VnmrJ Installation and Administration

User Guide

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VARIAN

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Contents

Chapter 1 Introduction

Varian MR systems provide unmatched productivity for diverse chemical applications by combining easy-to-use software with outstanding performance. Push-button experiments, along with straightforward processing and data export capabilities, make the MR the best choice for compound detection, quantification and structure confirmation.

1.1 About this Guide

This VnmrJ 3 Installation and Administration User Guide provides information for installing VnmrJ 3 and managing the system users.

Chapters in this user guide include:

- Chapter 1 Introduction
- Chapter 2 VnmrJ Installation
- Chapter 3 VnmrJ Administration
- Chapter 4 Spectroscopy Account Administration
- Chapter 5 Configuring Printers for VnmrJ
- Chapter 6 Automated Hardware
- Chapter 7 VnmrJ Accounting Administration
- Chapter 8 System Calibrations and Autotest

1.2 Warnings and Cautions

This user guide helps you establish operating conditions that permit safe and efficient use of your equipment. Special considerations and precautions shown in the form of **NOTES**, **CAUTIONS**, and **WARNINGS** are described below.

Observe the following precautions during installation, operation, maintenance, and repair of the instrument. Failure to comply with these warnings, or with specific warnings elsewhere in Varian documentation, violates safety standards of design, manufacture, and intended use of the instrument. Varian assumes no liability for customer failure to comply with these precautions. Contact Varian, Inc. if you have any questions regarding the safe and proper use of your equipment.

NOTE: Notes give additional and important information.

Table 1 Warning and Caution Symbols

Warning Symbol	Warning Description
	Alerts you to situations when failure to observe instructions could result in serious damage to equipment or loss of data.
	Alerts you to potentially hazardous situations that could result in serious injury or death to humans, animals, or significant property damage.
	Hazardous voltages are present inside instrument. Disconnect from main power before removing screw-attached panels. No user serviceable parts inside system.
	Very hot or cryogenically cold surfaces may be exposed. Use proper skin protection.
	Eye damage could occur either from flying particles, chemicals, or UV radiation. Use proper eye and face protection.
	Keep hands and fingers away.
	The potential for fire may be present. Follow user guide for safe operation.
	Hazardous chemicals may be present. Avoid contact especially when replenishing reservoirs. Use proper eye and skin protection.
	Class 1 invisible laser radiation present. Avoid long term viewing of laser.

1.3 Magnetic Medical Devices

	Remain outside the 5-gauss perimeter from the centerline of the magnet, if you have implanted or attached medical devices such as pacemakers and prosthetic parts must.

The superconducting magnet system generates strong magnetic fields that can affect operation of cardiac pacemakers, and harm implanted or attached devices such as prosthetic parts and metal blood vessel clips and clamps.

Pacemaker wearers should consult the documentation provided by the pacemaker manufacturer or contact the pacemaker manufacturer. Pacemaker wearers should always notify their physician and discuss the health risks of being in proximity to magnetic fields. Wearers of metal prosthetics and implants should contact their physician to determine if a danger exists.

Refer to the documentation supplied with the magnet for the size of a typical 5-gauss stray field. Check the gauss level after the magnet is installed.

1.4 Magnetic Media

	Keep magnetic media: ATM cards, credit cards, watches, outside the 5-gauss perimeter from the centerline of the magnet.

Refer to the documentation supplied with the magnet for the size of a typical 5-gauss stray field. Check this gauss level after the magnet is installed.

Chapter 2 VnmrJ Installation

This chapter provides information on VnmrJ installation requirements, installation procedures, installation options, software patches, and VnmrJ 2.3A restoration procedures. VnmrJ installations are able to accommodate both Varian and non-Varian distributed systems with pre-configured Red Hat Linux® RHEL 5.X OS.

Sections in this chapter include:

- 2.1 VnmrJ Installation Requirements
- 2.2 VnmrJ Installation
- 2.3 VnmrJ Installation Options
- 2.4 VnmrJ Patches
- 2.5 Restoring VnmrJ 2.3A After Installing VnmrJ 3

NOTE: After VnmrJ installation, documentation is located in the VnmrJ Help menu bar

2.1 VnmrJ Installation Requirements

2.1.1 Prior to VnmrJ Installation

- Verify that the firewall is disabled.
- Verify that SElinux is disabled.
- Verify that the console is connected and powered on.
- Verify that the network adapters are configured correctly. For more information, see "Configuring Network Settings" of the *Linux for VnmrJ User Guide*.

NOTE: For pre-installed RHEL systems, the console connects to the external network card. For re-loaded Linux systems, the console connects to the main internal network card.

	Firewalls and SElinux must be disabled for proper VnmrJ installation.

2.1.2 Required Items

- VnmrJ Installation DVD
- Red Hat Linux® — RHEL Installation DVD

2.2 VnmrJ Installation

Table 2 VnmrJ Installation Procedures

Section	Title	Description
2.2.1	Preinstallation – Checking Software Packages	Install the VnmrJ DVD to assess which RHEL OS software packages are needed.
2.2.2	Preinstallation – Installing Software Packages	Install the RHEL Installation DVD to obtain needed RHEL OS software packages
2.2.3	Installing VnmrJ Software	Install the VnmrJ Software.
2.2.4	Configuring Acquisitions Communications	Use the setacq command to establish communications between the host computer and the NMR console.
2.2.5	Creating the Acqproc User	Use the aqcqproc command to turn on/off information exchange between the host computer and the NMR console.
2.2.6	Configuring System Settings	Configure VnmrJ using the VnmrJ System Settings window.
2.2.7	Setting the Lock Frequency	Set the lock frequency on the system after VnmrJ and the magnet is installed.
2.2.8	Configuring Proton Experiments	Configure VnmrJ Proton Experiments using the Proton Experiments menu.

2.2.1 Preinstallation – Checking Software Packages

The initial phase of installation checks Red Hat RHEL OS for software packages required to install and run VnmrJ. If additional software packages are required, a message box will appear indicating that the RHEL installation DVD is needed. If no additional software packages are required, the Installation Window will appear.

NOTE: Users must be logged in as root. If the user is not root, “su” to root.

1. Insert the VnmrJ DVD.
2. Unmount then remount the VnmrJ DVD in the terminal window:
   a. `umount /dev/cdrom`
   b. `mkdir -p /media/vnmrj`
   c. `mount /dev/cdrom /media/vnmrj`
      (A write-protected message will appear)
   d. `cd /media/vnmrj`
   e. `./load.nmr`
3. A message box is displayed indicating that the RHEL installation DVD may be required for installation.
4. Click **Continue** on the message box.

5. If software packages are missing, a message box indicating that the RHEL Installation DVD may be required is displayed.
6. Click **OK** and continue to 2.2.2 Preinstallation – Installing Software Packages.
7. If no additional software packages are needed, continue to 2.2.3 Installing VnmrJ Software.

2.2.2 Preinstallation – Installing Software Packages

NOTE: Users must be logged in as root. If the user is not root, "su" to root.

1. Eject the VnmrJ DVD in the terminal window:

   a. `cd /`

   b. `eject`

2. Insert the RHEL Installation DVD and in the terminal window type

   `cd /tmp/varian_preinstall`

3. Wait for the DVD to be auto-mounted by the system and terminal window type:

   `./installpkgs`

NOTE: Installing packages may take a few minutes.

4. Eject the RHEL Installation DVD:

   `eject`

5. Continue to 2.2.3 Installing VnmrJ Software.

2.2.3 Installing VnmrJ Software

NOTE: Users must be logged in as root. If the user is not root, "su" to root.

1. Insert the VnmrJ DVD.
2. Unmount then remount the VnmrJ DVD. Enter the following in a terminal window:

   `umount /dev/cdrom`

   `mount /dev/cdrom /media/vnmrj`
   (A write-protected message appears)

   `cd /media/vnmrj`

   `./load.nmr`

3. The Installation window will appear. Configure VnmrJ installation options. For more information, see 2.3 VnmrJ Installation Options.
4. Click **Install**.

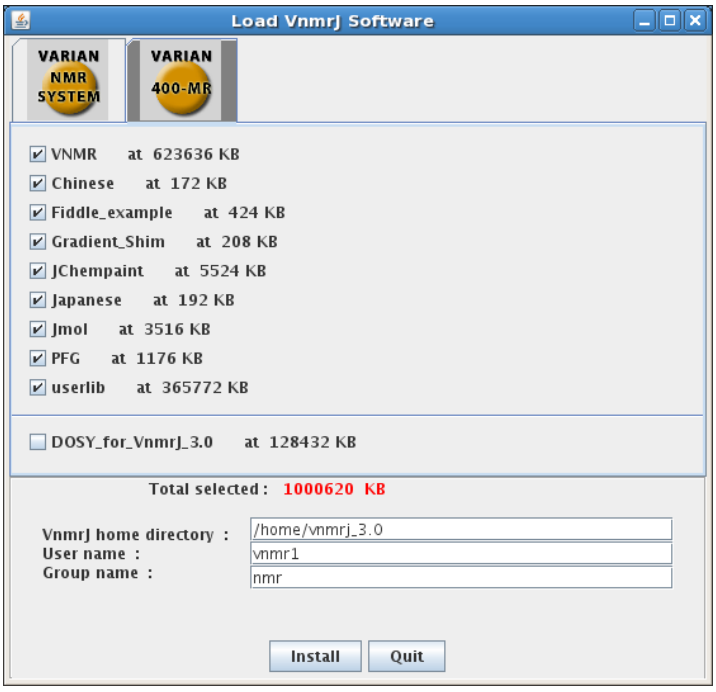


Figure 1 VnmrJ Installation Window

5. After VnmrJ installation is complete, click **Done** on the message box that pops up.
6. Continue to 2.2.4 Configuring Acquisitions Communications.

NOTE: VnmrJ automatically installs “vnmr1” as the administrator.

2.2.4 Configuring Acquisitions Communications

This section describes how to use the setacq command to establish communications between the host computer and the NMR console. Skip this section if VnmrJ is for a data station.

NOTE: Users must be logged in as root. If the user is not root, “su” to root.

1. After installing VnmrJ software, reboot the system (System–Shutdown–Restart).
2. Log in as vnmr1.
3. Run setacq by typing the following commands in a terminal window:

```
# cd /vnmr/bin
#./setacq
```

CAUTION	Do not reboot or reset the NMR console until setacq has finished. The process may take eight or more minutes.

4. Expproc will start and stop as needed. For more information see, 2.5.6 Sample Output of **`setacq`** When Changing from 2.3A to 3.0.
5. Wait for `setacq` to finish the update process.
6. Wait for the following message:
   Starting Acquisition communications
7. Reboot the system (System–Shutdown–Restart).

2.2.5 Creating the Acqproc User

Daemons, known as the proc-family, direct communications between the host computer and the console on systems that include a magnet installation (spectrometers systems, not data stations).

Create the user acqproc as follows:

1. Log in as **root**
2. Type the following command:
   ```
   # /vnmr/bin/makesuacqproc
   ```
3. The system prompts the user for the root password if the login is not root.

   All users can enable or disable the daemons once acqproc is created by typing the following command:
   ```
   user > su acqproc
   ```
4. Log in as vnmr1.
5. Install VnmrJ patches if needed. For more information, see 2.4 VnmrJ Patches.
6. Launch VnmrJ software by selecting the VnrmJ icon on the desktop.

2.2.6 Configuring System Settings

After VnmrJ is installed, configure VnmrJ using the VnmrJ System Settings window. Typically "vnmr1" is set as the VnmrJ administrator.

NOTE: When the interface is set to walkup, refer to the *Automation User Guide* for configuring system settings information.

1. Log in as the VnmrJ administrator, typically vnmr1.
2. Start **VnmrJ**.
3. Click Edit – System settings.
4. The System Settings window has two tabs: **System** and **Display/Plot**. Configure system settings for the spectrometer system.

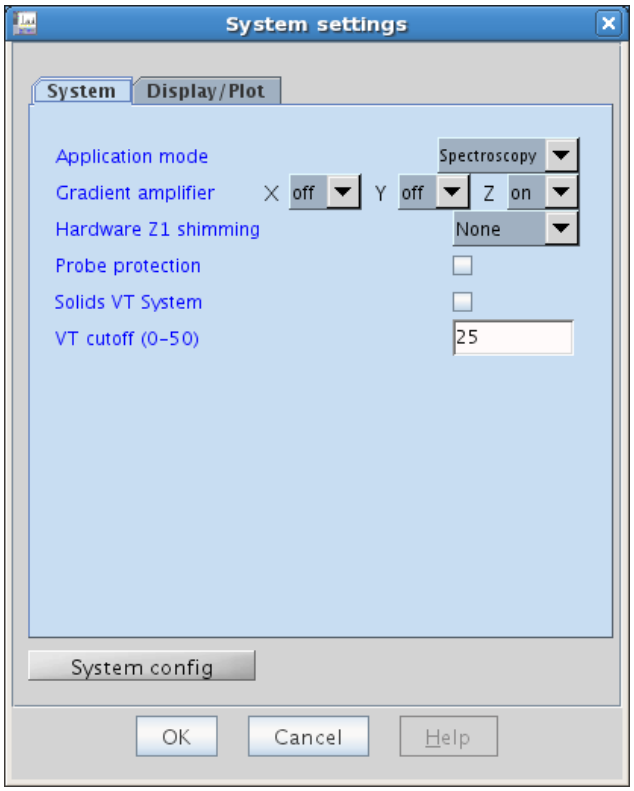


Figure 2 System Settings Window

Table 3 System Settings

Tab	Fields
System	Application mode —Spectroscopy, LC-NMR, and Imaging Autotest. Gradient amplifier — on/off selection for each installed gradient axis. Hardware Z1 shimming — none for no Z1 shimming, Delay for Z1 shimming enabled during delay time, or Presat for Z1 shimming enabled during delay time preceding presat. Probe protection — check to enable. VT cutoff (0-50) — specify VT cutoff temperature; 25°C recommended.
Display/Plot	Set display from plotter aspect ratio (wysisyg) — check to enable. Spectrum updating during phasing (0-100) — set the percentage of the display that is updated during interactive phasing. 100 is recommended. Max # of pens — number of plotter pens to use. Show Tooltips — check to enable. Max # of items to show in Locator - Set the number of locator items to show. A Setting greater than 2000 starts to diminish the performance. Display only matching items in locator — check to enable. Process data on drag-and drop from locator — check to enable.

2.2.7 Setting the Lock Frequency

This procedure is not required for imaging systems.

Set the lock frequency using the following procedure after VnmrJ and the magnet is installed on the system. Use the true ^{2}H frequency for this procedure. This procedure is required during installation and is repeated only if the magnet quenches or a large change in field strength occurs.

1. Make sure the magnet is at field.
2. Log in as the administrator, typically vnmr1.

   The setlockfreq macro will not use the values obtained to update /vnmr/conpar if the logged in user does not have administrative privileges.
3. Insert a water sample is in the magnet.

   Tap water is an acceptable sample.
4. Load the Proton experiment.
5. Set `sw = 5000000`
6. Set `tn='H1' lockfreq='n'`
7. Enter `ga`. The system is off resonance if no peaks are observed.

   Locate the water resonance by changing the value of tof (or array tof). Make changes of 200kHz- to 400-kHz for VNMRS and 400MR, so each spectral window overlaps its neighbors.
8. Center the located water resonance in the spectral window by placing the cursor on the line and typing `nl movetof.`
9. Acquire a spectrum with the line centered in the window.
10. Type the command `setlockfreq.`

    setlockfreq calculates and sets the lock frequency parameter lockfreq.

2.2.8 Configuring Proton Experiments

1. Log in as `vnmr1`.
2. From the **Experiment** menu, click **Proton**.
3. From the **Start** tab, click **Shim**.
4. In the File box, type "`reg0`".
5. Click the **Setup Hardware** button.

   When the message "Setup complete" appears, the system is ready.

2.3 VnmrJ Installation Options

VnmrJ offers general and password configuration options to be installed with VnmrJ.

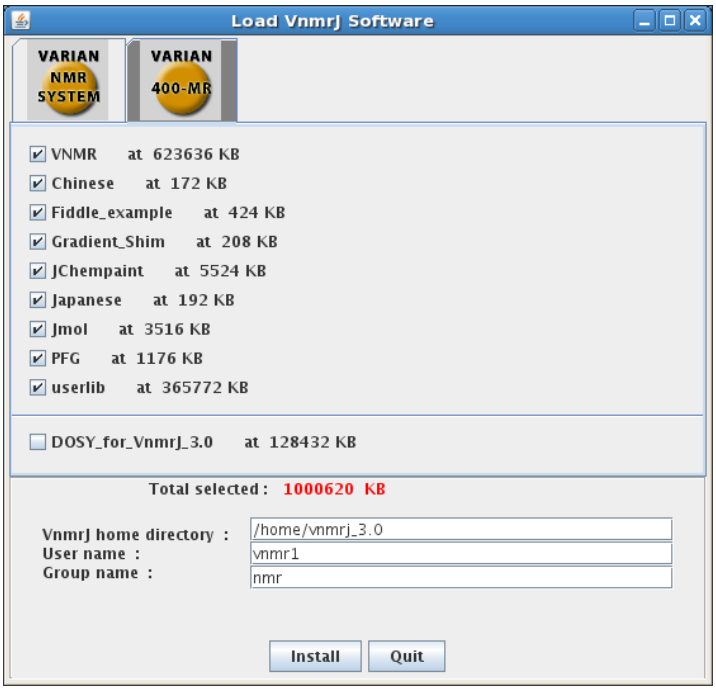


Figure 3 VnmrJ Installation Window

2.3.1 General Options

The following is a list of general options and descriptions. Select the check box next to each option you want to load..

Table 4 Installation Options

Option	Description
VNMR	Loads the basic VnmrJ and VNMR packages.
Fiddle_Example	Loads example of fiddle reference deconvolution.
Gradient_shim	Loads software for gradient shimming.
Jmol	Loads integrated Jmol molecular viewing software.
JChemPaint	Loads integrated JChemPaint molecular editing software.
Chinese	Loads Chinese language support.
Japanese	Loads Japanese language support
PFG	Loads files for PFG experiments.

2.3.2 Additional Varian NMR System Options

The Varian NMR System has the following options available:

Option	Description
Imaging_or_Triax	Loads software for imaging or triple axis gradient.

2.3.3 Options Requiring a Password

The following is a list of options (and descriptions) that require a password. A password field is visible when the option is selected. Enter the password in the field (passwords are case-sensitive). The list of options presented is system dependent.

Table 5 Password Required Options

Option	Description
Diffusion	Software for running diffusion experiments.
LC-NMR	Software for driving LC-NMR experiments.
STARS	A solids software simulation package.
CSI	Loads files for Chemical Shift Imaging.
BIR_shapes	Loads BIR-shaped pulse statements which provide variable tip-angle adiabatic pulses.
DOSY	Loads DOSY files to permit separation of resonances based on diffusion characteristics.
768_AS	Loads software for 768 AS sample changer accessory.
VAST	Loads software for VAST sample changing accessory.
Imaging_Sequences	Loads special pulse sequences for imaging.
Image_Sense	Loads software for parallel imaging reconstruction.

2.3.4 Spectrometer Configuration

Use the Spectrometer Configuration window to configure NMR spectrometer hardware.

1. Click the **System config** button in the System Settings window.
   A VnmrJ Spectrometer Configuration window similar to Figure 4 opens.

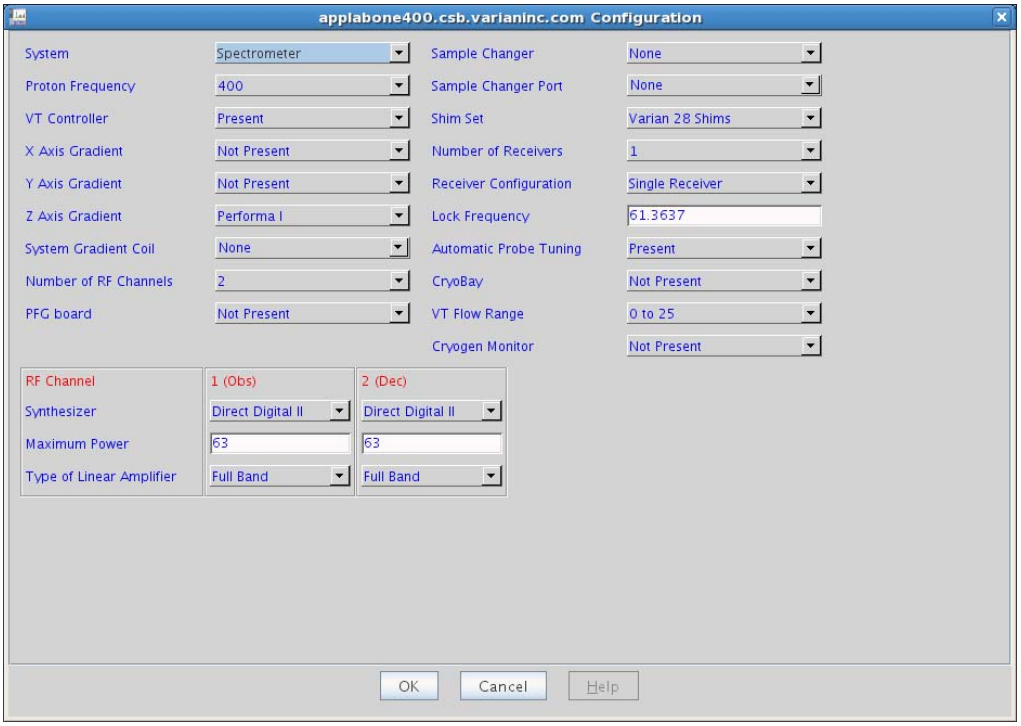


Figure 4 Spectrometer Configuration Window

2. Check that the configuration values are correct for your system.

   Refer to Table 6 General Configuration for more information on these values.

3. Configure each RF channel.

   Refer to Table 7 RF Channels Configuration for information on each selection.

4. Click **OK** to save the system settings or **Cancel** to make no changes and close the System Settings window.

5. Exit and restart VnmrJ to enable acquisition features in the main menu if the system is changed from a data station to a spectrometer.

Table 6 General Configuration

Label	Choices	Explanation
System	Spectrometer, Data Station	Sets whether function of the workstation is to control a spectrometer or to operate as a separate data station. If Data Station is selected, VnmrJ does not allow acquisitions (the *go* command, its aliases, and related commands do not work).
Proton Frequency	85, 100, 200, 300, 400, 500, 600, 700, 750, 800, 900, 3T, 4T	Sets ^{1}H frequency for spectrometer-type systems.
VT Controller	Not Present, Present	Sets whether a VT controller is present.

Label	Choices	Explanation
X Axis Gradient, Y Axis Gradient, Z Axis Gradient	Not Present, Gradient Coordinate Rotator Performa I, Performa IV, Performa XYZ, Homospoil	Sets value of the spatial axis. If the system has a waveform generator option with a gradient control unit, check the gradient values are correct next to the labels X Axis, Y Axis, and Z Axis. If the waveform generator is present for an axis, set the value to WFG+GCU. If the PFG option is installed, set the value to Performa I, Performa II, Performa III, or Performa IV; otherwise, set the value for the axis to None. Up to three gradients can be present, one for each spatial axis.
System Gradient Coil	None, Nano, Performa_1, Performa_2, Performa_XYZ	Selects the gradient coil configuration file that defines the current installed gradient coil (sysgcoil).
Number of RF Channels	1, 2, 3, 4, 5	Sets number of rf channels available (the lock channel is not included). Systems normally have 2, 3, or 4 rf channels: The first channel is for direct observation. The second channel allows decoupling or pulsing when decoupling. An optional third channel allows decoupling of a second nucleus. An optional fourth channel allows decoupling of a third nucleus. The minimum value you can select is 2. *Do not change this value to eliminate the use of a channel.* For information on how to disable a channel, refer to the descriptions of the parameters `dn2` and `dn3` in the *VnmrJ Command and Parameter Reference*.
PFG board	Present, Not Present Microimaging	Sets whether the MAS Controller is present. Sets software for both Gradient and PFG.
Sample Changer	None, Carousel, SMS 50 Sample, SMS 100 Sample, VAST, NMS, LC-NMR, 768 AS, 7510-AS, 7600-AS	Sets the type of optional sample changer. Select None if no sample changer is present or to disable an attached sample changer. Refer to Automated Hardware, for more information.
Sample Changer Port	None, Com1, Ethernet	Sets communications port used for the sample changer. Select Not Used if no sample changer is present.

