Agilent
VnmrJ 4

Administration Guide

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Notices

Safety Notices

CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

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Admin Quick Start

This Guide contains information on how to administer the Agilent VnmrJ 4.2 software, including

- Account administration
- Printer configuration
- Accounting administration
- Spectrometer calibration and autotest
- VnmrJ terminology
- Administration of the Locator

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Overview of Administrator Tasks

This chapter gives a description of typical Administrative tasks, including the creation and configuration of:

- user accounts
- operators
- printers
- probe files

Use the VnmrJ Admin interface to configure users, operators, and printers. Use the VnmrJ application to configure user account preferences and probe files.

Table 1   Summary of basic Administrator functions

Function	To do this	See
Creating accounts and adding operators		
	Set default operator password	"Setting the default operators password" on page 22
	Create a User Account	"Creating a single new user account" on page 22
	Create Multiple User Accounts	"Creating a single new user account" on page 22
		"Creating multiple new user accounts" on page 24
		"Creating multiple new user accounts" on page 24
	Set up User defaults, templates, and directories	"User Defaults and Directories" on page 48
	Delete a User Account	"Deleting a user account" on page 30
	Restore a User Account	"Restoring a user account" on page 30
	Add operators to a User Account	"Adding operators to a user account" on page 40

Table 1   Summary of basic Administrator functions (continued)

Function	To do this	See
	Remove operators from a User Account	"Deleting operators from a user account" on page 46
	Configure and modify operators profiles	"Creating, Editing, Viewing, and Deleting Profiles" on page 55
Creating User Types (persona) and Assigning Privileges		
	Create a user type	"Persona Manager - Administration" on page 56
	Set user preferences	"Persona Manager - Preferences" on page 58
	Set user privileges	"Persona Manager - Widgets and Rights" on page 59
	Set user parameter panel access	"Persona Manager - Parameter Panels" on page 60
	Set user access to experiments	"Persona Manager - Protocols" on page 61
Configuring printers		
	Set up Linusx printer	"Setting up a Linux printer" on page 72
	Set up a VnmrJ printer	"Setting Up a Printer for VnmrJ" on page 74
Configuring probe files		
	Adjust solvent lock power and gain values	"Adjusting solvent lock power and gain values in the probe file" on page 68
	Add or remove a nucleus in the probe file	"Adding and removing a nucleus in the probe file" on page 69

Starting the VnmrJ Admin Interface

VnmrJ Admin is used to perform the majority of the administrator tasks for VnmrJ. For more information on the VnmrJ Admin interface, see "The VnmrJ Admin Interface" on page 18.

1 Log in as the VnmrJ administrator, typically "vnmr1".

2 Double-click the VnmrJ Admin icon on the desktop.
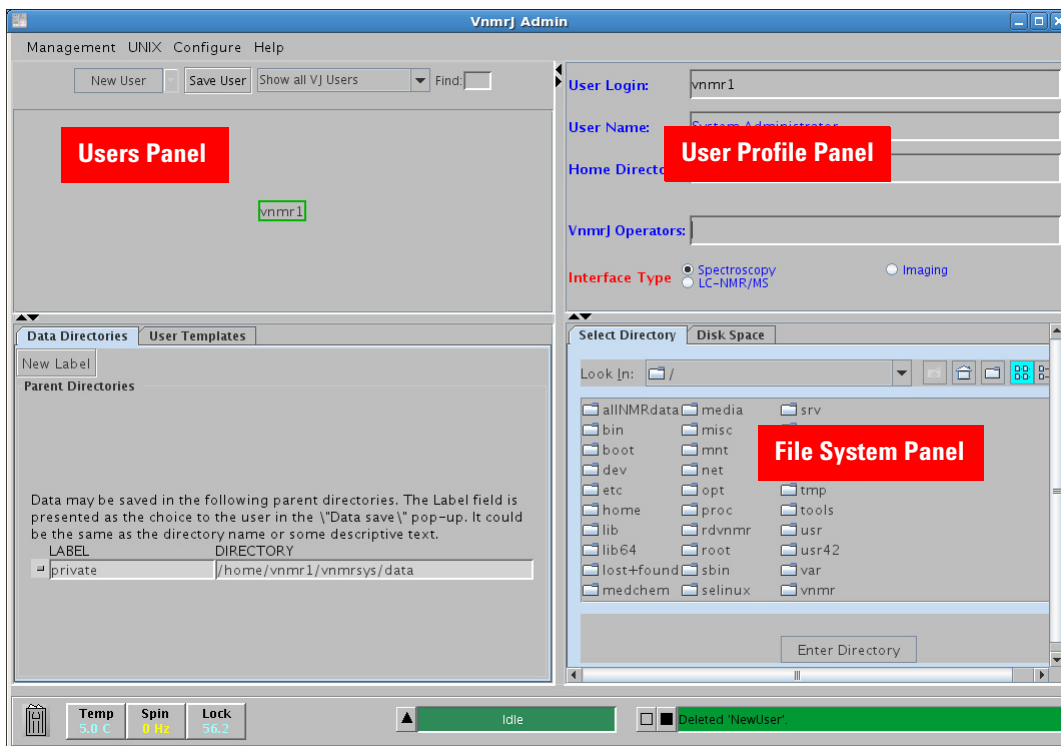
Figure 1   VnmrJ Admin window

System Configuration Window

For proper operation, the software must be configured to match the installed hardware. The system installer performs this task at the time of installing the spectrometer. The administrator should record the settings in the configuration for backup or reference, as there are no recording or backup capabilities in the software.

1 Log in as the VnmrJ administrator.

2 Double-click the VnmrJ desktop icon.

3 Click **Edit** in the main menu after VnmrJ starts.

4 Click **System Settings** to open the System Settings window.

5 Click **System config**.

The spectrometer Configuration window appears. See Figure 2 on page 14.

Record the settings for future reference and then click **Ok** to close the window.
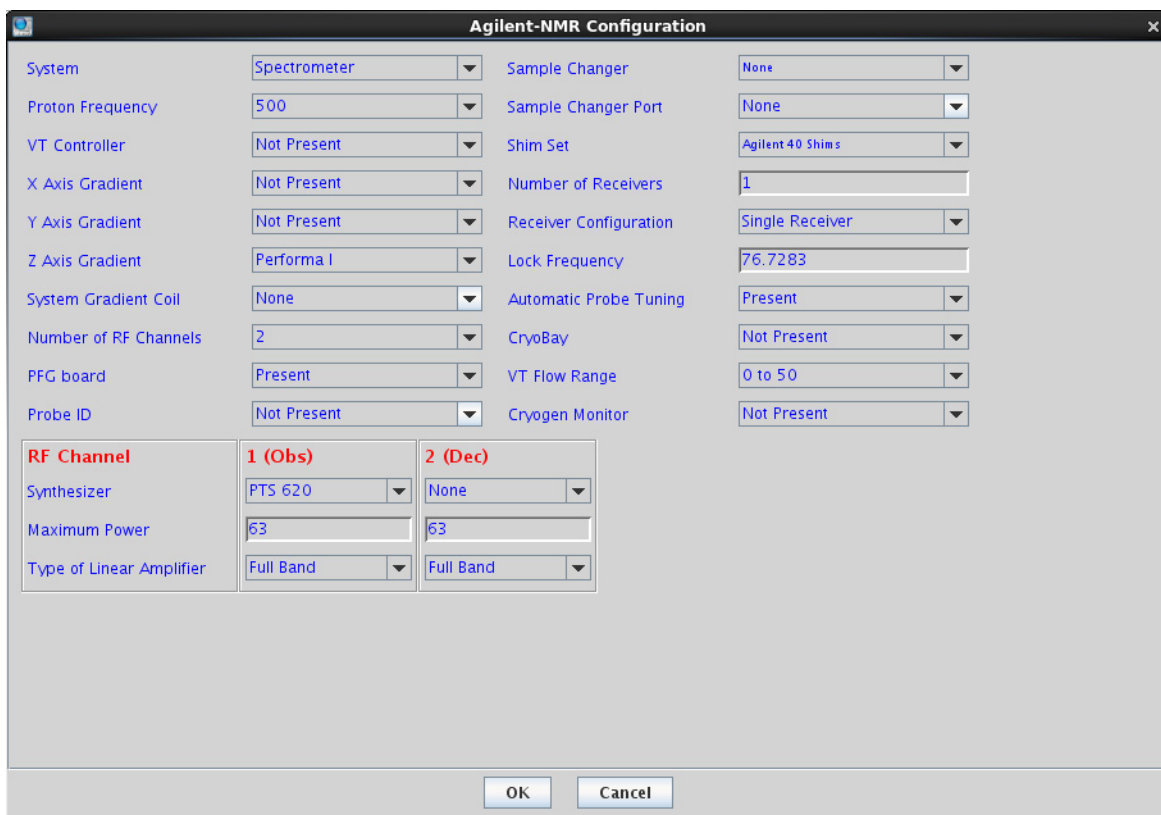
Figure 2   Spectrometer Configuration window

In time, the value of the Lock Frequency will need to be reduced to ensure z0 can be adjusted for all solvents used. This window is where the value of the Lock Frequency can be set for all users.

Getting Help

In addition to the online help provided in the VnmrJ software, Agilent supplies a variety of printed manuals. In addition, you can use the Agilent Spinsights website to access manuals, software patches, latest news, and more.

Agilent Spinsights on the Web

The Spinsights NMR and MRI community is a single online location where you can access a variety of resources to help you learn about and use your Agilent NMR/MRI system. In the Spinsights community, you can

- Help Yourself, by searching for: software patches, manuals, bug lists, application notes, videos, newsletters, and more.
- Help Each Other, by answering or posting questions in our discussion forums.
- Ask Agilent, by using the AskTAC link or making contact using the information in the Agilent Info area.

You must register the first time you access Spinsights.

To start using Spinsights, go to
https://spinsights.chem.agilent.com/

Contact Information

USA

Address:

Agilent Technologies, Inc.

5301 Stevens Creek Blvd.

Santa Clara, CA 95051

Telephone Numbers:
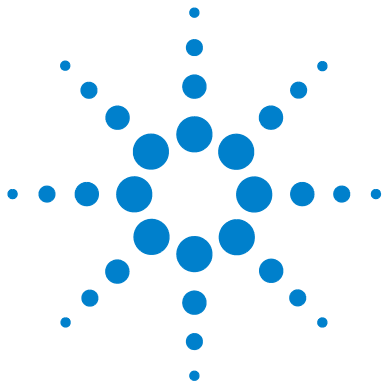
Toll Free: +1 (800) 227 9770

Agilent website (all countries)

To find contact information for your country, click the following link and then select your country.

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

2
VnmrJ Account Administration

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The VnmrJ Admin Interface

The VnmrJ Admin interface provides the tools for administering VnmrJ software and user accounts. (See Figure 1.) Select Administration functions from the menu bar.

Table 2   Management menu

Menu item	Description
Users	Displays users in the users panel and makes available all the administrative functions, see "User Account Administration" on page 21.
Printers	Displays printer functions using pop-up window, see Chapter 5, "VnmrJ Printer Configuration".
Cost/Time accounting	VNMR ACCOUNTING window. See Chapter 7, "VnmrJ Accounting Administration".
Console display sharing	Turns on sharing of display 0 for virtual network connections.
Export Log to CSV	Opens the Log to CSV Conversion pop-up, where you can export Administration Accounting log files to CSV (Comma Separated Value) format.
Exit	Exits and closes VnmrJ Admin.

