Setup EXP window or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.
3. Select the solvent by holding down the left mouse button on the solvent menu (Figure 59) and choosing the appropriate solvent from the solvent menu list.

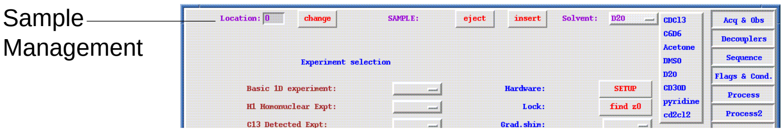
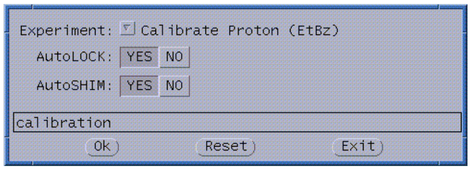

Location: 0
Solvent: D2O

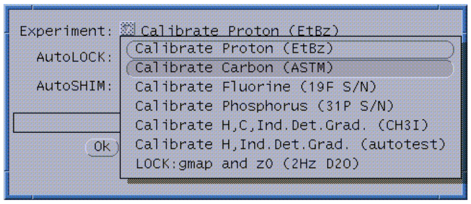
**Figure 59.** Setup EXP - Changing Calibration Samples

4. Type calibrate on the vnmr command line to display the interactive autocalibration menu (Figure 60A).

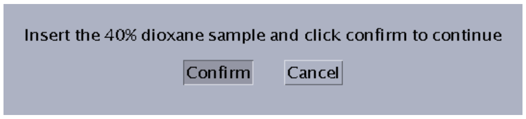

Experiment: Calibrate Proton (EtBz)

calibration

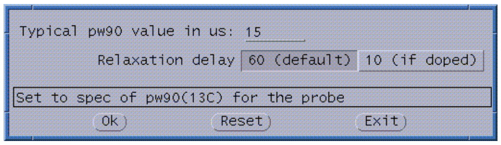
(A) Calibration Main Window



(B) Select “Calibrate Carbon (ASTM)”


Insert the 40% dioxane sample and click confirm to continue

(C) Confirm ASTM sample is inserted


Typical pw90 value in us: 15

Set to spec of pw90(13C) for the probe

(D) Enter Target $^{13}$C pw90 value

**Figure 60.** Calibrate Carbon.

5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Select the $^{13}$C calibration routine, from the **Autocalibration** menu (Figure 60B), by holding down the left mouse button on the **Autocalibration** menu and selecting **“Calibrate Carbon (ASTM)”** from the menu list.
7. Click the **Confirm** button (Figure 60C). If the current sample is not the correct sample, click **Cancel**.
8. In the target calibration window (Figure 60D), **Enter** a target pw90 value. The value is usually the $^{13}$C pulse specification for your probe.
9. **Select** the correct relaxation based on the ASTM sample used.
10. Click on **OK** to accept the value shown or the value you entered (or click **Reset** to return to the default value).
11. Click on **Exit**. Carbon sensitivity parameters are recalled.
12. If you set the **Autoshim** and **Autolock** options to **NO** in step 5, manually lock and shim your sample now. Tune the probe if needed.
13. Click on the **Setup EXP** button.
14. Click on the **Start ACQ** button to begin the calibration.

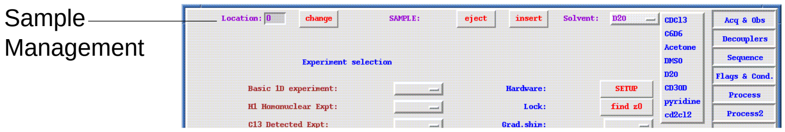
At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe calibration file.

## Calibrate Fluorine

1. Click the **Setup EXP** button in the right side of the Tcl/dg window.
2. **Eject** the current sample from the magnet and **insert** the $^{19}$*F sensitivity sample*. Click on the **Eject** and **Insert** buttons (Figure 61) in the sample management region

of the **Setup EXP window or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.

3. Select the solvent by holding down the left mouse button on the solvent menu (Figure 61) and choosing the appropriate solvent from the solvent menu list.



Location: 0

Solvent: D2O

**Figure 61.** Setup EXP - Changing Calibration Samples

4. Type *calibrate* on the vnmr command line to display the interactive autocalibration menu (Figure 62A).

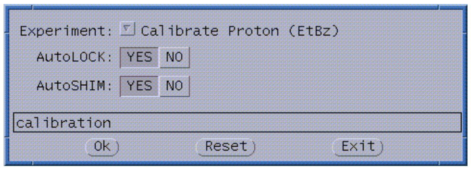
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.

6. Select the $^{19}$F calibration routine from the **Autocalibration** menu (Figure 62B) by holding down the left mouse button on the **Autocalibration** menu and selecting **"Calibrate Fluorine (19F S/N)"** from the menu list. The sample confirmation window opens.

7. Click the **Confirm** button Figure 62C. If the current sample is not the correct sample, click **Cancel**.

8. In the target calibration window (Figure 62D), **Enter** a target pw90 value. The value is usually the $^{19}$F pulse specification for your probe.

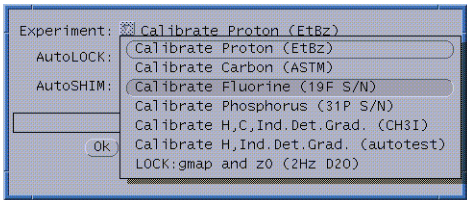
9. Click on **OK** to accept the value shown or the value you entered (or click **Reset** to return to the default value).



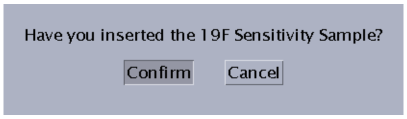
Experiment: Calibrate Proton (EtBz)

calibration

(A) Calibration Main Window

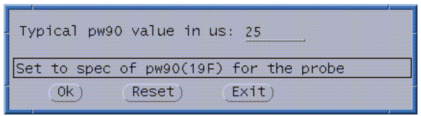


(B) Select "Calibrate Fluorine (19F S/N)"



Have you inserted the 19F Sensitivity Sample?

(C) Confirm 19F Sensitivity sample is inserted



Typical pw90 value in us: 25

Set to spec of pw90(19F) for the probe

(D) Enter Target $^{19}$F pw90 value

**Figure 62.** Calibrate Fluorine.

10. Click on `Exit`. Fluorine sensitivity parameters are recalled.

11. If you set the `Autoshim` and **Autolock** options to **NO** in step 5, manually lock and shim your sample now. Tune the probe if needed.

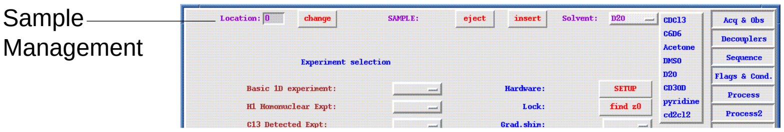
12. Click on the **Setup EXP** button. Click on the **Start ACQ** button to begin the calibration.

At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

## Calibrate Phosphorus

1. Click the **Setup EXP** button in the right side of the Tcl/dg window.

2. **Eject** the current sample from the magnet and **insert** the *$^{31}$P sensitivity sample*. Click on the **Eject** and **Insert** buttons (Figure 61) in the sample management region of the **Setup EXP window or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.
3. Select the solvent by holding down the left mouse button on the solvent menu (Figure 61) and choosing the appropriate solvent from the solvent menu list.