Label	Choices	Explanation
Shim Set	Varian.13.Shims, Varian.14.Shims, Varian.15.Shims, Oxford.15.Shims, Oxford.18.Shims, Varian 18.Shims, Varian 20.Shims, Varian 23.Shims, Varian 26.Shims Varian 28.Shims, Varian 29.Shims, Varian 35.Shims, Varian 40 Shims, Ultra 18 Shims, Ultra 39 Shims Whole Body	Sets type of shims on the system.
Number of Receivers	1, 2, or 4	Sets the number of receivers available in the system.
Receiver Configurations	Single Receiver Parallel Multi Nuclear	Standard receiver configuration. Multi receiver configuration for Imaging. Multi receiver configuration for simultaneous multi nuclear observation..
Lock Frequency	1 Hz to 160 MHz, in 0.1 Hz steps (enter the number directly)	The value should be the same as found in the procedure in sec, which is the nominal ^{2}H observe frequency. To observe NMR signals, the value of Lock Frequency must be set correctly**.**
Automatic Probe Tuning	Present, Not Present	Select present if ProTune hardware is installed and in use, see also Setting Up Automatic Probe Tuning.
CryoBay	Present, Not Present	Select present if CryoBay hardware is installed and in use.

Table 7 RF Channels Configuration

Label	Choices	Explanation
RF Channel		Number of rf channels displayed is determined by the value set in Number of RF Channels. Channels are RF Channel 1 (Obs) and RF Channel 2 to 5 (Dec).

Label	Choices	Explanation
Synthesizer	None, PTS320, PTS500, PTS620, PTS1000, Direct Digital, Direct Digital II	Sets the model of the PTS frequency synthesizer if present on the current rf channel. The model number is written on the front of the synthesizer. To make a selection for the Decoupler RF Channel with a fixed-frequency decoupler, select PTS*** for RF channels 1 and 2 (and all others, if present), where *** is the number written on the front of the synthesizer.
Maximum Power	0 to 63 for 63-dB attenuator, or -16 to 63 for 79-dB attenuator (enter number directly)	Sets the maximum power (upper limit) to the current rf channel to prevent damage from high power rf. The decoupler channel is usually set to **45** or **50** to prevent damage to the probe.
Type of Linear Amplifier	Full band, Low band, Broadband Shared	Sets type of amplifier on the current rf channel. Full Band indicates the channel uses a linear full-band amplifier. Low Band indicates the channel uses a linear low-band amplifier. Broadband indicates the channel goes to one amplifier for all frequencies, which is the usual selection from ^{UNITY}INOVA Direct Drive horizontal NMR imaging systems. Shared means that the amplifier is fully declared with the third channel and that the fourth channel shares this amplifier with the third channel. Contact your field service engineer if you have any questions about what class amplifiers are in your system. Refer to the **`amptype`** parameter in the VnmrJ Command and Parameter Reference.

2.4 VnmrJ Patches

The latest VnmrJ patches can be downloaded from the NMR User Pages. For more information, see VnmrJ User Pages on the Web.

Patches for the VnmrJ software are available at the Varian NMR User Page at ww.varianinc.com.

1. Click **NMR** in the list of Scientific Instruments,
2. Click **User Page** in the *NMR Resources* section
3. Click **Software**,
4. Click on the appropriate software version,
5. Type the login name and password when requested.
   Follow the on-screen instructions.

2.4.1 Check the Patch Level

1. Log in as vnmr1.
2. Open a terminal window and type:
   `vnmr1> ls /vnmr/adm/patch`
3. The installed patches are listed.
   The system returns “No such file or directory” if no patches are listed.

2.4.2 Download and Install a Patch

1. Log in as vnmr1.
2. Go to the VnmrJ User Pages Web page.
3. Navigate to the Software Patches page and find the appropriate patch.
4. Read the **Readme** file for the patch before downloading and installing the patch.
   Any patch specific instructions are specified in this file.
5. Follow the instructions in the **Readme** file.
6. Click on the patch name to download it.
   Use the patchinstall script to install the patch (as specified in the Readme file).

2.5 Restoring VnmrJ 2.3A After Installing VnmrJ 3

CAUTION	The system will not function correctly if these procedures are not followed. VnmrJ 3 upgrades inter-process communication software.

2.5.1 Initial Restore to VnmrJ 2.3

The first time the system is reverted to VnmrJ 2.3, the program restore3x must be ran. The script prompts the user for the full path to the version of VnmrJ version restore.

1. Run restore3x.
2. Re-establish the `/vnmr` symbolic link to point to VnmrJ 2.3.
3. Reset the master controller on the console.
4. Run setacq as per the standard installation process.
5. Run dbsetup.

2.5.2 Subsequent Switches

Make subsequent switches between VnmrJ versions as follows:

1. Switch the link /vnmr to VnmrJ 2.3.
2. Reset the master controller.
3. Run setacq.
4. Run dbsetup.

NOTE: Do not run restore3x.

2.5.3 Sample output of `restore3x`:

```
vnmr1> restore3x
This version of VnmrJ is in /vnmr:
VNMR VERSION 3.0 REVISION A
DATE .., 2009
Enter the full path of the VnmrJ version you want to
restore: /home/vnmrj_2.3A
This will restore /home/vnmrj_2.3A
VNMRJ VERSION 2.3 REVISION A
DATE .., 2008
Done
```

2.5.4 Changing the Link

```
root# rm /vnmr
rm: remove symbolic link `/vnmr'? y
root# ln -s /home/vnmrj_2.3A /vnmr
root# ls -l /vnmr
lrwxrwxrwx 1 root root 20 Feb 6 09:14 /vnmr -> /home/
vnmrj_2.3A
```

2.5.5 Sample Output from `setacq` When Changing from 3.0 to 2.3A

```
root# /vnmr/bin/setacq
The Network Port to console = eth1, subnet = 172.16.0
The Network Port to main net = eth0, subnet = 10.190.42
One moment please...
Please make sure both console and PC are connected.
The download step may take four to eight minutes
Do not reboot the console during this process
Testing console software version, will try up to 10 seconds
NDDS Version Query Response: 'ndds4.2e_rev0
downloading 10 files to the acquisition console.
download file 1 of 10.
…
…
```

2.5.6 Sample Output of `setacq` When Changing from 2.3A to 3.0

```
Log in as the system's root user,
or enter cntrl-C to exit.
```

```
Please enter this system's root user password
Password:
The Network Port to console = eth1, subnet = 172.16.0
The Network Port to main net = eth0, subnet = 10.190.42
One moment please...
Please make sure both console and PC are connected.
The download step may take four to eight minutes
Do not reboot the console during this process
Testing console software version, will try up to 20 seconds
Master Failed to connect to publication.
downloading 10 files to the acquisition console.
download file 1 of 10
download file 2 of 10
download file 3 of 10
download file 4 of 10
download file 5 of 10
download file 6 of 10
download file 7 of 10
download file 8 of 10
download file 9 of 10
download file 10 of 10

25 second pause
downloading 10 files to the acquisition console.
download file 1 of 10
download file 2 of 10
download file 3 of 10
download file 4 of 10
download file 5 of 10
download file 6 of 10
download file 7 of 10
download file 8 of 10
download file 9 of 10
download file 10 of 10
```

Chapter 3 VnmrJ Administration

This chapter describes VnmrJ administration procedures, administrative functions, and account administration.

Sections in this chapter include:

- 3.1 VnmrJ User Pages on the Web
- 3.2 Starting the VnmrJ Admin Interface
- 3.3 VnmrJ Admin Interface
- 3.4 User Account Administration
- 3.5 User Defaults and Directories
- 3.6 User Directories and Data Saving Templates
- 3.7 Console Display Sharing

3.1 VnmrJ User Pages on the Web

The VnmrJ User Pages offer the following information for registered VnmrJ users:

- Software patches
- Online manuals
- Varian MR and MRI News — current issue and searchable archive
- User library — also provides additional software such as BioPack
- Magnetic Moments newsletter archive
- Upgrade information
- FAQs
- Bug lists

3.1.1 Registering as a VnmrJ User

Use the following procedures to register as a VnmrJ user:

1. Go to 2.2.4 Configuring Acquisitions Communications.
2. Register as a VnmrJ user to be eligible to access the User Pages.
3. Click **Registration Form.**
4. Fill in the form and click **Submit.**

3.2 Starting the VnmrJ Admin Interface

1. If the current user is the administrator, click on the VnmrJ Admin icon on the desktop and log in to the workstation using the VnmrJ administrator login.
2. If the current user is not the administrator, open a terminal window and change users to the VnmrJ administrator account.

   Enter **`vnmrj admin`** at the prompt.
3. If prompted, enter the administrator password to start VnmrJ Admin, see Figure 5.

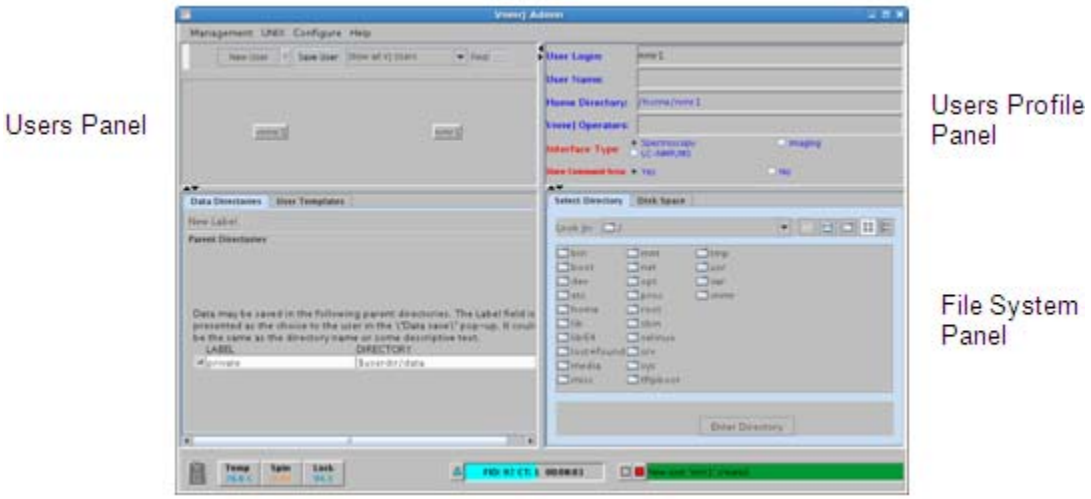


Figure 5 VnmrJ Administrator Window

3.3 VnmrJ Admin Interface

The VnmrJ Admin interface provides the tools for administering VnmrJ software and user accounts, see Figure 5. Select administration functions from the menu bar.

Table 8 VnmrJ Admin Menu

Menu Item	Description
Users	Displays users in the users panel and makes available all the administrative functions, refer to User Account Administration.
Printers	Displays printer functions using popup window, refer to Configuring Printers for VnmrJ.
Cost/Time Accounting	VNMR ACCOUNTING window. Refer to VnmrJ Accounting Administration.
Console Display Sharing	Turns on sharing of display 0 for virtual network connections
Exit	Exits and closes VnmrJ Admin.

Table 9 UNIX Menu

Menu Item	Description
File System	Popup window displays file system information; refer to Viewing the File System, for more information and instructions.
Command window	Opens an operating system terminal window.

Table 10 Configure Menu

Menu Item	Description
Users	Select additional functions using popup windows: • Convert users—opens the Change vnmr users to VnmrJ user window. Refer to Converting User Accounts to VnmrJ. • Defaults—open the default values window. For more information, see User Account Defaults. • Update users—opens the Update VnmrJ Users window. Refer to Updating User Accounts.
Operators	• Edit operators—opens the Modify Operators window (Modify Operators tab). Refer to Adding Operators to a User Account. • Delete operators—opens the Modify Operators window (Delete Operator tab). For more information, see Deleting Operators from User Accounts. • Reset password—opens the Reset Operators Password window. For more information, see Resetting Operator Password. • Preferences—open the Preferences window for setting the default operators password and for selecting a default login icon. For more information, see Setting Operator Default Password.
Automation	Calls the automation configuration popup window, see Setting Up Sample Reuse.
Edit Profiles	Create and assign user profiles containing the protocols, rights and tools. For more information, see Creating, Editing, Viewing, and Deleting Profiles.
Investigator	List Enter investigators in the popup window.
Background Colors	Change the default background colors of the VnmrJ Admin windows.

Table 11 Help Menu

Menu Item	Description
VnmrJ Help	Opens the VnmrJ HTML help pages in a browser.
Admin Help	Opens the VnmrJ Administration HTML help pages in a browser.
Online Manuals (PDF) …	Opens the VnmrJ online manuals in PDF format.

3.4 User Account Administration

User accounts are created or set up using the VnmrJ Admin interface. You can use the VnmrJ interface to set up new accounts and configuration, assign a group of operators to a single user account.

For liquids systems, the user and operators are working with an automated sample changer system—use the VnmrJ Admin interface to assign a group of operators and user to a single user account.

3.4.1 VnmrJ Interfaces

Each VnmrJ account can be set up with an interface and appropriate privileges. The main interfaces are listed in the below table.

Table 12 VnmrJ Interface Menu

Interface	Description
Spectroscopy	The spectroscopy interface is designed for both automated and manual operation, with or without a sample changer. There can be two types of users of the spectroscopy account, the account owner and the operator.
Account owner	The account owner is the operating system (OS) login user, and therefore the owner of the account and any acquisitions and data while logged in. The VnmrJ login window (if displayed) sets the operator parameter and other properties set by VnmrJ Admin, such as the user profile, panellevel, etc. The account owner sets up the preferences and settings of the account.
Operator	The operator is a user of the account but is not the OS login user of the account, therefore does not own any of the files in the account. The operator has VnmrJ access via a name and password entered on the VnmrJ login window and can operate the software.
Imaging	The imaging interface provides the user with the full range of functions necessary for the acquisition of MRI data, the design of imaging sequences, building study protocols, and processing of imaging data.

3.4.2 Creating a Single New User Account

Use this procedure to create a single new user account. New user accounts will contain default values set in User Account Defaults, see User Account Defaults. To create multiple new user accounts, see Creating Multiple New User Accounts.

1. Select **Management.**

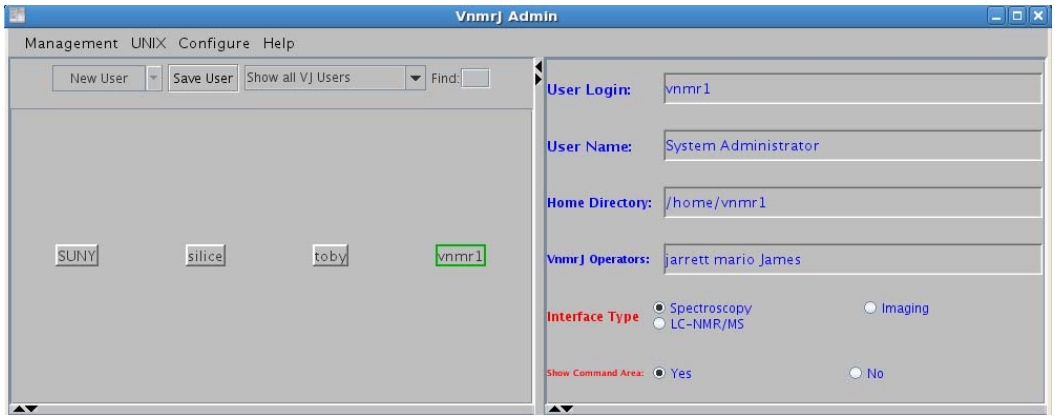


Figure 6 VnmrJ Admin Window

2. Select **Users**.
3. Select **Show all VJ Users**.
4. Click **New User**.

   New User appears with a box around it and the account's profile is displayed in the User Profile Panel.
5. Fill in the **User Profile Panel** as appropriate.

   The User Profile Panel (by default) has five sections; see User Account Defaults page to view other fields, data dir, and so on.

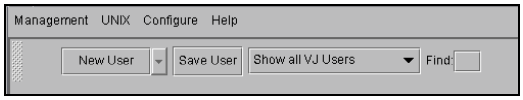
Field	Description
User Login	Type login name and select TAB prompt is displayed in the user login field.
User Name	Optional. Enter a user name.
Home Directory	New users with no operating system account: Setup is automatic and applies the user defaults (see User Account Defaults). Current users with an operating system account: The user's operating system account home directory is used.
VnmrJ Operators	Optional. List other users with VnmrJ operation privileges.
Interface Type	Click the option button to select the interface type, Refer to VnmrJ Interfaces.
Show Command Area	Click a **Yes** or **No** option button to show or hide the command area.

6. Click **Save User.**

3.4.3 Creating Multiple New User Accounts

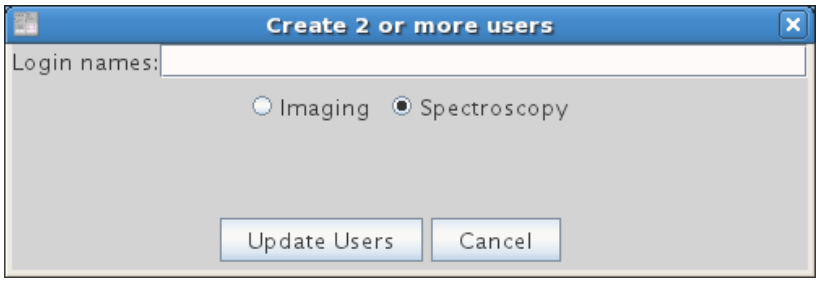
Use this procedure to create multiple new user accounts. The new user accounts will contain default values set in User Account Defaults, see User Account Defaults. To create a single new user account, see Creating a Single New User Account.

1. Select **Management** from the main menu bar.



2. Select **Users**.
3. Click the **New User** arrow.
4. Select **Multiple Users** from the drop- down menu.
5. Click **New Users** (2 or more).

   The Create 2 or more users window opens.
6. Enter the **login name** for each user. Separate each user name by a space.
7. Select the interface assigned to the multiple users. For more information, see VnmrJ Interfaces.



8. Click **Update Users**.

The home directory is automatically setup (new users - no operating system account) based upon the user defaults (see User Account Defaults). Or if the user was first set up as an operating system account, the user's operating system account home directory is used.

3.4.4 Deleting a User Account

Use this procedure to delete a user account.

1. Select **Management**.
2. Select **Users**.
3. Select **Show all VJ Users**.
4. Right-click on the user's account and select **Delete**.

Only the user account is deleted—operators assigned to the account are not deleted. Operators can be assigned to other user accounts, see Adding Operators to a User Account, or deleted, see Deleting Operators from User Accounts.

The home directory and VnmrJ files can be restored from the trash can if the trash can has not been deleted.

3.4.5 Restoring a User Account

A deleted user account can be restored if the trash can has not been emptied.

1. Double-click the **Trash Can** icon.

   The Trash Can window appears.

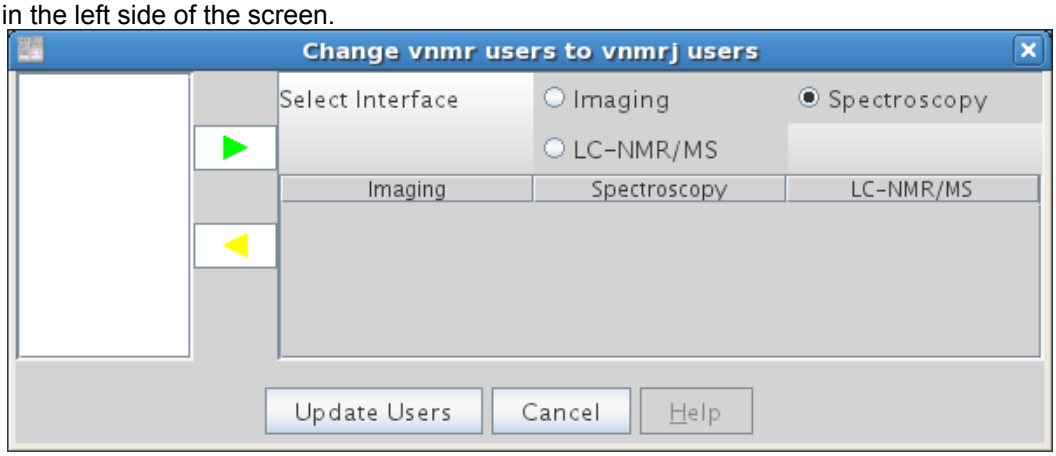
2. Select the account to be restored by clicking it once.
3. Select **Restore**.
4. Exit the **Trash Can** window.

3.4.6 Converting User Accounts to VnmrJ

Use this procedure to convert VNMR users to VnmrJ users.

1. Select **Configure** from the VnmrJ Admin interface.
2. Select **Users**.
3. Select **Convert** users.

   The Change vnmr users to vnmrj users window appears. VNMR user accounts are listed in the left side of the screen.



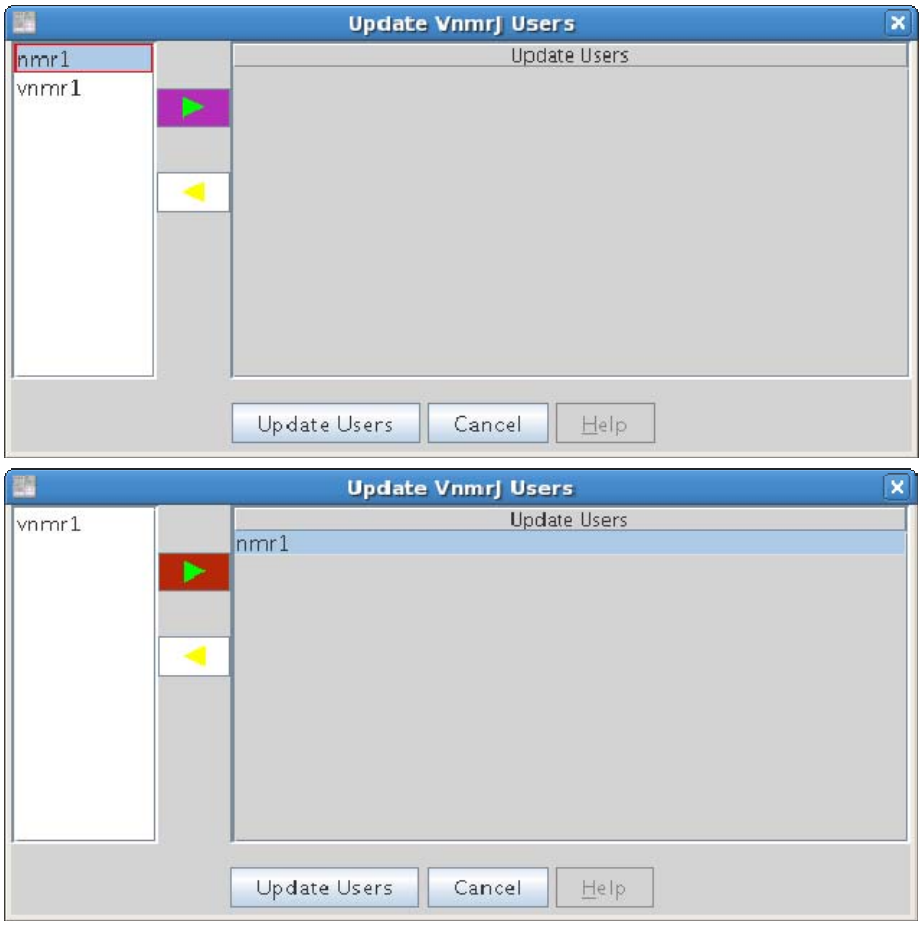
4. Click on an interface type to sort by interface type.
5. Select the **VNMR account** to be converted.
6. Select the **interface type** and click the **green arrow**.
7. Hold the **Control** and **Shift** keys to make multiple selections of accounts with the same interface.
8. Repeat the previous step for other accounts using other interfaces.
9. Click **Update Users**.

3.4.7 Updating User Accounts

Use this procedure to update multiple VnmrJ user accounts.

CAUTION	Update user accounts after upgrading or reloading software.

1. Select **Configure**.
2. Select **Users**.



3. Select **Update users**.

   The Update VnmrJ users' window appears with VnmrJ user accounts listed on the left side of the window.
4. Click on an interface to sort by that interface.
5. Select the accounts to be updated.
6. Hold the **Control** and **Shift** keys to select multiple accounts with the same interface.
7. Click the highlighted, green arrow to move the accounts to Update Users.
8. Click **Update Users**.

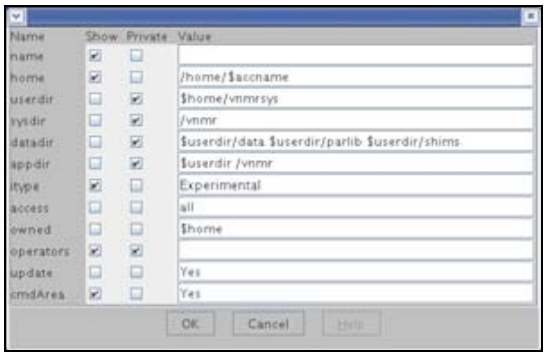
3.5 User Defaults and Directories

Use the VnmrJ Admin interface to set up user account defaults, templates, and directories.

