VnmrJ 3 QUICKSTART GUIDE

Administrator Tools

NMR SOFTWARE

This VnmrJ Administration Quickstart Guide covers typical day-to-day tasks, including the creation and configuration of:

- user accounts
- operators
- printers
- probe files

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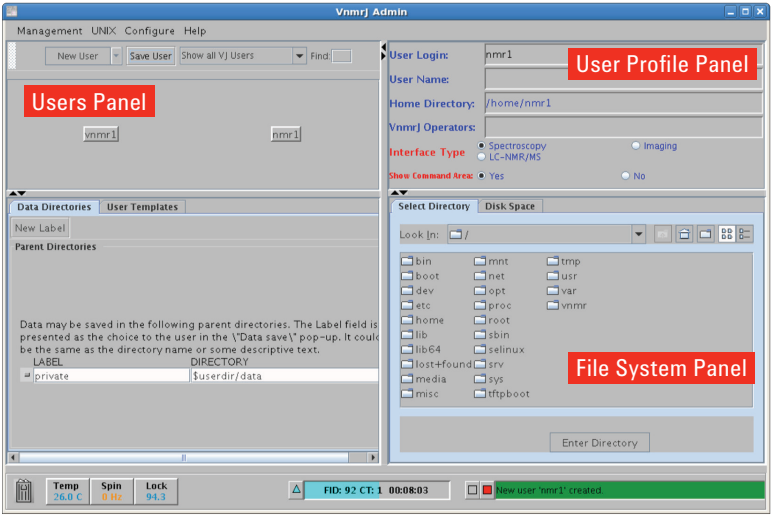
Administration of users, operators and printers are executed using the VnmrJ Administration interface. Adding printers requires the Linux root password and accessing the VnmrJ Administration interface. Configuration of the probe file is done through the VnmrJ interface.

Table of Contents Page

Starting the VnmrJ Admin Interface

1. Log in as the VnmJ administrator, usually vnmr1.
2. Click on the **VnmrJ Admin** icon on the desktop.



User Account Creation and Administration

A typical administration function is setting up new accounts and configuration of the VnmrJ interface according to the needs of the users. Another administration function is assigning a group of operators to a single user account. If operators will be used, then the default password should be set first, before creating operators.

Setting the Operator Default Password

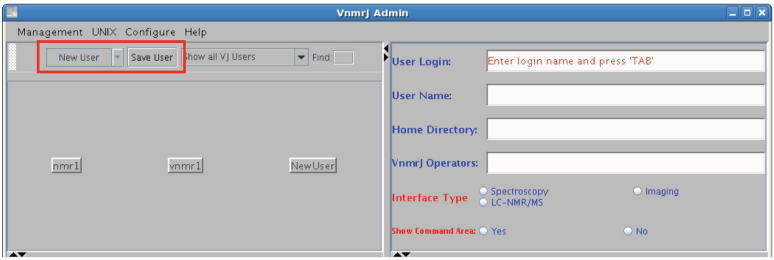
Set the default password for VnmrJ operators that *do not have* an operating system login as follows:

1. From the VnmrJ Admin interface, click Configure.
2. Click Operators.
3. Click Preferences.
4. The Preferences window appears.
5. Enter a password in the **Default Password for VnmrJ Operators** box.
6. Click **OK**.

Creating a New User Account

This procedure creates a single new user account.

1. From the VnmrJ Admin interface, click **Management.**
2. Click **Users**.
3. Click **New User**.
   NewUser appears with a box around it and the account's profile is displayed in the User Profile Panel.
4. Fill in the **User Profile Panel** as appropriate. Usually the User Login (Linux Login Name), User Name (*Optional* - User's Full Name), VnmrJ operators (*Optional* - one word per operator separated by a space) Interface Type and Show Command Area are modified.
5. Click **Save User**. You must configure newly created user accounts. Refer to the section Configuring the User's Account.



Creating multiple new user accounts from a .csv file

The .cvs file must follow a specific format. In the first line, enter a list of column keywords separated by commas. Keywords are login, itype, name, home, email, profile. 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. The .csv file's comment lines must start with a number.