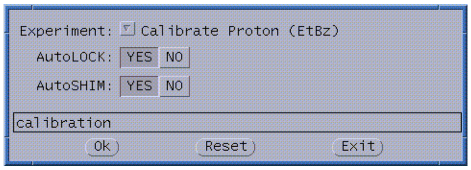


Location: 0

Solvent: D2O

**Figure 63.** Setup EXP - Changing Calibration Samples

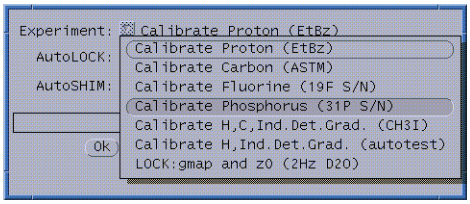
4. Type *calibrate* on the vnmr command line to display the interactive autocalibration menu (Figure 62A).
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Select the $^{31}$P calibration routine from the **Autocalibration** menu (Figure 62B) by holding down the left mouse button on the **Autocalibration** menu and selecting **"Calibrate Phosphorus (19F S/N)"** from the menu list. The sample confirmation window opens.
7. Click the **Confirm** button Figure 62C. If the current sample is not the correct sample, click **Cancel**.
8. In the target calibration window (Figure 62D), **Enter** a target pw90 value. The value is usually the $^{31}$P pulse specification for your probe.
9. Click on **OK** to accept the value shown or the value you entered (or click **Reset** to return to the default value).



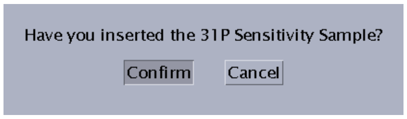
Experiment: Calibrate Proton (EtBz)

calibration

(A) Calibration Main Window

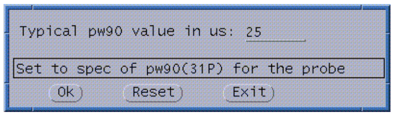


(B) Select "Calibrate Phosphorus (31P S/N)



Have you inserted the 31P Sensitivity Sample?

(C) Confirm 31P Sensitivity sample is inserted



Typical pw90 value in us: 25

Set to spec of pw90(31P) for the probe

(D) Enter Target $^{31}$P pw90 value

**Figure 64.** Calibrate Phosphorus.

10. Click on **Exit**. Phosphorus sensitivity parameters are recalled.
11. If you set the **Autoshim** and **Autolock** options to **NO** in step 5, manually lock and shim your sample now. Tune the probe if needed.
12. Click on the **Setup EXP** button. Click on the **Start ACQ** button to begin the calibration.

At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

## Calibrate H, C, Ind. Det., and Gradients ($CH_3I$)

This procedure calibrates H1 and C13 observe, H1 and C13 decouple (pulses as well as γH2), and gradients using the $^{13}$C enriched $CH_3I$ in $CDC1_3$ sample.

1. Click the **Setup EXP** button in the right side of the Tcl/dg window.
2. **Eject** the current sample from the magnet and **insert** the $^{13}$*C enriched CH3I sample*. Click on the **Eject** and **Insert** buttons (Figure 65) in the sample management region of the **Setup EXP window or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.
3. Select the solvent by holding down the left mouse button on the solvent menu (Figure 65) and choosing the appropriate solvent from the solvent menu list.

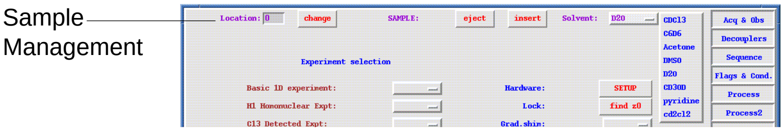
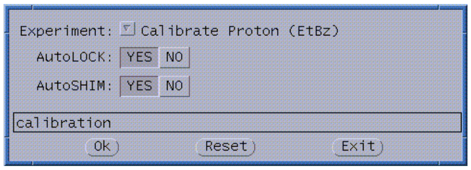


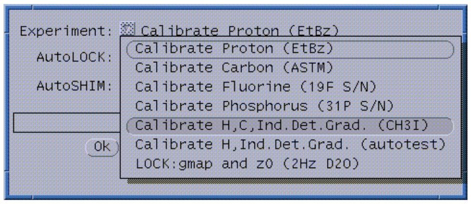
**Figure 65.** Setup EXP - Changing Calibration Samples

4. Type calibrate on the vnmr command line to display the interactive autocalibration menu (Figure 66A).
5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Select the **Indirect Detection** calibration routine, from the **Autocalibration** menu (Figure 66B), by holding down the left mouse button on the **Autocalibration** menu and selecting **"Calibrate H, C, Ind. Det. Grad (CH3I)"** from the menu list.
7. Click the **Confirm** button (Figure 66C). If the current sample is not the correct sample, click **Cancel**.
8. In the calibration window (Figure 67), select the calibration(s) to be run, **H1 Observe, C13 Decouple, C13 Observe, H1 Decouple, Gradient (g/cm/dac),** and **C/H gradient ratio**.

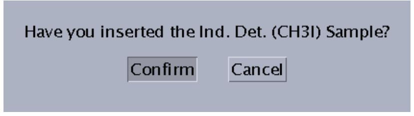

Experiment: Calibrate Proton (EtBz)

calibration

(A) Calibration Main Window



(B) Select "Calibrate H, C, Ind. Det. Grad. (CH3I)"


Have you inserted the Ind. Det. (CH3I) Sample?

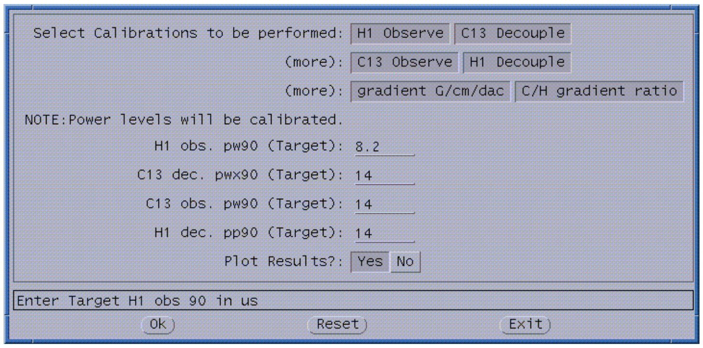
(C) Confirm CH3I sample is inserted

**Figure 66.** Calibrate Using $CH_3I$.

9. **Enter** the following target calibration values for the observe and decoupler calibrations:
   a. $^{1}$H observe pw90
   b. $^{13}$C dec pwx90
   c. $^{13}$C observe pw90
   d. $^{1}$H dec pp90

   The target values are typically the pulse specifications for your probe.

10. Click on **OK** to accept the value shown or the value you entered (or click **Reset** to return to the default value).