3.5.1 User Account Defaults

Review and configure user account default properties before creating a new user account. These properties apply to all new VnmrJ user accounts.

1. Select **Configure**.
2. Select **Users**.
3. Select **Defaults**.
4. The Defaults window appears and shows the defaults that will be used when a new user account is established.



Field	Description
name	Full name of a user.
home	Home directory of a user.
userdir	Directory that contains private VnmrJ files for a user.
sysdir	System directory for VnmrJ.
datadir	Path of the directories where user data is stored.
appdir	Directory search path used to search for application-specific files.
itype	The `itype` field specifies the user interface; Spectroscopy for automation and manual operation systems.
access	User's access level to other users' data
owned	Directories that are owned by the user
operators	Authorized account users. A system login is not required.
update	When creating users, `makeuser` is automatically run to update user preferences if the value is set to Yes. This setting is only for operating system or VnmrJ users who are already in the system
cmdArea	Show or do not show a command line.

5. Review the home field, which shows the path of a new user's home directory.

   The default is set to `/home/$accname`.

   The account name is `$accname` and `/home` is where the home directory of a new user account is located. This path is only used if the user is not a defined operating system user. The current home directory of existing operating system user is used.

   Replace `/home` with the directory path to the user's home directory if `/home` does not exist or if the home directory of the user is located in another directory.

6. Review the `itype` field (the default interface type) for new VnmrJ users.

7. Click **OK** to save your changes or **Cancel** to leave the settings unchanged.

3.6 User Directories and Data Saving Templates

User Directories and Data Saving Templates are now set up in the user preferences interface.

3.7 Console Display Sharing

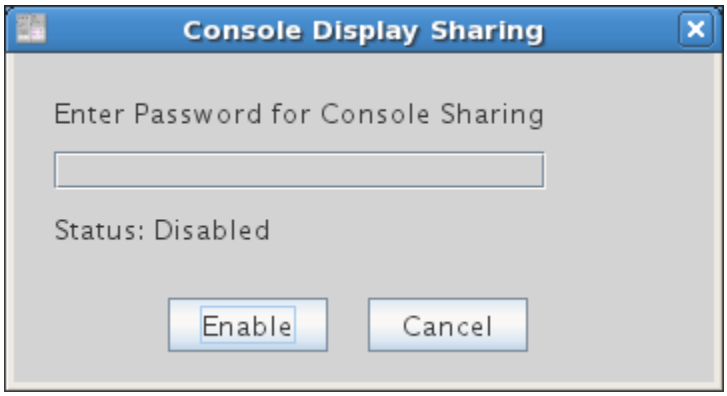
Use this procedure to share the console display with the virtual network connection (VNC) viewers.

To enable:

1. From the VnmrJ admin interface, click Management

2. Click **Console Display Sharing…**

   The Console Display Sharing window will appear.



   The status field shows if sharing is enabled or disabled. If disabled, a password entry box is present. This is the password one will use to remotely access and view the shared display (display 0).

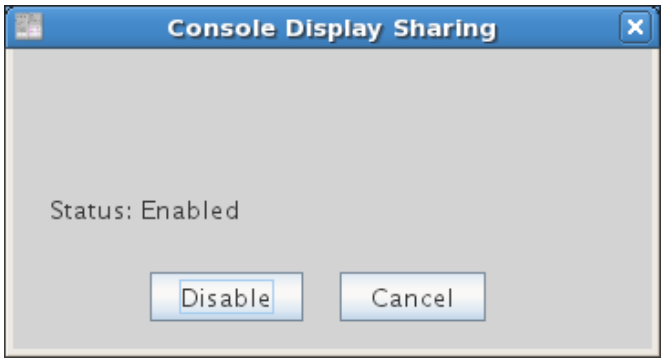
3. Enter a password and click **Enable**.

   The window will now update. If this is the first time display sharing is turned on, the workstation needs to be rebooted.

   To access the shared display, a new vnc viewer is needed, which will require the IP address of the workstation, the display (display 0) and the password provided in step 3.

To disable:

1. To disable Display Sharing, click the **Disable** button



Chapter 4 Spectroscopy Account Administration

VnmrJ administrative functions are controlled at the VnmrJ Admin level. Additional Spectroscopy administration functions are controlled by the Spectroscopy account owner; see Preferences in the *Automation User Guide*.

Sections in this chapter include:

4.1 Adding Operators to a User Account

VnmrJ operators can be added to user accounts. Operators are typically added to a Spectroscopy account owner—a Spectroscopy account with an operating system login. Typically, a Spectroscopy account owner sets up an automation run for operators to use. Operators can be VnmrJ-only operators or established VnmrJ users.

1. Click **Show all VJ Users** and select the user account to which operated are to be added.
2. Enter the name of each operator, who has NMR privileges in the selected account in the VnmrJ Operator field on the right panel.

   Separate each operator with a space. The operators can have a mixture of VnmrJ only operators and operators with both an operating system and VnmrJ account.

   Operators with no operating system account are assigned the default password, see Setting Operator Default Password.

   Operators that have an operating system account use their operating system account password to access the VnmrJ operator interface
3. Click **Save User**.

4.2 Creating Profiles - Spectroscopy Accounts

4.2.1 Implementing Profiles

Implement the operator profile for the Spectroscopy account owner and operator. The system administrator creates and assigns a profile containing the protocols, rights, and tools that are available to a specific operator or assigned to several operators.

Protocols are selected from the available list of protocols or from the Profile popup, see Figure 7.

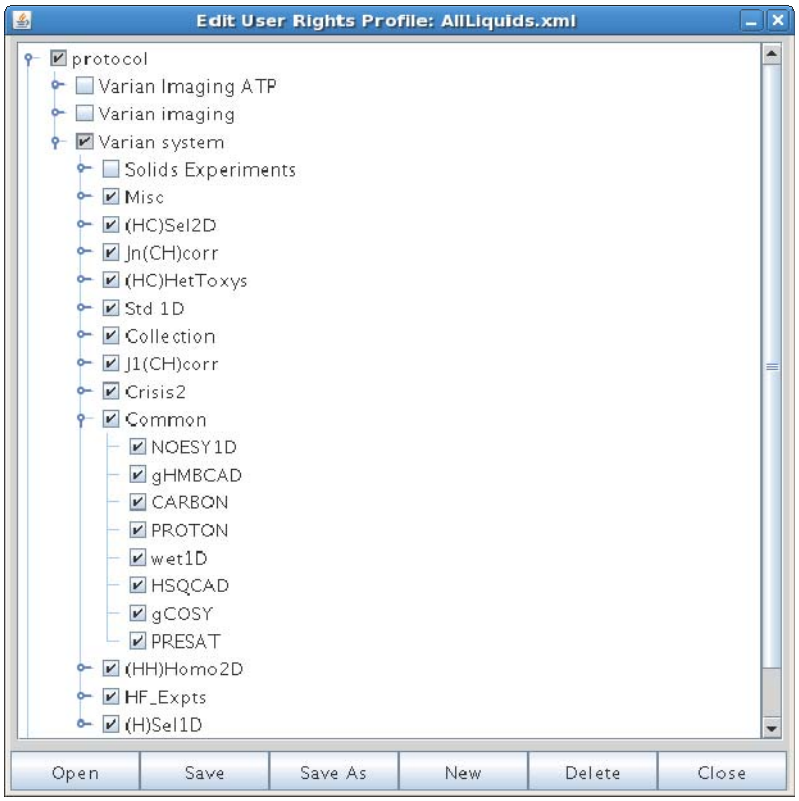


Figure 7 User Rights Profile Window

Rights are selected from the available rights listed in Table 13.

Table 13 User Profile Rights and Options

Right	Function or Action Allowed
May Edit Password	Show the Edit Password item in the Tools menu.
Can Browse Anywhere	Give the operator access to all files in the file browser.
Enable Locator Update	Show the following items in the Tools menu: Update locator submenu, Import files to locator, Save/Delete custom locator statement.
Enable All Editors	Show all items in the Edit menu, and show the Create protocols submenu in the Tools menu.
Edit Own Profile	Show the Edit config profile item in the Edit menu.

Right	Function or Action Allowed
Show Molecular Structures	Show the Molecular Structures submenu in the Tools menu.
Show All Acquisition Menus	Show the Acquisition menu.
Show All Processing Menus	Show the Process menu.
Enable Calibrations	Tools menu, show the Standard Calibration Experiments, Probe Tuning, and Gradient Shimming menus.
May Tune Probe	Show the Manual Tune Probe item in the Tools menu.
Enable Automation Setup	Show the New Workspace, Save data setup, New automation run, and Create Plot Design items in the File menu; Show the Experiments menu; Show Update night queue start time and Auto Tune Setup in the Tools menu.
Show All Operators Studies	Show studies for all operators in the study queue.
Edit All Operators Studies	May edit studies for all operators. If selected, Show All Operators Studies must also be selected.
Remove New Sample Node	When a study is cleared using New sample in the Study Options menu, do not create a new sample node.
Can Edit Protocols	May edit or customize protocols in the study queue.
Can edit application directories	Allows application edits.
Select All Prescans	Select all prescans when an operator logs in.
Select minsw	Enable or disable minimize sweep width by default.
Priority Sample	Show the priority sample check box in the study queue panel.
Can Exit VnmrJ	Operator may exit VnmrJ.

Table 14 User Tools

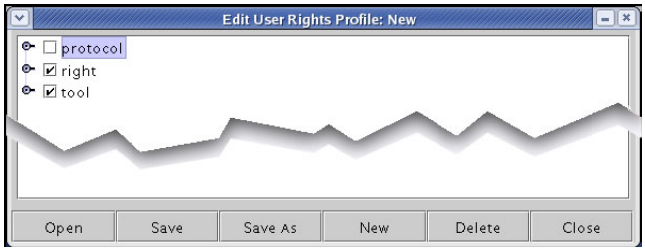
Tools	Description
Locator	Accesses database search interface.
Browser	Accesses user file retrieval interface.
Study Queue	Displays queue area in the vertical panel.

Table 15 User Profiles

User Profile	Description
AllLiquids	Contains all liquid protocols, all rights, and available tools.
BasicLiquids	Contains only a few protocols, a few rights, and available tools.
CommonLiquids	Contains common liquid protocols.
BasicLiquidsSecure	Contains a few protocols, a few rights, and available tools.
AllImaging	Contains imaging protocols, all rights, and all tools.
AllSolids	Contains all solids protocols, all rights, and all tools.

4.3 Creating, Editing, Viewing, and Deleting Profiles

1. Start **VnmrJ Admin**.



2. Click **Configure** in the main menu.
3. Select **Edit Profile**.

   The Edit User Rights Profile window opens and displays the Profile named at the top of the window.

4.3.1 Creating a New Profile

1. Select **New** to create a new profile.
2. Use the file tree controls to expand or contract the file tree:
   - Expand — click on the to change it to .
   - Collapse — click on the to change it to .
3. Set Rights as follows:
   - Allow: Select the check box.
   - Not Allow: Clear the check box.
4. Use the controls at the bottom of the Edit User Profile window to **Save** (uses existing file name), **Save As** (prompts for new file name), or **Close** (no change) the Edit User Profile window.

4.3.2 Editing or Viewing an Existing Profile

1. Select **Open** to edit an existing user rights profile.
2. Use the file tree controls to expand or contract the file tree:
   - Expand — click on the to change it to .
   - Collapse — click on the to change it to .
3. Do one of the following:
   - Close after viewing the profile — Go to Step 5 and click **Close**.
   - Continue and edit the profile by going to next step (Set Rights).
4. Set Rights as follows:
   - Allow: Select the check box.
   - Not Allow: Clear the check box.
5. Use the controls at the bottom of the **Edit User Profile** window to **Save** (uses existing file name), **Save As** (prompts for new file name), or **Close** (no change) the **Edit User Profile** window.

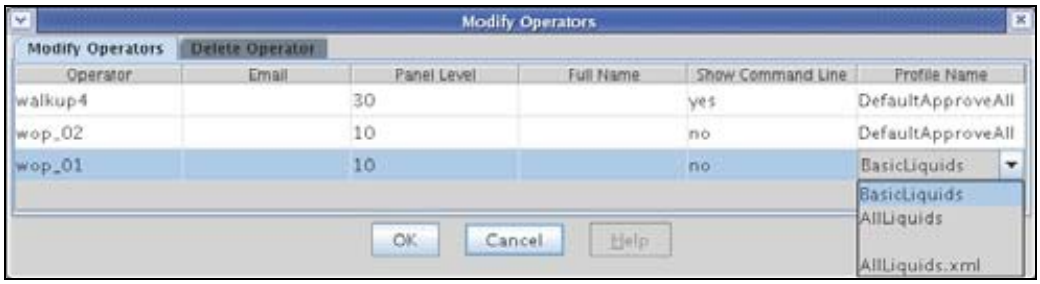
4.3.3 Deleting an Existing Profile

1. Click the **Delete** button to bring up a profile browser.
2. Select the user profile to be deleted.
3. Click the **Delete** button to delete or click the **Cancel** button to exit without deleting any profiles.*-*/*-

4.4 Assigning Operator Profiles

Assign a named profile to an operator using the VnmrJ Admin interface as follows:

1. Start **VnmrJ Admin**.
2. Click **Configure** on the main menu.
3. Select **Operators**.



4. Select **Edit Operators…**to open the Modify Operators window. The last column in the Modify Operators window is for assigning the operator or account owner a Profile Name. The default is AllLiquids.
5. Click in the field under Profile Name for an operator to access the drop down menu of profiles.
6. Select a **Profile** for operator rights. For custom profiles, see Creating, Editing, Viewing, and Deleting Profiles.
7. Click **OK** to apply the selected profile.

4.5 Setting Rights to Edit Applications Directories Search Paths

The user AllLiquids, BasicLiquids, and AllSolids profiles supplied with VnmrJ set many rights including the canEditAppdir right. AllLiquids user profile enables the canEditAppdir right and the BasicLiquids user profile disables the canEditAppdir right. The AllSolids profile replaces the liquids experiments in the experiment panel with the full set of solids related experiments.

1. Start **VnmrJ Admin**.
2. Click **Configure** in the main menu.
3. Select **Edit Profile**.

4. Expand the list under right by clicking on the to change it to .

5. Do one of the following:
   - Select the check box next to canEditAppdir right to allow the operator to edit the applications directory (default for experimental and walkup account owners).
   - Clear the box next to canEditAppdir right, to remove the right to edit the applications directory.
   - Account login users with write permission to the /vnmr/adm/users directory and subfiles can set applications directories for all users. Account login users without these systems write permissions and having the canEditAppdir right can edit and customize their private applications directories. Account login users operators that are not granted the canEditAppdi right can not change their applications directories.
6. Save the profile with new name or overwrite the current profile. Assign the profile to the operators associated with the spectroscopy account.
   a. Click **Configure**.
   b. Select **Operators**.
   c. Select **Edit operators…**
   d. Click in the **Profile Name** field for the operator.
   e. Select a **Profile** from the drop-down menu list. Continue for each operator.
   f. Click **OK** to set the assignments of the profiles and close the Modify Operators window.
7. Click **Save User**.
8. Click **Management**.
9. Click **Exit** to close the VnmrJ Admin window.

4.6 Setting Operator Default Password

Set the default password for VnmrJ operators that do not have an operating system login as follows:

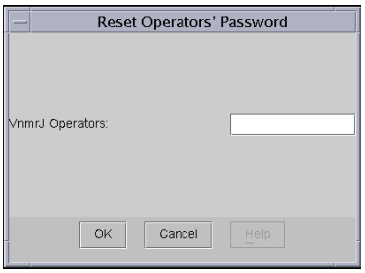
1. Select **Configure**.
2. Select **Operators**.
3. Select **Preferences**.

   The Preferences window appears.
4. Enter a default password in the password field for operators that do not have an operating system login.

   Operators with an operating system account login use the operating system account password to access the walkup operator interface. Operators, both with and without an operating system account, can change their passwords by selecting Change Password from the Tools menu on their interface. Change Password will change the both the Operator and operating system login password, if an operating system account exists.
5. Click **OK**.

4.7 Resetting Operator Password

This applies only to operators that do not have an operating system (OS) account login. Refer to the OS manual(s) to reset the password for an operator/OS account.



Reset an operator's password to the default password set in, Setting Operator Default Password, by entering the operator name and clicking OK.

4.8 Modifying Operators

4.8.1 Opening the Modify Operators Window

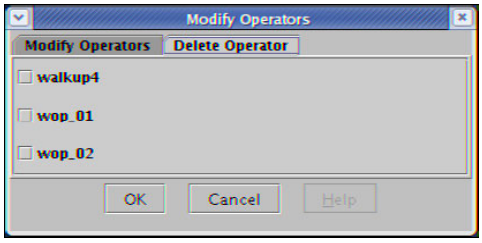
1. Start the **VnmrJ Admin** interface.
2. Select **Configure**.
3. Select **Operators**.
4. Select **Edit** operators.

   The Modify Operators window appears.
5. Select the **Modify Operators** tab.

4.8.2 Adding or Editing Operator's Email

If the operator's email is added, the operator is notified when a sample is finished.

1. Refer to Opening the Modify Operators Window.



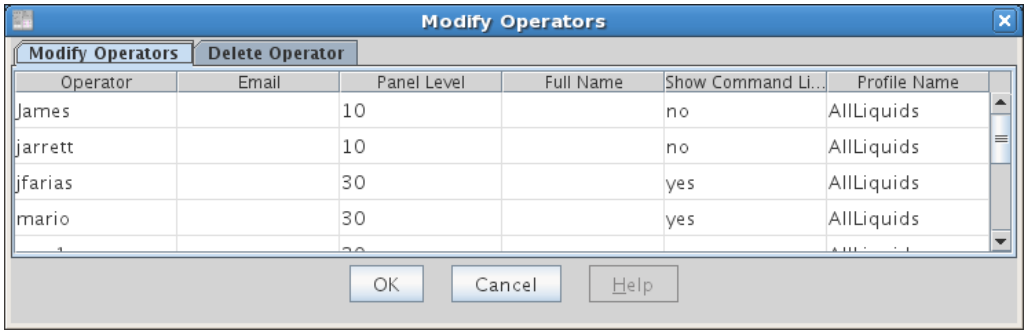
2. Edit or add an e-mail address.
3. Do one of the following:
   - Continue with Setting Panel Levels and Command Line Access.
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit from the Modify Operators window and make no changes.

4.9 Setting Panel Levels and Command Line Access

Panel levels are set by the VnmrJ Administrator and determine which VnmrJ interface pages are available under the tabs in the parameter page area. Setting panel levels applies only to walkup account owners and walkup account operators. The default is 10 for operators and 30 for the account owner. Setting the panel level higher allows for more pages to be available. The experimental VnmrJ account has a fixed panel level of 100.

NOTE: Panel levels can only be changed during the operator login process in the Walkup interface.

1. Refer to Opening the Modify Operators Window.
2. Change the panel level for any operator by entering a value in the Panel Level cell for the operator.



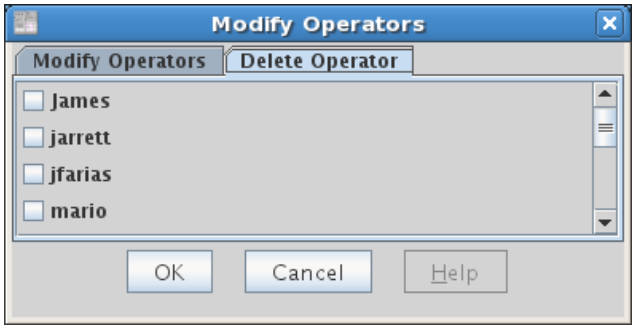
Panel level values and displayed pages are:

Value	Display
0-9	Show minimum number of pages
10-29	No shim, lock, or processing, and minimal parameter control is available. This may be used for routine automation users and is typical for a basic user Shim and lock are available only if there is a no sample changer. Basic processing is available. Pages are not fully populated, allowing control of a few basic parameters.
30-49	All pages are available and fully populated.
50-100	All pages and menu options are available and fully populated. Typical setting for the system owner.

3. Type **Yes** in the field under Show Command Line to give each operator command line access. The default is no command line access.
4. Do one of the following:
   - Continue to next section.
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

4.9.1 Adding Operators Full Name

1. Refer to Opening the Modify Operators Window.

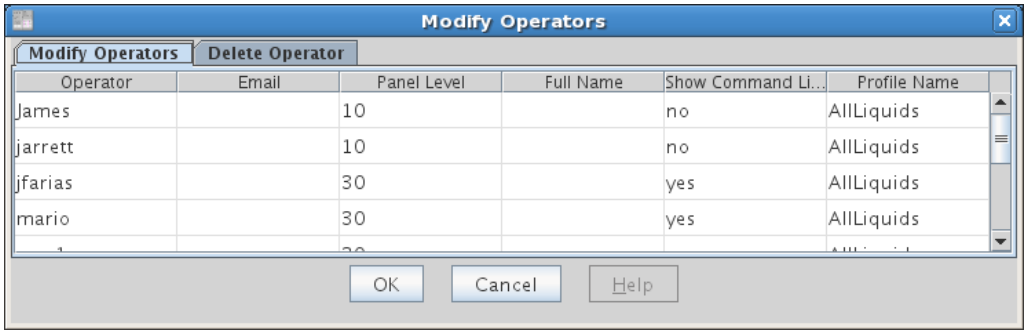


2. Edit or add the full name of the operator in the field below Full Name.
3. Do one of the following:
   - Continue with Viewing Command Line Access.
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

4.9.2 Viewing Command Line Access

1. Refer to Opening the Modify Operators Window.

   The command line access is displayed in the field below Show Command Line in the operator's row.

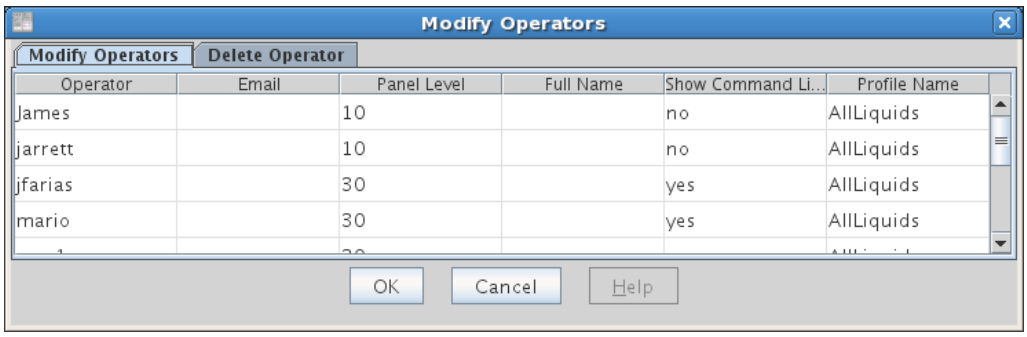


2. Access to the command line is set by Setting Panel Levels and Command Line Access or by Adding or Editing User Profiles.
3. Do one of the following:
   - Continue with Adding or Editing User Profiles.
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

4.9.3 Adding or Editing User Profiles

1. Refer to Creating Profiles - Spectroscopy Accounts
2. Create or edit an existing user profile.
3. Close the Edit User Rights Profile window.

4. Write down the name or names of the user profiles that will be assigned to the operators.
5. Refer to Opening the Modify Operators Window.
6. Type the name of the profile (with no extension) in the field below Profile in the operator's row.



7. Do one of the following:
   - Click **OK** to close the Modify Operators window.
   - Click **Cancel** to exit the Modify Operators window and make no changes.

4.10 Deleting Operators from User Accounts

Operators can be removed from all accounts or from a single account.

4.10.1 Deleting Operators from All Assigned Accounts

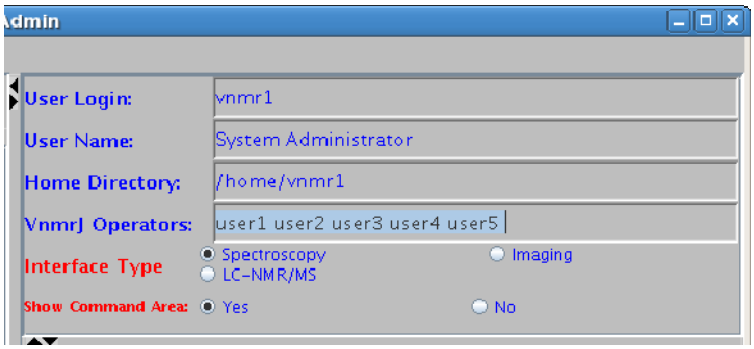
1. Select **Configure**.
2. Select **Operators**.
3. Select **Delete Operator**.
   The Modify Operators window appears displaying the Delete Operators tab.

4. Select operators to be removed and click **OK**.

4.10.2 Deleting an Operator from a Single Account

1. Select a user account.
   The operators are listed in the right panel, in the VnmrJ Operators field.
2. Delete the operator(s) from the list.