Table 3   UNIX menu

Menu item	Description
File system	Pop-up window displays file system information; see "" on page 65, for more information and instructions.
Command window	Opens an operating system terminal window.

Table 4   Configure menu

Menu Item	Description
Users	Select additional functions using pop-up windows:
	• Convert users-opens the Change vnmr users to VnmrJ user window. See "Converting user accounts to VnmrJ" on page 31.
	• Defaults-opens the default values window. See "User account defaults" on page 48.
	• Update users-opens the Update VnmrJ Users window. See "Updating user accounts" on page 32.
Operators	• Edit operators-opens the Modify Operators window (Modify Operators tab). See "Creating Profiles-Spectroscopy Accounts" on page 54.
	• Delete operators-opens the Modify Operators window (Delete Operator tab). See "Changing the Icon on the Operator Login Screen" on page 65.
	• Reset password-opens the Reset Operators Password window. See "Resetting the operator password" on page 40.
	• Preferences-opens the Preferences window for setting the default operators password and for selecting a default login icon. See "Resetting the operator password" on page 40.
Edit profiles	Creates and assigns user profiles containing the protocols, rights and tools. See "Creating, Editing, Viewing, and Deleting Profiles" on page 55.
Investigator list	Enter investigators in the pop-up window.
Locator Config	Lets you set an age limit on files so that only more recent files are kept in the Locator database. This enables the Locator to run faster. You can also turn off the Locator.
Background colors	Changes the default background colors of the VnmrJ Admin windows.

Table 5 Help menu

Menu item	Description
Manuals	Opens the VnmrJ help, where you can open VnmrJ manuals in PDF format.
Spinsights Community Help Site	Opens the Agilent Spinsights help site in a browser. From Spinsights, you can access various downloads, manuals, and get help from different sources. https://spinsights.chem.agilent.com
About VnmrJ	Opens information about the VnmrJ software.

User Account Administration

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

Review and configure user account default properties before creating a new user account. These properties apply to all new VnmrJ 4 user accounts. See "User Defaults and Directories" on page 48

Basic administrative User account tasks include:

• setting the default password (do this first) — see "Setting the default operators password"

• setting up new accounts — see "Creating a single new user account"

• assigning operators to a user account — see "Adding operators to a user account" on page 40

• assigning operators e‑mail account and levels — see "Assigning operators an e‑mail address" on page 42

• assigning profiles — see "User Defaults and Directories" on page 48

Setting the default operators password

To set the default password for a group of VnmrJ operators:

1 Launch the VnmrJ Admin interface.

2 Click **Configure > Operators > Preferences**. The Preferences window appears.

3 Enter a password in **Default Password for VnmrJ Operators**.

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 both the Operator and operating system login password, if an operating system account exists.

4 Click **OK**.

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 Defaults and Directories" on page 48. To create multiple new user accounts, see "Creating multiple new user accounts" on page 24.
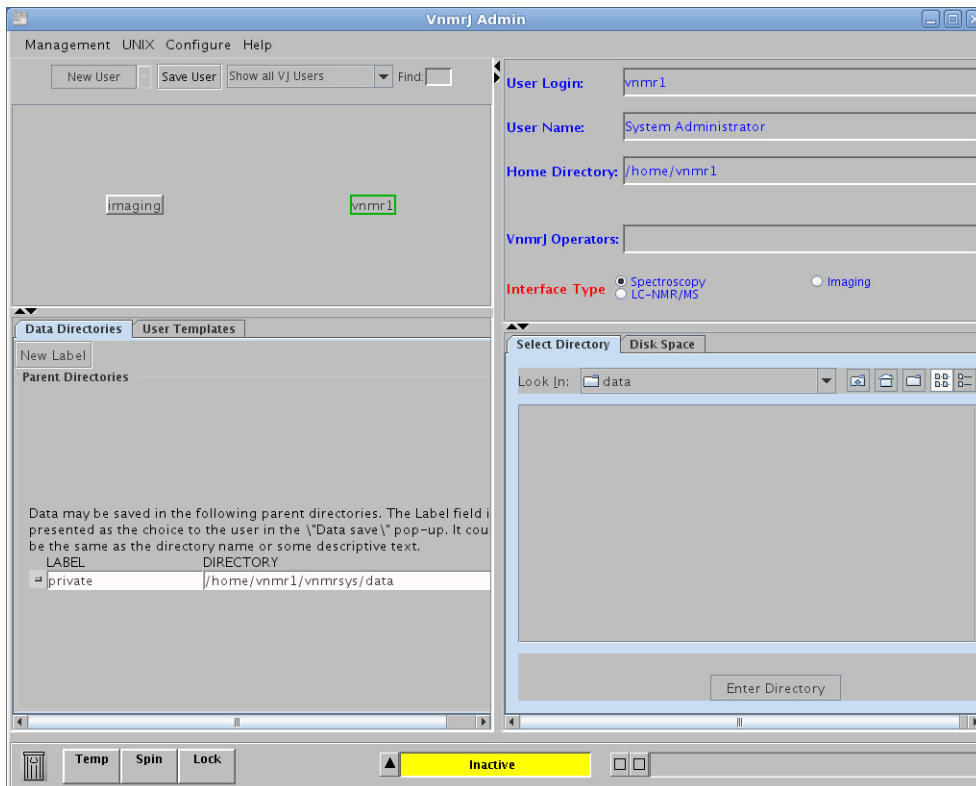
Figure 3   VnmrJ Admin window

1 Select **Management**.

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" on page 48 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, See "Assign VnmrJ interface to a user account" on page 28.

6 Click **Save User**.

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 Defaults and

Directories" on page 48. To create a single new user account, see "Creating a single new user account" on page 22.

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

Management UNIX Configure Help

    New User ▾ │ Save User │ Show all VJ Users ▾ Find:
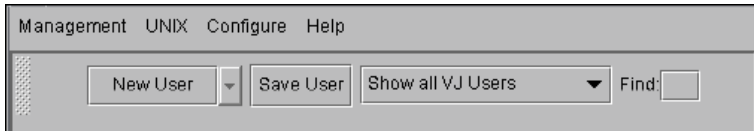
2 Select **Users**.

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. See "Assign VnmrJ interface to a user account" on page 28.

Create/Delete 2 or more users ✕

Login names:
☐ **Use File for User list input**

○ Imaging ● Spectroscopy

Add Users   Cancel
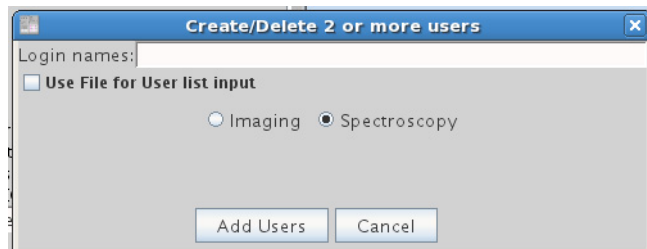
8 Click **Update Users**.

The home directory is automatically setup (new users - no operating system account) based upon the user defaults (see "User account defaults" on page 48). Or if the user was first set up as an operating system account, the user's operating system account home directory is used.

You can also create multiple new user accounts using a .csv file. For information, see "Using a .csv file to add multiple user accounts" on page 26

Using a .csv file to add multiple user accounts

Requirements for the .csv file

- The comment lines in the .csv file must start with a number.
- In the first line, enter a list of column keywords separated by commas. The only required columns are login and itype. Column keywords can be listed in any order on the first line. List subsequent lines of values, separated by commas, in the same order as the column keywords listed on the first line.

Column keyword	Description
login	required-user login
itype	required-Spectroscopy or Imaging
name	full name or description
home	home directory for user
email	user email address
profile	basic liquids, all liquids, common liquids, all imaging

- Default user information will be used for Information not defined in the .csv file, see "User Defaults and Directories" on page 48.

- For each subsequent line, enter a list of values separated by commas in the same order of column keywords listed in the first line.

Example:

```
login,name,home,itype,email,profile
```

```
myuser1,My User 1,/home/myuser1,Spectroscopy,
user1mai@abc.com,BasicLiquids
```

```
myuser2,My User 2,/home/myuser2,Spectroscopy,
user2mai@abc.com,CommonLiquids
```

To create multiple new user accounts from a .csv file

1 From the menu bar, go to **Management > Users**.
2 Select **New User**.
3 Select **Multiple Users** from the drop-down menu.
4 Select **New Users (2 or more)**.
5 Select the **Use File for User list input** check box.
6 Select the **Create** button.
7 Enter the file path for the .csv input file.
8 Select the **Add Users** button.

To delete multiple users through inputting a .csv file:

The input file format is technically the same as for adding users. The only required keyword and value are for "login". That means the file must have the word "login" in the first non-comment non-empty line.

1 From the menu bar, go to **Management > Users**.
2 Select **New User**.
3 Select **Multiple Users** from the drop-down menu.
4 Select **New Users (2 or more)**.
5 Select the **Use File for User list input** check box.
6 Select the **Delete** button.
7 Enter the file path for the .csv input file.
8 Select the **Delete Users** button.

Assign VnmrJ interface to a user account

Each VnmrJ account can be assigned an interface and appropriate privileges. The main interfaces are listed in the following table.

Table 6 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.

Setting data directories for the Locator

The Data Directories tab (Figure 4) is used to set the directories to be searched and displayed in the Locator for the selected user.
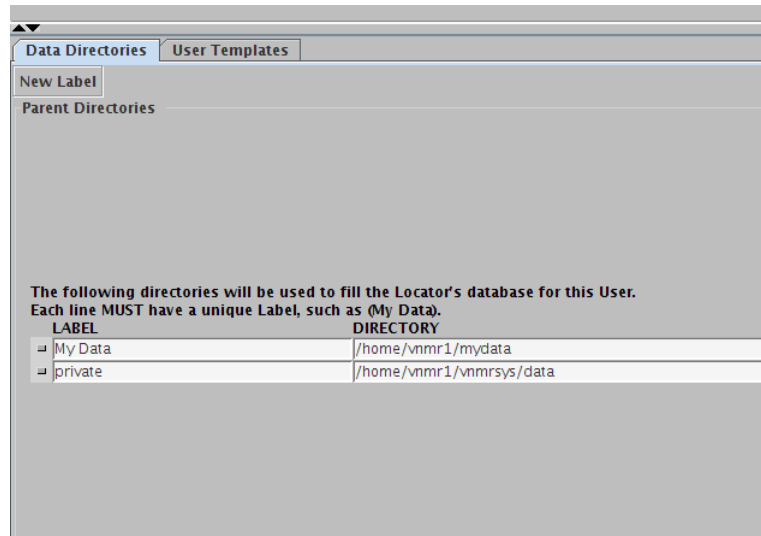
Figure 4   Data Directories tab in VnmrJ Admin

1 Select a user from the list of buttons in the upper left of the VnmrJ Admin window.

2 Click the Data Directories tab in the lower left corner of the VnmrJ Admin window.

3 Click **New Label** to add a new directory.

A row is added to the list of directories.

4 Type a label for the new directory. The label for each directory must be unique for this user. For example, you cannot have two directories with labels of "My Data". Instead, label them "My Data 1" and "My Data 2". These directories are searched recursively when filling the database. It is usually best not to include a user's home directory (eg., /home/vnmr1) because the locator will have to search a large number of files to populate the database.

5 To remove a directory, edit the directory line to be blank.

6 After adding or removing directories, click **Save User** to save this information.

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 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 "Creating Profiles-Spectroscopy Accounts" on page 54, or deleted, see "Changing the Icon on the Operator Login Screen" on page 65.