Select Calibrations to be performed: H1 Observe C13 Decouple
(more): C13 Observe H1 Decouple
(more): gradient G/cm/dac C/H gradient ratio
NOTE:Power levels will be calibrated.
H1 obs. pw90 (Target): 8.2
C13 dec. pwx90 (Target): 14
C13 obs. pw90 (Target): 14
H1 dec. pp90 (Target): 14
Plot Results?: Yes No
Enter Target H1 obs 90 in us

**Figure 67.** CH3I Calibration Target Values

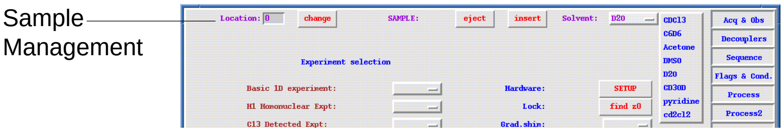
11. Click on **Exit**.
12. If you set the **Autoshim** and **Autolock** options to **NO** in step 5, manually lock and shim your sample now. Tune the probe if needed.
13. Click on the **Setup EXP** button.
14. Click on the **Start ACQ** button to begin the calibration.

At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe calibration file.

## Calibrate H, Ind. Det., and Gradients ($CH_3OH$)

This procedure calibrates H1, C13 decouple (pulse as well as $\gamma$H2), and gradients using the AutoTest sample ($^{13}$C enriched $CH_3OH$ in doped $D_2O$). Specific calibration routines can be selected in the customization menu.

1. Click the **Setup EXP** button in the right side of the Tcl/dg window.
2. **Eject** the current sample from the magnet and **insert** the *AutoTest sample*. Click on the **Eject** and **Insert** buttons (Figure 68) in the sample management region of the **Setup EXP window or, from the command line,** use the `e` command to eject the sample and the `i` command to insert a new sample.
3. Select the solvent by holding down the left mouse button on the solvent menu (Figure 68) and choosing the appropriate solvent from the solvent menu list.

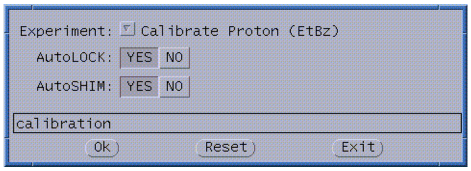


Location: 0
Solvent: D2O

**Figure 68.** Setup EXP - Changing Calibration Samples

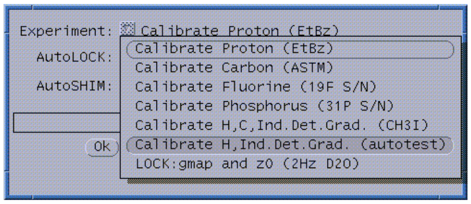
4. Type calibrate on the vnmr command line to display the interactive autocalibration menu (Figure 69A).

5. Set **Autoshim** and **Autolock**. Click the **NO** button if your sample is already locked and shimmed or if you would prefer to lock and shim manually.
6. Select the **Indirect Detection** calibration routine, from the **Autocalibration** menu (Figure 69B), by holding down the left mouse button on the **Autocalibration** menu and selecting **“Calibrate H, Ind. Det. Grad (autotest)”** from the menu list.
7. Click the **Confirm** button (Figure 69C). If the current sample is not the correct sample, click **Cancel**.
8. In the calibration window (Figure 70), select the calibration(s) to be run, **H1 Observe, C13 Decouple, Gradient (g/cm/dac),** and **C/H gradient ratio**.

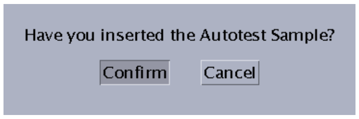


Experiment: Calibrate Proton (EtBz)

(A) Calibration Main Window



(B) Select “Calibrate H, Ind. Det. Grad (autotest)”



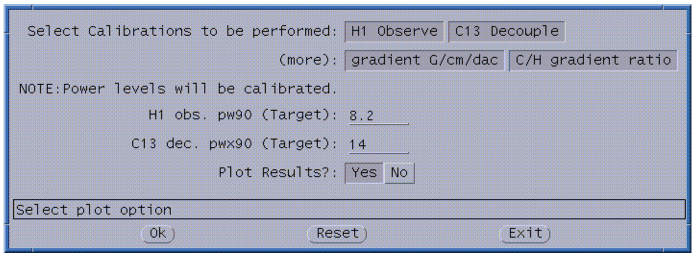
Have you inserted the Autotest Sample?

(C) Confirm AutoTest sample is inserted

**Figure 69.** Calibrate Using AutoTest Sample.

9. **Enter** the following target calibration values for the observe and decoupler calibrations:
   a. $^{1}$H observe pw90
   b. $^{13}$C dec pwx90

   The target values are typically the pulse specifications for your probe.
10. Click on **OK** to accept the value shown or the value you entered (or click **Reset** to return to the default value).



Select Calibrations to be performed: H1 Observe C13 Decouple
(more): gradient G/cm/dac C/H gradient ratio
NOTE:Power levels will be calibrated.
H1 obs. pw90 (Target): 8.2
C13 dec. pwx90 (Target): 14
Plot Results?: Yes No
Select plot option

**Figure 70.** Calibration Target Values Using AutoTest Sample

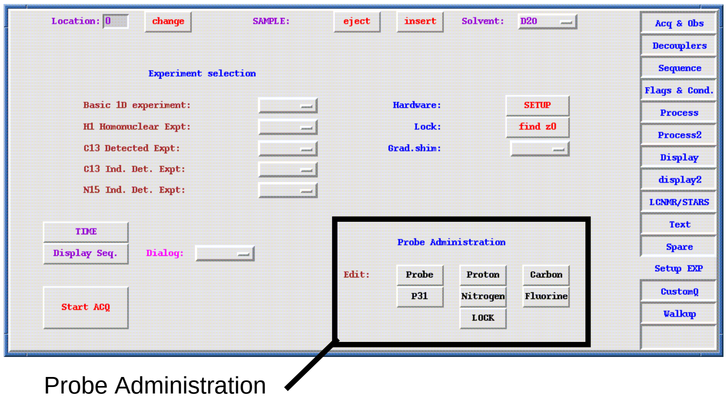
11. Click on **Exit**.
12. If you set the **Autoshim** and **Autolock** options to **NO** in step 5, manually lock and shim your sample now. Tune the probe if needed.
13. Click on the **Setup EXP** button.
14. Click on the **Start ACQ** button to begin the calibration.

At the end of the calibration routine, the power and pulse width values are automatically incorporated into the probe file.

## 8.3 Manually Editing the Probe File

You can manually edit the probe file by using the edit buttons shown in the *probe administration region* of the Setup Exp Window (Figure 71).

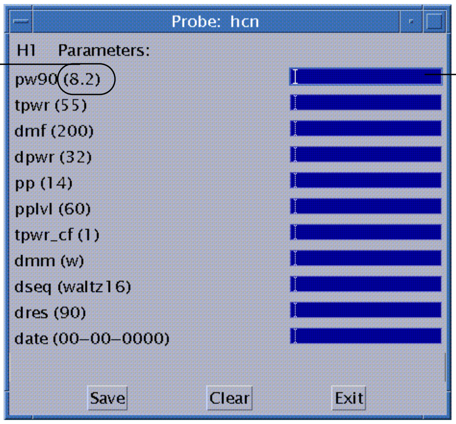
For example, to edit H1 calibrations for the current probe, click on the **Proton** button. The window shown in Figure 72 opens.