3. Click **Save User**.



4.11 Changing the Icon on the Operator Login Screen

The Default Operator Login window contains the Varian, Inc. logo, which is a GIF file. Change the logo as follows.

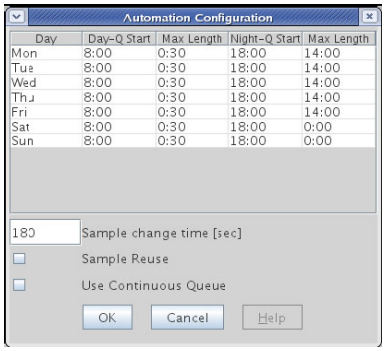
1. Select **Configure**.
2. Select **Operators**.
3. Select **Preferences** to display the Preferences window.
4. Enter the complete path to the GIF file.
5. Click **OK**.

4.12 Setting Up Sample Reuse

This procedure applies to the Automation Queue used with the Spectroscopy interface.

1. Select Configure.
2. Select Automation.

   The Automation Configuration window has the following columns:

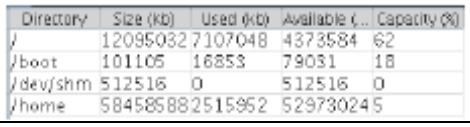


3. Select **Sample Reuse** to reuse sample numbers during an automation run.
   Only the Sample Reuse is used from this interface, all other options are set from within the Preferences window of the VnmrJ account.
4. Do one of the following:
   - Click **OK** to save the automation queue (changes and closes the window)
   - Click **Cancel** to close the window without saving changes.

4.13 Viewing the File System

The lower right panel of the VnmrJ Admin interface shows information about the operating system.

The Select Directory tab has the following icons:

Instruction/Button/Icon	Description or Window
1. Select **UNIX**. 2. Select **File System**. The View Directories window opens.	
Disk space window	
Disk space window displays information about mounted network directories, disk partitions, size, space used, space available, available capacity. This same information is also shown from Disk Space tab in the VnmrJ Admin Interface.	
	Change directory to selected directory.
	Go to admin's /home directory.
	Create a new directory in the current directory.
	List files with small icons.
	List files with small icons and details.
Look In drop down menu	Select a directory from the drop down list. Click on a directory in the directories window to select a directory. The directory is inserted in the empty directory field of user directories; see User Directories and Data Saving Templates.

Chapter 5 Configuring Printers for VnmrJ

Use the Linux Printer Set window, wizard, and Vnmr Plotter Configuration window to add or manage a printer.

NOTE: Adding or managing a printer is done by the Linux or VnmrJ administrator.

Sections in this chapter include:

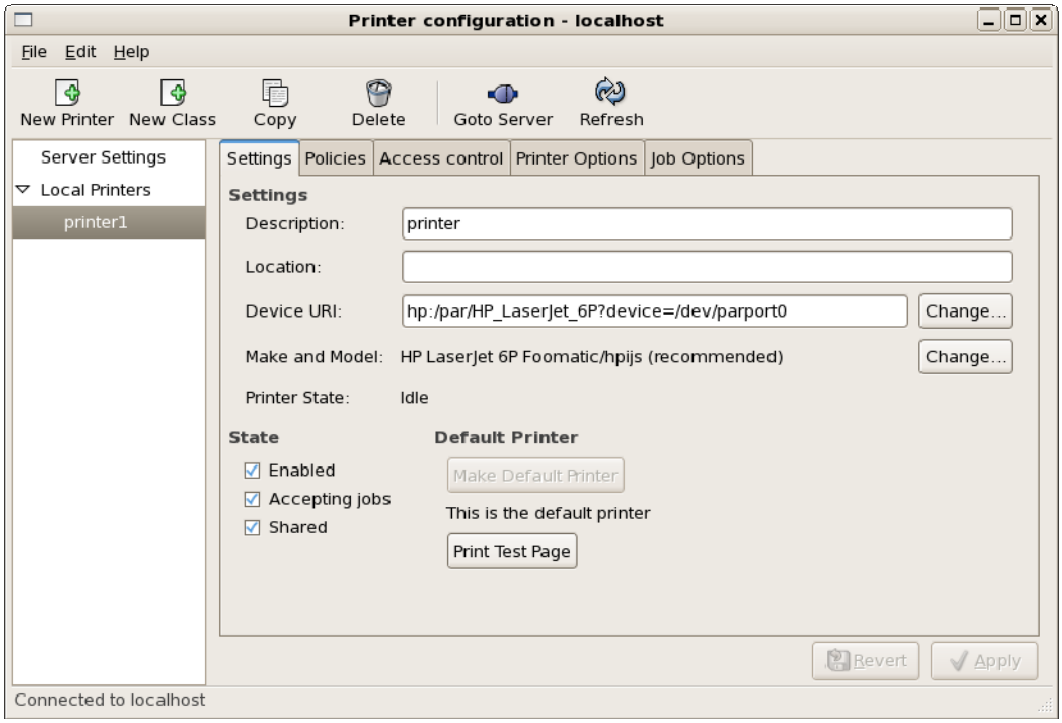
- 5.1 Setting Up a Linux Printer
- 5.2 Setting up a Printer for VnmrJ

5.1 Setting Up a Linux Printer

As the Linux or VnmrJ administrator, use this procedure to set up a printer.

1. Click the Linux **System** menu.
2. Select **Administration**.
3. Select **Printing**.
4. Enter the root user's password in the popup window.

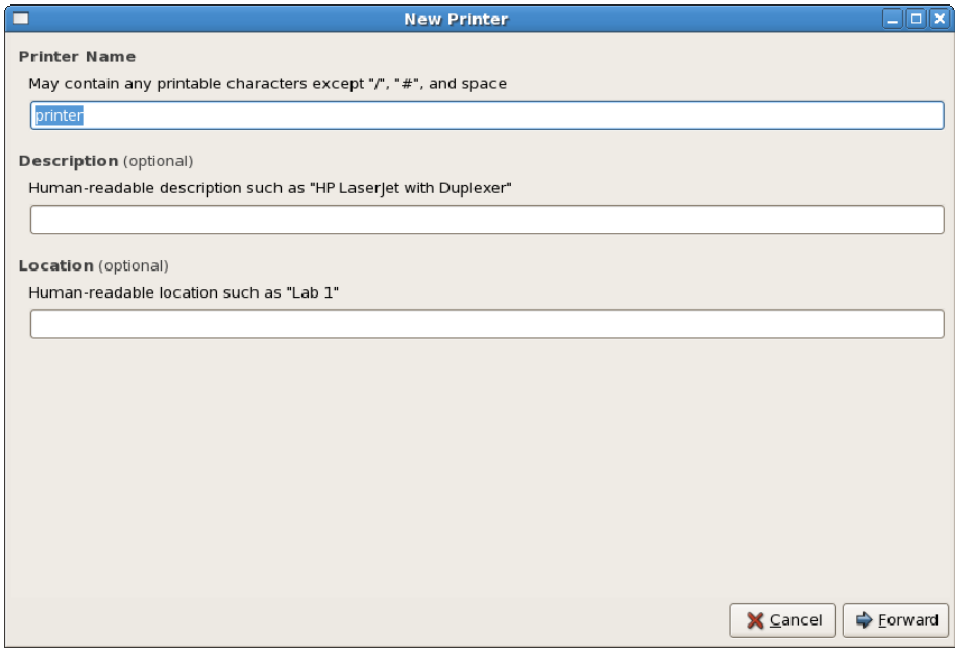
   The Printer Configuration window appears. Use this window to configure, add, or remove Linux printers.
5. Click **Print Test Page** to verify proper printer configuration.



6. To add a new printer, click **New Printer**.

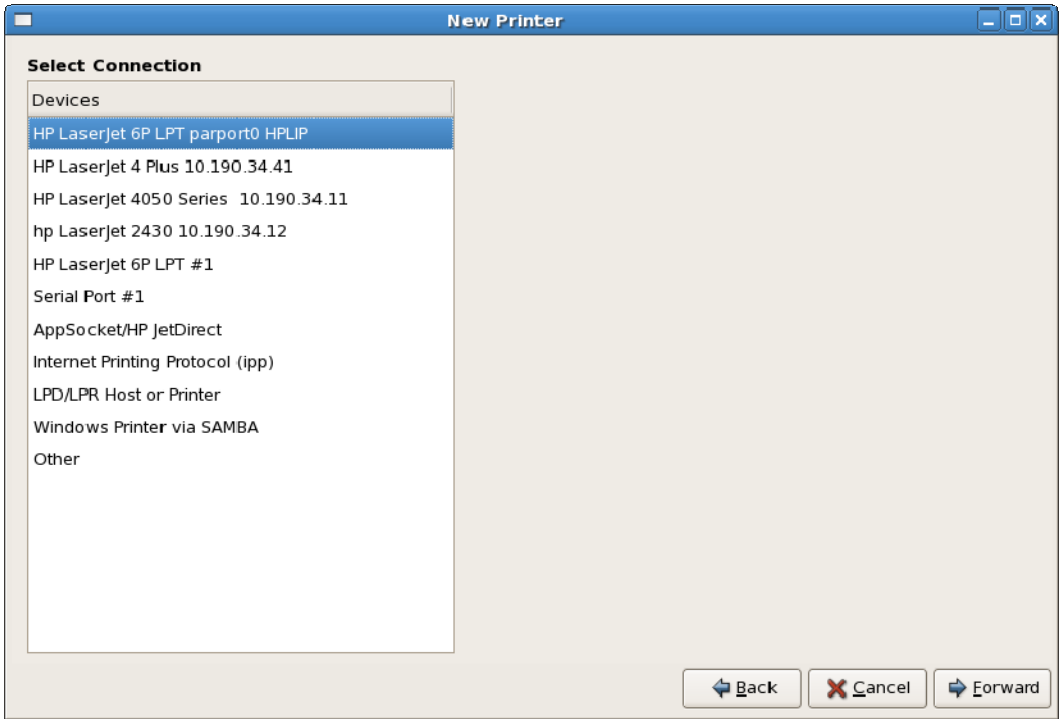
   A New Printer wizard is displayed to assist in adding a printer.

7. Enter a **Printer Name**, **Description**, **Location,** and click **Forward**.



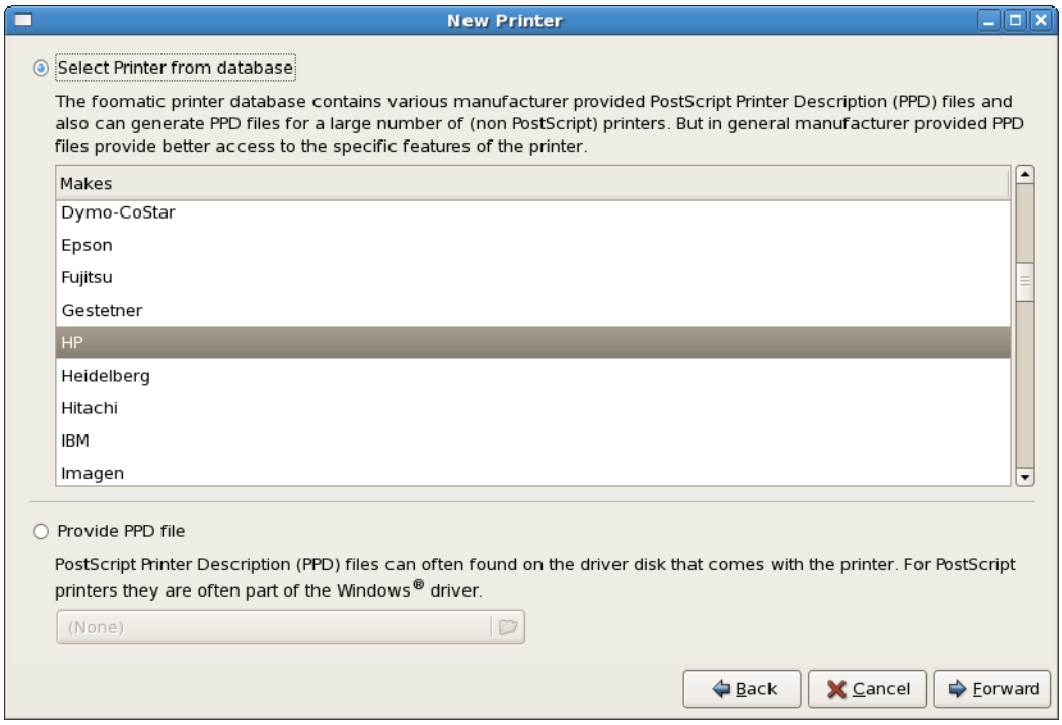
8. Select the printer connection then click **Forward**.

   The wizard detects and lists printers that are turned on and connected to the workstation.

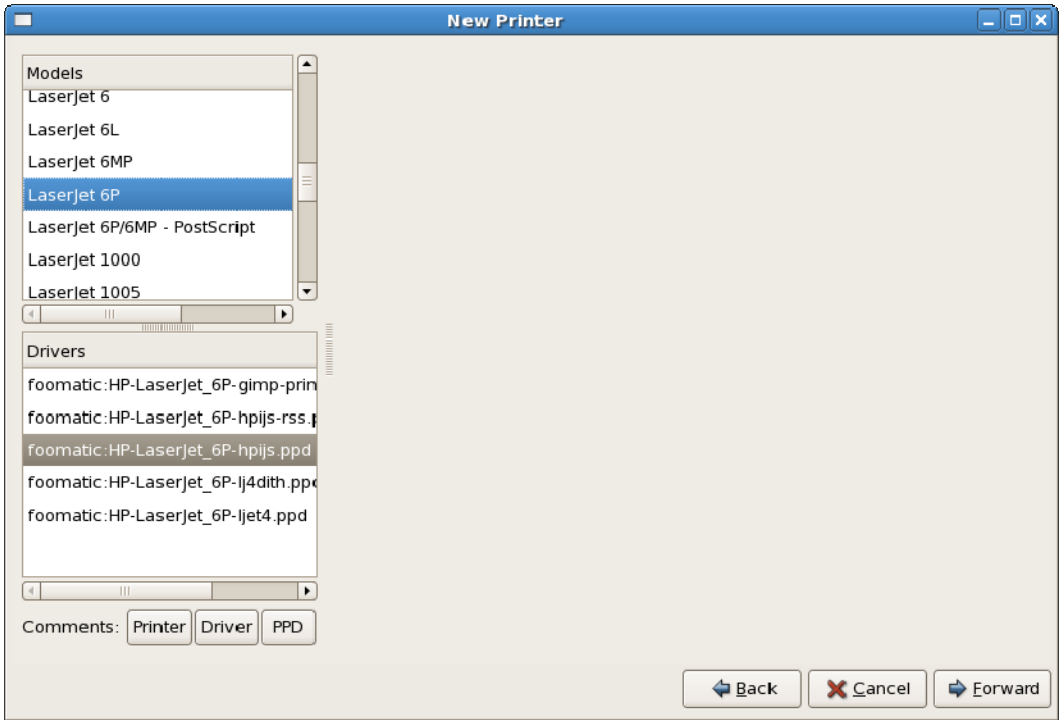


9. Select a PostScript Printer Description then click **Forward.**

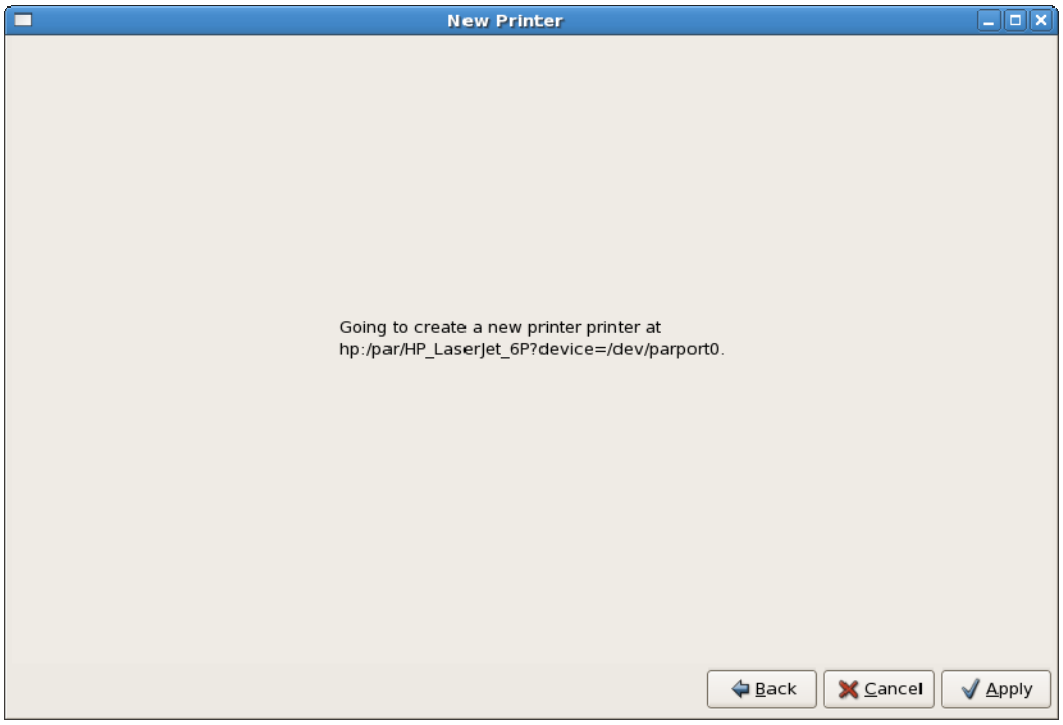
10. Select the printer. The wizard highlights the detected printer.



11. Select the printer model and driver, and then click **Forward**. The wizard highlights the detected printer's model and default driver.



12. Click **Apply** to create the new printer.



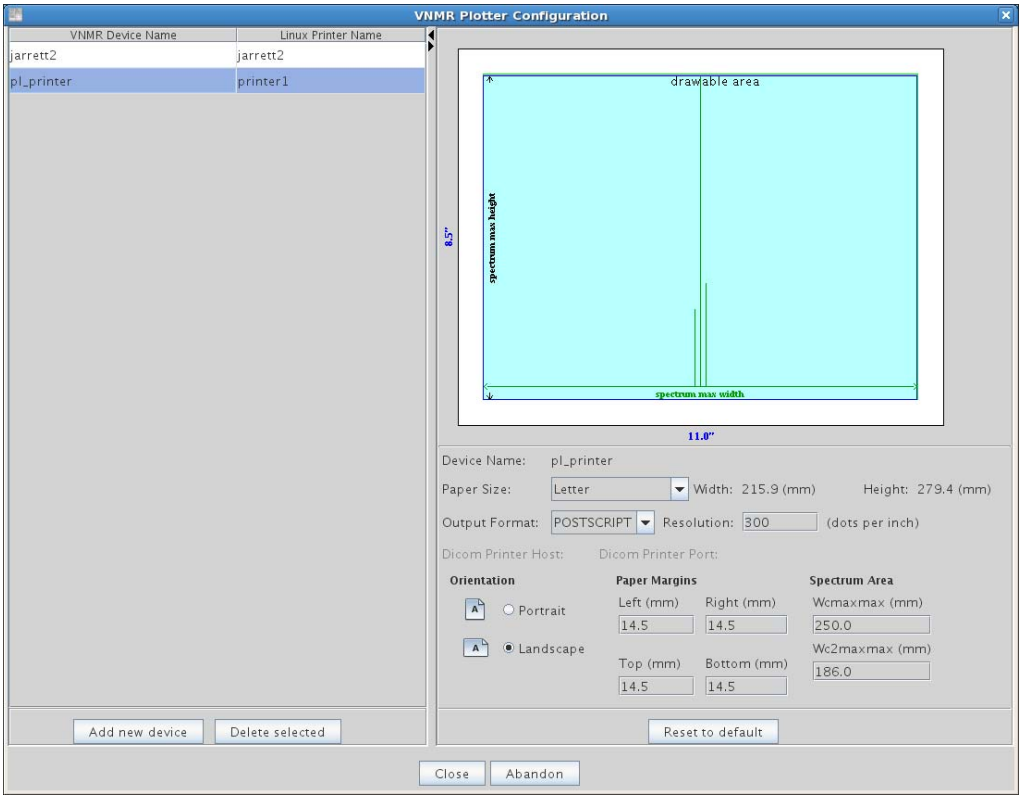
13. Print a test page from the Printer Configuration window to verify proper configuration of the printer.

NOTE: To delete a printer, select the printer in the Printer Configuration window and click the Trash Can icon.

5.2 Setting up a Printer for VnmrJ

Set up a VnmrJ printer using the VNMR Plotter Configuration window.

1. Click the **VnmrJ Admin** icon.
2. Click **Management**.
3. Select **Printers...** to open the VNMR Plotter Configuration window.



4. Select an available printer from the Linux Printer Name pull down menu.
5. Enter in a Name that VnmrJ will use to recognize this printer in the VNMR Device Name entry window.
6. Configure VnmrJ page settings on the right of the **VNMR Plotter Configuration** window: paper size, output format, dots per inch (dpi), paper orientation, and printable area.

   NOTE: The **Reset to default** button resets the printer configuration to the last saved settings. It does not restore the settings to a "factory default."

7. Click **Close** to save and close the VNMR Plotter Configuration. To abandon all changes, click **Abandon**.
8. To delete a printer, select the printer in the **VNMR Device Name** column.
9. Click **Delete selected**, then click **Close** to save the deletion and close the VnmrJ Plotter Configuration window.

   NOTE: To use a non-standard device type, create a printer with the VNMR Plotter Configuration window then edit that printer entry in the /vnmr/devicenames file to contain the appropriate type. See Table 16 for various types and descriptions.

Table 16 VnmrJ Printer and Plotter Types with Descriptions

VnmrJ Device Type	Description
HP7475A	HP7475 plotter
HP7550A	HP7550 plotter using 11x17 inch paper

VnmrJ Device Type	Description
HP7550A8	HP7550 plotter using 8 1/2 x 11 inch paper
DeskJet_300	HP DeskJet using 300 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
DeskJet_300R	HP DeskJet using 300 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
DraftPro_C	HP DraftPro plotter using size C paper
DraftPro_D	HP DraftPro plotter using size D paper
DraftMaster_A	HP DraftMaster plotter using size A paper
DraftMaster_B	HP DraftMaster plotter using size B paper
DraftMaster_C	HP DraftMaster plotter using size C paper
DraftMaster_D	HP DraftMaster plotter using size D paper
DraftMaster_E	HP DraftMaster plotter using size E paper
LaserJet_150	HP LaserJet (or DeskJet) using 150 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
LaserJet_150R	HP LaserJet (or DeskJet) using 150 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LaserJet_300	HP LaserJet (or DeskJet) using 300 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
LaserJet_300R	HP LaserJet (or DeskJet) using 300 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_B_300R	HP LaserJet (or DeskJet) using 300 dpi, B-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_300R	HP LaserJet (or DeskJet) using 300 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_300R	HP LaserJet (or DeskJet) using 300 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LaserJet_4550	HP Color LaserJet using 600 dpi.
LaserJet_600R	HP LaserJet (or DeskJet) using 600 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.

VnmrJ Device Type	Description
LJ_B_600R	HP LaserJet (or DeskJet) using 600 dpi, B-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_600R	HP LaserJet (or DeskJet) using 600 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
PS_A	PostScript printer using vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value is not recommended.
PS_AR	PostScript printer (e.g., PS4069) using horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
PS4079_HPGL	Lexmark PS4079 or PS4079plus using 11x17 inch paper in HPGL mode. HPGL mode is required for color output.
QuietJet_96	HP QuietJet using low 96 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
QuietJet_96R	HP QuietJet using 96 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
QuietJet_192	HP QuietJet using 192 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
QuietJet_192R	HP QuietJet using 192 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
ThinkJet_96	HP ThinkJet using 96 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
ThinkJet_96R	HP ThinkJet using 96 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
ThinkJet_192	HP ThinkJet using 192 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
ThinkJet_192R	HP ThinkJet using 192 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.

Chapter 6 Automated Hardware

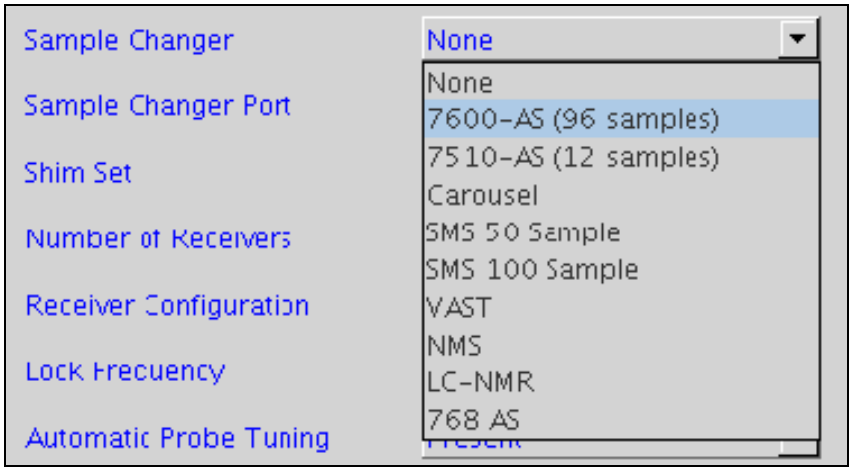
This section describes how to configure software to control automated hardware. Set up procedures require system hardware administration access, typically vnmr1, and may require VnmrJ system administrator access.