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

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 on it once.

3 Select **Restore**.

4 Exit the **Trash Can** window.

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 on the left side of the screen.
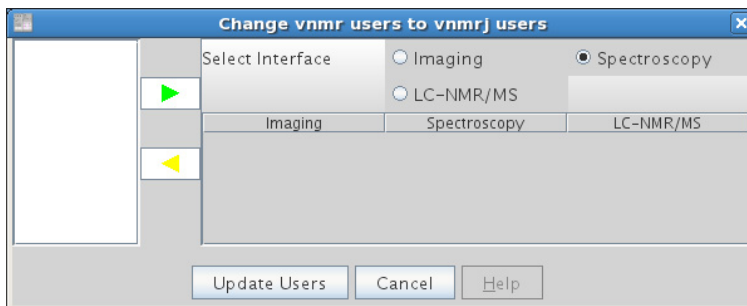
4 Click an **interface type** to sort by **interface type**.

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**.

Updating user accounts

Use this procedure to update multiple VnmrJ user accounts.

CAUTION	Update user accounts after upgrading or reloading software.

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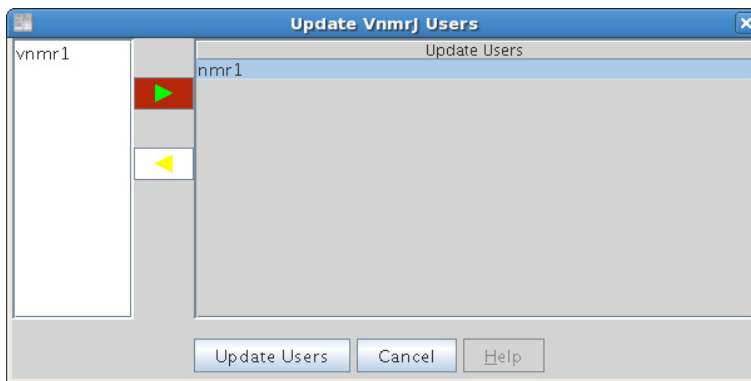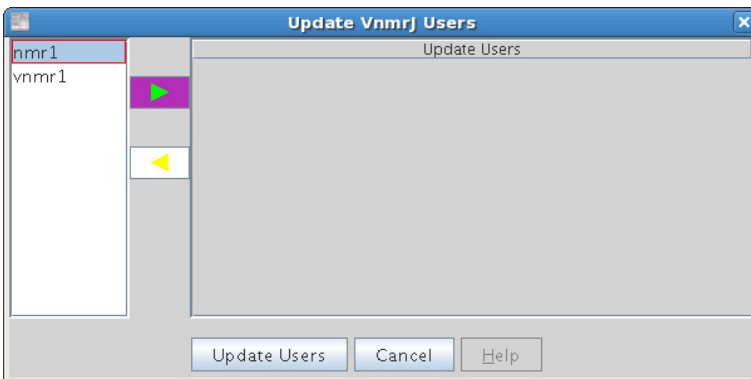
2 Select **Users**.

3 Select **Update Users**.

The Update VnmrJ Users window appears with VnmrJ user accounts listed on the left side of the window.

4 Click 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**.

Deleting a user account

A user account can be deleted by selecting the user account and dragging it to the Trash Can or by using a .csv file. Once the Trash Can is emptied, the account cannot be restored.

Setting User Preferences

Each VnmrJ account can be further customized in the VnmrJ program. These preferences control only that user account and any operator using that account; it does not affect any other VnmrJ account. The Preferences pop-up and all of its contents are described in detail in the *Agilent VnmrJ Familiarization Guide*.

- Data saving templates
- Default automation functions
- Day and night queues
- Study Queue display configuration
- Settings for all sample queues
- E-mailing options
- Data mirroring
- Parameters to preserve during a queued acquisition (Sample tags)
- The ability to define parameters to be stored and recalled for the user
- Operator rights
- Adaptive NMR

To access the Preferences pop-up, in the main VnmrJ menu bar, click **Edit > Preferences...** The Preferences window appears.

Templates
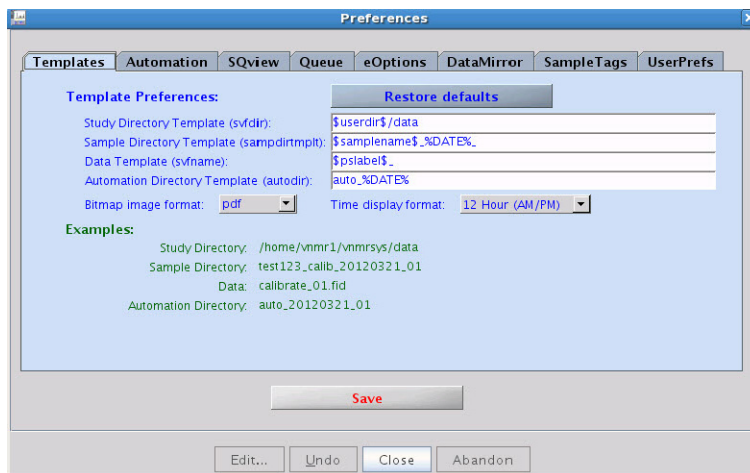
Figure 5 Preferences — Templates tab

Preferences found in the Templates tab are usually customized to the user's needs and several common examples are provided here (although the default naming and saving convention can be used.) Parameters are placed between dollar symbols (example: $pslabel$), time and date substitutions are placed between percent symbols (example: %DATE%), and appending a numeral on the end that increments to prevent names from being identical can also be added (example: %R3%) in the templates. Entering man('Svfname') in the VnmrJ command line will provide a detailed description of other substitution identifiers, usage, and examples.

NOTE The Study Directory Template is a path. The three remaining templates are directories and do not contain a path ("/" forbidden). Any changes done on this window should be saved before exiting the pop-up by clicking **Save**. Changes do not affect submitted studies, only future studies. If the Automation Directory Template is changed, a new automation run needs to be started for the template to become effective.

In the example above, all study data is directed to /home/vnmr1/vnmrsys/data/<study owner>, accomplished by the use of the $studyowner$ argument. The data for each sample will further be saved in a directory named <notebook>_<page>, where notebook and page are the notebook and page numbers that were entered in the Start tab of the parameter panel. The actual FID directory will be saved as <pslabel>_<samplename> with a three digit revision after it.

Other sample templates are shown below:
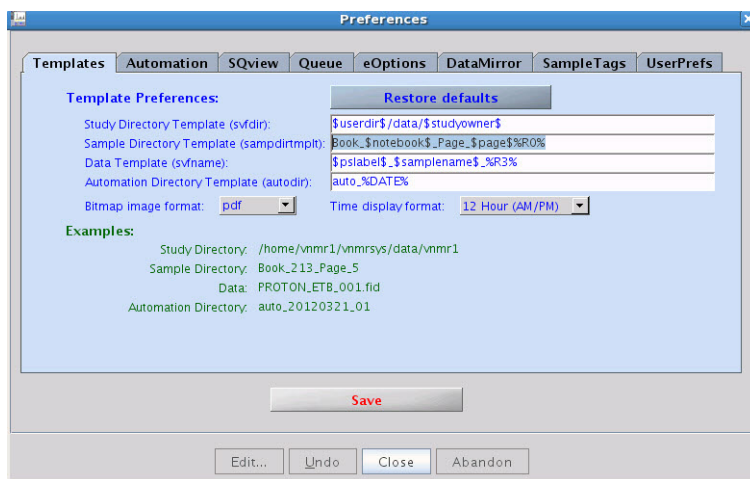
Figure 6   Fixed text (Book and Page) are included in the Sample Directory Template
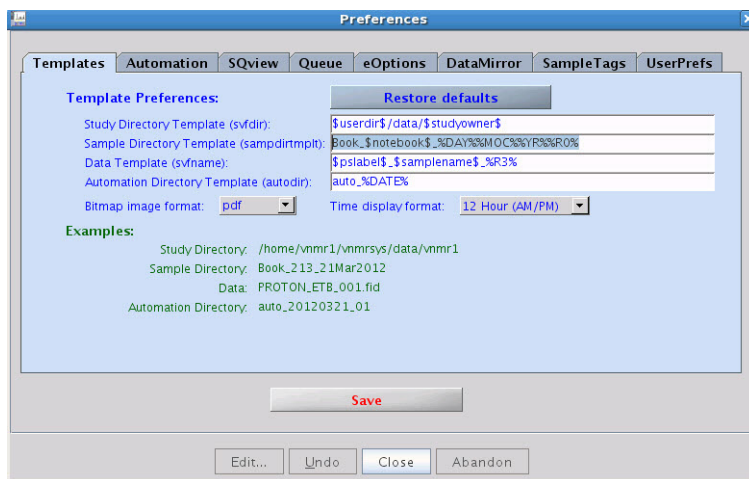
Figure 7   Date in the format of day-month-year is included in the Sample Directory Template
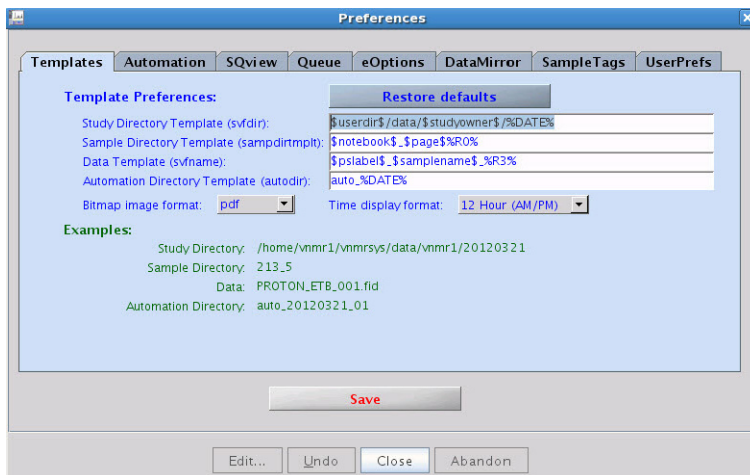
Figure 8   Date in the format of numerical year-month-day is included in the Study Directory Template

Queue

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

eOptions

Actions that will be taken to produce an electronic output of the recorded spectra are defined here. The default options set on this tab will be the default option with every new study queue. Each operator has the option to override these in the Start parameter panel during the submission of the queue.

UserPrefs

The UserPrefs tab allows the account administrator to set up operator options. The account administrator can define the interface personality at the time of operator login from here, as well as the action to be taken after sample submission.

| **NOTE** | The Preferences pop-up and all of its contents are described in detail in the VnmrJ Automation User Guide, Chapter 7. |

Spinner and temperature configuration

The temperature and spinner control can be set from the Start Spin/Temp parameter panel. If "Control ... from this panel only" is selected, then the configuration on this page is applied to all operators and experiments, and can only be

reset/changed from this panel. If it is unchecked, then users may have the option to change the temperature and/or regulate spinner as desired.