Probe Administration

**Figure 71.** Setup EXP Window - Probe Administration Region

Current parameter value



H1 Parameters:

pw90 (8.2)
tpwr (55)
dmf (200)
dpwr (32)
pp (14)
pplvl (60)
tpwr_cf (1)
dmm (w)
dseq (waltz16)
dres (90)
date (00–00–0000)

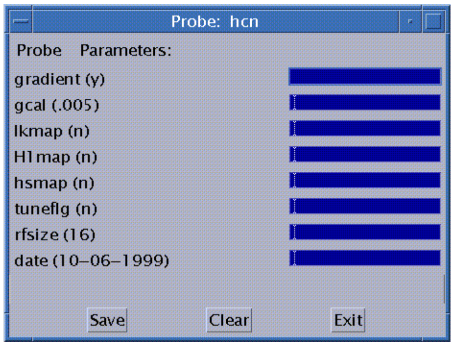
Enter new values in these fields

**Figure 72.** H1 Calibrations Window

Enter the new calibration values in the appropriate field and click **SAVE** and **EXIT**. The new calibration value is incorporated into the current probe file.

Gradient, maps, and other related information are accessed by clicking on the **Probe** button (Figure 73).

All the calibration widows access the local probe calibration files in `userdir+/probes`. To store the probe file in the system directory (`/vnmr/probes`), you must log in as `vnmr1` or `root`, and copy the probe directory from the "local" directory to the system directory.



Probe Parameters:

gradient (y)
gcal (.005)
lkmap (n)
H1map (n)
hsmap (n)
tuneflg (n)
rfsize (16)
date (10–06–1999)

**Figure 73.** Probe Gradient and Map Window

# Chapter 9. Processing and Plotting Saved Data

Sections in this chapter:

- 9.1 "Retrieving Stored Data," this page
- 9.2 "Plotting Retrieved Data Using GLIDE," page 139
- 9.3 "Plotting Spectra Using Plot Designer," page 141

You retrieve and process saved data using the File Manager and the Common Desktop Environment (CDE) interface or VNMR and GLIDE in the OpenLook Environment. The processed data is displayed on the VNMR screen ready for you to plot. Plot Designer provides you with tools to customize the way the data is presented. Plot Designer also provides different formats (GIF, JPEG, and other) for saving the plotted data to a file for later plotting or display.

## 9.1 Retrieving Stored Data

### Common Desktop Environment.

Steps 1 and 2 need to be done only once during a VNMR session.

1. Click the *GLIDE* button in the Permanent Menu to bring the VNMR input window to the front (Figure 74).

**Figure 74.** VNMR Permanent Menu

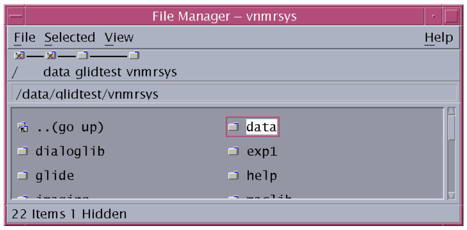
2. Enter the command `listenon` in the input window
3. Click the file drawer icon in the CDE Front Panel(Figure 75).

**Figure 75.** CDE Front Panel

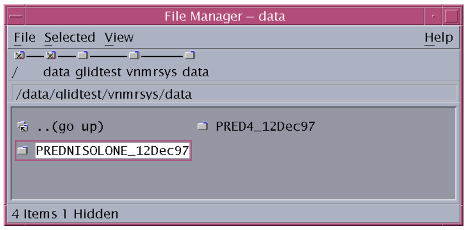
4. Using the File Manger navigate to the directory `~/vnmrsys/data`/<directory containing fids>/ and double click on the FID file you want to process. A Step by Step example is given in Figure 76.

A File Manager windows appears. Double-click on `vnmrsys` to change to the directory `~/vnmrsys`

Double-click on `data` to change to the directory `~/vnmrsys/data`



Change to the directory where the FIDs are stored.



Double-click on the FID file you want process. The FID is loaded to the current experiment and automatically processed. After that, the final spectrum is displayed.

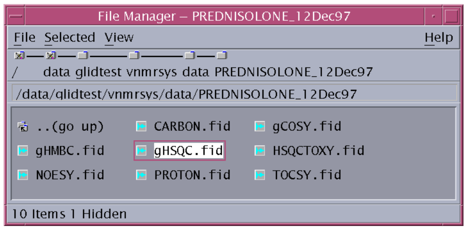
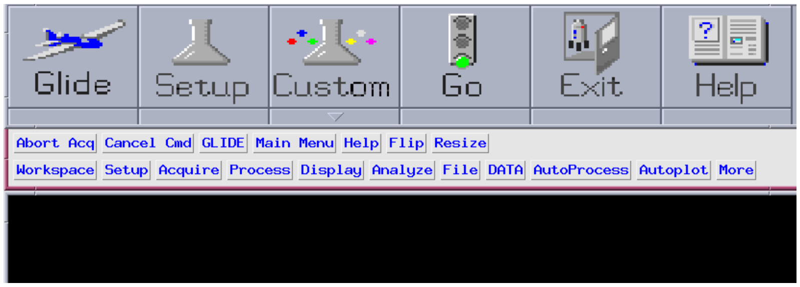


**Figure 76.** Processing With *GLIDE* in the CDE Environment

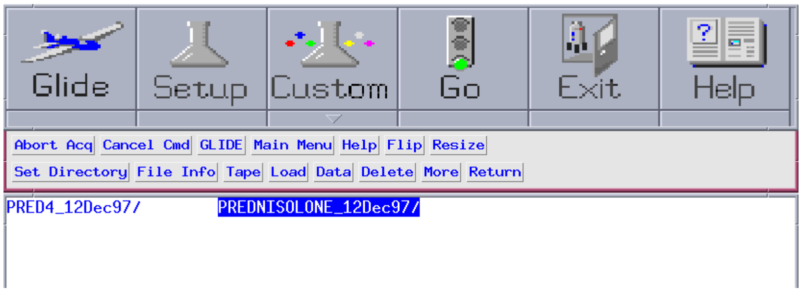
## OpenLook Environment.

1. Click the Main Menu button in the Permanent menu, and then click on the DATA button in the Main menu, Figure 77A.
2. Find the name of the directory where the FIDs are stored, highlight the name (click on the name with left mouse button), and then click the Set Directory button, Figure 77B.

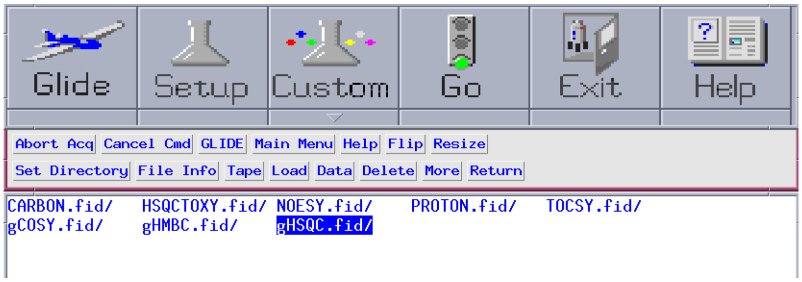
3. Highlight the FID file and click the Load button. The FID is loaded to the current experiment, Figure 77C.