Sections in this chapter include:

- 6.1 Setting Up Automated Sample Handling
- 6.2 Setting Up Automatic Probe Tuning
- 6.3 Setting / Resetting the Phase for Automatic Probe Tuning

6.1 Setting Up Automated Sample Handling

1. Log in as the system hardware administrator.
2. Click **Edit** on the main menu.
3. Select **System settings**.
4. Click the **System config** button.
5. Click the drop down menu next to the Sample Changer field and select a sample changer option.



6. Click the drop-down menu next to the Sample Changer Port field.
7. Select a sample changer port.

8. Click the drop- down menu next to the Sample Changer Port field.

SMS 50, 100, NMS, Carousel	Select Com1
7600-AS, 7510-AS, 768AS	Select Ethernet
Not used or no sample handler	None

Operating and other instructions specific to an automated sample handing option are contained in the Automation manual and their corresponding hardware manuals.

9. Click **OK**.

6.2 Setting Up Automatic Probe Tuning

6.2.1 Configuring the Software for ProTune

1. Log in as the system hardware administrator, typically vnmr1.
2. Click **Edit** on the main menu.
3. Select **System Settings**.
4. Click the **System config** button.
5. Select **Present** from the drop down menu next to the Automatic Probe Tuning field.
6. Click **OK.**
7. Continue with Loading chan# and motor# Persistence Files.

6.2.2 Loading chan# and motor# Persistence Files

AutoX and PZT compatible probes ship with a CD containing Persistence files (chan# and motor# files) specific to that probe. These files characterize the probe for the Automatic probe tuning accessory and are used the first time the probe is automatically tuned.

Load the Persistence files as follows:

1. Insert the CD with probe Persistence files into the CD ROM drive.
2. Open a terminal window and do one of the following:

   Locate the system probe file.

   g. Type:
   ```
   cd /vnmr/probes
   ls
   ```
   h. Write down the <name of probe file>.

   i. Continue with step 3.

   Create a probe system file.

   a. Follow the procedure in Setting Up, Selecting, and Creating a Probe Calibration File.

   b. Type:
   ```
   cd /vnmr/probes
   ls
   ```
   c. Verify and write down the <name of probe file>.

d. Continue with step 3.

3. Type:

   ```
   cd /vnmr/tune
   mkdir <name of probe file>
   ```

4. Change to the CDROM directory and enter one of the following:

   ```
   cd /media/cdrecorder
   ```

5. Copy the Persistence files from the CDROM to the created probe directory:

   Type: `cp * /vnmr/tune/<name of probe file>`

6. Verify that the files were copied.

   Type: `ls /vnmr/tune/<name of probe file>`

   The new ProbeName directory should contain six chan# files (chan#0 through chan#5) and six motor# files (motor#0 through motor#5).

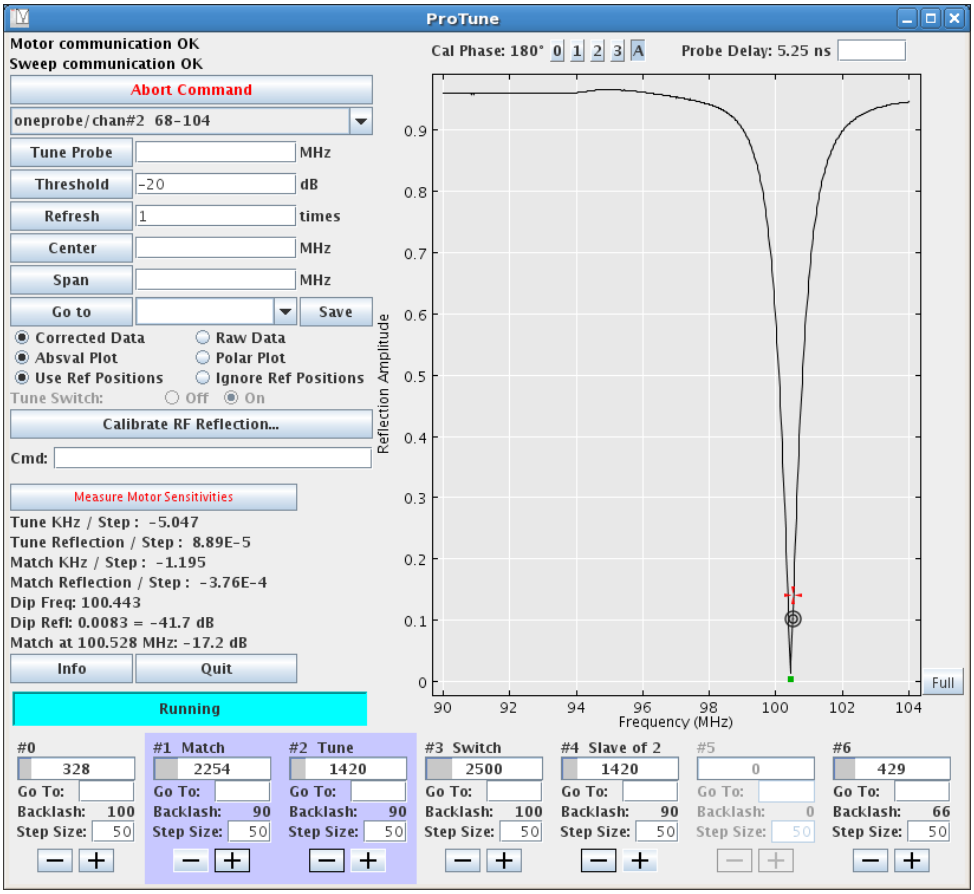
ProTune software copies the probe Persistence files to the directory ~user/vnmrsys/tune the first time it is run by a user. If the directory has not been created, the directory is created. A database of reference values is maintained in the local directory.

6.3 Setting / Resetting the Phase for Automatic Probe Tuning

This section provides instructions for setting or resetting the phase for ProTune. It may be necessary to reset the phase if the NMR console has been power cycled.

6.3.1 Starting the ProTune GUI

1. Log in as the system hardware administrator, typically vnmr1.
2. Start the VnmrJ by clicking on the **VnmrJ** icon.
3. From the command line type `protune('calibrate')`
   The ProTune GUI appears.



4. Click the **A** button located in the top center of the ProTune GUI for the program to automatically find the best phase.

NOTE: One can manually set the phase by clicking on the 0, 1, 2, 3 buttons and observing the displayed reflection. The phase which provides the flattest base is the phase to save.

Chapter 7 VnmrJ Accounting Administration

The VnmrJ Accounting tool provides NMR administrators an effective way to keep a log of VnmrJ users. Use VnmrJ Accounting to create groups of console users with single-rate or multi-rate billing, show and print invoices and accounting reports.

Sections in this chapter include:

7.1 Starting VnmrJ Accounting

Start VnmrJ Accounting from:

- VnmrJ Admin
  a. Log in as the system administrator, typically vnmr1.
  b. Start **VnmrJ Admin**
  c. Click **Management** in the menu bar.
  d. Select **Cost/Time Accounting**.
- Terminal Window
  a. Open a terminal window.
  b. Change users to the system administrator if the terminal window as not opened while logged in as the system administrator.
  c. Type **vnmr_accounting**

7.2 VnmrJ Accounting Window Interface

7.2.1 Billing

Click the **Billing** tab to open the Billing window, see Figure 8.

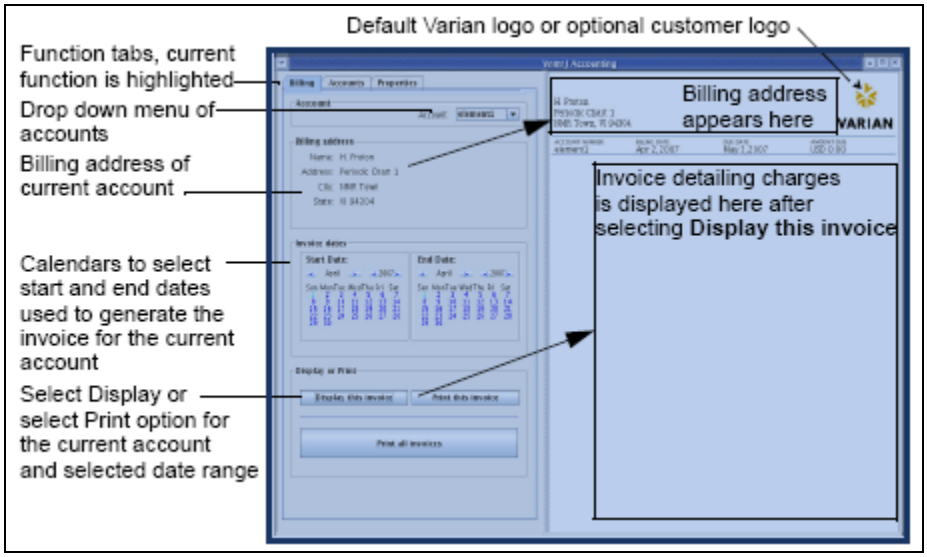


Figure 8 VnmrJ Accounting Billing Window

7.2.2 Accounts

Click the **Accounts** tab to open the Accounts window, see Figure 9.

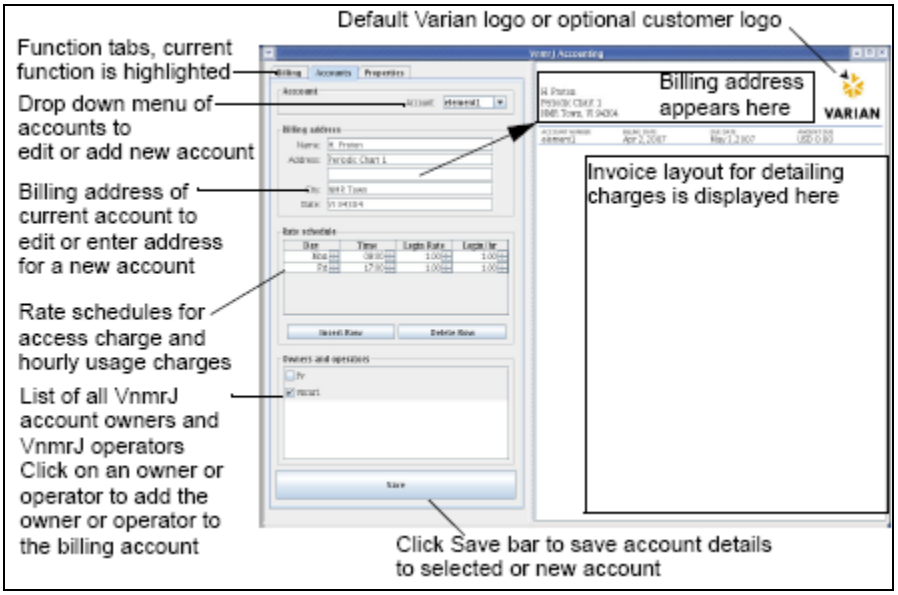


Figure 9 VnmrJ Accounting Accounts Window

7.2.3 Properties

Click the **Properties** tab to open the Properties window, see Figure 10.

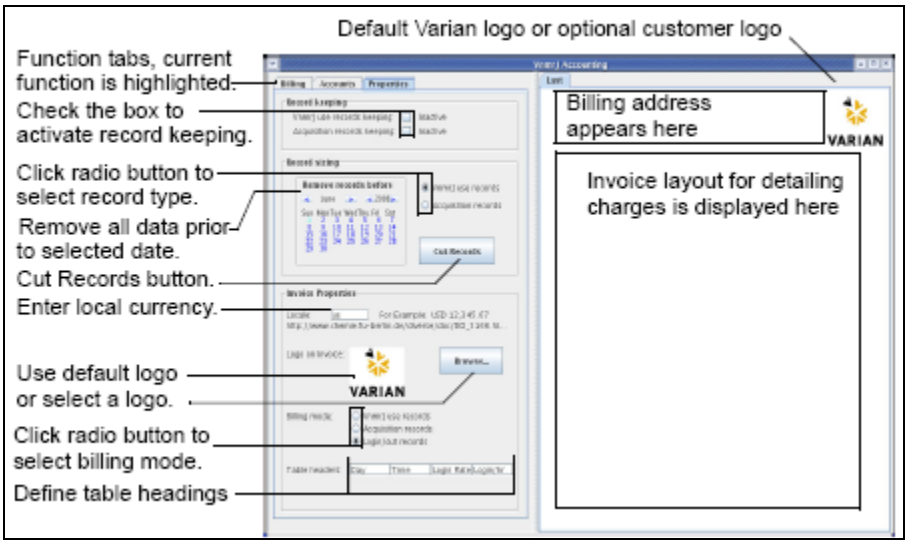


Figure 10 VnmrJ Accounting Properties Window

7.3 Generating Invoices

1. Start VnmrJ Accounting if it is not running.
2. Select the **Billing** tab.
3. Select an account number from the drop down list of accounts in the Account: field.
4. Select the start day using the Start Date: calendar controls as follows:
   a. Select a month and year using the calendar controls.
   b. Select a date by clicking on the calendar date in the selected month and year.
5. Select the end day using the End Date: calendar controls as in step 4.
6. Do one of the following:

   Print Invoice for currently displayed account

   a. Click **Display** this invoice button to display the invoice on the right side of the Billing tab, see Figure 8.
   b. Click **Print this invoice** to print the displayed invoice.

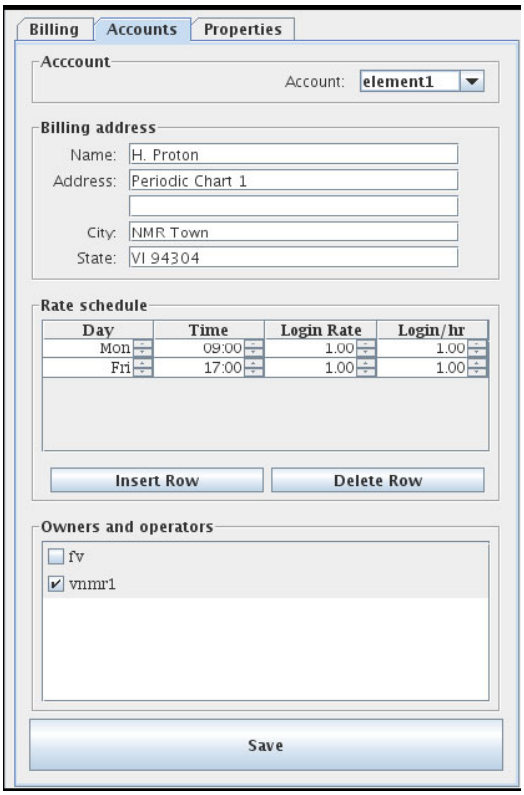
   Print invoices for all accounts on system.

   a. Click **Print all invoices** to generate an invoice for each account on the system.
   b. Click **Print Summary** button to print out the summary page.

      The summary can be saved as a comma separated value (.csv) file for use with other software.

7.4 Creating or Editing an Account

A billing account gathers the time and use charges for system login account owners and any operators with privileges to use the system login account.



1. Create any required system login accounts that are required, see User Account Administration,.
2. Add any required operators to each system login in account; see Adding Operators to a User Account,
3. Start VnmrJ Accounting, see Starting VnmrJ Accounting,.
4. Select the Accounts tab.
5. Enter an account name in the Account: field in the Account region or select an existing account number from the drop down menu.

   Account name can be alpha, numeric, a combination, and can contain dashes or underlines. Do not use spaces, special characters, or non printing characters. Any string that is a legal filename may be used.
6. Complete the Billing address information work sheet for a new account or edit the information as required to update of an existing account.
7. Create or edit the billing rate, see Establishing or Editing a Billing Rate Schedule, Add owners and operators whose usage is tracked and billed to this new account by placing a check mark in the box next to the owner or operator.
8. Click **Save** to save the new or updated account information.

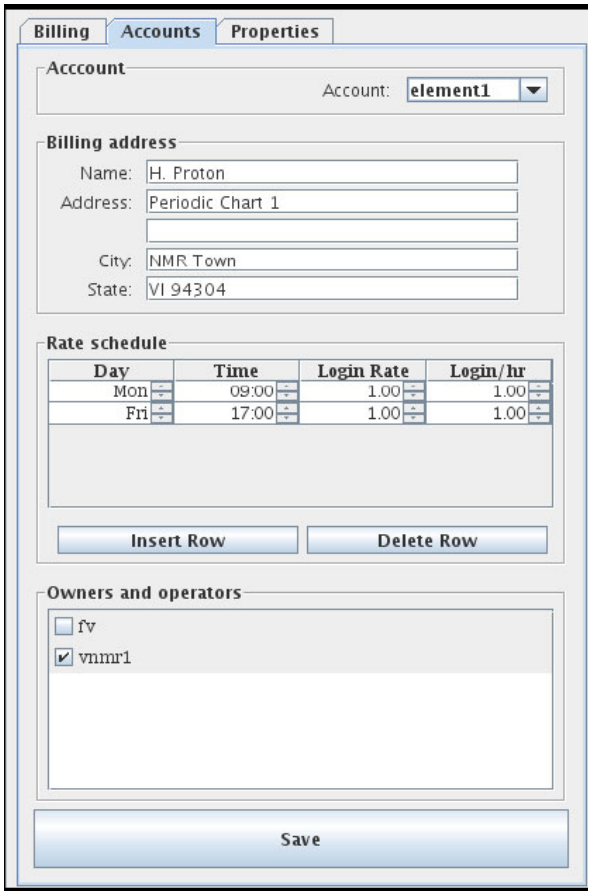
7.5 Establishing or Editing a Billing Rate Schedule

7.5.1 Billing Rates

Usage is billed at the sum of the hourly rate times the number of hours plus the login or go rate charge.

The rate schedule for the current account is shown in the Rate schedule region A new account will have only one billing row. An existing account will have one or more billing rows.

1. Enter account values for: Set the day, time, login rate, and hourly rate (Login billing default) or set the day, time, Go rate, Go hourly rate (Acquisition billing default) by using the control to set the required value or enter the information into the fields.



2. Insert or delete rows as required:

   Insert a new row:

   a. Place the cursor in any field in the row below which a new row is required.

   b. Click on the Insert Row bar to add a row below the row with the cursor.

   Delete a row:

   a. Place the cursor in any field in the row to be deleted.

   b. Click on the Delete Row bar to delete the row.

3. Click on the Save bar to save the new rate schedule for the current account.

7.5.2 Billing Rates Example

The billing period and rate begins on the day specified in the Day field at the time specified in the Time field and continues at the specified rate until a new time (on the same day) or new time and day are encountered. The rate of the last row applies until the time specified in the first row.

Set up a weekday / weekend schedule as follows:

1. Set the day on the first row to Mon.
2. Set the Time to 06:00 (6 AM). Change the hours using up and down arrows by double clicking on the hours first. Change the minutes using up and down arrows by double clicking on the minutes first. The time can also be entered.
3. Set a Rate for Login or Go.
4. Set the hourly rate.
5. Add a new row below the current row.
6. Set the day on the new row to Sat.
7. Set a new time of 00:01 (12:01 AM Saturday morning)
8. Set a new Rate
9. Set a new hourly rate.

The weekday rate in this example begins at 06:00 hours on Monday and continues until one minute past midnight on Friday or 00:01 hours Saturday morning. The weekend rate continues until 06:00 hours Monday morning when the weekday rate starts.

7.6 Controlling Properties

Properties apply to all system accounts.

7.6.1 Enable/Disable Record Keeping

1. Select the **Properties** tab to display the current account properties.
2. Activate the record keeping type by placing a check in the box next to the type of record keeping:
   - Login/out records keeping
   - Acquisition records keeping

   The label changes from inactive or on hold to active when the box is checked.
3. Type the command `su acqproc` twice if the Acquisition record keeping is (re)activated.

7.6.2 Reducing Record Size

The accounting record files can be large over time. To reduce their size:

1. Select a month and year using the calendar controls.
2. Select a date by clicking on the calendar date in the selected month and year.
3. Select Log/out records or Acquisition records.
4. Click the Cut Records button.

7.7 Invoice Properties

7.7.1 Locale

Enter a two letter local code in the **Locale:** field to establish the billing currency correct currency format. Local codes and currency formats are available at:
http://www.chemie.fu-berlin.de/diverse/doc/ISO_3166.html.

7.7.2 Logo

Keep the default Varian logo or select a custom logo using the **Browse** button. Place any custom logos in /vnmr/adm/accounting/ as .gif files. The default logo is 87x70 pixels. The logo does not have a size limit and the invoice layout can adjust to accommodate logo size.

7.7.3 Billing Modes

Account billing is determined by one of three billing modes:

- **Acquisition Time**
  Tracks time from start to completion and processing of an experiment.
  This is tracked in:
  /vnmr/adm/accounting/accounts/goes.txt
- **VnmrJ Use**
  This was called login/out use.
  Tracks the time the owner or operator starts or logs in to VnmrJ. This implementation is used to track operator time during walkup and owner time in walkup or experimental mode or both. If more than one VnmrJ is opened, both are tracked and invoiced.
  This is tracked in:
  /vnmr/adm/tmp/macros.txt
  This is the only way to track operator time.
- **Login/out**
  Tracks Linux login/logout time. The operating system tracks the Login/logout time using the file:
  /var/log/wtmp

  NOTE: The file /var/log/wtmp must exist for tracking time.

  The file, if it does not exist, must be created by root using the command:
  ```
  prompt>touch /var/log/wtmp
  ```
  The accounting software does not provide a way to create, enable, or disable this file. Linux tracks the current and previous months and automatically deletes older login/logout times at midnight on the 1st. Write all invoices on time.
  Linux creates entries for each terminal opened when tracking login/logout. Only one charge for the longest entry is on the invoice. Overlapping entries are ignored.
  Linux creates some entries that are not complete. Incomplete entries are ignored by the accounting software. The software creates the following ASCII file to make the invoice:
  /vnmr/adm/tmp/last.txt
  Any text editor can be used to inspect this file.

7.7.4 Table Headers

Enter the table headers in the **Table headers:** fields to reflect the billing mode. The text in the headers does not alter the billing mode.

7.8 File Locations

- Account information —
  /vnmr/adm/accounting/accounts/<account>.txt
- Records —
  /vnmr/adm/accounting/gorecords.txt
  /vnmr/adm/tmp/macrorecords.txt
- Logo —
  /vmnr/adm/accounting/*.gif
- Properties file —
  /vnmr/adm/accounting/accounts/accounting.prop

7.9 Properties File Contents

The /vnmr/adm/accounting/accounts/accounting.prop file contains the properties and keyword-value pairs required to customize the accounting software. Use the controls under the **Properties** tab to maintain this file. Each keyword-value pair appears on a separate line and is formatted as:
keyword<space>=<space>value
Lines starting with the # character are treated as a comment and ignored.

7.9.1 Currency

Enter the two-letter name for the country (e.g.us for United States, de for Germany) to set the number format and currency symbol for the local. Refer to the following Web site for a complete list: http://www.chemie.fu-berlin.de/diverse/doc/ISO_3166.html. The currency keyword defines currency symbol used in the invoice Amount Due and determines the use of the decimal period or comma in numbers.

7.9.2 Billing mode

Invoices are written based on the billing mode; Login time or Acquisition time, the choices are mutually exclusive.

billingmode = macros

Time is tracked by the operatorlogin and operatorlogout macros. When the file /vnmr/adm/accounting/macrorecords exists, these macros will record one line for each login and logout. The file is in ASCII and has world read/write permissions.

billingmode = goes

Time is tracked for any `su, go, ga, au, shim, lock, spin, change,` or `sample` command. One data line is written for each acquisition when the file
/vnmr/adm/accounting/gorecords.xml
exists and the following are recorded:

- account — usually ""
- operator — the operator name
- goflag — whether su, go, au, etc.
- result — ""

- seqfil — the name of the pulse sequence
- submit — time of submit action
- start — time the acquisition started
- done — time the acquisition stopped, including data handling, plotting, etc.

The difference between the last two dates is invoiced.