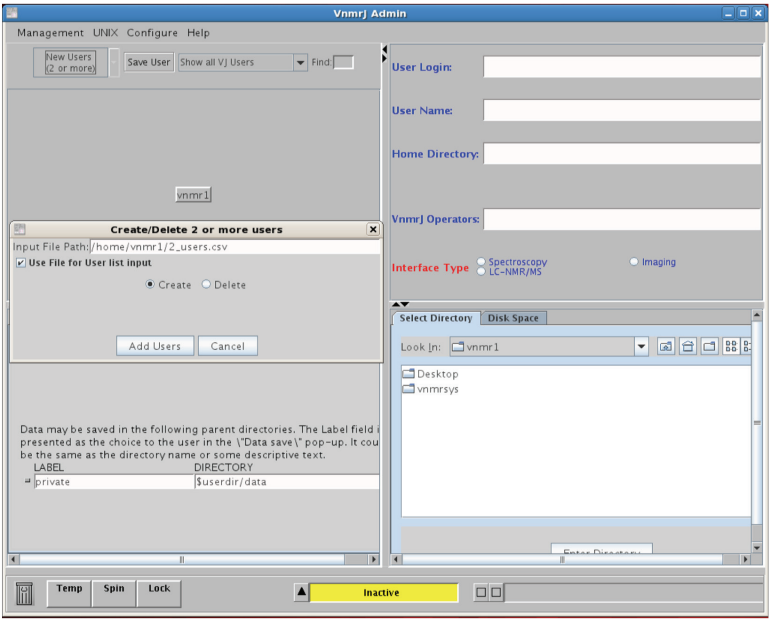
Example: login,name,home,itype,email,profile
myuser1,My User 1,/home/myuser1,Spectroscopy,user1mail@abc.com,BasicLiquids
myuser2,My User 2,/home/myuser2,Spectroscopy,user2mail@abc.com,CommonLiquids

To create multiple new user accounts from a .csv file

1. From the VnmrJ Admin interface, click **Management - Users.**
2. Click **Multiple Users** from the drop-down menu next to the **New User** button.
3. Click **New Users (2 or more)**.

The Create/Delete 2 or more users windows appears.

4. Select **Use File for User list input**.
5. Select **Create**.
6. Enter the file path for the .csv input file.
7. Click **Add Users**.



NOTE: To create multiple new users accounts at once without using a .csv file, refer to the VnmrJ Installation and Administration User Guide.

Deleting a User Account

User accounts can be deleted as necessary by moving accounts to the trashcan or using a .cvs file. Once the trashcan is emptied, the account cannot be restored. See the VnmrJ Installation and Administration User Guide for further account manipulation details.

Adding Operators to a User Account

1. From the VnmrJ Admin interface, select **Show all VJ Users** and click on the user account to which operators are to be added.
2. Type the name of each operator in the **VnmrJ Operators** box in the User Profile Panel.
3. Operators with no operating system account are assigned the default password, those that have an operating system account use their operating system account password to access the VnmrJ operator interface
4. Click **Save User**.

Resetting the Operator Password

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

1. From the VnmrJ Admin interface, click **Configure**.
2. Select **Operators**.
3. Select **Reset Password**.
4. The Reset Operator's Password window appears.
5. Enter the operator or operators in the **VnmrJ Operators** box.
6. Click **OK**.

Modifying Operators

The system administrator assigns operators an email address, a panel level, a full name, access to the command line, a profile, and even removes an operator.

Opening the Modify Operators Window

1. From the VnmrJ Admin interface, click **Configure**.
2. Click **Operators**.
3. Click **Edit Operators**.
4. The Modify Operators window appears.

Assigning Operators an Email Address, Panel Level, Full Name and Command Line Access

The operator can be assigned a default email address. The panel level determines which VnmrJ interface pages are available under the tabs in the parameter page area. The default is 10 for operators and 30 for the account owner. Setting the panel level higher makes more pages available (Default panel level groups are **0-9, 10-29,** and **30-100.**) Edit the above fields as follows.

1. From the Modify Operators Window, click **Modify Operators**.
2. Click the box to edit.
3. Type or edit the email address, panel level, and full name.
4. Select **yes** or **no** from the **Show Command Line** list.
5. Click **OK** to accept changes and close the **Modify Operators** window.

Assigning Profiles to a User and an Operator

A profile controls the buttons that appear in the Experiment Selector, rights, and tools that are available to a user(s) and operator(s). (To create, edit, view or delete a profile, as well as an explanation of rights and options, refer to the VnmrJ Installation and Administrator User Guide.)

1. Click **Modify Operators**. The last column in the Modify Operators window is for assigning the profile.
2. From the **Profile Name** list, click on the box and scroll to the profile for the operator.
3. Click **OK** to apply.

Additional operator rights are assigned from within the users account, and explained in detail in the Automation User Guide, Chapter 9.