Temperature can also be set from the Automation section of the Preferences pop-up but will not supersede the temperature setting in the Spin/Temp panel if "Control temperature from this panel only" is selected.
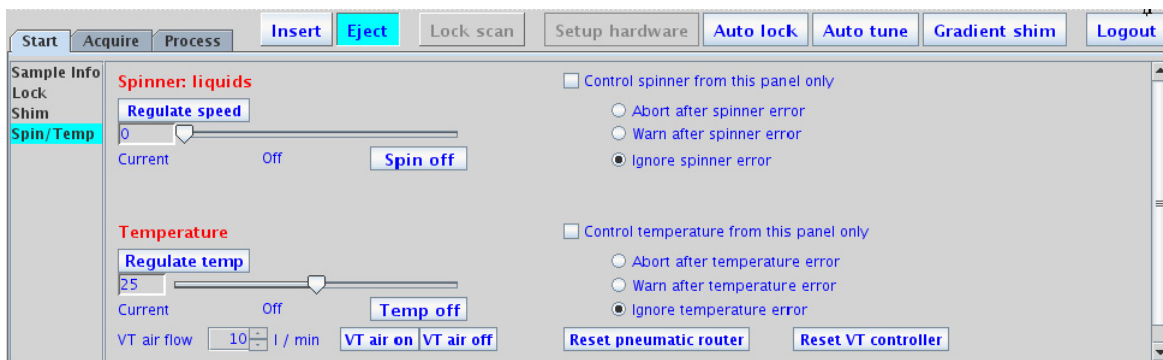
Figure 9   Spin/Temp panel

Operator Administration

Administration of operators includes adding or deleting operators, resetting operator password, assigning e-mail address, panel level, and command line access.

Adding operators to a user account

1 From the VnmrJ Admin interface, select **Show all VJ Users** and select the desired user account.

2 Type the name of each operator in the VnmrJ Operators box in the User Profile Panel, separated by a space.

   Operators with no operating system account are assigned the default password. Operators with an operating system account can use their operating system account login to access the VnmrJ operator interface.

3 Click **Save User**.

Resetting the operator password

This section only applies to operators that do not have an operating system login.

1 Double-click the VnmrJ Admin desktop icon.

2 Click **Configure > Operators > Reset Password.** The Reset Operators' Password window appears.

3 Enter the operator or operators in **VnmrJ Operators**.

4 Click **OK**.

Figure 10   Reset Operators' Password dialog box

Modifying operators

In the Modify Operators pop-up, a system administrator assigns operators an email address, a panel level, a full name, access to the command line, a profile, and can also remove an operator.

Opening the Modify Operators window

1 From the VnmrJ Admin interface, click **Configure**.

2 Click **Operators**.

3 Click **Edit Operators**.

The Modify Operators window appears.
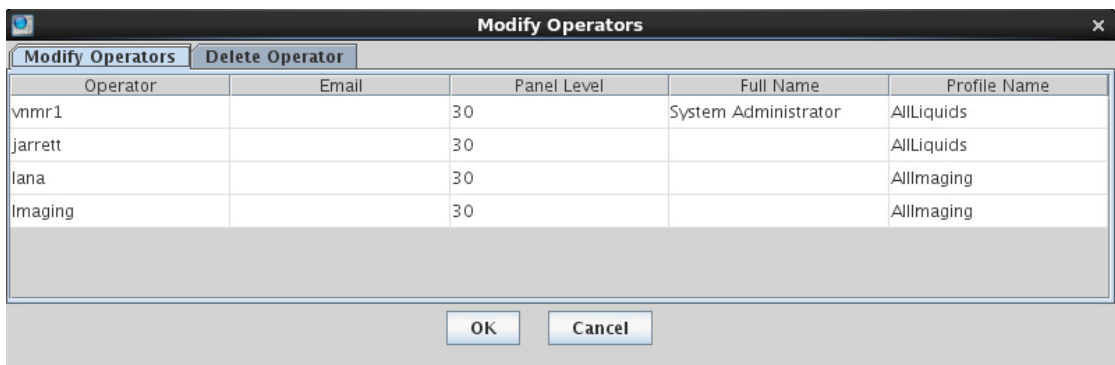
Figure 11   Modify Operators window

Assigning operators an e-mail address

The operator can be assigned a default email address. If the operator's email is added, the operator is notified when a sample is finished.

1 From the VnmrJ Admin interface, click **Configure**.

2 Click **Operators**.

3 Click **Edit Operators**.

The Modify Operators window appears.

4 From the Modify Operators Window, click **Modify Operators**.

5 Click the Email box to edit.

6 Type or edit the email address.

7 Click **OK** to accept changes and close the Modify Operators window.

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 From the VnmrJ Admin interface, click **Configure**.

2 Click **Operators**.

3 Click **Edit Operators**.

The Modify Operators window appears.

4 From the Modify Operators Window, click **Modify Operators**.

5 Change the panel level for any operator by entering a value in the Panel Level cell for the operator.
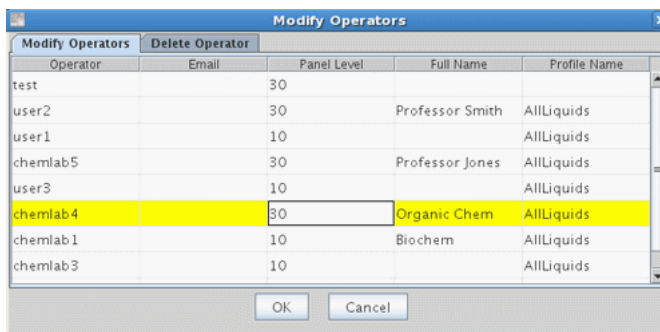
Panel level values and displayed pages are:

Value	Display
0-9	Shows 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.

6 Type Yes in the field under Show Command Line to give each operator command line access. The default is no command line access.

7 Do one of the following:

  • Continue to the next section.

  • Click **OK** to close the Modify Operators window.

  • Click **Cancel** to exit the Modify Operators window and make no changes.

Adding operators full name

1 From the VnmrJ Admin interface, click **Configure**.

2 Click **Operators**.

3 Click **Edit Operators**.

The Modify Operators window appears.

4 From the Modify Operators Window, click **Modify Operators**.
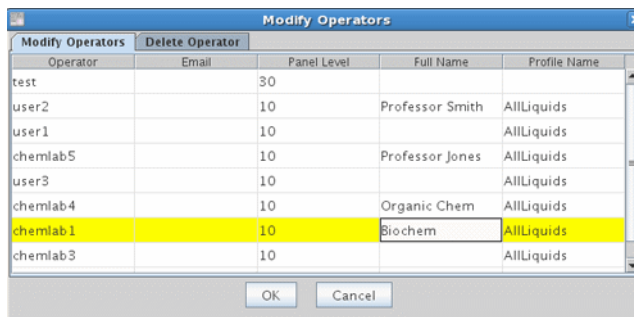
5 Edit or add the full name of the operator in the field below Full Name.

6 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.

Changing the icon on the Operator Login screen

The default Operator Login window contains the Agilent Technologies, 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**.

Deleting operators from a user account

To delete an operator from a single account:

1 Click the user account from the **Users Panel**.

   The operators of that user are listed in the User Profile Panel.

2 Edit the VnmrJ Operators box to remove the operators from the list.

3 Click **Save User**.

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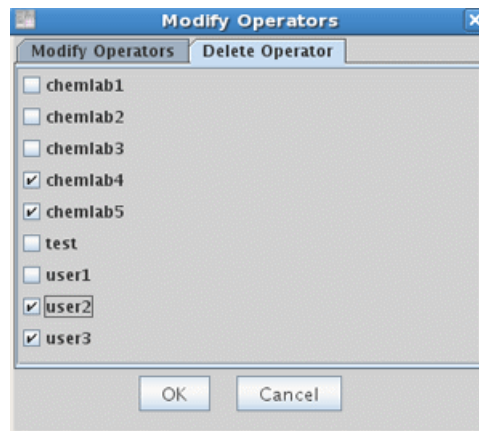
4 Select the operators to be removed and click **OK**.

User Defaults and Directories

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

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**.

The Defaults window appears and shows the defaults that will be used when a new user account is established.
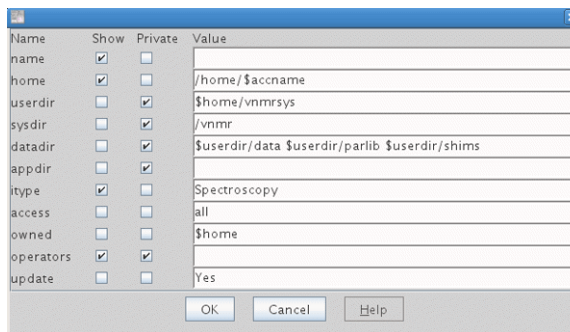
Field	Description
Name	Full name of a user.
Home	Home directory of a user.
Userdir	Directory that contains private VnmrJ files for a user.

Field	Description
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

4 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.
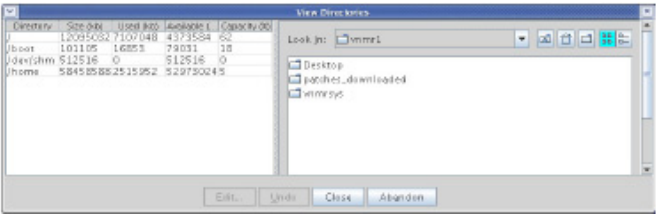
Replace `/home` with the directory path to the user's home directory if `/home` does not exist or if the home directory of the user is located in another directory.

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

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

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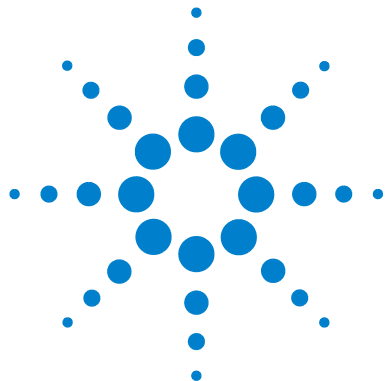
The lower right panel of the VnmrJ Admin interface shows information about the operating system.

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 4 Admin Interface.	
	Change the 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 a directory in the directories window to select a directory. The directory is inserted in the empty directory field of user directories.

3
VnmrJ Persona Administration

Agilent Technologies

Persona Manager

Use the Persona Manager to customize user preferences, permissions, user types (persona), and create users from the current VnmrJ login account.

There are two levels of persona in VnmrJ:

- The Administrator can create persona and assign them to Users. This is done using **Edit > System Settings > Persona Manager**. This option is only available if you are a VnmrJ system administrator. The Persona Manager for VnmrJ system administrators is shown in .

- The Administrator or User can assign persona to Operators. This is done using **Tools > Persona Manager**.