7.9.3 Table header

Enter table headers. For example:

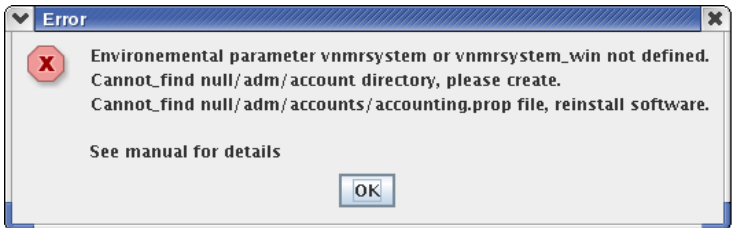
- If billingmode = goes
  Use tableheaders = "Day" "Time" "Go Rate" "Go/hr"
- If billingmode = macros or login
  Use tableheaders = "Day" "Time" "Login Rate" "Rate/hr"

7.10 Error Messages

7.10.1 Messages Displayed at Start Up

The software checks if certain items exist at start up and displays error messages provided a required item is missing. Only some of the error messages are shown in this section.

If the first message is as follows:



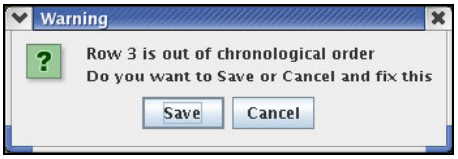
Other messages that are displayed:

- Environment parameter **`vnmrsystem`** or **`vnmrsystem_win`** not defined.
- In Linux this parameter is normally defined in the .login or .cshrc file using the line:
  `setenv vnmrsystem /vnmr`
- The line must be added to the .login or .cshrc file when VnmrJ accounting is run by an operating system login (local or remote) account that was not created by VnmrJ Admin.
- Cannot find the nulladm/accounting/accounts directory, please create.
- This is the directory where the accounts' information is stored. It must exist for the software to store and retrieve the information. In this example the path starts with null because vnmrsystem or vnmrsystem_win was not defined either. The correct directory path is /vnmr/adm/accounting/accounts. Create the path manually if it is not present.
- Cannot find the 'nulladm/accounts/accounting.prop' file, reinstall software.
- The software needs the properties file to determine logos, currency, and billing mode. The path starts with null, because vnmrsystem was not defined. The correct file path is /vnmr/adm/accounts/accounting.prop. Reinstalling the software is the method to recover this file, unless you can copy it from another place. The file is installed with the VnmrJ software.

7.10.2 Account Information Error Message

Times in the rate table must be in chronological order to generate accurate and correct invoices. The software checks that the times in the rate table are in chronological order when the Save button in the account panel is pressed.

A warning message is displayed if the rate table is not in chronological order.



Do one of the following:

- Click the **Cancel** button, correct the order, and click the **Save** button.
- Continue with clicking the **Save** button — the invoices may not be correct. The software searches for the first entry beyond a login or go time. If the entries are not in chronological order the wrong entry may be used.

7.10.3 Comma Separated Value (or Comma Delimited)

Write the printer output to a CSV text file for an individual invoice or all invoices. This file can be imported into an Excel spreadsheet for further processing.

Create the following file to write the printer output to a CSV file:

/vnmr/adm/accounting/account/CSV_yes

The file can be a file or directory. Create this file on Linux using:

```
vnmr1>cd /vnmr/adm/accounting/accounts
vnmr1>touch CSV_yes
```

Return to normal printing by renaming the file to CSV_no or by deleting the CSV_yes file.

7.11 Accounting Limitations

- VnmrJ Accounting is only run on systems that create billing records. Records are created and invoices generated by the VnmrJ Accounting package running on the system where the VnmrJ software is installed. Accounts are invoiced by the system. A billing account on multiple systems will have an invoice for each system. Merging records from different systems is not supported.
- Pruning large record files is supported.
- The files /vnmr/adm/accounting/gorecords.xml and /vnmr/adm/tmp/macrorecords grow larger and larger with time. The VnmrJ Administrator must periodically delete records in these files. The gorecords.xml file grows the fastest. Use the Properties tab and the Cut Records button to reduce the file size or use any ASCII editor to delete records.
- Billing modes of **Acquisition** (goes) and **Login** (macros) are mutually exclusive. Records for both billing methods can be kept at the same time. Invoices are written based on one or the other mode. Create an invoice using one mode then change the billing mode and create a second invoice in the other mode.
- VnmrJ macros write to the macrorecords.txt file from different user accounts and set the file access permission to rw-rw-rw-. This leaves a lack in the security that allows anyone to modify records. Keep a local copy of the macros that do not write these records.

- Expproc writes the gorecords.xml file. Access permission for this file is rw-------. Expproc executes with root permission and does not need general access permission to write to gorecords.xmlmaking to make it more secure.

Chapter 8 System Calibrations and Autotest

This chapter describes the liquids NMR system calibration procedures for a newly installed Varian Inc. NMR Spectrometer system. These calibrations and system test procedures can be used for routine system calibration maintenance. Procedures described here cover pulse width calibration, decoupler field strength, decoupler 90° pulse width, and decoupler pulse calibration. Additional calibration procedures are described in various probe installation and acceptance test procedure manuals, accessory test and installation manuals, and other test manuals.

Sections in this chapter include:

8.1 Procedure Requirements

- Magnet is installed and ready for normal operation.
- System operating software is installed.
- All required network issues and connections are completed.
- VnmrJ software is installed, printers setup, and hardware configuration set.
- All accessories are installed and ready for calibration.

8.2 Referenced Manuals

This system calibration procedure references the following manuals:

- Probe Installation and Acceptance Test manual(s)
- AutoTest
- Spectroscopy User Guide

8.3 Calibrating the System

1. Install the primary system probe and complete all the acceptance test procedures.

   Typically this configuration consists of a conventional probe using 5 mm sample tubes, VT system, and gradient(s) (if present). Sample changers, flow systems and probes, cryogenic probe and system, and other specialized accessories are installed and calibrated last.

   Refer to gradient shimming in the *Spectroscopy User Guide*.

2. Run AutoTest

   Refer to the *AutoTest* manual for instructions and the console acceptance test and installation procedures manual for specifications.

3. Calibrate the probe and create a calibration file.

   Choose all the calibration procedures that are appropriate for the probe. A new system or probe installation requires the creation of a system level probe calibration file. Refer to Calibrating a Probe for instructions – choose the calibration procedures that are compatible with the probe functions.

4. Install any additional probes - follow the instructions in the Probe Installation and Acceptance Test manual.

5. Calibrate and create a calibration file for each additional probe.

   Choose all the calibration procedures that are appropriate for the probe. A new system or probe installation requires the creation of a system level probe calibration file. Refer to Calibrating a Probe for instructions – choose the calibration procedures that are compatible with the probe functions.

6. Edit the probe calibration file for each probe as necessary and add any manually determined calibrations, e.g., add the15N calibrations for an HCN probe.

   Refer to Adding Calibrations for 15N Calibrations.

7. Calibrate any installed accessories such as:
   - Cold Probe – refer to the Cold Probe Installation and Cryogenic Systems Installation manuals
   - Sample Changers – refer to the related manual
   - LC-NMR and LC-NMR/MS systems – refer to related manual
   - VAST – refer to related manual
   - ProTune – refer to Calibrating ProTune.

8.4 Calibrating ProTune

This section applies only to systems equipped with ProTune.

8.4.1 Changing Probes

1. Remove the current probe – do one of the following:

   Currently installed probe is a ProTune or PZT compatible probe.

   a. Eject the sample if one is present.

   b. Turn OFF the master module or probe tuning controller.

   c. Disconnect cables to ProTune controllers from the probe.

d. Remove rf cables and pneumatics lines.

e. Remove the probe from the magnet.

Currently installed probe is not a ProTune or PZT compatible probe.

a. Eject the sample if one is present.

b. Remove rf cables and pneumatics lines.

c. Remove probe from the magnet.

2. Install the next probe in the magnet.
3. Set the system probe name to the currently installed probe.
4. Do one of the following:

Installed probe will use ProTune or PZT.

a. Connect flexible shafts or controller cable to the probe.

b. Connect the RF cables and turn the Master module or probe tuning controller ON.

c. Set or verify that the system hardware option, ProTune, is set to **present** — see Spectrometer Configuration.

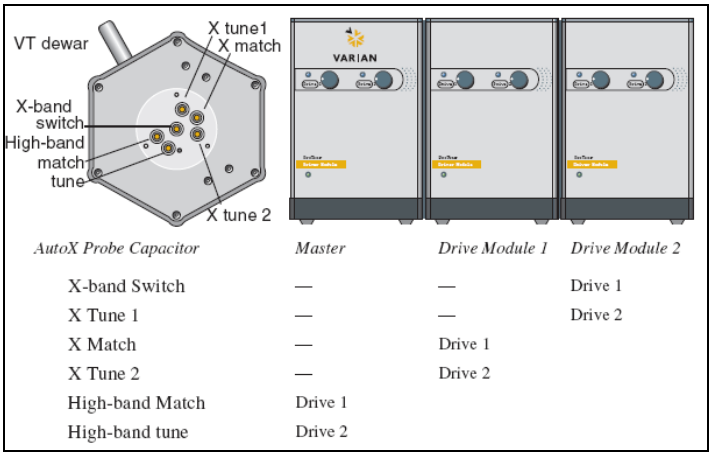
Installed probe will not use ProTune or PZT.

a. Set system hardware to ProTune not present — see Spectrometer Configuration.

b. Connect all cables and pneumatics lines to the probe.

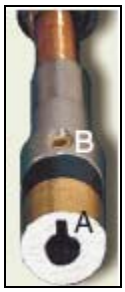
8.4.2 Connecting ProTune Modules to the Probe

1. Connect the cables from the ProTune module to the probe in the order shown, using the procedure in the next step.



AutoX Probe Capacitor	*Master*	*Drive Module 1*	*Drive Module 2*
X-band Switch	—	—	Drive 1
X Tune 1	—	—	Drive 2
X Match	—	Drive 1	
X Tune 2	—	Drive 2	
High-band Match	Drive 1		
High-band tune	Drive 2		

2. Connect each cable from the ProTune modules to the probe as follows:



   a. Align the slot on the cable end with the pin on the knob of the probe.
   b. The slot (A) lines up with the set screw (B) on the flex shaft.
   c. Push the shaft on to the knob and compress the spring in the knob.
   d. Turn the capacitor knob approximately 90º clockwise to lock.
   e. Repeat this procedure for each capacitor and cable pair.

8.4.3 Connecting the Probe Tuning Controller to the Probe

Connect the cable from the Probe Tuning Controller to the Probe Tuning Module Driver with the red dot on the connector cable facing up.

8.5 Motor Index

This section applies only to those systems equipped with ProTune or PZT. The ProTune or PZT motors might need to be indexed after the following:

- The probe has been changed.
- The Master Driver Module or probe tuning controller has lost power, has been power cycled, or is going through initial installation.

NOTE: The motors will be automatically indexed with the current probe if power to the controlling unit has been interrupted since the last time the ProTune command was executed.

8.5.1 Indexing all the ProTune Motors and PZT

1. Log in as administrator, typically vnmr1.
2. Set the system probe name to the name of the currently installed probe.
3. Verify all ProTune connections are correct.
4. Turn the ProTune modules On and the system is Idle.
5. Type `protune('calibrate')` at the VnmrJ command line.

   The ProTune Interface window appears.

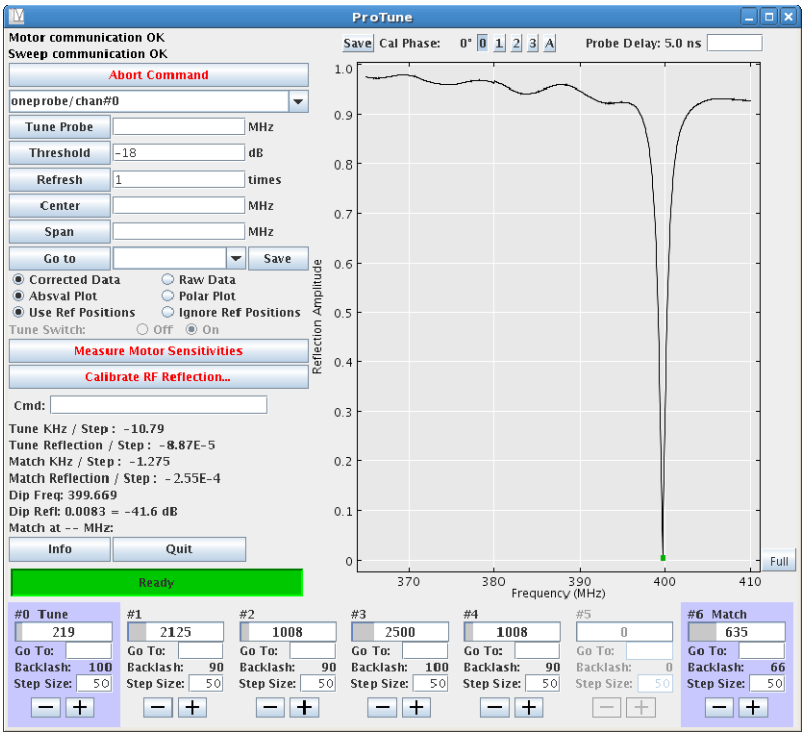


Figure 11 ProTune GUI

6. Verify that the Motor and Sweep communication show **OK** in the top left corner of the ProTune Interface window.
7. Type **index all** in the ProTune window Cmd field.

   Each motor will be indexed automatically.Wait for the indexing process to complete.
8. Exit from the ProTune Interface.

8.5.2 Indexing Individual ProTune Motors

1. Log in as administrator, typically vnmr1.
2. Set the system probe name to the name of the currently installed probe.
3. Verify all ProTune connections are correct.
4. Turn the ProTune modules On and the system is Idle.
5. Enter `protune('calibrate')` on the VnmrJ command line.

   The ProTune Interface window appears.
6. Verify that the Motor and Sweep communication show OK in the top left corner of the ProTune Interface window.
7. Enter index <motor number> in the ProTune window Cmd field, refer to Table 17.

   The motor will be indexed automatically.

Table 17 Module and Motor Designations

	Master Module		Dual Module 1		Dual Module 2	
Alternate name	**Box 1**		**Box 2**		**Box 3**	
Motor number	1	0	3	2	5	4
Drive number	1	2	1	2	1	2
Probe connection	HB Match	HB Tune	X Match	X Tune 2	X Switch	X Tune 1

8. Wait for the indexing process to complete.
9. Repeat steps 7 and 8 for next motor to be indexed.
10. Exit ProTune Interface.

8.5.3 Clearing Motor Stuck Message with ProTune (not PZT compatible probe)

The software displays the motor stuck warning if the indexing process does not reach an end or if the motor cannot turn the capacitor. The message will specify a box or a motor number or both; see Table 17 for module and box number correlation. Clear the error message using the following procedures:

1. Indexing does not reach an end.
   - Check and tighten all the screws on corresponding flexible shaft. Use the non-magnetic tools provided with ProTune Tool Kit.
   - Re-index the motor.
2. Tune knob is stuck.
   - Disconnect flexible shaft from the probe's tune knob. Use the non-magnetic tools provided with ProTune Tool Kit.
   - Use the tuning stick provided with the probe and turn the knob in the opposite direction as indexing to free the knob.
   - Re-connect flexible shaft and re-index the motor.

8.6 Calibrating Sweep Range

This section applies only to systems equipped with ProTune. The sweep range must be calibrated if parts of the RF path, cables or filters, are changed. Sweep range calibration is probe independent.

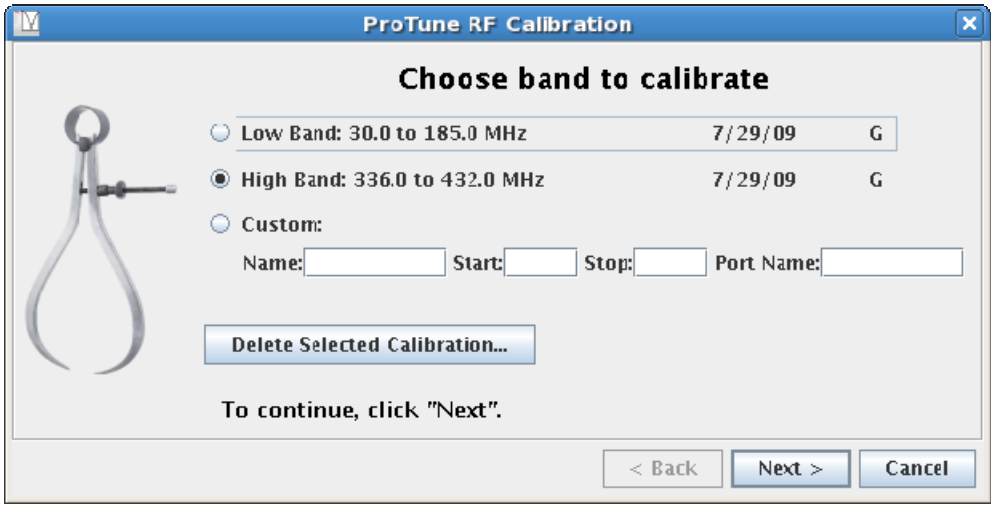
Calibrate the ProTune sweep range by measuring the RF reflection using the following procedure:

1. Log in as the VnmrJ administrator (typically vnmr1) and start VnmrJ.
2. Type `ProTune('calibrate')` at the VnmrJ command line.

   The ProTune Interface window is displayed.
3. Verify that for both Motor and Sweep communication **OK** is displayed (upper left corner of the window).

4. Click the **Calibrate RF Reflection** button.

   The following pop-up wizard appears. Choose High Band or Low Band, the sweep width is set for you. Then click **Next** to continue.



5. Follow the directions in the subsequent pop-ups to complete calibration of the selected band.
6. Repeat steps 4 through 6 for the other band.

8.6.1 Calibration Verification

Verify the calibration of this channel as follows:

1. On the commad line, type the command `setCalSweep` along with the sweep range to check. For example, the range for the low band from the graphics above is 30 to 185 MHz, so the command `setCalSweep` 30 185 is entered.
2. A flat line at reflection=1 is the ideal response.

8.6.2 Exiting the Calibration Mode

1. Remove the shorting plug and reconnect the Probe.
2. Connect the proton and X channels to the probe.
3. Close the **ProTune Interface** window.

8.7 Calibrating a Probe

This procedure uses the VnmrJ Spectroscopy interface. A complete list of samples and calibration tests are in AutoCalibration.

8.7.1 Logging In and Installing the Probe

Completion of these steps is required for all the procedures that follow.

1. Log in to VnmrJ as the administrator, typically vnmr1, to create a system probe file (typical for initial installation).

NOTE: Write permission to /vnmr/probes/probe_name is required to create a system level probe file.

2. Install the probe to be calibrated.

   Probe installation instructions are provided in the *Installation and Operations* manual for the probe.

8.7.2 Setting Up, Selecting, and Creating a Probe Calibration File

Set up the probe calibration file before calibrating a probe for the first time, using the procedure described below.

1. Click the **Probe** button in the hardware bar in the VnmrJ interface or Click Tools on the VnmrJ menu bar, select **Standard Calibration Experiments**, and select **Calibrate probe.**

   The probe selection window will appear, see Figure 12.

2. Select **Edit** check box

   Editing options appear in the Probe window.

3. Do one of the following based upon the operating system login:

   - VnmrJ system administrator (typically vnmr1) or user with equivalent write permissions – select from the Level drop down menu either:

     System — writes the calibrations into: /vnmr/probes/probe_name
     and makes all calibration available to all users — typical for new system and probe installation.

     – OR –

     User — writes the calibrations into:~/vnmrsys/probes/probe_name
     and is available only to the logged-in user creating the calibration file.

     The User level calibration file can be written to the system level directory, if the user has write permission to the system level directory, by clicking on the Copy to system button, see Figure 12.

   - Logged in as a user (most users) without write permission to /vnmr/probes files.
   - Continue with the next step – the Level option is not displayed and all calibrations will automatically be saved to:
     ~/vnmrsys/probes/*probe_name*.

4. Do one of the following (refer to Figure 13 as needed):

   New probe

   a. Type the name of the probe in the Probe name field (letters first followed by numbers and no spaces, e.g. abc456).

   b. Select system or user from the **Level** drop down menu.

   c. Press **Enter** (must press the enter key to add the new probe name).

   d. Click the **Add probe** button.

e. Do the following for nano and AutoMAS probes:

Enter `tach` in the field next to **Probespintype** (do not use the nano option).

Enter an approximate maximum spinning speed based on the probe:

Nano probe — 2500 is typical

MAS probes — Maximum value for the spinner that will be used most often. Refer to the probe manual for specifications of spinner speed, material, and temperature.

Update the parameters after adding an MAS type probe by entering **probe=probe** on the VnmrJ command line. Selecting the new MAS type probe will now automatically set the spintype and the maximum speed.

The Spin/Temp panel will require updating if it was open while the new probe was added. Select any other panel then select the Spin/Temp panel.

f. Continue with Starting a Calibration.

Existing probe

a. Click the **Select Probes** drop-down menu.

b. Select the probe.

If this probe file was NOT created from VnmrJ 3, then the probefile should be updated so that it will contain additional parameters for use in VnmrJ 3. Take note of the lock power and lock gain values stored in the probe file .

Click Edit, then click on the lk tab in the Probe edit window, then from the command line type `updateprobe` to update the probe. Then re-enter the lock power and gain values for the various solvents in the probe file.

NOTE: The new / updated probefile will contain the parameters **`Probewtune`** and **`Probetunemethod`**. If the probe is a ProTune compatible probe, these parameters should be set for the desired operation. The directory /vnmr/tune/methods contains the entries valid for Probetunemethod. The parameter **`Probewtune`** takes the same parameters and has the same usage as the parameter wtune. (See the *Command and Parameter Reference* entry for wtune.)

---

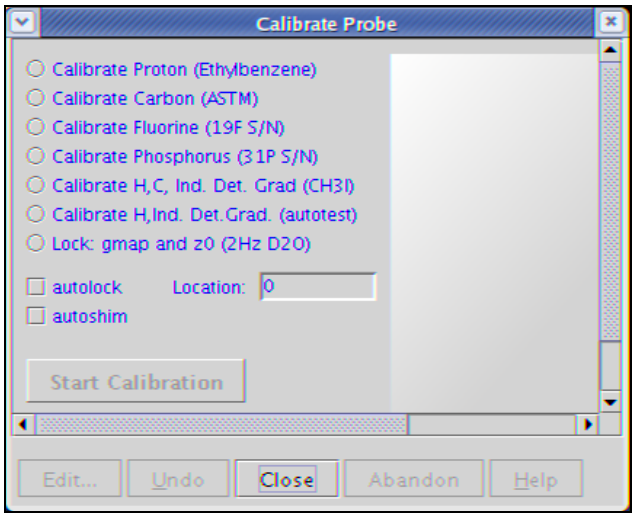
c. Continue with Starting a Calibration.

8.7.3 Tuning Probes

Probe tuning is covered in the *NMR Spectrometer User Guide*. Tuning operations and tuning ranges specific to each probe are covered in the manual provided with the probe.

8.7.4 Starting a Calibration

1. Click the **Do Calibration** button in the **Probe Calibration** popup window.
2. Select **Calibrations** from the **Calibration** popup window.



a. Click an option button in the calibrate probe window to select the calibration experiment.

b. Enter the location of the calibration sample.

   No entry field appears if a sample changer is not attached to system.

c. If a sample change system is not present or not used, insert the sample into the magnet manually using the **Insert** and **Eject** buttons. It is located on the **Lock** page of the **Start** tab

d. Select the **autolock** check box to have the system automatically lock the sample.

e. Clear the **autolock** check box if your sample is already locked or if you would prefer to lock manually.

f. Select the **autoshim** check box to have the system automatically shim the sample.

g. Clear the **autoshim** check box if the sample is already shimmed or to shim manually.

3. Follow the procedure in AutoCalibration for the autocalibration procedure that was selected in Starting a Calibration, step 2a.

   - Verify the correct sample is present in the probe.

     Probe calibration will begin.

   - The calibration files are created and written to the locations determined by the level that was selected in Setting Up, Selecting, and Creating a Probe Calibration File.

   Some probes, like the Autoswitchable and 4 nucleus probes, require additional calibrations not covered in this manual. For information on the calibration of these probes, see the *Installation and Operations* manual for the probe.

4. Select autoshim to have the system automatically shim the sample.

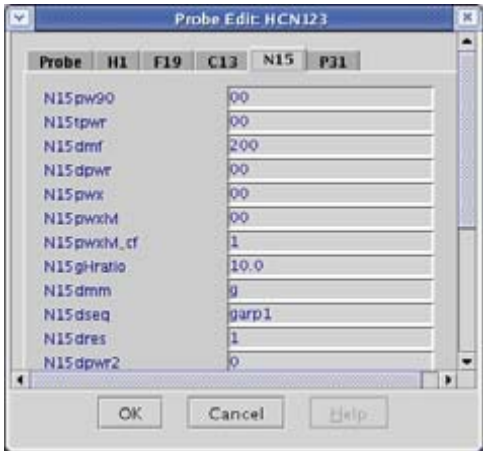
5. Click the button if your sample is already shimmed or if you would prefer to shim manually.