(A) GLIDE and the Permanent VNMR Menu



(B) GLIDE and VNMR File List



(C) GLIDE and FID Selected for Processing

**Figure 77.** Processing with *GLIDE* in the Openlook Environment

4. Click the Main Menu button in the Permanent menu.
5. Click the AutoProcess button.

   The FID is automatically processed and the final spectrum is displayed.

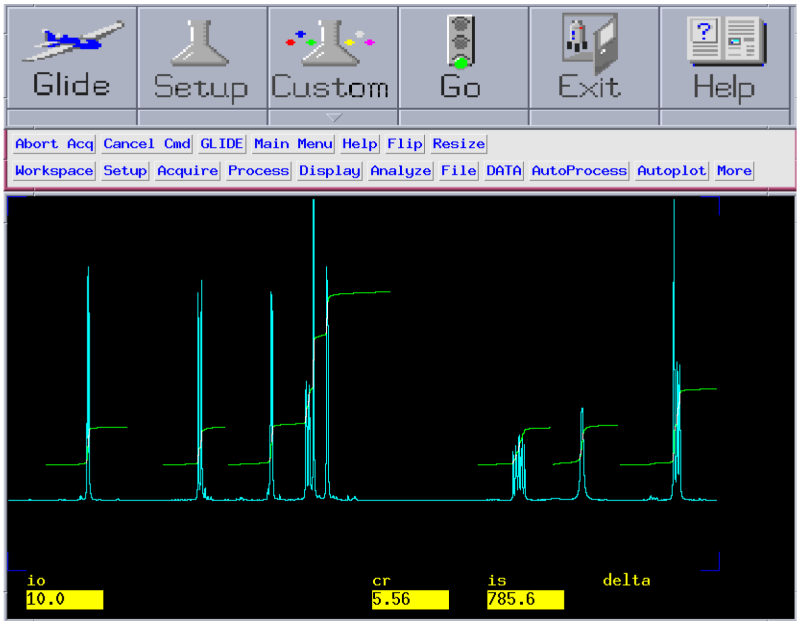
## 9.2 Plotting Retrieved Data Using GLIDE

After processing, the 1D or 2D spectrum are displayed in the Interactive mode so you can adjust the vertical scale, expansion, and threshold. To plot the spectrum:

1. Click the Main Menu button in the Permanent menu.

2. Click the Autoplot button (Figure 78). This generates a 1D plot or 2D plot. 2D plots are plotted with appropriate high-resolution 1D spectra and/or skyline projections.

1D
Plot



io 10.0
cr 5.56
is 785.6

2D
Plot

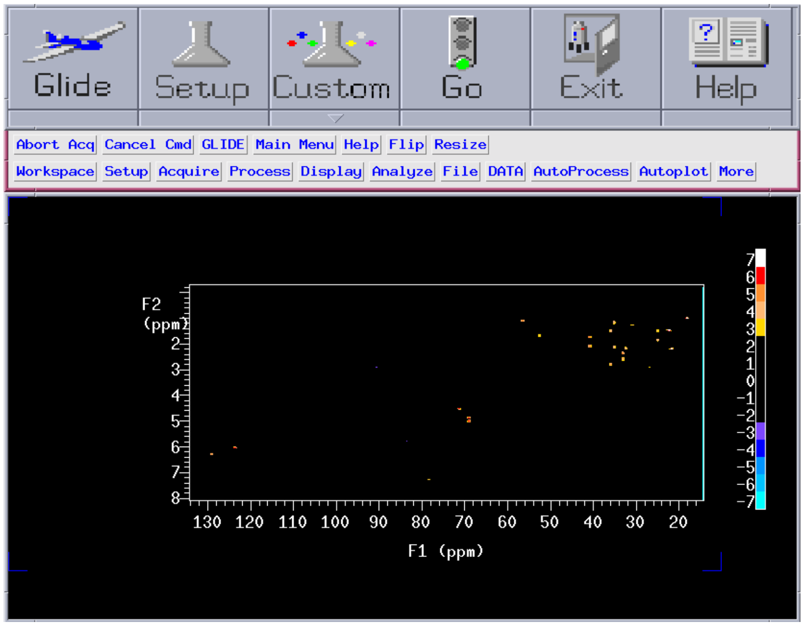


**Figure 78.** Plotting from *GLIDE*

## 9.3 Plotting Spectra Using Plot Designer

Plot Designer allows you to see and design a plot before you print it. It provides templates, drawing tools, and a text editor that give you the capability of positioning spectra, parameters, axes, and other plot output on a page.

### System Requirement

Plot Designer is a Java-based application.You must have Solaris 2.6 or later installed in order to use Plot Designer. The Java$^{TM}$ Runtime Environment (JRE) for Solaris$^{TM}$ from Sun Microsystems provides an environment in which you can run Java applications. Plot Designer requires at least JRE 1.1.6. You can download the latest version of JRE for Solaris$^{TM}$ from the Sun Microsystems Web site at **http://www.sun.com/solaris/jre/index.html**.

### Creating a Plot Design

1. Start the Plot Designer program by entering `jdesign` in the VNMR input window. The window shown in Figure 79 appears.
2. In the main menu, click on **Region**, then **New** to create a region on the workspace. The cursor arrow changes to cross-hairs.

   Regions are smaller workspaces. For more information about regions, see "Working with Regions" on page 147.

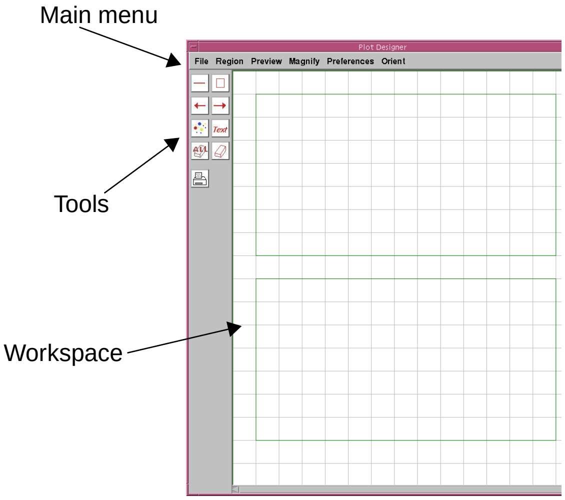


**Figure 79.** Plot Designer Window

3. Draw a region by pressing and holding down the left mouse button and dragging the cursor across the workspace. Release the mouse button when the region is the size that you want it.

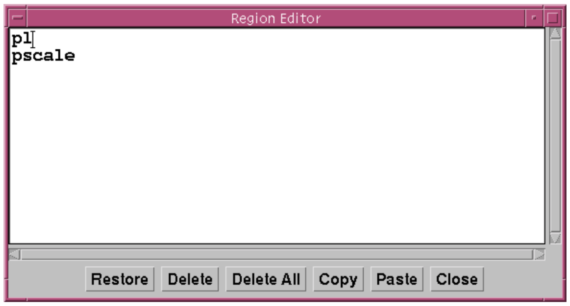
### *Importing a Plot into a Region*

After you have created a region, you can use the Region Editor, shown in Figure 80, to import a plot from the VNMR graphics window into the workspace. Region Editor is a text editor in which you can enter commands to change the look of a plot and then import it. For more information about using Region Editor, see the section **"Editing a Plot" on page 150.**

To open the Region Editor, do the following procedure:

1. Click on **Region** in the main menu, then **Edit**.

   If you created multiple regions and do not select one, when you click **Region-Edit**, the first region created is automatically selected.
2. Enter a VNMR command (such as `pl` or `pscale`) in the text input area. For more information about commands, see "Storing Commands" on page 150.



```
pl
pscale
```

**Figure 80.** Region Editor Window

3. Click on **Preview** in the main menu, then **Selected** to import the plot into the region. If you created multiple regions, click **Preview-All** to import plots into all regions.