Removing Operators from User Accounts

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

To delete an operator for all accounts:

1. Click **Delete Operator**.
2. Click the box(es) next to the operator(s).
3. Click **OK** to apply.

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 operator(s) from the list.
3. Click **Save User**.

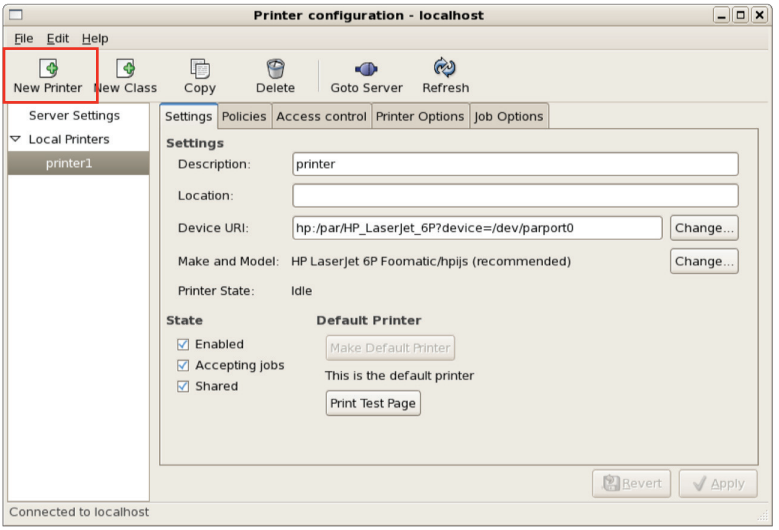
Configuring Printers

To add and manage printers, access to the Linux administrator permissions (root) and the VnmrJ Admin interface (typically vnmr1) are needed, and can be done using the Linux Printer wizard and the VNMR Plotter Configuration window.

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 root user's password in the popup window. The Printer configuration window appears.



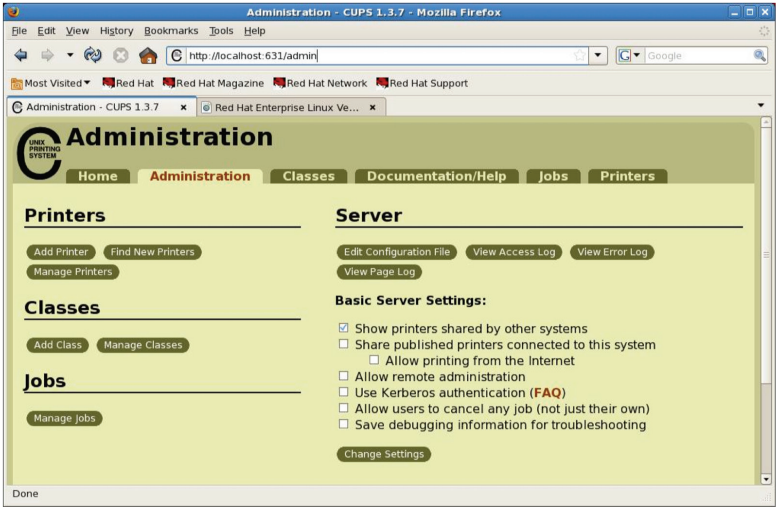
5. Click **New Printer** in the Printer configuration window.

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

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

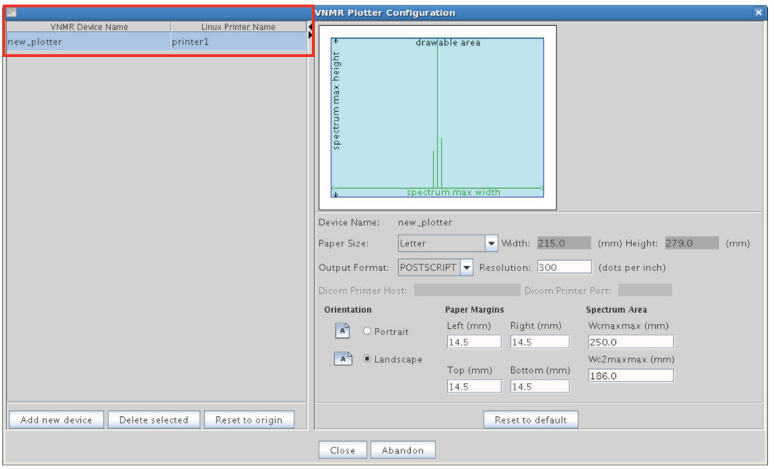
   NOTE: To delete a printer, highlight or select printer in the Printer Configuration window and click the **Delete/trash** can icon.