The Persona Manager window has three panels: Widgets and Rights, Parameter Panels, and Protocols.
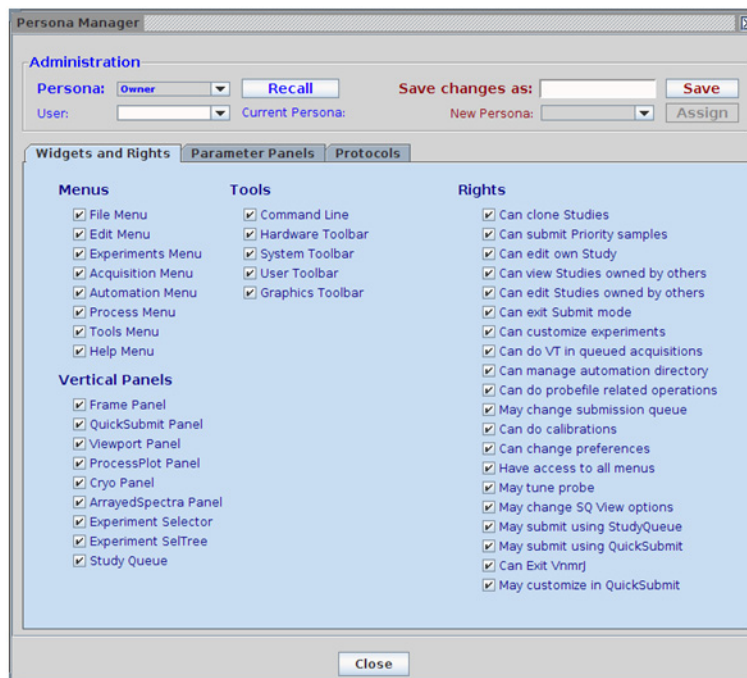
Figure 12   Persona Manager for VnmrJ system administrators

Persona Manager - Administration

Use the Persona Manager Administration tools to create and assign persona to Users (if you are a VnmrJ system administrator) or Operators (if you are a VnmrJ system administrator or User).
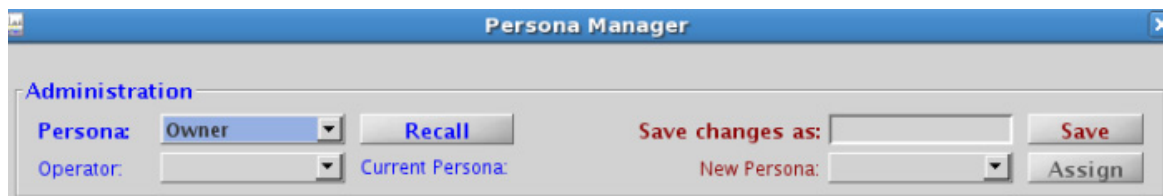
Figure 13 Persona Manager — Administration

Persona

VnmrJ comes with four predefined user types, called "persona". Owner has all permissions and no restrictions, and the other three have increasingly limited access.

- Owner
- Spectroscopist
- Chemist
- Student

These user types have been provided as examples or templates for easy customization.

Creating a new persona

To create a new persona:

1 Configure settings appropriately.

2 Enter the new persona type in **Save changes as:** and click **Save**.
The persona types are stored in the directory *vnmr/personalib*. User types can be assigned to an operator by selecting the appropriate name from the Operator pull-down list.

3 Select the persona type from **New Persona** pull-down and click **Assign**.
The operator will then be assigned the preferences and privileges of that persona after the next login.

NOTE The default persona is "Owner," and includes all privileges. Owner is assigned if the type was not defined or a type name has been assigned that does not exist.

Managing a Large Numbers of Users

When managing large numbers of users, it may be easier to assign persona types directly from the file *vnmrsys/persistence/PersonaManager/PERSONAassignment*. This is simply a text file with a two column list containing operator names in the first column and the persona type assigned in the second. This file can be edited with a text editor, or generated from an excel file as tab- or space-delimited text and placed in the appropriate directory. Alternatively, the file could exist on a central server with pointers to it. This allows for easy management of users on multiple instruments.

Persona Manager - Preferences

The Preferences panel contains a subset of preferences that can be applied on a per-user basis. For example, inputs to manage the limits for experiment time and priority samples, queue submission controls, and instructions for after login and/or sample submission. These preferences can be applied to a specific user or user type. General preferences, such as sample change time and automation directories, should be managed from **Edit > Preferences**.
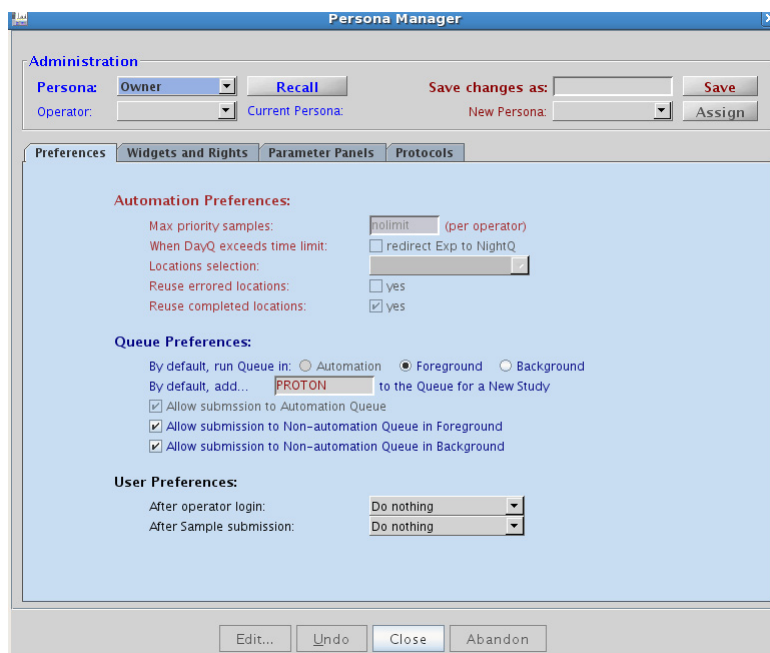
Figure 14   Persona Manager — Preferences

Persona Manager - Widgets and Rights

The Widgets and Rights panel contains lists of menus, tools, vertical panels, and rights. Accesses are granted from the check box to the left of each item. This list allows for a great deal of flexibility to manage user privileges.
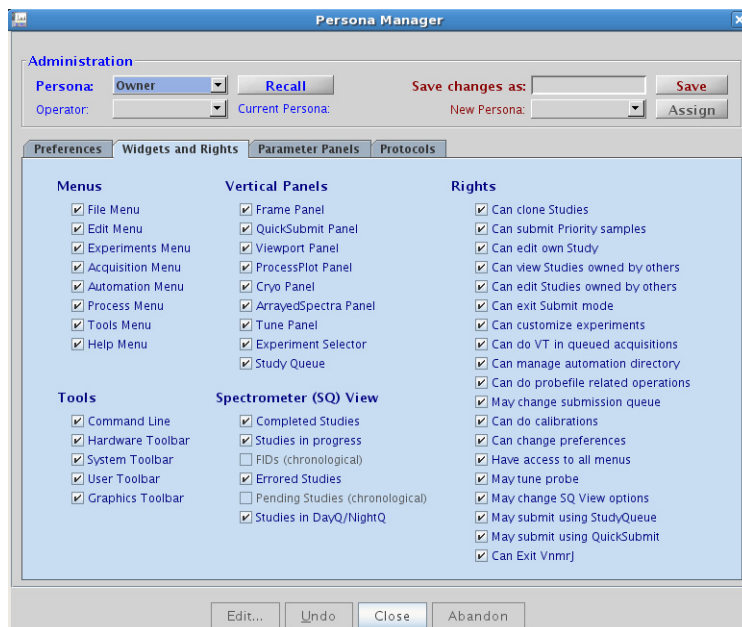
Figure 15   Persona Manager — Widgets and Rights

Persona Manager - Parameter Panels

Use Parameter Panels to control access to the parameter panels beneath the spectrum window.
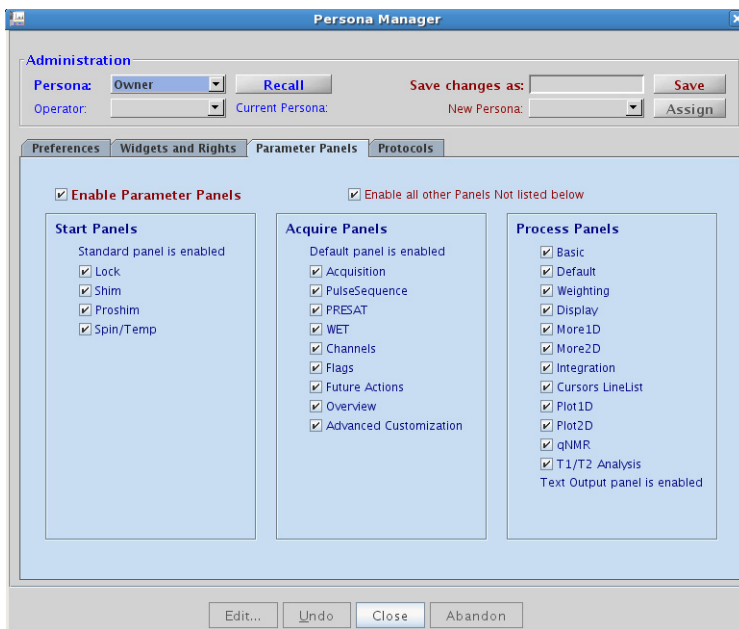
Figure 16   Persona Manager — Parameter Panels

Persona Manager - Protocols

The Protocols panel is where access to experiments in the Experiment Selector can be managed. Access can be managed either by individual experiments, or by entire protocol groups or subgroups. At the top of the panel are pull-down menus to view the four different experiment protocol groups and the subgroups. Next to the pull-down menus are check boxes to allow or restrict access to the entire group or subgroup currently selected. Below these menus, each experiment for the current group/subgroup selected is listed and access to the individual protocols can be controlled from the check box to the left of the experiment name.

NOTE Custom protocols will automatically appear in the list. All users and user types will be granted access to newly created protocols.
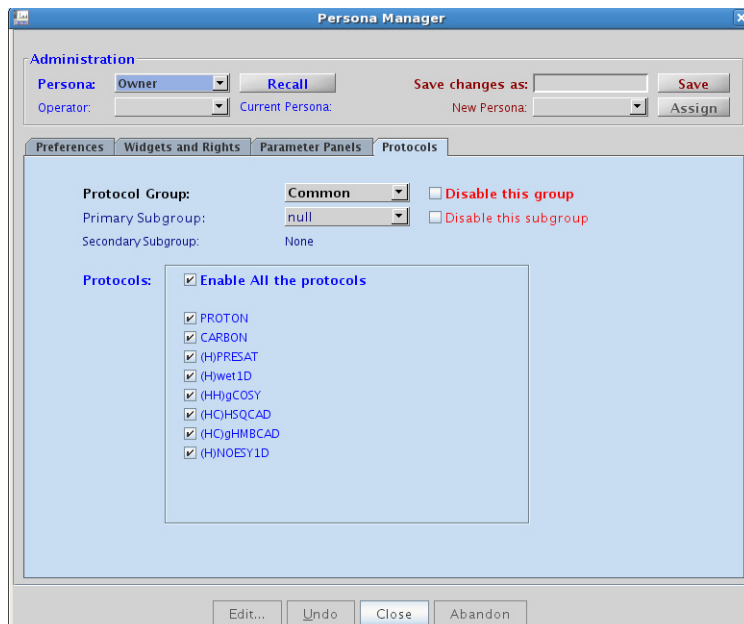
Figure 17   Persona Manager — Protocols
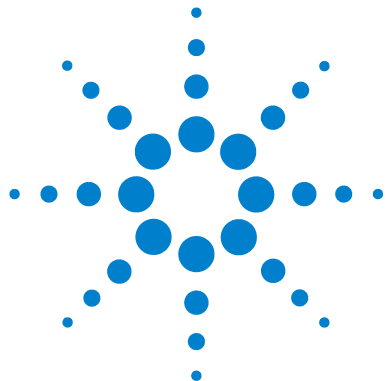
4

VnmrJ Probe Administration

Agilent Technologies

Configuring Probe Files

A probe file contains 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 may 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. A probe file that corresponds to the installed probe must be selected for proper functioning of protocols within VnmrJ.

Setting up, selecting, and creating a probe calibration file

Create a 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 of the VnmrJ 4 interface.