8.7.5 Adding Calibrations for ^{15}N Calibrations

The calibrations for ^{15}N can be added to the probe calibration file following the manual calibration for probes with an X channel that can tune to 15N or that have a pre-tuned ^{15}N channel.

To add Calibrations for ^{15}N:

1. Click the **Probe** button on the hardware bar in the VnmrJ interface, or
2. Click **Tools** on the VnmrJ menu bar, select **Standard Calibration Experiments**, and select **Calibrate** probe.
3. Select the **Edit** check box — editing options appear in the Probe window.
4. Click the **Select Probes** drop down menu and select the probe.
5. Click **Edit Probe**.



A pop up window appears with calibration names and fields to enter values.

6. Select the **N15** tab.
7. Add the calibration values in the provided fields – current calibration values are next to the parameter name e.g. pw90 (14).

   Leave the field if a calibration is not available — do not enter a zero.
8. Click **Save**.
9. Click **Exit**.

8.7.6 Viewing or Editing Calibration Values

Each of the probe calibration files can be viewed and edited. Editing individual parameters is best done at the user level probe file and not at the system level. This is appropriate for specialized calibrations such as high salt concentrations, biological samples, and low temperature calibrations etc. that are specific to an individual user but not appropriate for all users.

To edit or view a calibration value:

1. Click the **Probe** button in the VnmrJ interface or click the **Utilities** button in the VnmrJ menu bar.
2. Select a probe from the **Select Probe** drop down menu.
3. Select the check box next to Edit.

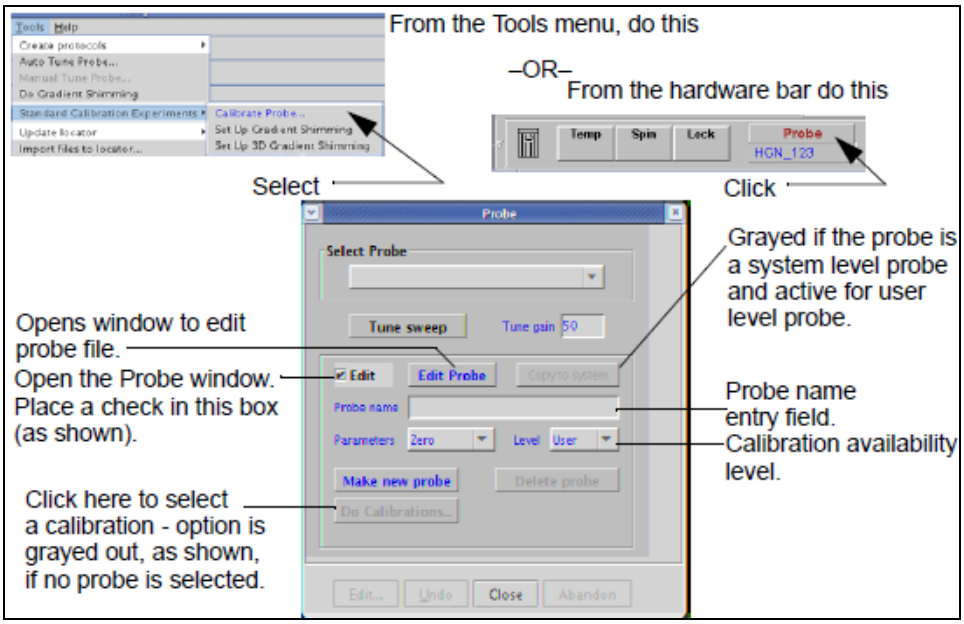


Figure 12 Calibrating a Probe

4. Click to check the **Edit** button — editing options appear in the Probe window, see Figure 13.

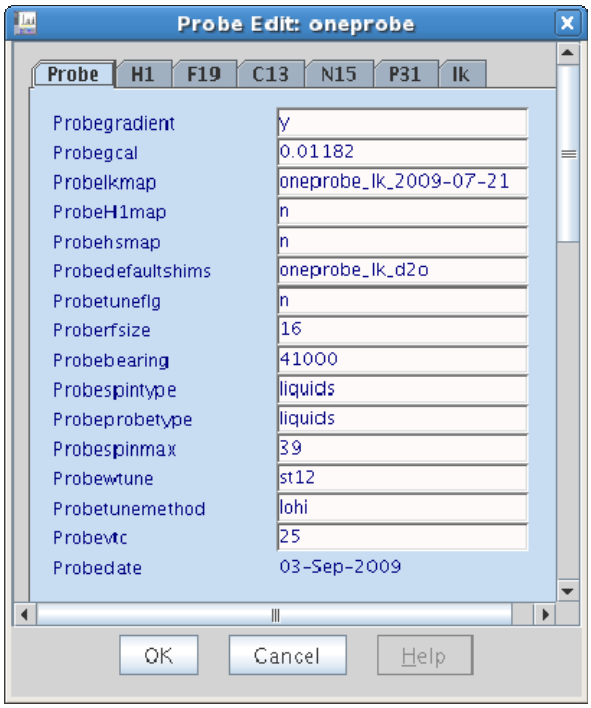


Figure 13 Probe File Edit Window

5. Select the tab to modify a probe calibration entry.
6. Change the calibration values in the fields provided.

   Leave the field blank if a calibration is not available — do not enter a zero.
7. Click **OK**.
8. Click **Exit**.

9. Repeat for each probe calibration file as required.
10. Click **Close** to exit the Probe calibration pop up window.

Optional – create a new version of the probe calibration file that will contain any special calibrations (typically a user level requirement):

1. Open a terminal window.
2. Do one of the following:
   - User level probe file:

     Type cd ~/vnmrsys/probes – this is the probes directory of the current operating system log in user.
   - System level probe file:

     Type cd /vnmr/probes.
3. Copy the directory for the probe of interest to a new directory name.
4. Change directories to the probe name directory.
5. Rename the probe file in the directory to exactly the same name as the directory.

8.8 AutoCalibration Samples

The samples listed in Table 18 can be used for auto calibration. Not all samples are provided with each system. The required samples for the acceptance test procedures during system installation will include one or more of these samples.

Table 18 AutoCalibration Samples

Sample	Calibrate Option	Part Number
0.1% ethylbenzene in CDCl3 1H sensitivity	Proton	00-968120-70
40% dioxane in C6D6 13C sensitivity	Carbon	00-968120-69
0.485 M triphenylphosphate in CDC13 31P sensitivity	Phosphorus	00-968120-87
0.05% trifluorotoluene in benzene~~d~~6 19F 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% 13C-enriched methanol, 0.1% ^{15}N-enriched acetonitride, and with 0.30 mg/ml GdCl3 in 1% H2O/99% D2O (AutoTest Sample)	Proton, Carbon, ID, and Gradients (aqueous solvents)	00-968120-68
2 Hz D_2O	LOCK, gmap and Z0	01-901855-01

8.9 AutoCalibration

1. Click any one of the following calibration option buttons
   - Calibrate Proton (Ethylbenzene)
   - Calibrate Carbon (ASTM)
   - Calibrate Fluorine (19F S/N)
   - Calibrate Phosphorus (31P S/N)
   - Calibrate H, C, Ind. Det. Grad (CH3I)
   - Calibrate H, C, Ind. Det. Grad (autotest)
   - Lock:gmap and z0 (2Hz D2O)
   - Calibrate H1 Dec. for F19 Obs.(Ethylbenzene)
   - Calibrate F19 Dec. for H1 Obs. (19F S/N)
2. Follow the prompts, enter any required values, select options, and proceed according to the instructions presented in the Calibrate probe window; see Figure 14 for an example of the prompts presented:
3. Click the **Start Calibration** button.

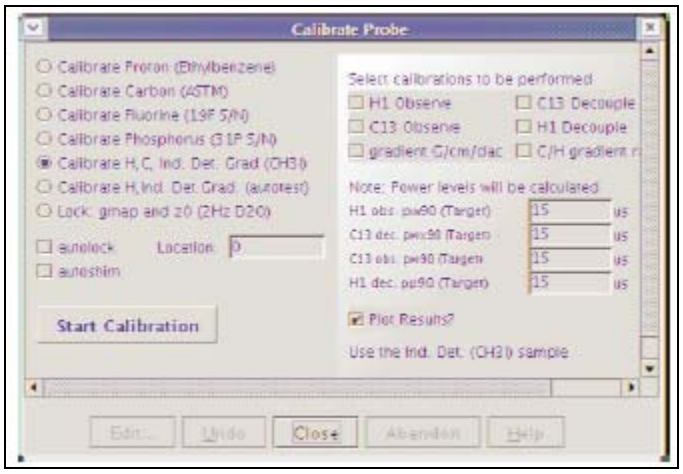


Figure 14 Prompts for Calibrate H, C, Ind. Det. Grad (CH3I)

8.10 Calibrating - Manual Methods

The manual calibrations are run from the command line. Parameter arrays are general examples and may need to be adjusted for individual probes and systems.

8.10.1 Calibrating Pulse Width

Sample	Any sample
Parameter set	None

1. Set up parameters to obtain a spectrum on the sample of interest.
2. Arrange the spectral window so that at least one resonance falls relatively near the center of the spectral window using either the macro movetof or the macro movesw.

   Estimate the relaxation time *T* of the sample so that any experiments using intervals between pulses several times greater than that *T*an be repeated.
3. Acquire one transient (nt=1) with no steady-state (ss=0) in absolute intensity mode (ai) using a transmitter power and pulse estimated at less than 90°.
4. Phase that spectrum properly.
5. Estimate the 90° pulse width, multiply by 4 to get the 360° pulse width, and enter an array around the 360° pulse width.
6. Make sure d1 is greater than 3 times *T*, and acquire data using ga.

   The signals should be negative if the pulse is shorter than 360°, zero if the pulse is 360°, and positive if the pulse is longer than 360°.
7. Select a value of pw that gives the result nearest to zero, using rough mental interpolation if none of your results were exactly zero.

   Divide this value by 4 to give the 90° pulse width and enter this value in pw90 as well as in your log book. To be sure you were not off by a factor of two, set pw equal to a 180° pulse and obtain a spectrum—the result should be near zero. Now set pw to a 90° pulse and the result should be a maximum.

The peak is rarely *exactly* zero but instead shows a dispersive signal with some signal positive and some negative. Do *not* readjust the phase in this case. This is normal behavior. Simply select the value of pw that gives “equally balanced” up and down resonances.

8.10.2 Calibrating Decoupler Field Strength

Sample	60% C_6D_6/40% dioxane (5-mm probe, Part No. 00-968120-69; 10-mm probe, Part No. 00-968123-69; 16-mm probe, Part No. 00-949134-69)
Parameter set	**`/vnmr/tests/gammaH2`**

The strength of the decoupler field, known as γH, is important to know for a number of reasons:

- **`dmm='f'`** (swept fm or fm-fm modulation) decoupling, the decoupler field strength gives a rough measure of the range over which protons will be efficiently decoupled. Thus at 200 MHz, one might want a 10 ppm or 2 kHz decoupler field, at 300 MHz, a 3 kHz decoupler field, etc.
- **`dmm='w'`** (WALTZ-16) decoupling, protons are efficiently decoupled over roughly twice that range; that is, efficient decoupling over a 2 kHz range can be achieved using only a 1 kHz decoupler field strength.
- For WALTZ-16 decoupling, the decoupler field strength must be known because the modulation frequency parameter **`dmf`** must be set to equal 4•γH2.
- Various experiments that require the use of decoupler pulses will also require knowledge of the decoupler field strength.

Decoupler field strength is a function of the decoupler power level (controlled by the parameters dpwr or dhp/dlp) and the probe. To a lesser extent, though more so when using highly ionic samples that can detune the probe, the decoupler field strength depends on the sample. For most organic solvents, calibrate the decoupler field strength for each probe at a variety of settings and repeat the calibration every few months. For polar solvents, and samples in water at high buffer concentrations, it may become necessary to calibrate the decoupler on a sample or a comparable sample.

The standard method of calibrating the strength of the decoupler field is off-resonance decoupling. Two experiments are performed, one with the decoupler at a higher frequency than the proper decoupling frequency for a particular proton, and one with the decoupler at a lower frequency.

This technique produces two carbon spectra with “reduced” couplings—multiplets that mostly have the same pattern as in a coupled spectrum (doublets, triplets, etc.), but the coupling constant is reduced. With these two spectra plus knowledge of the full coupling constant, an appropriate equation can be used (see K.G.R. Pachler, *J. Magn. Reson.* 7:442 (1972) to determine the value of γ. Use the following procedure:

1. Insert the standard ^{13}C sensitivity sample (60% C_6D_6 and 40% dioxane).

   The dioxane produces a single resonance, a triplet with 1:2:1 amplitude, when coupled (from the carbon in dioxane). This pattern will change when decoupling is used.

2. Retrieve an appropriate parameter set (assuming that dpwr or dhp is set correctly) by typing `rtp('/vnmr/tests/gammaH2')`.

3. Acquire two spectra by typing `ga`.

4. Display the first spectrum with two cursors by typing `ds(1)`.

5. Position the cursors on the outer lines of the triplet.

6. Read the value delta from the screen.

   Divide the result by 2 (because we really want just the value of a single splitting) and write down that number.

7. Display the second spectrum by typing ds(2).

8. Position the cursors in a similar fashion, and read the value of delta.

9. Write down half that difference.

10. Start the program to calculate the strength of the decoupler field by typing: h2cal.

11. When the system prompts for the low-field residual coupling value, enter the result from step 6.

12. When the system prompts for the high-field residual coupling, enter the result from step 8.

13. When the system prompts for the full coupling constant, enter 142, the value for dioxane.

The system displays the calculated value of the decoupler field strength γH, the predicted coalescence point (the frequency at which single-frequency decoupling would collapse the dioxane to a singlet), and the pulse width for decoupler pulses if this decoupler level is to be used for pulsed decoupling.

8.10.3 Calibrating Decoupler 90º Pulse Width with Polarization Transfer

Sample	30% menthol in CDCl3 (Part No. 00-968120-94)
Parameter set	/vnmr/stdpar/C13

The decoupler 90° pulse width value (parameter pp) from the test above should be appropriate for polarization transfer experiments. To calibrate pp separately, use a polarization transfer pulse sequence directly on the sample of interest. Use a sample such as menthol having CH, and CH carbons to test. If menthol is unavailable, use any small molecule organic compound that is highly soluble.

1. Type **`jexp2 setup('C13','CDCl3') nt=4 ga`**.
2. Phase the spectrum and place the two cursors around the aliphatic region.
3. Type **`movesw ga`** to narrow the spectral window. Phase the new, narrowed spectrum.
4. Type **`jexp1 setup('H1','CDCl3') nt=4 ga`**.
5. Place the cursor in the center of the aliphatic region and type **`sd`**. Note the value of dof (decoupler offset) after typing sd.
6. Type jexp2 and set **`dof`** to the value just found by sd.

   The follow is an alternative to this step:

   a. Set the decoupler offset dof to –2.5 times the spectrometer frequency of the system (e.g., on a 200-MHz system.

   b. Set dof=–500; on a 400-MHz, set dof=–1000).
7. Type `DEPT`.
8. Type an estimate of the decoupler 90° pulse width that was obtained previously, or some other conservative estimate, after the help file is displayed.
9. Type `mult=0.5 d1=1 ss=2 nt=16 ga.`
10. Phase the data when finished. All resonances should be positive.
11. Type `pp=10,20,30,40,50,60,70` and rerun the experiment.
12. Type dssh after the data are transformed.
13. Select the value of **`pp`** that gives the maximum peak heights (use da to check the array).
14. Type a new array of **`pp`** values, bracketing the value determined in step 12 by ±20%, using about six smoothly-spaced values. Rerun the experiment and determine the pp value for maximum intensity, the same as step 12. This value is a reasonable estimate of the decoupler 90° pulse width.

    Very accurate value of the decoupler 90° pulse width is required for spectral editing. Determine the decoupler 90° pulse Obtain this by observing pp dependence of CH_3 and CH_2 carbons for mult=1.0 (CH selection).
15. Type `mult=1`.
16. Make an array of pp in steps of 1 ∝s, from –5 to +5 ∝s around the pp value determined above.
17. Type ga and when finished, type `dssh`.

18. Phase the CH carbons vertically.

    The CH_2 carbons go from positive to negative with increasing pp. The CH_3 carbons decrease to zero and then increase. The pp value corresponding to a decoupler 90° pulse is the value that nulls the CHs. Use the J value in the parameter set is correct for the type of CH in the molecule: 125 Hz for menthol. Reset the pp range to cover a smaller span with smaller steps in pp if a more precise 90° pulse is required.

19. Update the system log book and probe file.

8.10.4 Calibrating ^{1}H Decoupler Pulse Width with PPCAL

The PPCAL pulse sequence is used to calibrate the proton decoupler pulse width for experiments such as DEPT, INEPT, and HETCOR. Figure 15 shows the sequence.

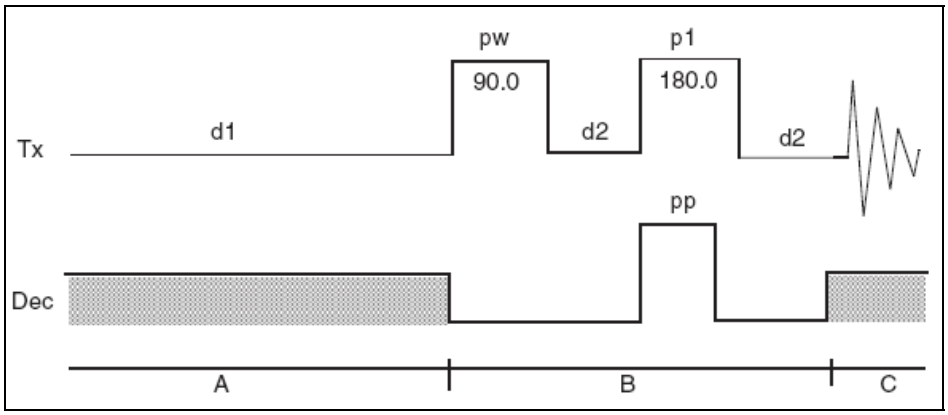


Figure 15 PPCAL Pulse Sequence

The ppcal macro sets up the parameters for PPCAL as follows:

Table 19 Parameters

pp	Proton 90° decoupler pulse (in μs).
d2	Delay that should equal $1/(2*J_{CH})$ (in sec).
pw	90° pulse on ^{13}C (in μs).
p1	180° pulse on ^{13}C (in μs).
dm	Decoupler mode. The value should be 'yny'.
Dmm	Decoupler modulation mode. Its value should be 'wcw' or 'fcf'.
Pplvl	Power level for the proton decoupler pulse. dpwr is the power level for broadband proton decoupling if the decoupler channel uses a linear amplifier.

The following technique is recommended:

1. Array parameter pp, starting at 0.

   Make sure that delay d1 is reasonably long compared to the ^{13}C relaxation times.

2. Phase the first spectrum (pp=0). CH and CH_3 carbons should go from positive to negative and CH_2 from positive to zero and again positive.

   All peaks should null when pp is a 90° pulse. The CH carbons are the most sensitive.

8.10.5 Calibrating ^{13}C (or X) Decoupler Pulse Width with PWXCAL

The PWXCAL pulse sequence is used to calibrate the pulse width characteristics of the probe's decoupler channel(s) in indirect detection or triple resonance experiments. PWXCAL can also be used to determine the rf field homogeneity of the decoupler. This calibration is a more sensitive measure of the decoupler X pulse widths than the first increment of HMQC.

The pwxcal macro sets up the parameters for PWXCAL as follows:

Table 20 Parameters for PWXCAL

pw	proton pulse width (in μs).
pwx1	90° pulse on X (in μs) for the first decoupler.
pwx2	90° pulse on X (in μs) for the second decoupler.
pwx3	90° pulse on X (in μs) for the third decoupler.
jC13, jN15, or jP31	should be set to the appropriate coupling constant.
jname	set by the pwxcal macro to indicate which nucleus has been selected.
dm	decoupler modulation and must be 'nnn'.
dmm	decoupler modulation mode and should be 'ccc'.
dof	X-nucleus resonance location (note: CH_3I dof is –14800 for a 500-MHz system at 11.4 T).
dpwr (or dpwr2)	power level of the "X" decoupler pulse, and tpwr is the power level for proton observe if the decoupler channel uses a linear amplifier.

Use the following technique:

1. Starting from a 1D proton parameter set, type `pwxcal` and answer the questions "use decoupler 1, 2, or 3 [1]" and "calibrate C13, N15, or P31 [C13]".
2. Press the Return key in response to either of the questions selects the default response enclosed in square brackets.
3. Array parameter pwx1, starting at 0, making sure that delay d1 is reasonably long compared to the 1H relaxation times.
4. Phase the first spectrum (pwx1=0). All peaks null when pwx1 is a 90º pulse.

   If a second decoupler is present, the parameter pwx2 is arrayed to calibrate the 90º pulse width on that decoupler. If a third decoupler is present, the parameter pwx3 is arrayed to calibrate the 90º pulse width on that decoupler.

8.11 Running Autotest

Refer to the *Autotest* manual for details on how to run and work with Autotest.

1. Set the applications directory to enable autotest.
2. Click **Tools**
3. Select **Standard Calibration Experiments**.
4. Select **Autotest Settings…**
5. Make any required changes.

6. Close the **Autotest Setting** window and save the changes by clicking **OK** or click **Cancel** to exit form the window without making any changes..
7. Click on **Tools.**
8. Select **Standard Calibration Experiments**.
9. Select **Start Autotest….**
10. Select the Autotest experiments to run from the choices in the Auto Test window (click Clear Selection to start over).
11. Click **Begin Test** to start Autotest using the selections or click **Exit** to close the window and not start Autotest.

Appendix A VnmrJ Terms

Sections include:

- A.1 Liquids
- A.2 Imaging
- A.3 Administrator
- A.4 General

A.1 Liquids

Account-Owner, Account-Administrator or User

Account-owner, administrator or user is the user that owns the operating system login account. User privileges include access to the command line, all parameter panels and all protocols, and right to create new or edit protocols for operator use. The user (account owner) is the head of a group of operators that share the particular login account. User responsibilities include maintaining special protocols and probe files for this group of operators.

Acqlog

The acqlog file (in /vnmr/tmp) allows the spectroscopist to monitor an automation run as it progresses in background. The acqlog is a simple text file that (if it exists) is updated automatically as a study is submitted to the acquisition queue or Study Queue.

Application Directory

VnmrJ application directories are directories where VnmrJ looks for directories such as templates, maclib, manual, menulib, parlib, probes, seqlib, shims, tablib, shapelib, gshimlib, and mollib. These are directories that VnmrJ uses during its normal operation.

Application Type

Application types (apptype) define how related experiments or a family of experiments, are set up, acquired, processed and plotted.

Background Acquisition

A background VnmrJ process is spawned for this acquisition when one or more experiments are submitted for acquisition from the Study Queue if background or automation is selected. All workspaces are available for data analysis while VnmrJ collects NMR data in a background process.

DayQ

The DayQ is typically between the hours of 8:00 a.m. and 6:00 p.m. and provides 30 minutes of NMR time for each sample submitted by the operator. Submitted samples are accepted to the DayQ provided the sample data acquisition time does not exceed the time limit. See also NightQ.

Direct Acquisition

Direct acquisition is carried out as a foreground acquisition and the Study Queue is not used. Select an experiment/ protocol from the vertical experiment panel in direct acquisition mode or from the list of experiments accessed by clicking on Experiments on main menu. Parameters are loaded directly into the current workspace for manual data acquisition.

Experiment

See Workspace.

File types

NMR data sets have the file extension .fid. The .fid file (FID free induction decay data) contains all of the raw data and parameters of an acquired data set.

A parameter file or set has the .par extension and contains the parameters necessary to set up and acquire an NMR experiment. Parameter files may be both local and global.

A shim file contains a list of shims and their values. Both .fid directories and .par directories contain a file called procpar, which includes the shim settings.

Foreground acquisition

When working in direct acquisition mode, the workspace is tied to a particular manual acquisition. No other NMR data set may be loaded into the active workspace while data acquisition is in progress.

Minimize spectral window

The minsw (minimize spectral window) process is often executed before a 2D experiment. First a full spectral width 1d is acquired. The software detects where the highest and lowest field peaks are, recalculates the spectral width, and reacquires the 1d experiment with the new spectral width. The minsw process is automatically turned on if a proton, presat or wet1d protocol precedes a 2D protocol.

NightQ

The NightQ is typically between the hours of 6:01 p.m. to 7:59 a.m. and provides 3 hours of NMR time for each sample submitted by the operator. Submitted samples are accepted to the nightQ provided the sample data acquisition time does not exceed the nightQ time limit. See also DayQ.