You can also import a plot into a region by doing the following procedure:

1. Select the region by double-clicking anywhere inside it.
2. Press the right mouse button anywhere in the workspace to open the plot menu window shown in Figure 81.
3. Choose a command to import the plot.

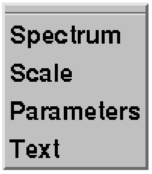


**Figure 81.** Plot Menu Window

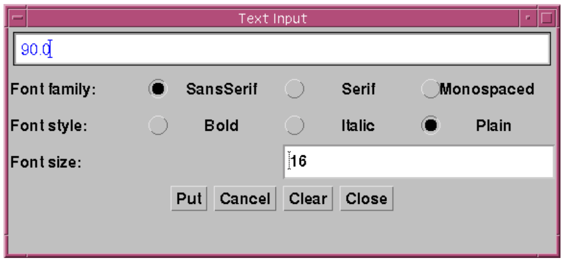
## Customizing a Plot

You can customize the plot by adding simple graphics and text to it and changing its size and appearance with the tools listed in Table 1.

## Adding Text to Your Design

To add text to your design, do the following procedure:

1. Click on the text input tool Text to open the Text Input window shown in Figure 82.



90.0

Font family: ● SansSerif ○ Serif ○ Monospaced

Font style: ○ Bold ○ Italic ● Plain

Font size: 16

**Figure 82.** Text Input Window

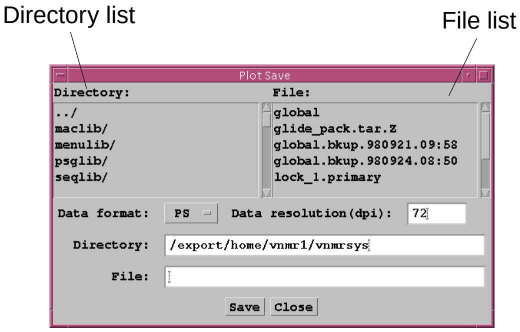
2. Type text in the input area in the top of the window.

   Click on the desired **Font family** and **Font style** selections and enter a **Font size.**
3. Click on **Put** and drag the cursor (and the text) into the workspace.
4. Click once to paste the text.

**Table 1.** Plot Designer Tools

| | | |
|---|---|---|
| — | **Line** | Draws a line.<br>To draw a line, place the cursor in a region or anywhere in the workspace. Press and hold down the left mouse button, then drag the cursor. Release the mouse button to complete the drawing. |
| ☐ | **Box** | Draws a box.<br>To draw a box, place the cursor in a region or anywhere in the workspace. Press and hold down the left mouse button, then drag the cursor down diagonally. Release the mouse button to complete the drawing. |
| ←<br>→ | **Arrow** | Drawing an arrow is similar to the procedure for drawing a line.<br>The left-pointing arrows places the arrowhead at the point in which you START to draw the arrow. The right-pointing arrow places the arrowhead at the point in which you END drawing the arrow. |
| ⁂ | **Item Preferences** | Sets the color and size of lines and fonts. You can also choose three styles of fonts: monospaced, SansSerif, and serif. To edit an object, select it by double-clicking on it. For instructions and a description of Item Preferences properties, see "Customizing Objects" on page 149.<br>You can also open this tool by clicking on **Region** in the main menu, then **Preferences**. |
| *Text* | **Text Input** | Allows you to add text into your design. Several options allow you to control the size and appearance of the text. To use this tool, see "Adding Text to Your Design" on page 142. |
| ⌫<br>ALL | **Eraser** | The eraser tool removes only selected objects.<br>The **ALL** eraser clears the workspace. To remove all objects and regions, click on **Region** in the main menu, then **Delete All**. Objects removed with **Delete All** cannot be restored to the workspace. For more information about removing and restoring regions and objects, see page 149. |
| 🖶 | **Print** | Prints a file.<br>No window opens; your plot design is automatically printed. |

## Saving Your Design



Directory:
../
maclib/
menulib/
psglib/
seqlib/

File:
global
glide_pack.tar.Z
global.bkup.980921.09:58
global.bkup.980924.08:50
lock_1.primary

Data format: PS
Data resolution(dpi): 72
Directory: /export/home/vnmr1/vnmrsys
File:

**Figure 83.** Plot Save Window

1. When you are satisfied with the plot that you have created, click on **File** in the main menu, then **Save Data** to open the Plot Save window shown in Figure 83.
2. Scroll down the list of directories and choose a directory. You can also enter a path for your file in the text input area of the **Directory** field.
3. Label your file by clicking on a name in the **File** list or entering a name in the text input area of the **File** field.
4. Click on the **Data format** button to select a format for your file. Table 2 lists the formats that are available.
5. Enter a **Data resolution**.
6. Click **Save** to store the data.
7. Click **Close** to exit the window.

## Printing Your Design

Print your plot by clicking on the print tool . No window appears; your design is automatically printed.

## Exiting Plot Designer

To exit Plot Designer, click on **File** in the main menu, then click on **Quit**.

**Table 2.** Formats Available in Plot Designer

| *Format* | *Description* |
|---|---|
| AVS | AVS X image file |
| BMP | Microsoft Windows bitmap image file |
| EPS | Adobe Encapsulated PostScript file |
| FAX | Group 3 FAX |
| FITS | Flexible Image Transport System |
| GIF | Compuserve Graphics Interchange Format (version 89a) |
| GIF87 | Compuserve Graphics Interchange Format (version 87a) |
| JPEG | Compressed format from Joint Photographic Experts Group |
| MIFF | Magick image file format |
| PCD | Photo CD |
| PCX | ZSoft IBM PC Paintbrush file |
| PDF | Portable Document Format |
| PICT | Apple Macintosh QuickDraw/PICT file |
| PGM | Portable gray map |

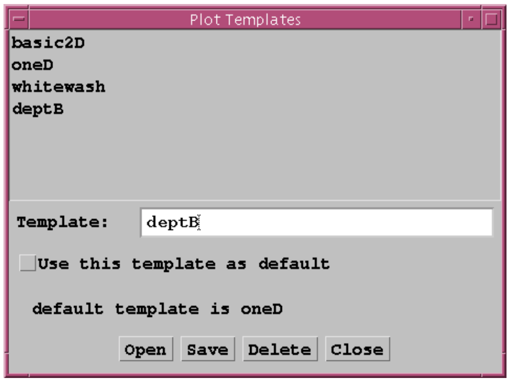
**Table 3.** Formats Available in Plot Designer (continued)

| *Format* | *Description* |
|---|---|
| PNG | Portable Network Graphics |
| PS | Adobe PostScript file |
| PS2 | Adobe Level II PostScript file |
| SGI | Irix RGB image file |
| SUN | Sun Rasterfile |
| TGA | Truevision Targa image file |
| TIFF | Tagged Image File Format |
| VIFF | Khoros Visualization image file |
| XBM | X11 bitmap file |
| XPM | X11 pixmap file |
| XWD | X Window System window dump image file |

If you leave a design in the window when you exit Plot Designer, your design will automatically appear in the workspace the next time that you use the program.