NOTE: Printers can be managed from the Common UNIX (and Linux) Printing System interface by typing http://localhost:631/ in the browser address line. The Administration tab allows for addition of printers, while the Administration, Jobs and Printers tab provides addition tools to manage printing jobs and print queues. More information can be found by visiting the official CUPS site http://www.cups.org/ for printer drivers and printers.



Setting up a Printer for VnmrJ

1. Click on the **VnmrJ Admin** icon.
2. Click on **Management**.
3. Click **Printers...** to open the tool. The VNMR Plotter Configuration window appears.



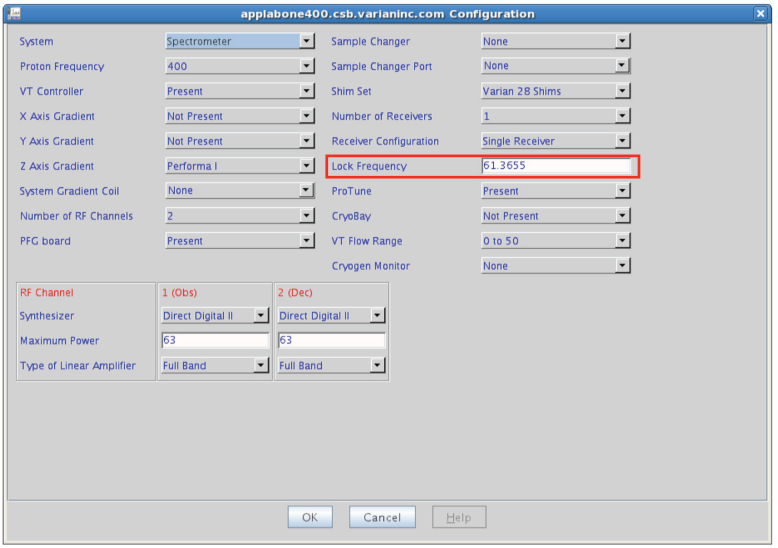
4. Select an available printer from the **Linux Printer Name** list.
5. Type a name that VnmrJ will use to recognize this printer in the **VNMR Device Name** box.
6. To the right of the **VNMR Device Name** and **Linux Printer Name** columns are the page settings VnmrJ will use to print. These are to be set for appropriate paper size, output format, dots per inch (dpi), paper orientation, and printable area.
7. Click **Close** to save and close the VNMR Plotter Configuration. To abandon **ALL** changes, click **Abandon**.

Accessing the Hardware Configuration Window

The software must be configured to match the installed hardware for proper operation. This system installer performs this task at the time of installing the spectrometer. The administrator may want to record the settings in the configuration for backup or reference.

1. Log in as the Vnmrj administrator.
2. Click on the **VnmrJ** icon on the desktop.
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.
6. Record the settings for future reference and then click **Cancel** to close the window.

   In time, value of the Lock Frequency may 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. (Refer to the VnmrJ Installation and Administration User Guide for details.)



Adjusting Solvent Lock Power and Gain Values in the Probe File

The solvent lock power and gain values in the probe file are generated when the gradient shim map was automatically created and are based on the lock power and gain values of the D_2O 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. Click the **VnmrJ** icon on the desktop.
3. Click the **Probe** button 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 put calculated values of lock power and gain in the new probe file. A backup of the old profile file with previous values is located in the probe's direcotory.
7. Scroll to the bottom of the page and click the **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" except click the **Si29** tab rather than the **lk** tab.