Operator

The administrator (vnmr1) creates operators as subservient users of a particular user's account. The operator does not own the login account. The operator may be considered a spectroscopist within a group where the group's head owns the login account. The operator privileges such as limited access to parameter panels (panellevel), command line, or NMR experiments are defined by the VnmrJ administrator.

Panel Level

The VnmrJ parameter, panellevel, defines the number of pages an operator has access to in the horizontal panels. The VnmrJ administrator (vnmr1) determines the panellevel for each operator.

Probe File

A probe file is a list of parameters that change with each probe: pulse widths, powers, decoupling patterns or shapes for proton, carbon and other nuclei (if applicable). The probe files are maintained in either local directories or globally in the probes directory of /vnmr. Users have a local probe file (vnmrsys/probes) that they keep current with the latest calibrations and gradient shimming files. The global probe file is maintained by the administrator's (vnmr1). A probe file that corresponds to the installed probe must be selected for proper functioning of protocols within VnmrJ.

Priority Sample

A priority sample is submitted to the Study Queue by checking the Priority Sample box before submission. The sample is run after data acquisitions for current sample is completed, and before the other samples submitted to the Study Queue are run. The ability to run a priority sample can be assigned to an operator by the VnmrJ administrator.

Protocol

A protocol consists of any single or series of NMR acquisitions. A protocol may be a simple NMR experiment or involve a series of shorter acquisitions that are acquired but not stored in order to establish necessary parameters (such as solvent location) for the desired NMR experiment.

Required Experiment / Protocol

A required experiment / protocol is an experiment / protocol consisting of one or more required experiments that are executed before the desired data set is acquired. All 2D protocols in the walkup interface require that a proton apptype protocol is run before the 2D protocol is run. Selecting a 2D protocol, such as the Cosy protocol, automatically adds a proton protocol ahead of the 2D protocol. The requirements for running a proton apptype protocol is met if a proton apptype protocol (proton, presat or wet1d) already exits in the list of experiments before the 2D. A required proton experiment, that is part of the 2D protocol, is not added to the Study Queue. Solvent suppression parameters are carried forward to the 2D experiment if the proton apptype protocol is presat or wet1d and the 2D experiment is acquired with these parameters. A minsw process executed if proton, presat, or wet1d listed ahead of any 2D experiment and, if it is not desired, must be turned OFF before the experiment is submitted.

Spectroscopy Interface

The walkup is primarily designed for point and click acquisition of NMR experiments with or without a sample handler (SMS, Carousel, VAST, 768AS).

Study

A study consists of a one or more NMR experiments collected on one or more NMR samples.

Study Queue

The Study Queue is an area in VnmrJ where a list of protocols (NMR experiments) to be acquired on a single sample or a series of samples is created. This area can reflect the sample that is active, the sample that is displayed, or a queue.

Traymax

The parameter **traymax** is used define the type of autosampler or sample handler associated with the NMR system and can have the following values.

traymax =	Sample handler
0	No sample handler
1	LC-NMR or LC-NMR/MS
9 12	Carousel 7510-AS
50	SMS with a rack for 50 samples
100	SMS with a rack for 100 samples
96 97	VAST 7600-AS
768	768AS robot

Viewport

Activating viewports allows the user to view more than one workspace at a time. Each viewport must be linked to a specific workspace. Up to nine viewports can be open in VnmrJ at a time. Viewports allow the user or operator to look at one or more spectra (with or without linking cursors) at a time.

Workspace

The terms workspace and experiment are used interchangeably. Either one refers to a directory in the user's local vnmrsys directory called exp1, exp2, exp3, etc., which correspond to workspace 1, workspace 2, workspace 3, or equivalently, experiment 1, experiment 2, experiment 3 and so on. The exp directory contains parameters and, potentially, data for any given NMR experiment or protocol.

Data is directly acquired into a defined workspace or experiment corresponding to an exp directory in direct acquisition mode and must be stored into a FID file or it will be overwritten by the next direct, user-executed acquisition. The workspace or experiment can also act as a holding pen for processed data that is already stored on the disk.

A.2 Imaging

Applications Type

Experiments are grouped in types of applications such as: 3D fast spin echo, localized spectroscopy (1D), global spectroscopy (1Dglobal), or EPI-like. Each application type has, a generic set-up, processing, and prescan procedure.

Composite Protocol

A composite protocol is a series of protocols, required protocols, prescans, or a series of NMR data acquisitions, clustered together into one unit.

Exec-parameters

The exec-parameters (string parameters) define how a particular protocol is prepared for scan (execprep), processed (execprocess), or run in the prescan mode (execprescan). Typically, the exec-parameters contain just the name of a single macro, but generally they can be anything that could be typed on the command line or typed in a macro.

File Types

Spectroscopy data is stored with the raw data is saved a single file (fid) accompanied by an ASCII file listing all parameters in the subdirectory name.fid. Image data is stored with the processed images saved as individual files for each slice in a 2D experiment or as a single file in a 3D experiment in the subdirectory `name.fdf`.

Protocol

A protocol can either be a basic or composite. A basic protocol is a single parameter set, e.g., sems or gems, whereas a composite protocol is a collection of basic protocols.

Study

A study consists of one or more scans run on a single subject in a single session.

Study Queue

The Study Queue is a list of protocols to be acquired. These protocols are coded with different colors and fonts to distinguish between active, completed and new protocols. The protocols move to the top as scans are acquired.

Viewport

There are usually three available Viewports: Plan, Current, and Review. Each viewport is a separate work-area with different functions. Use the Plan Viewport to set up experiments and graphically plan the slices or volume. The data will be acquired and displayed in the Current Viewport, which therefore always has the most recent data. Use the Review Viewport to view and analyze previously acquired data.

A.3 Administrator

Administrator (vnmr1)

The administrator of VnmrJ (both hardware and software) is generally called vnmr1 and is the owner of all files and directories of the VnmrJ software. Typical functions of the VnmrJ administrator are: creating new users and operators, assigning appmodes and various privileges such as access to panels and NMR experiments, and hardware configuration through the vnmr1 user login.

Application mode (appmode)

The application mode determines what features are displayed in the VnmrJ window. The application modes are Spectroscopy, LC-NMR and Imaging. The administrator (vnmr1) defines each user's application mode upon the creation of that user's operating system login account.

A.4 General

Folder

The user interacts with the parameters through panels in one of the four folders: Start, Acquire, and Process. Each folder can have a number of pages. The folders are found in the bottom horizontal region of the VnmrJ interface.

Global files

Global parameters, templates, experiments, file and so forth are available to all users and are stored in the /vnmr directory, which is owned by the system administrator (vnmr1).

Local files

Local files (parameters, templates, experiments, probe files, and so forth) are stored in the user's directory (~/user/vnmrsys). Local files typically are specified as the first application directory to search.

Locator

The locator is a database manager that helps spectroscopists keep track of the location of automation runs, shim files, protocols, acquired data and so forth.

Node in Study Queue

Each entry in the study queue is termed a node. A node is either a parent node (the name of the sample or a child node (the actual scan).

Pages

The sub-panels in each folder are called pages, panels, or templates. These pages have entry fields, menus, check boxes, and so on, for setting up sample-specific, acquisition, or processing parameters.

Prescan(s)

A prescan is a short acquisition generally not saved to disk that can be part of or precede protocols. Prescans that are integrated into protocols include solvent suppression optimization routines (presat in 90% water), and scout scans to find solvents for suppression. Prescans that precede protocols or data acquisition are automatic tuning, locking and gradient shimming. These prescans are set-up from the "Standard" page found in the "Start" folder.

Push-pin

A small icon that looks like a tack or a push-pin is located in the upper right of the folders and vertical panels. By untacking the push-pin, the user can hide the folders or vertical panels. A tab to the side of VnmrJ is created. When the mouse is rolled over the tab, the vertical panel or folder will be temporarily redisplayed. If permanent redisplay of the panel or folder is desired, the push-pin may be tacked in place.

Vertical panels

The vertical panels are located on the left-hand side of the screen. They provide easy access to general cross-applications functions, which is particularly useful when the horizontal folders are hidden.

Appendix B Printers and Plotters Troubleshooting

This appendix contains troubleshooting and setup information for printers and plotters. It describes a number of printers and plotters tested as compatible with VnmrJ. Check the Varian Web site for new printers that work with VnmrJ. Refer to the original system manuals supplied with the printer or refer to the on-line manuals for printers supplied with older spectrometers.

The following printers and plotters are covered in this manual:

B.1 Hewlett-Packard LaserJet 840C Printer

Printer I/O	HP IEEE-1284-B Parallel Universal serial bus 1284-B receptacle
Printer Language	HP PCL 3
Printer Memory	2 MB standard memory
Cartridges	black and color
Resolution	Black – 600 x 600 dpi with black pigmented ink Color – HP color layering technology
Pages per Minute	Black – 4 ppm Black and color – 0.8 ppm
Configuration Control	Software controlled

There are two buttons and three lights on the front panel of the printer. The lights indicate if the printer is operating correctly or indicate the time when the printer requires attention from the user..

B.1.1 Self-Test Procedure

1. Turn the HP DeskJet 810C and 830C series printer off and remove the cable that connects the printer to the computer.
2. Turn the printer back on.
3. Press and hold the Power (top) button. Press the Resume button 4 times and then release the Power button.
4. The self-test page will print with a report containing the printer model name, serial number and a diagonal self-test pattern. The test pattern verifies that all nozzles on the print cartridge are firing. If a gap appears along the diagonal self-test pattern, one or more nozzles are not firing.

B.1.2 Operation

1. Turn off the power.
2. Connect the interface and power cables.
3. Press go to turn the power on. The ready light should come on.
4. Open a terminal window, log in as root, and activate LaserJet_150, LaserJet_150R, LaserJet_300, LaserJet_300R, LaserJet_600, and LaserJet_600R using the procedures in the beginning of this chapter.
5. Set the parameter printer, from within VnmrJ, to the name you typeed in the previous step, for example, printer='LaserJet_300' or printer='lj'. Type printon dg printoff to produce a test print.

   To use as a plotter, set the parameter plotter to the name you typeed in the previous step, for example, plotter='lj 300' (If you activated more than one resolution, there will be different names corresponding to the different resolutions). To test, type pl page.

B.2 Lexmark Optra Color 45 Inkjet Printer

Printer I/O	IEEE 1284 ECp compliant,1284-B receptacle, Internal Solutions Port (6 options).
Printer Language	PostScript Level and PCL 5c emulation.
Printer Memory	8 MB.
Cartridges	Dual head thermal inkjet
Resolution	600 x 600 dpi
Pages per Minute	Black - 8 ppm Color - 4 ppm
Configuration Control	Software controlled.

The Varian supplied customized Optra Color 45 printer/plotter includes special software and is HPGL, PS, and PCL compatible. This custom printer is not available from other sources. The optional tri-port serial port board is installed in the Varian Optra Color 45 allowing either serial or parallel port mode. The Optra Color 45 replaces the Lexmark 4079, HP 7475, and the HP 7550A plotters.

B.2.1 Self-Test Procedure

1. Follow the set up instructions in the printer manual and then plug into ac power.
2. The print display shows Ready, and the green light is on.
3. Click the **Menu** button until TESTS MENU is displayed; and click **Select**.
4. Click the **Menu** button until Print Demo is displayed and click **Select** twice.

   A multi-color page should be printed, and the Menu returns to Ready.

B.3 Hewlett-Packard DeskJet 5550 Printer

Printer I/O	Centronics Parallel Universal serial bus
Printer Language	HP PCL 3, PostScript
Printer Memory	512 KB standard memory sufficient for full page graphics at 600 dpi
Cartridges	Black and color
Resolution	Black – 600 x 600 dpi Color – depends on paper type
Pages per Minute	Black – 12 ppm Black and color – 10 ppm
Configuration Control	Software-controlled

The Hewlett-Packard 5550 features 600 dpi color printing and is software-controlled. It has a color cartridge and a black cartridge. The control panel has two switches. Refer to the *Hewlett-Packard* manual for operating procedures.

There are three buttons in the user interface:

Power button and light should always be used to turn the printer on and off.

Using a power strip, surge protector, or a wall-mounted switch to turn on the printer may cause premature printer failure.

Cancel button stops the print task.

Resume button and light is used when the light above the resume button is flashing. Press the button to continue printing.

Varian software does not support two-sided printing.

B.4 Hewlett-Packard DeskJet 970Cxi Printer

Printer I/O	Centronics Parallel Universal serial bus 1284-B receptacle
Printer Language	HP PCL 3
Printer Memory	512 Kbyte standard memory sufficient for full page graphics at 600 dpi.
Cartridges	black and color
Resolution	Black – 600 x 600 dpi Color – depends on paper type
Pages per Minute	Black – 12 ppm Black and color – 10 ppm
Configuration Control	Software controlled

The Hewlett-Packard 970CXI features 600 dpi color printing and is software-controlled. It has a color cartridge and a black cartridge. The control panel has two switches. Refer to the Hewlett-Packard manual for operating procedures.

There are three buttons in the user interface to control the printer:

Power button and light should always be used to turn the printer on and off. Using a power strip, surge protector, or a wall-mounted switch to turn on the printer may cause premature printer failure.

Cancel button stops the print task.

Resume button and light is used when the light above the resume button is flashing. Press the button to continue printing.

Varian software does not support two-sided printing.

B.5 Hewlett-Packard LaserJet 2300 Printer

Printer I/O	Centronics Parallel, USB port
Printer Language	HP PCL 6
Printer Memory	4 MB standard memory (expandable to 52 MB
Cartridges	black
Resolution	1200 x 1200 dpi
Pages per Minute	10 ppm
Configuration Control	Software controlled.
Devicetable entry	LaserJet_600 and LaserJet_600R

The Hewlett-Packard LaserJet 2100 features 1200 dpi printing and is software controlled. The control panel has two switches and two lights. Refer to the Hewlett-Packard manual for operating procedures.

B.5.1 Self-Test Procedure

To print the configuration page, press and release the **go** (large button at bottom of control panel) and **job cancel** (button at top of control panel with upside down triangle) buttons simultaneously when the printer is in the ready mode.

B.6 Hewlett-Packard LaserJet 2100 Printer

Printer I/O	Centronics Parallel, 1284-B receptacle LocalTalk port
Printer Language	HP PCL 6
Printer Memory	4 MB standard memory (expandable to 52 MB
Cartridges	black
Resolution	1200 x 1200 dpi
Pages per Minute	10 ppm
Configuration Control	Software controlled.

The Hewlett-Packard LaserJet 2100 features 1200 dpi printing and is software-controlled. The control panel has two switches and two lights. Refer to the Hewlett-Packard manual for operating procedures.

B.6.1 Self-Test Procedure

To print the configuration page, press the GO button (at bottom of control panel) and JOB CANCEL button (at top of control panel with upside down triangle buttons) simultaneously when the printer is in the Ready mode.

B.7 Hewlett-Packard Color LaserJet 4550 Printer

Printer I/O	Bidirectional parallel port (requires a “C” connector), Two Enhanced Input/Output (EIO) slots; paper handling accessory port; infrared receiver port. IEEE compliant, 1 open EIO slot, HP JetDirect EIO print server for fast Ethernet 10/100Base-TX in second EIO slot. (optional) HP JetDirect 600N and 610N (EIO) internal print servers, external print servers, connectivity card
Printer Language	HP PCL 5C, PostScript Level 3 Emulation, HP PCL 6
Printer Memory	64 MB standard memory (expandable to 192 MB)
Resolution	600 dpi
Pages per Minute	16 ppm (black); 4 ppm (color)
Configuration Switches	Expanded Control Panel

B.7.1 Operation

Set up the printer as described in the Hewlett-Packard manual. Specify the printer as a PostScript printer. On the Name and Type lines in the file /vnmr/devicenames, type PS for a printer and PS_AR for a plotter. In the user's global file, set `maxpen=8`.

B.8 Hewlett-Packard LaserJet 5000 Series Printers

Printer I/O	IEEE 1284-compliant bidirectional parallel, RS-232 9-pin serial, 2 PCI-based EIO slots
Printer Language	HP PCL 5e, HP PCL 6, and Postscript Level 2 emulation
Printer Memory	4 MB standard memory (expandable to 100 MB)
Resolution	1200 dpi
Pages per Minute	16 ppm
Configuration Switches	Control Panel

B.8.1 Overview

The Hewlett-Packard 5000 provides large format (11 x 17") printing at 16 pages per minute.

The control panel has an LCD display, three LEDs and six buttons.

The LaserJet 5000 features 1200 dpi resolution, but for NMR typical applications the plot lines are too fine. You may even fail to plot a full page at this resolution without expanding the printer memory since a full 11 x 17" page takes up to 32 MBytes of pixel information. Also even in parallel interface applications transferring data is unacceptably slow. For good plot resolution, 600 dpi is a good choice; for publication quality spectra and reproduction, 300 dpi is a better option since the plot looks darker.

Switching between large and standard formats requires changing the paper size in the printer configuration menu on the LaserJet 5000.

B.8.2 Self-Test Procedure

1. Load paper and toner cartridge. Press the **Go** button to turn printer on.

   Wait until the printer warms up.

   The READY message should be displayed.
2. Press **Menu** until the display reads **INFORMATION MENU**.
3. Press **Item** until the display reads **PRINT CONFIGURATION**.
4. Press **Select** to print the configuration page.

   The configuration page shows the printer's current configuration.

B.8.3 Operation

Set up as described in the Hewlett-Packard printer manual.

B.9 Hewlett-Packard Color Inkjet CP1700 Printer

Printer I/O	Bidirectional parallel port (requires a “C” connector) Two Enhanced Input/Output (EIO) slots Paper handling accessory port Infrared receiver port. USB, IEEE-1284 (parallel), Infrared, and network LIO. (optional) HP JetDirect 600N and 610N (EIO) internal print servers, external print servers, connectivity card
Printer Language	HP color Inkjet cp1700: HP PCL 3 enhanced HP color Inkjet cp1700d: HP PCL 3 enhanced HP color Inkjet cp1700ps: HP PCL 3 enhanced
Printer Memory	16 megabyte (MB) built-in random access memory (RAM), cannot be upgraded. 4 megabytes (MB) built-in read only memory (ROM), cannot be upgraded
Resolution	1200 x 1200 dpi (black); 2400 x 1200 dpi (color)
Pages per Minute	16 ppm (black); 14.5 ppm (color)

B.9.1 Overview

The control panel has an LCD display representing ink levels and printer status. There are also three push buttons to control power on/off, resume, and cancel. The resume and power switches have a LED associated with them.

The CP1700D features 1200 dpi resolution for black and white printing and 2400 dpi for color, but for NMR typical applications the plot lines are too fine. It might not be possible to plot a full page at this resolution without expanding the printer memory because a full 11 x 17 page takes up to 32 Mbytes of pixel information. Also, even in parallel interface applications, transferring data is unacceptably slow. For good plot resolution, 600 dpi is a good choice; for publication quality spectra and reproduction 300 dpi is a better option since the plot looks darker.

B.9.2 Self-Test Procedure

1. Load paper, ink tanks, and print heads.
2. Click the **Power** button to turn printer on.

   Wait until the printer initializes and reports Ready.
3. Press and hold down the **Resume** button in the control panel for three seconds until the LCD display reports processing Job.

   A test page is automatically printed.

B.9.3 Operation

Set up as described in the Hewlett-Packard printer manual.

Appendix C Locator Administration

Sections in this appendix include:

- C.1 Restricting User's Data Viewing Privileges in Locator
- C.2 Configuration Files
- C.3 Large Database Recommendations
- C.4 Network Database
- C.5 Database Hints

C.1 Restricting User's Data Viewing Privileges in Locator

The system administrator can restrict how files appear in the Locator for each user. An access list controls the data that is visible to the users.

C.1.1 Show the Access List

Use these steps to show the Access field in the User Information panel on the right side of the VnmrJ Admin interface.

1. Open the **VnmrJ Administration** interface, if is not already open.
2. Click the button with the user's name to select the user.
3. Open the Users Defaults window:
   a. Click **Configure**
   b. Select **Users**
   c. Select **Defaults**
4. Select the **access** check box under the Show column.
5. Click **OK**.

An Access line appears in the user information panel on the right side of the VnmrJ Admin interface.

C.1.2 Access List

The following steps describe how to set up an access list for a user.

1. Select a user account by clicking the user's name button.
2. Type a space-separated list of users whose files the selected user can access.
   For example, if user1 will be allowed to view files for user2, user3, and user99, type: user2 user3 user99.
3. Click **Save User**.
4. Repeat for each user.

C.2 Configuration Files

Configuration files for the Locator are contained in the following directories for the different appmode types:

Interface	Directory
Spectroscopy	/vnmr/shuffler
Individual users	$vnmruser/shuffler

C.3 Large Database Recommendations

The maximum number of items to display in the Locator can be controlled by setting its value in Systems Settings window.

Do one the following:

1. Select **Edit**.
2. Select **System settings**.
3. Click the **Display/Plot** tab.
4. Type a value for Max # of items to show in Locator.

Setting the value in **Max # of items to show in Locator** higher than 2000 slows down the response of the Locator by filling Locator table with a large number of rows. A value between 1000 and 2000 gives optimal performance. A row is shown with the word Truncated if the database returns more items than the limit. The message indicates that more items returned but are not shown in the Locator to save time.

Use the following guidelines if the database contains more than 10000 items:

- Set the Locator to show only items that match the criteria of the statement as follows:
- Imager Interface
    a. Select **Tools**.
    b. Select **System settings**.
    c. Click the **Display/Plot** tab.
    d. Check the box next to Display only matching items in locator.
- Liquids **Interface** (Spectroscopy):
    a. Select **Edit**.
    b. Select **System** settings.
    c. Click the **Display/Plot** tab.
    d. Check the box next to Display only matching items in locator.

    Do not type values in the Locator statement of all, etc.
- Set values in the Locator statement to match 1000 or 2000 items.
- Do not type values in the Locator statement of *all*, etc.
- Use the File Browser to limit the directory scope. The Locator only matches items that are in and under the directory the browser defines if the File Browser is displayed.
- Set Max # of items to show in Locator between **1000** to **2000**.

C.4 Network Database

Several computers running VnmrJ can access the same Postgres database server. This way, all of the VnmrJ users will have immediate access to data saved on other machines (if the user has access to that data).

This access requires that all computers running in network database mode be mounted to any directories of other computers containing data that is intended to be accessed. The mounts can be hard mounts listed in the vfstab file or automount, but they must be mounted to gain access.

Set the environment variable PGHOST to the host name of the machine to use for the DB server in every user account. The default is the local host. Different users can use different DB servers, or some computers can use their own database server. A computer which is to be a DB server will need the Postgres postmaster daemon running on it. Even if it is running, if PGHOST is set to a remote computer, the remote computer will be used.

Non DB server computers default to network mode DB access by comparing PGHOST with the local host name. Specifying a remote host sets the non DB server computer in network mode. The DB server computer has itself as PGHOST, and the VnmrJ administrator on the server computer must create an empty file

/usr/varian/config/NMR_NETWORK_DB

to force it into network mode. Data access from other computers will not work correctly if this is not done. Setting this variable on non server computer will force it into network mode.

The file /usr/varian/config/NMR_NETWORK_DB, if it is used, must be in place before dbsetup is run during installation, or the DB will not be set up correctly.

The attribute 'hostdest' in the database contains the host name where the file actually resides (destination) when a computer is set up for network mode. The attribute 'host_fullpath' contains hostdest:fullpath where fullpath is the path as it looks on the machine, hostdest. It does show the mounted path from the current machine.

Pushing automount relations from a server makes the following necessary:

VnmrJ must be able to translate between the mounted path and the actual path on the destination computer. It will first look for a file

'/usr/varian/mount_name_table'

It only uses this file if it is found. An example of this file is as follows:

```
# Table of remote system mount names and paths
# One line per entry, Syntax:|
#host:direct_path  mount_path
mongoose:/export/home/mongoose_home
voyager:/export/home/home
```

If 'mount_name_table' is not found, it looks in '/etc/mnttab' and in '/etc/auto_direct' to get relationships. If automount relations are pushed from a server, they will not always be available in these files and will need to be put into a 'mount_name_table file'. Mounts from the vfstab file and from the local auto_direct file, should work properly without a 'mount_name_table' file.

Changing the UNIX port number is not normally necessary, but might be done if more than one Postgres daemon is to run on the system at one time. The port will default to 5432 unless specified otherwise in every user's. login file with the environment variable, PGPORT. It should be possible for different users (and thus different groups) to use entirely different database daemons and databases on the same computer. If PGPORT is set to something other than 5432, then every user on every computer using that DB server will need PGPORT set in their accounts.

C.5 Database Hints

If the Locator shows Error under the column headings, or if the error message, DataBase contents version is not correct, appears on the bottom of the screen, exit VnmrJ and run `dbsetup` in a terminal window.