## Using Templates

After you have created a plot design, you can save your design as a template. To create a template, do the following procedure:



basic2D
oneD
whitewash
deptB

Template: deptB

☐ Use this template as default

default template is oneD

**Figure 84.** Plot Template Window

1. Click on **File** in the main menu, then click on **Templates** to open the Plot Templates window shown in Figure 84.
2. Enter a name in the **Template** field. If you want the file to be the default template, click on the box next to **Use this template as default**.
3. Click **Save** to store the template in `$vnmruser/templates/plot` directory.

   If you try to save a template with the same name as an already existing template, a warning notifying you that the file will be overwritten appears. If you do not want the file replaced, click on **Cancel**.
4. Quit the Plot Templates window by clicking on **Close**.

If you close Plot Designer with a template in the workspace, the next time that you start Plot Designer, it will open with the template and any changes that you made to it automatically loaded on the workspace.

### Specifying Templates

You can plot a page with a specific template by typing the `jplot` command and the template name. For example, entering `jplot('t1')` starts a plot with the t1 template automatically loaded.

When you open Plot Designer with the `jdesign` macro, the workspace is either empty or it contains the design that was being worked on the previous time Plot Designer was used. Do the following procedure to load a template file:

1. Click on **File** in the main menu, then **Templates** to open the Plot Templates window.
2. Select a template by either clicking on a file in the list in the upper region of the window or by entering the file name in the **Template** field. If you want the file to be the default template, click on the field **Use this template as default**.
3. To insert the template into the Plot Designer window, click on **Open**.
4. Click **Close** to exit the window.

### Removing Templates

To remove a template from the list in the Plot Templates window, click on the file then click on **Delete**. A warning appears notifying you that the template will be deleted. Click **Cancel** if you do not want to delete the template.

## Customizing Plot Designer

You can customize Plot Designer by changing the orientation and size of the window and the appearance of, and properties in, the workspace.

### Changing Window Orientation

Plot Designer can be viewed in either a landscape or a portrait (the default) orientation. To change the orientation of the Plot Designer window, click on **Orient** in the main menu, then click on **Landscape** or **Portrait**.

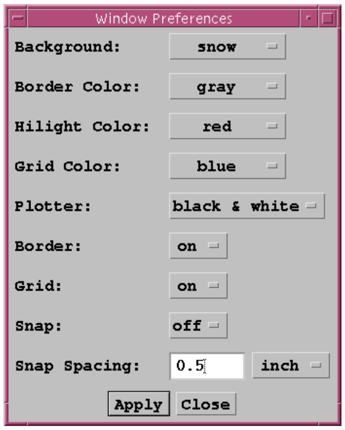
### Changing Window Size

You can shrink or enlarge the Plot Designer window. To increase or decrease the size of the window, click on **Magnify** in the main menu, then select a percentage by which you want to reduce or expand the size of the window.

### Customizing the Workspace

You can change the look and properties of the workspace by doing the following procedure:

1. In the main menu, click on **Preferences**, then **Set Up** to open the Workspace Preferences panel shown in Figure 85.
2. To change an aspect of, or property in, the workspace, click on its corresponding control button; a pull-down list appears. See Table 4 for a description of each control.
3. After you have entered all of your preferences, click on **Apply** to execute the changes.
4. Click **Close** to exit the window.



Background: snow
Border Color: gray
Hilight Color: red
Grid Color: blue
Plotter: black & white
Border: on
Grid: on
Snap: off
Snap Spacing: 0.5 inch

**Figure 85.** Workspace Preferences Panel

Figure 86 is an example of the workspace without visible region borders and a grid.

## Working with Regions

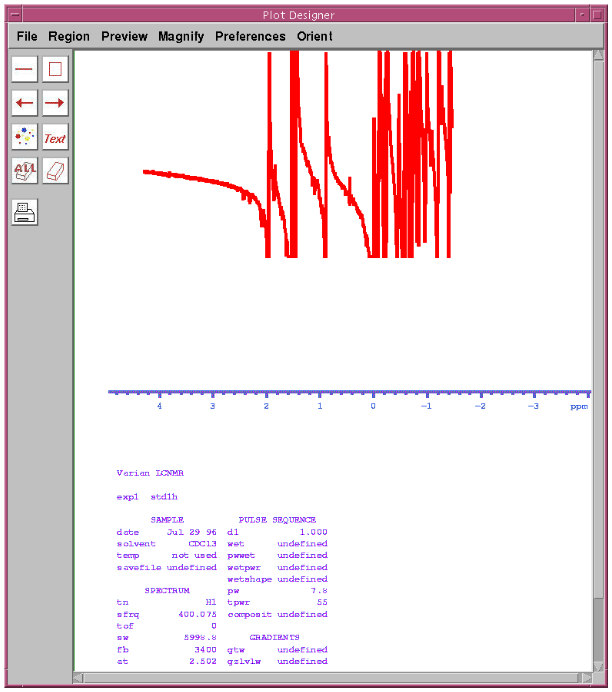
Regions on the workspace are smaller workspaces in which you can create designs. This section describes how to adjust plot parameters within regions, manipulate regions and objects on the workspace, and customize regions.

### *Adjusting and Restoring Plot Parameters in a Region*

When you draw a region, the scaling parameters of the plotting area (`wcmax` and `wc2max`) are adjusted by the macro `jplotscale`. `jplotunscale` is a macro that restores the original parameters of the current experiment to the plot. The scaling parameters (`io`, `is`, `vs`, `wc`, and `wc2`) of a plot that is imported into a region are automatically adjusted according to `wcmax` and `wcmax2`.

**Table 4.** Workspace Preference Controls

| *Control* | *Function* |
|---|---|
| **Background** | Changes the background color of the workspace. |
| **Border Color** | Changes the color of the border surrounding the workspace. |
| **Highlight Color** | When you double-click on an object, its color changes to indicate that it is selected (or highlighted). This option controls the highlight color. |
| **Grid Color** | Changes the color of the grid. |
| **Plotter** | Allows you to choose a black and white or color plotter. |
| **Border** | Shows (**on**) and hides (**off**) region borders. |
| **Grid** | Turns on and turns off the grid in the workspace. |
| **Snap** | The grid is magnetic. When it is turned **on**, the path of an object (the center of its border) automatically snaps (is magnetized) to the grid whenever you draw or move the object or change its size or shape. Turning **off** Snap demagnetizes the grid. |
| **Snap Spacing** | Controls the amount of space on the grid to which an object snaps. Spacing can be in inches, centimeters, or points. |



```
Varian LCNMR

exp1  std1h

      SAMPLE          PULSE SEQUENCE
date      Jul 29 96  d1            1.000
solvent       CDCl3  wet       undefined
temp       not used  pwwet     undefined
savefile  undefined  wetpwr    undefined
                     wetshape  undefined
     SPECTRUM        pw              7.8
tn               H1  tpwr             55
sfrq        400.075  composit  undefined
tof               0
sw           5998.8      GRADIENTS
fb             3400  gtw       undefined
at            2.502  gzlvlw    undefined
```

**Figure 86.** Workspace with Data and Without Borders and a Grid

If you want to use the adjusted parameters, enter the following command string, which first restores the parameters of the current experiment (`n`) to the plot, then applies the adjusted parameters to the plot:

```
jplotunscale jexpn jplotscale
```

If you do not want to use the adjusted parameters, enter the following command:

```
jplotunscale jexpn
```

## Moving Regions and Objects

To move a region, double-click the left mouse button anywhere inside it, then drag the mouse. Double-click anywhere outside the region to deselect the region.