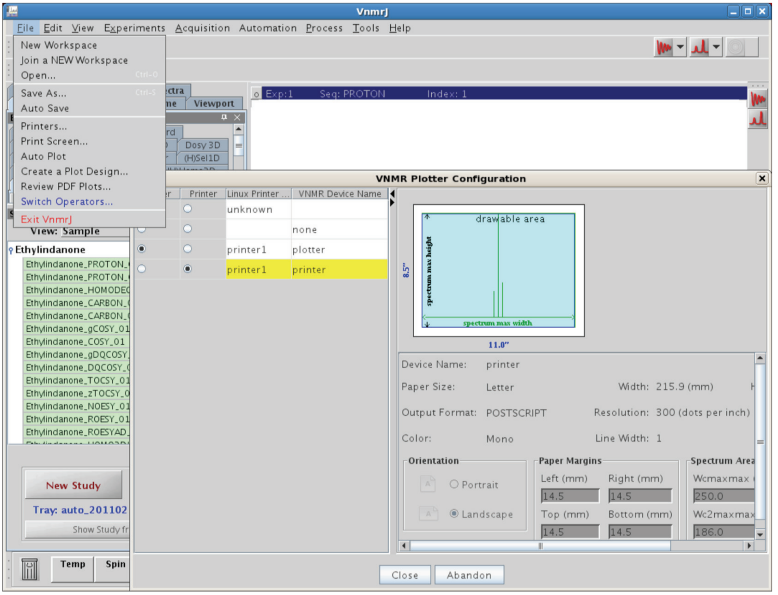
Configuring the User's Account

These settings refer to a single user's account. Each user will need to log in to their own account and set their printer and preferences. These changes affect only that user's account.

Setting Printers for Users

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

1. Click on the **VnmrJ** icon on the desk top.
2. Click **File** in the main menu after VnmrJ starts.
3. Click **Printers...** to open the VNMR Plotter Configuration window.
4. Select a default printer and plotter to be used then click **Close** to save the setting.



Setting User Preferences

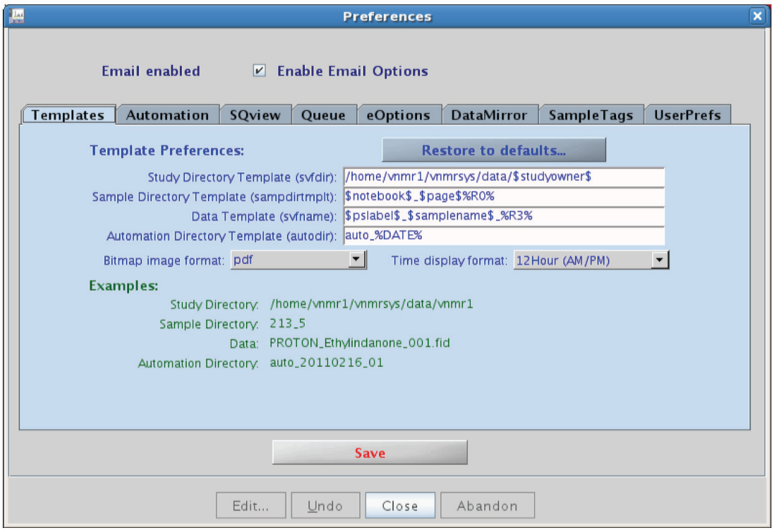
Each VnmrJ account can be further customized through the Preferences popup. These preferences control only that user's account and any operator using that account; it does not affect any other VnmrJ account. The Preferences popup and all of its contents are described in detail in the VnmrJ Automation User Guide, Chapter 7.

- The Preferences configures:
- 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 popup:

1. Click **Edit** in the main menu.
2. Click on **Preferences...** to open the Preferences popup.

Template Preferences

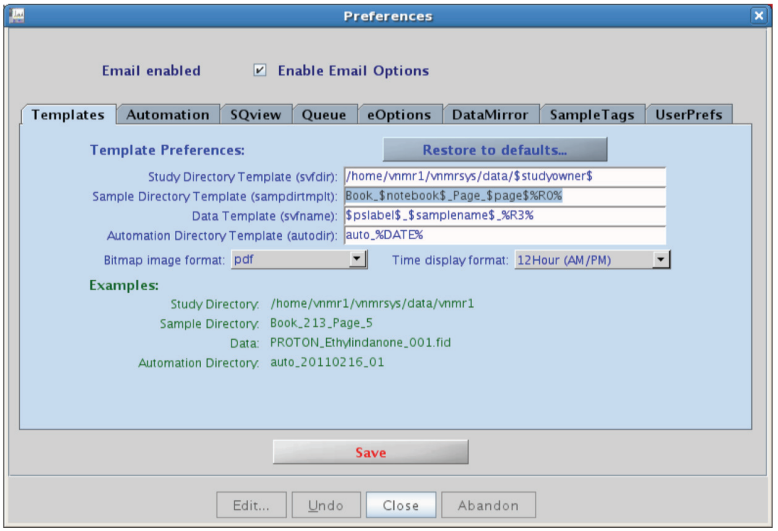


The Template Preferences found in the **Templates** tab are usually customized to the user's needs and several common examples are provided here (although the default naming and saving convention can be used.) Parameters are placed between dollar symbols (example: $pslabel$), time and date substitutions 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. Typing man('Svfname') from the VnmrJ command line will provide a detailed description of other substitution identifiers, usage, and examples.