The probe selection window appears. (See Figure 18 on page 65.)
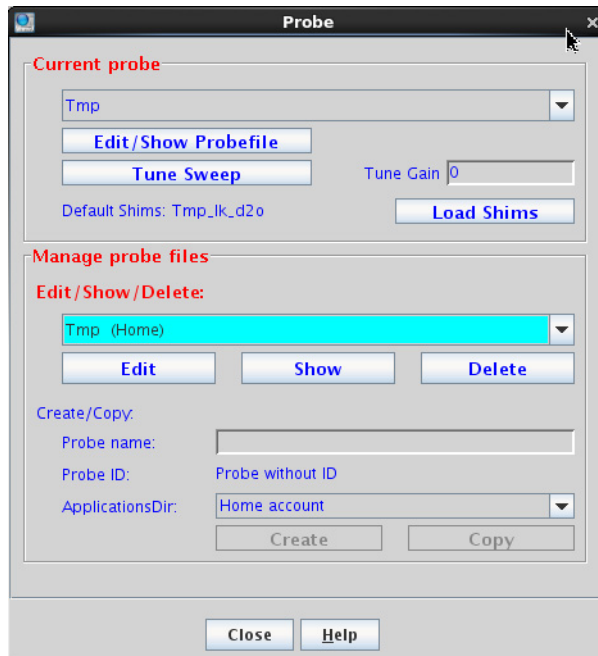
Figure 18   Probe window

2 In the **Manage Probe Files** section of the probe pop-up window, type the new probe name into the field for Probe name (letters first, followed by numbers and no spaces, e.g. abc456) and press the Return key.

3 From the **Probe ID** pull-down menu choose either **Probe without ID** to create a blank probe file or choose the probe ID that corresponds to the desired probe. This creates a probe file that is pre-populated with approximate calibration values for that style of probe.

4 Do one of the following based upon the operating system login:

- VnmrJ administrator or user with equivalent write permissions – select the appropriate radio button to choose either:
  Systemdir– writes the calibrations into:
  `/vnmr/probes/probe_name`
  and makes all calibration available to all users — typical for new system and probe installation.
  – OR –
  Userdir – 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 entering the desired file name and clicking **Copy**. See Figure 18 on page 65.

- 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`.

5 Click the **Create** button.

a 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.

b Run a calibration. See "Starting a calibration in Experiment Selector" section in the *Agilent VnmrJ System Calibrations Guide*.

For an existing probe

a Select the probe from the drop-down menu.

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

Click **Edit**, then click 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.)

b Run a calibration. See "Starting a calibration in Experiment Selector" section in the *Agilent VnmrJ System Calibrations Guide*.

Adjusting solvent lock power and gain values in the probe file

The solvent lock power and gain values are written to the probe file the first time a gradient shim map is automatically generated. The values are based are based on the lock power and gain values of the D2O sample used. These values should be adjusted for typical samples used in the probe after the automated routine has been run, so as to not replace your manually adjusted values for calculated values.

1 Log in as the VnmrJ administrator.

2 Double-click the **VnmrJ** desktop icon.

3 Click **Probe** at the bottom of the VnmrJ interface. The Probe window appears.

  The Current probe and Manage probe files sections display pull down menus of probes available for showing and editing.

4 Select the probe to edit from the appropriate section from the pull down menu.

5 Click either the **Edit/Show Probefile** if editing the current probe displayed in the pull down menu or **Edit** if editing a probe in the Manage probe files section. The probe file is displayed.

6 Click the **lk** tab to display and edit the lock power and gain values of various solvents under automation.

NOTE   If the autocalibration routine for gmap and z0 is run, the new/updated probe file will contain calculated values of lock power and gain. A backup of the old profile file with previous values is located in the probe's directory.

7 Scroll to the bottom of the page and click **Save Changes** to accept changes.

8 Click the **Close** button to close the Probe edit window.

9 Click the **Close** button to close the Probe window.

Adding and removing a nucleus in the probe file

A new entry (example: Si29) can be added to the probe file by typing on the command line:

```
addnucleus('Si29')
```

The probe file will then need to be edited to contain appropriate values for the new entry. Follow the directions in the "Adjusting solvent lock power and gain values in the probe file" on page 68, except click the **Si29** tab rather than the **lk** tab.

Alternatively, a new entry can be added by scrolling to the bottom of an opened probe file, then entering the nucleus in the Nucleus box and clicking **Add**.
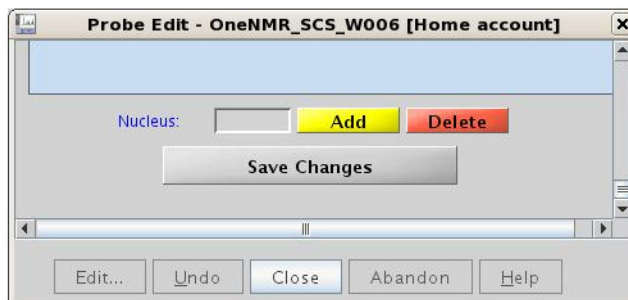
Figure 19   Adding nucleus in an opened probe file

| NOTE | The Save Changes button is located at the bottom of every tab. If it is not visible, then scroll down to the bottom of the displayed tab. |
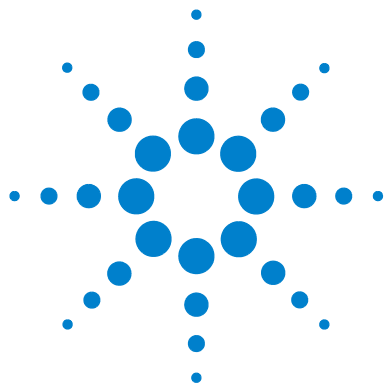
5
VnmrJ Printer Configuration

To configure printers for VnmrJ, first set up the printer in Linux using standard Linux system tools. Then use the Vnmr Plotter Configuration window to add or configure a printer for VnmrJ.

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

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Configuring Printers

The general steps to add and manage printers are:

1 Ensure the printer is connected and powered on.

2 Use the Linux desktop tools (with root permission) to find and create the printer.

3 Use VnmrJ Admin (as vnmr1) to set the printer up for VnmrJ.

4 Each user must select the printer from their account using the File->Printers menu in VnmrJ

Setting up a Linux printer

Follow this procedure for each printer to be accessible by VnmrJ.

1 Click on the Linux **System** menu.

2 Select **Administration**.

3 Select **Printing**.

4 Enter the root password in the pop-up window. The Printer configuration window appears.

5 Click **New > Printer** in the Printer configuration window.

A New Printer wizard is displayed to assist in adding a Printer. Follow the wizard to completion.

NOTE	If the correct print driver is not in the list of pre-installed drivers, then selecting one of the same manufacture and model/style will usually work. VnmrJ writes PostScript or PCL print files.

6 Print a test page from the printer configuration window to verify proper configuration of the printer.

| NOTE | Printers may also be managed from the Common UNIX Printing System (CUPS) interface accessed by going to http://localhost:631 in a browser.   More information can be found by visiting the official CUPS web site. |

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.
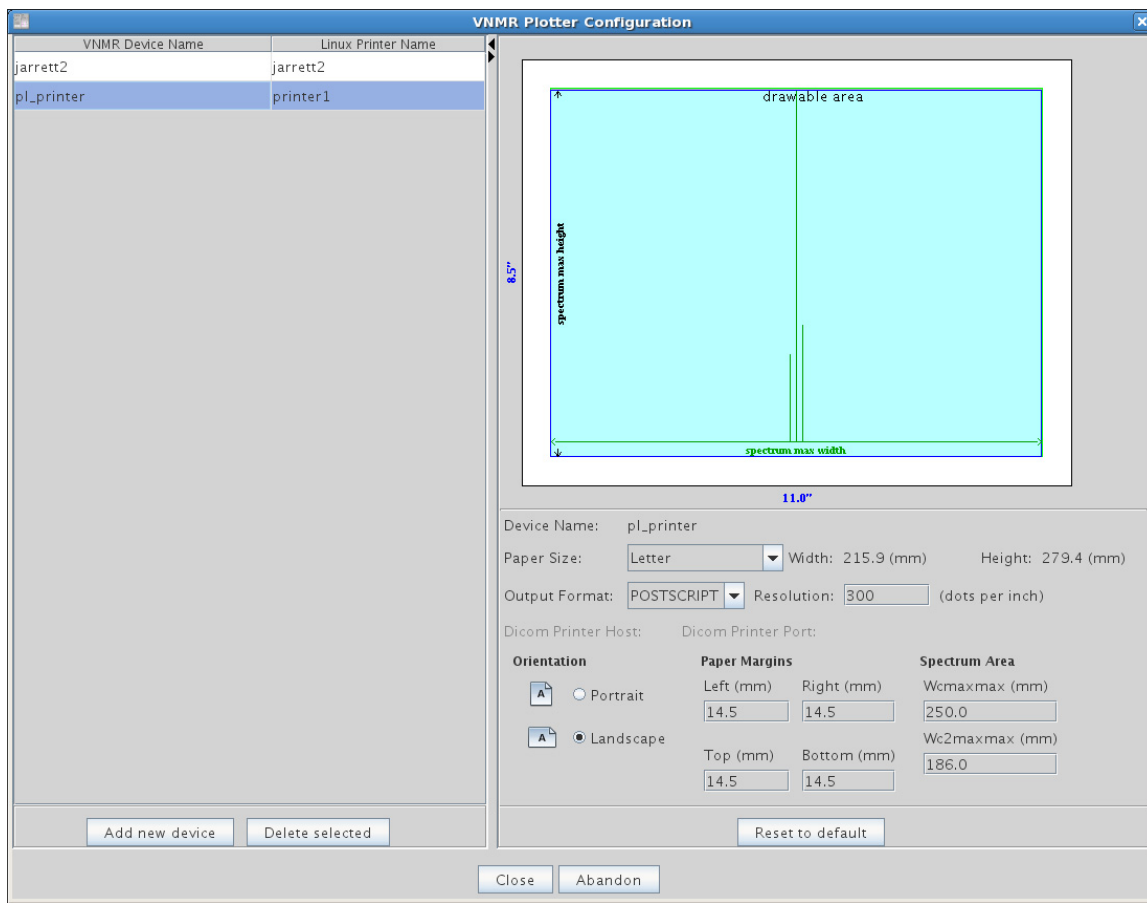
4 Select an available printer from the Linux Printer Name pull-down menu.

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	Creating plots with resolution of 1200 dpi and above will usually result in plot lines that are too fine or too light for presentation-quality results.

NOTE	Refer to the original manuals supplied with the printer or refer to online manuals for printers with older spectrometers.

Setting printers for users

Each user will need to set their default printer and plotter from the list created in the Plotter Configuration window in their own account in order to print from VnmrJ.

1 Double-click the **VnmrJ** desktop icon.

2 In the VnmrJ menu bar, click **File > Printers.** The Plotter Configuration window appears.

3 Select a default printer and plotter to be used then click **Close** to save the setting.
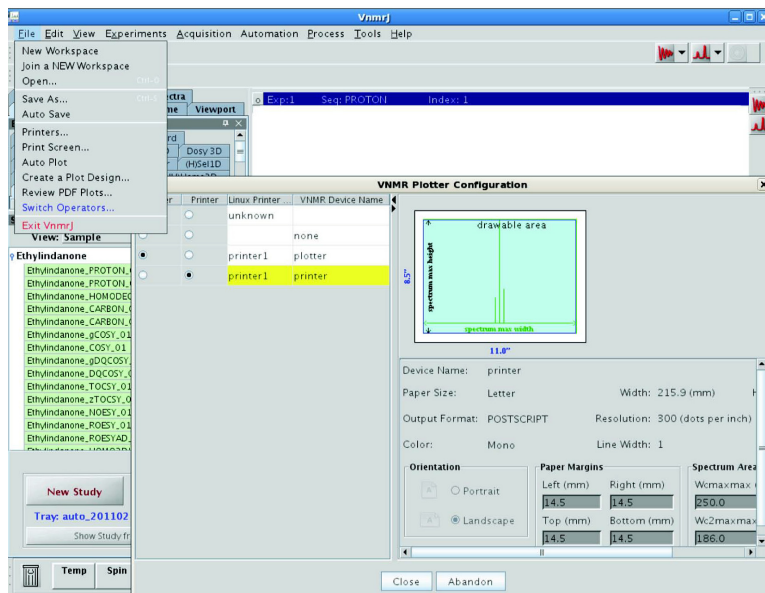
Figure 20   Configuring printers in VnmrJ

6
VnmrJ Automated Hardware Administration

This section describes how to configure software to control automated hardware.