To move an object, double-click the left mouse button on it and drag the mouse. Release the mouse button to deselect the object.

After you select an object or region, you can also use the arrow keys on your keyboard to move regions and objects.

## Changing the Size of a Region

You can shrink or enlarge a region by double-clicking on it, placing the cursor on a border anchor, and dragging the cursor up, down, or diagonally.

## Deleting a Region

To delete a region from the workspace, double-click anywhere inside the region. In the main menu, click on **Region**, then **Delete**.

To remove all regions from the workspace, click **Region**, then **Delete All**.

*Note:* Regions removed with **Delete All** are not stored in a buffer and cannot be restored to the workspace.

### Restoring a Deleted Region

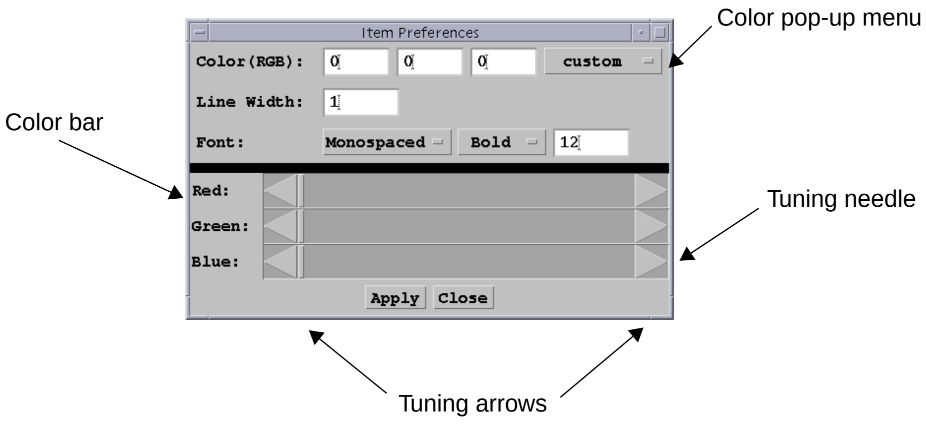
To restore a region deleted from the workspace, click on **Region** in the main menu, then **Undelete**.

#### *Clearing the Workspace*

To *permanently* remove all regions from the workspace, click **Delete All**. Remember, when you remove all regions, you cannot restore them with **Undelete**.

## Customizing Objects

You can change the line width and color of objects and the family, style, and size of fonts with the Item Preferences window, shown in Figure 87. To open the window, either click on **Region** in the main menu, then **Preferences** or click on the Item Preferences tool described on page 143.



Color(RGB): 0 0 0 custom
Line Width: 1
Font: Monospaced Bold 12
Red:
Green:
Blue:

**Figure 87.** Item Preferences Window

### Changing Line Color

You can change the color of a line by doing the following procedure:

1. Double-click on the line to select it.
2. In the Item Preferences window, click on the color button `green` to open a pop-up list showing a range of colors.
3. Click on a color. The color appears in the color bar.

   Move the tuning needle left or right to change a color. You can also change a color by clicking on the left or right arrows in the **Red**, **Green**, and **Blue** fields; the values in the **Color(RGB)** field automatically change as you move a needle.
4. When you are satisfied with a color, click **Apply**.
5. Place the cursor anywhere in the workspace and click once to see the color change.

### Changing Line Width

Change the width of a line by doing the following procedure:

1. Highlight the line by double-clicking on it.
2. Enter a new width in the **Line Width** field.
3. Click **Apply** to change the line.
4. Click anywhere in the workspace to deselect the line.

#### *Changing Fonts*

Plot Designer has three font families: SansSerif, `Monospaced`, and Serif. Fonts can be Plain, **Bold**, or *Italic*. To change fonts, do the following procedure:

1. Double-click on the text to select it.
2. Click on the Item Preferences tool to open the Item Preferences window.
3. Choose a family, style, and enter a size in the **Font** field.
4. Click **Apply** to change the text.

### Changing Font Color

You can change the color of text that you add to your design. To change the color of fonts, repeat the procedure for "Changing Line Color" on page 149.

## Editing a Plot

You can edit a plot by using the Region Editor shown in Figure 80. To edit a plot, do the following procedure:

1. Double-click anywhere inside a region to select it.
2. In the main menu, click on **Region**, then **Edit** to open the Region Editor window.
3. Enter a command (such as `pl` or `pscale`) in the text input area. Use the buttons listed in Table 5 to edit text.
4. Exit Region Editor by clicking **Close**.

## Storing Commands

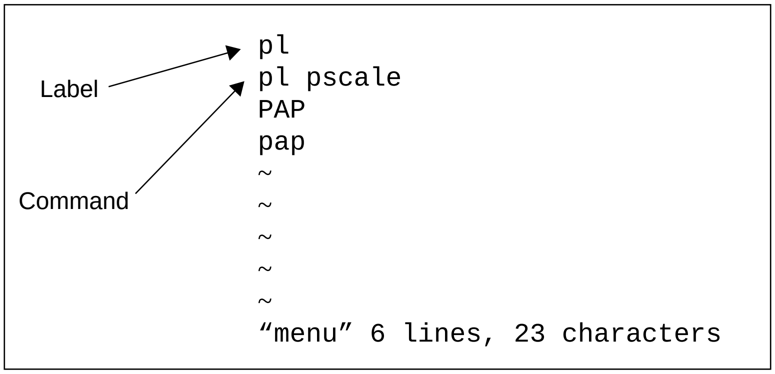
Commands are stored in the `/$vnmruser/templates/plot/menu` file or /`$vnmrsystem/user_templates/plot/menu` file. You can edit both of these files to add or delete commands. In the `menu` file, the command is indicated by the following two lines:

- The first line is the label of the command that appears in the plot menu window.
- The second line is the command itself.

In Figure 88, the label `pl` identifies the command line `pl pscale`. The label PAP identifies the `pap` command.

**Table 5.** Region Editor Buttons

| *Button* | *Function* |
|---|---|
| **Restore** | Applies the original template to a region. If you opened a template and made changes to it, you can restore your design to the original template design by using this button. |
| **Delete** | Removes text. This option is not similar to **Copy**. Deleted text is not stored in a buffer; do not use **Delete** to cut and paste text. |
| **Delete all** | Clears all text from the input area. |
| **Copy** | Duplicates text. |
| **Paste** | Inserts copied text in the text input area. |



```
pl
pl pscale
PAP
pap
~
~
~
~
~
“menu” 6 lines, 23 characters
```

**Figure 88.** menu File

# Index