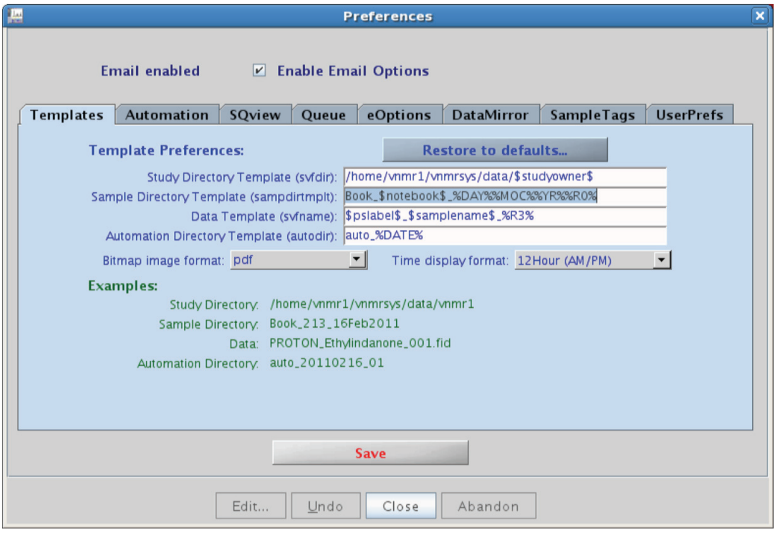
NOTE: The **Study Directory Template** is a path. The three remaining templates are directories and do not contain a path. Any changes done on this window should be saved before exiting the popup by clicking **Save**. If the **Automation Directory Template** is changed, a new automation needs to be started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

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 revision number is suppressed here. The actual FID directory will be saved as <pslabel>_<samplename> with a three digit revision after it.

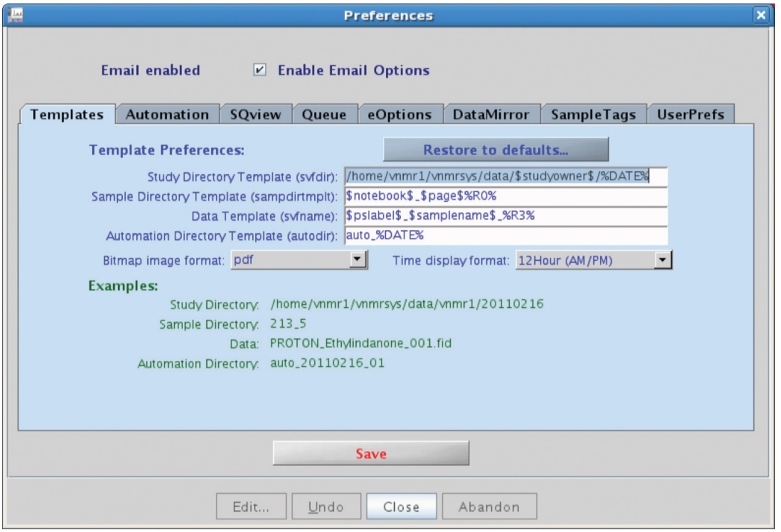
Several other samples templates are shown below:



Fixed text (Book and Page) are included in the Sample Directory Template.



Date in the format of day-month-year is included in the Sample Directory Template.



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

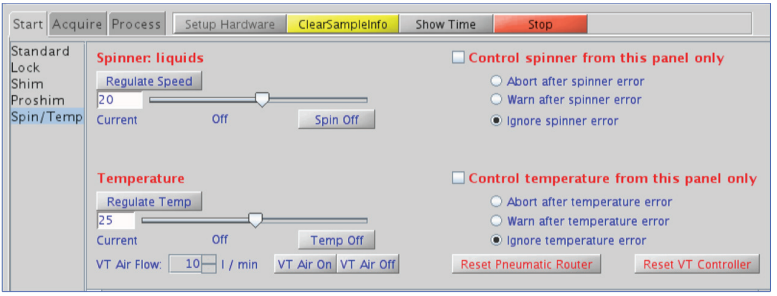
The **UserPrefs** tab allows the account administrator to set up operator options. The account administrator can define the interface personality at the time of operator login from here, as well as the action to be taken after sample submission.

NOTE: The Preferences popup 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 users 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** popup but will not supersede the temperature setting in the **Spin/Temp** panel if "**Control temperature from this panel only"** is selected.



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