Setup procedures require administrator access.

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Setting Up Automated Sample Handling

1 Log in as the 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.
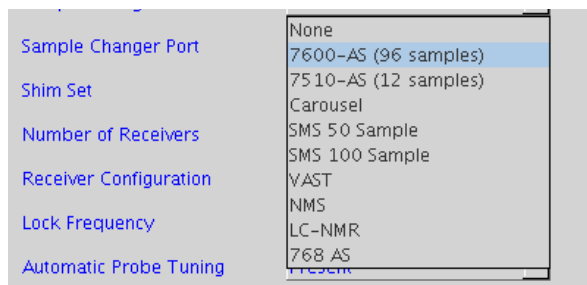
6 Click the **drop-down** menu next to the Sample Changer Port field.

7 Select a sample changer port.

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

SMS 50, SMS 100, Carousel, VAST	Select Com1
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**.

Setting Up Automatic Probe Tuning

Use the procedures in this section to set up automated probe tuning.

Configuring the Software for ProTune

1 Log in as the administrator.

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".

Loading chan# and motor# Persistence Files

AutoX-compatible probes ship with a CD or are on a probeID 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.

To load the Persistence files from a CD:

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.

a Type:
```
cd /vnmr/probes
ls
```

b Write down the <name of probe file>.

c Continue with step 3.
If no probe file exists, follow the procedure for setting up, selecting and creating a probe calibration file in the *VnmrJ 4 NMR System Calibrations User Guide*.

d Type:
```
cd /vnmr/probes
ls
```

e Verify and write down the <name of probe file>.

f Continue with step 3.

3 Type:

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

4 Type:

```
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) for standard AutoX and OneNMR probes.

To load the Persistence files from probeID:

Install and enforce probe ID. If probeID will not be used, copy the persistence files from `/vnmr/probeid/cache/<ID>/Varian/Tune be file>`

to

`/vnmr/tune/<name of probefile>` then disable probeID. See steps 1-3 and 5 from to create and copy the persistence files.

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.

Configuring Default Tuning Parameters for Autotuning in Automation

1 Click **Probe** in the Hardware Toolbar > **Edit/Show Probefile**.
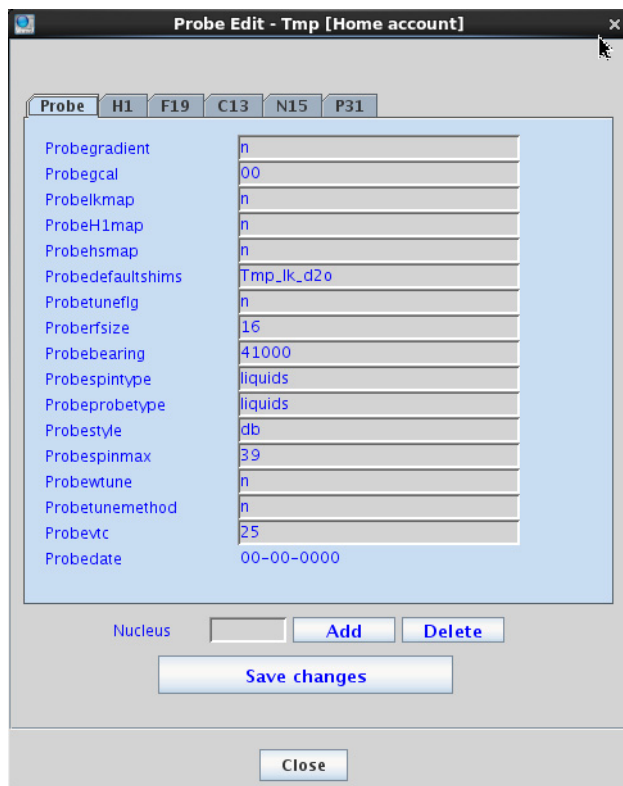
Figure 21   Probe Edit window

2 Recommended parameters for OneNMR and AutoX probes:

- Probewtune = st12
- Probetunemethod = lohi

For more information about these parameters, see the *User Programming Guide* and the *Command and Parameter Reference Guide*.

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.

Agilent Technologies

Starting VnmrJ Accounting

VnmrJ Accounting is managed from within a separate user interface in VnmrJ Admin.

NOTE	In order to do cost and time accounting, you must first enable the record keeping log. (See "To enable record keeping".)

To open the VnmrJ Accounting interface

1 Log in as the administrator.

2 Start **VnmrJ Admin**.

3 In the menu bar, click **Management**.

4 Select **Cost/Time Accounting**.

To enable record keeping

In order to activate record keeping,

1 Open the VnmrJ Accounting interface. (See "To open the VnmrJ Accounting interface".)

2 In the VnmrJ Accounting interface, click the **Properties** tab.

3 Under Record keeping, click to select the check box next to **Acquisition & Use record keeping**. When selected, the label on the check box changes from Inactive to Active (Figure 22 on page 85).
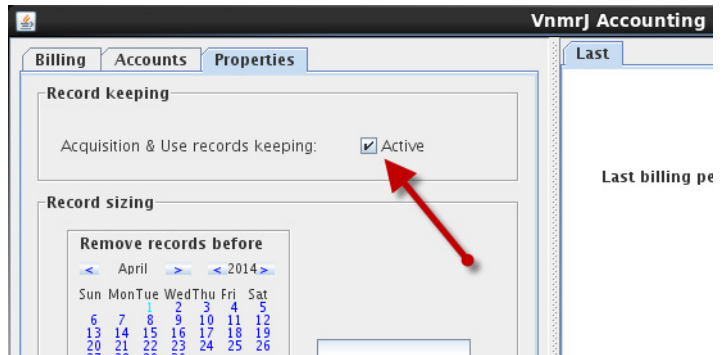
Figure 22 Enable record keeping in VnmrJ Accounting

VnmrJ Accounting Window Interface

The VnmrJ Accounting interface contains three tabs, where you set up Billing, Accounts, and Properties.

Billing

Click the **Billing** tab in the VnmrJ Accounting window to open the Billing window. See Figure 23. See also "Generating Invoices" on page 89.

Default logo or optional customer logo

Select account from drop-down list

Billing address of selected account

Invoice details for selected dates is displayed in this area when you click Display this invoice.

Calendars are used to select start and end dates for generating invoice

Options for printing invoices
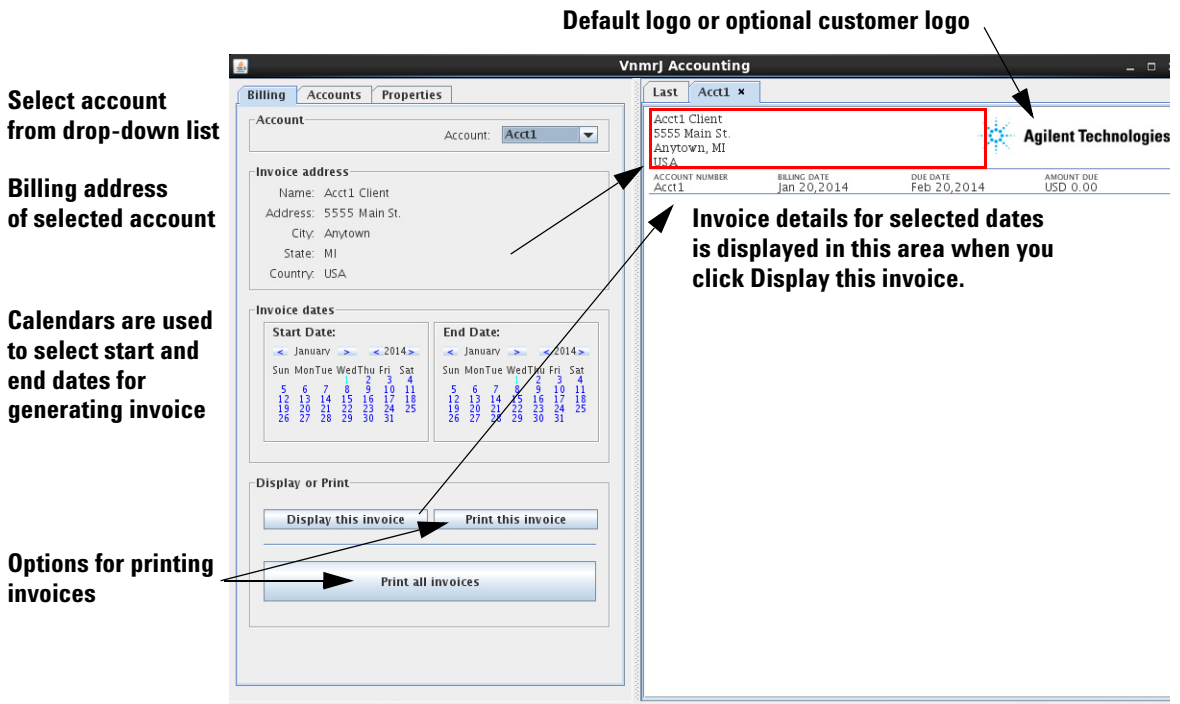
Figure 23   VnmrJ Accounting Billing tab

Accounts

Click the **Accounts** tab in the VnmrJ Accounting window to open the Accounts window; see Figure 24. See also "Creating or Editing an Account" on page 90 and "Establishing or Editing a Billing Rate Schedule" on page 92.

Figure 24   VnmrJ Accounting Accounts tab

Properties

Click the **Properties** tab of the VnmrJ Accounting window to open the Properties window; see Figure 25. See also "Controlling Properties" on page 95.

Default logo or optional customer logo

Select to enable records keeping

Select a date and click Cut Records to remove records prior to selected date

Select currency

Use default logo or browse to select custom logo

Select billing mode

Customize rate schedule table headers

Billing address
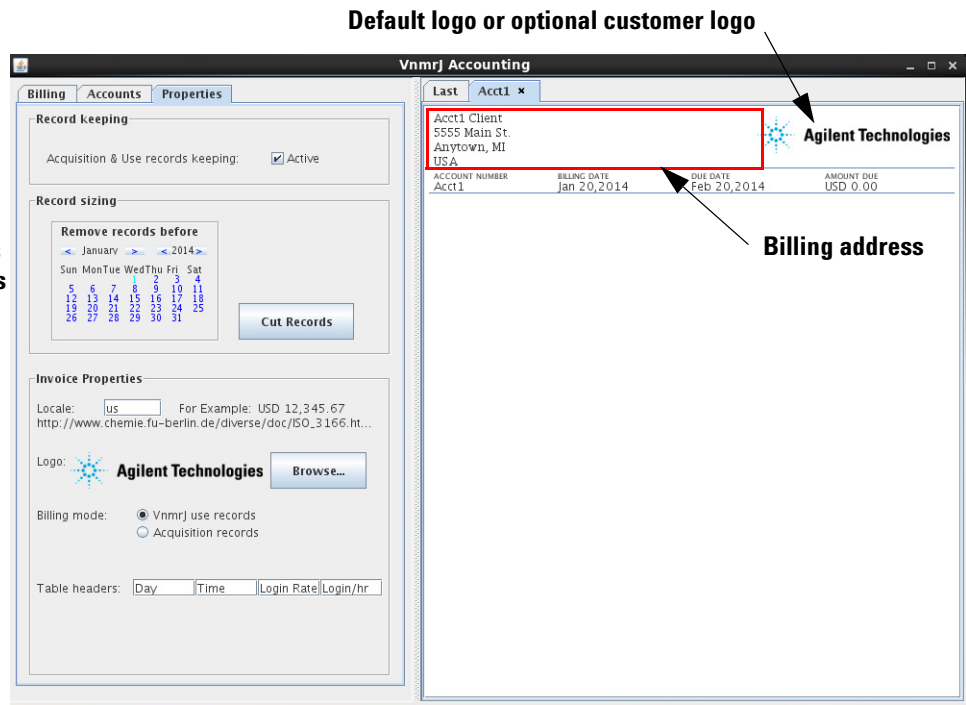
Figure 25   VnmrJ Accounting Properties tab

Generating Invoices

1 Start the VnmrJ Accounting interface if it is not running ("Starting VnmrJ Accounting" on page 84).

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 the **Display this invoice** button to display the invoice on the right side of the Billing tab; see Figure 23 on page 86.

  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.

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" on page 21.

2 Add any required operators to each system login in account; see "Creating Profiles-Spectroscopy Accounts" on page 54.

3 Start **VnmrJ Accounting**, see "Starting VnmrJ Accounting" on page 84.

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 alphanumeric, 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" on page 92.
Add owners and operators whose usage is tracked and billed to this new account by selecting the check box next to the owner or operator.

8 Click **Save** to save the new or updated account information.

Establishing or Editing a Billing Rate Schedule

Use the Accounts tab to create and edit a billing rate schedule. See "Billing rates" on page 92 and "Billing rates example" on page 94.

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.

   To insert a new row:

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

   b Click the **Insert Row** button to add a row below the row with the cursor.

   To delete a row:

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

   b Click the **Delete Row** button to delete the row.

3 Click the **Save** button to save the new rate schedule for the current account.

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.

Controlling Properties

Properties apply to all system accounts. Use the Properties tab of the VnmrJ Accounting window to Enable/disable record keeping, Reduce record size, and set Invoice Properties.

Enable/disable record keeping

To enable record keeping,

1 From VnmrJ Administration, select **Management > Cost/Time Accounting**.

2 In the VnmrJ Accounting window, select the **Properties** tab.

3 In Record keeping, make sure the check box next to **Acquisition & Use record keeping** is selected.

The label changes from inactive or on hold to active when the check box is selected.

4 From a terminal, type the command su acqproc twice if the Acquisition record keeping is (re)activated.

When record keeping is enabled, a log file is created /vnmr/adm/accounting/acctLog.xml. Login/Logout and Acquisition (go) record logging are both entered in this file.

NOTE	If the acctLog.xml file does not exist, no logging will take place. This log file is in XML format with date and time in easy to read format.

Parameters that are automatically logged:

```
type (login/logout/gorecords), start, startsec,
end, endsec, operator, owner, seqfil (for
gorecords only), systemname, vnmraddr
```

To have other vnmr parameters included in the log files, the vnmrj admin can add parameters to the file /vnmr/adm/accounting/loggingParamList.

Entries should be in two columns where the first column is the parameter name and the second column is the "tree" where the parameter is located.

For example:

```
# paramName    tree

   tn           current

   sw            current
```

This example adds the nucleus and sweep width to the log file. Some parameters will not make much sense for login/logout nor others for acquisition. However, the parameters will be dutifully logged as requested in this configuration file.

Reduce 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 **Logout records** or **Acquisition records**.

4 Click the **Cut Records** button.

Invoice Properties

Invoice properties are set on the Properties tab.

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

Logo

Keep the default Agilent logo or select a custom logo using the **Browse** button. Place any custom logo 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.

Billing modes

Account billing is determined by one of two billing modes: Acquisition Time, VnmrJ Use.

Acquisition Time

Tracks the time from start to completion and processing of an experiment. This is tracked in: `/vnmr/adm/accounting/acctLog.xml`.

VnmrJ Use

Tracks the time the owner or operator starts or logs into VnmrJ. This implementation is used to track operator time during walkup, owner time in walkup or experimental mode, or both. If more than one VnmrJ 4 is opened, both are tracked and invoiced. This is tracked in: `/vnmr/adm/accounting/acctLog.xml`. This is the only method to track operator time. This was previously referred to as Login or Logout Use.

File Locations

- Account information —

  `/vnmr/adm/accounting/accounts/<account>.txt`

- Records —

  `/vnmr/adm/accounting/acctLog.xml`

- Logo —

  `/vmnr/adm/accounting/*.gif`

- Properties file —

  `/vnmr/adm/accounting/accounts/accounting.prop`

- Logging parameters

  `/vnmr/adm/accounting/loggingParamList`

NOTE	Gorecords and login/logout are both in the `acctLog.xml` file.

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.

Currency

Enter the two-letter name for the country (for example, us
for United States, de for Germany) to set the number format
and currency symbol for the local. Refer to the following
Website 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.

Billing mode

Account billing is determined by one of two billing modes:
Acquisition Time or VnmrJ Use.

`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/acctLog.xml exists and the following are recorded:

- account — usually "vnmr1"
- 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.

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"

Error Messages

Possible messages in VnmrJ Accounting include Messages displayed at start up and Account information error message.

Messages displayed at start up

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

If the item exists, the message is as follows:
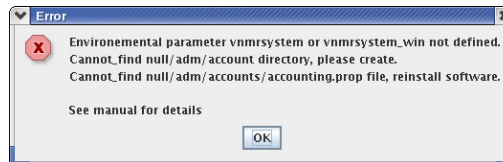
Other messages that are displayed:

- 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 4 software.

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.
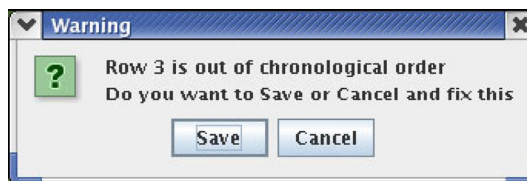
Do one of the following:
- Click the **Cancel** button, correct the order, and click the **Save** button.

- Continue with clicking on 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.

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.

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/acctLog.xml` and `/vnmr/adm/tmp/macrorecords` grow larger and larger with time. The VnmrJ 4 Administrator must periodically delete records in these files. The `acctLog.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.

- `Expproc` writes the `acctLog.xml` file. Access permission for this file is rw-------. `Expproc` executes with root permission and does not need general access permission to write to `acctLog.xml`, making it more secure.

Converting Log Files to CSV

You can export the login/logout and acquisition log files to CSV (Comma Separated Values) format. This enables you to import the CSV file into excel or access for further manipulation and display.

To convert the log files to CSV (Comma Separated Values)

1 Open VnmrJ Admin.

2 On the menu, click **Management > Export Log to CSV.**

The Log to CSV Conversion pop-up appears.
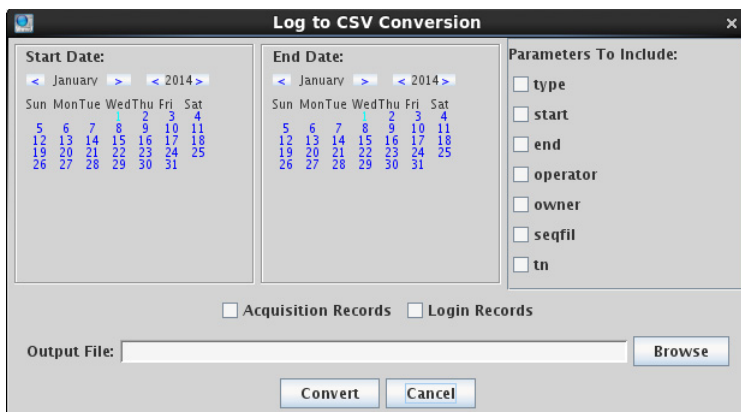
Figure 26   Log to CSV Conversion pop-up

3 On the Start Date and End Data calendars, select start and end date (inclusive) for the log data to export. Only entries within that date range are converted.

4 Under **Parameters to Include**, select the parameters that you want transferred to the output file.

5 Select **Acquisition Records**, **Login Records** or both to be converted.

6 Browse to select an output file location and filename.

7 Click **Convert**.

Using the xmlToCsv command

The `xmlToCsv` command can be used by scripts and automated cronjobs for the conversion of the login/logout and acquisition log files to Comma Separated Values (CSV) files. The intent is to allow the user to then import the CSV file into excel or access for further manipulation and display. It allows for limiting the conversion to

    specific date ranges

    specific parameters

    acquisition/login/both entries

Usage: `xmlToCsv inputLogFilePath outputCsvPath`

    `[-type acq/login/all] [-paramlist p1 p2 p3 p4 ...]`

    `[-startdate "Month Date Year"]`

    `[-enddate "Month Date Year"]`

    `[-debug]`

- `type` can have values of "acq", "login", or "all".
- `paramlist` should be followed by a space separate list of parameters that are desired in the csv file.
- `startdate` specifies the beginning of the date range to be included in the output file. The dates must be in the form "Month Date Year" and surrounded by double quotes.
- `enddate` specifies the end of the date range to be included in the output file. The dates must be in the form "Month Date Year" and surrounded by double quotes.
- `debug` Causes the command to output all of the values it will be operating with. It is basically a verbose output to the command line.

8
VnmrJ Terms

Agilent Technologies

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 4 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 **Experiments** on main menu. Parameters are loaded directly into the current workspace for manual data acquisition.

Experiment

See "Workspace" on page 117.

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`, `preset`, 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 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 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. 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`, `preset`, 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 `preset`, 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
9	Carousel
50	SMS with a rack for 50 samples
100	SMS with a rack for 100 samples
96	VAST

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.

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, for example, 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.

Administrator

Administrator

The administrator of VnmrJ (both hardware and software) is generally called "vnmr1" and is the owner of all files and directories of the VnmrJ 4 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 defines each user's application mode upon the creation of that user's operating system login account.

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 administrator.

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.
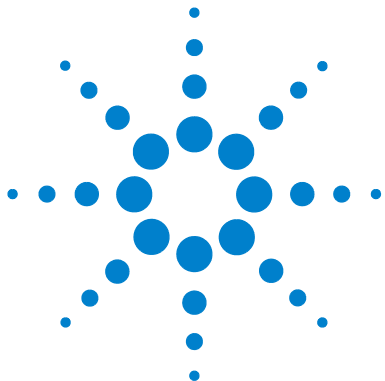
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Locator Administration

Agilent Technologies

Restricting User's Data Viewing Privileges in Locator

The Locator is a database browser that provides access to data sets, experiments, shim sets, commands, and so on. The administrator can restrict how files appear in the Locator for each user. An access list controls the data that is visible to the users.

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.

Access list

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

1 Select a user account by clicking on 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.

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

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**.

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. If PGHOST is set to a remote database computer, that remote database will be used even if there is a local instance of a database running.

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. Creating this file on a non-server computer will force the database 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.

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.

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