## 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.

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## **Starting the VnmrJ Admin Interface**

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

🛅 Vnmrj A	Admin 💶 🗆 🗙
Management UNIX Configure Help	
New User V Save User Show all VJ Users V Find	User Login: nmr1 User Profile Panel -
Users Panel	Home Directory: //home/nmr1
vnmr1 nmr1	Interface Type • Spectroscopy • Imaging LC-NMR/MS
	Show Command Area:  Yes No
Data Directories User Templates	Select Directory Disk Space
New Label Parent Directories Data may be saved in the following parent directories. The Label field is presented as the choice to the user in the \'Data save\' pop-up. It could be the same as the directory name or some descriptive text.	Look In: /  Look In: / Look In: Trap boot Inet Usr dev Opt Var etc proc Vnmr home root libb 4 selinux
ABEL DIRECTORY	File System Panel
Temp         Spin         Lock           26.0 C         0 Hz         94.3	1 00:08:03

### **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.

🖺 Vnmrj A	dmin _ D ×
Management UNIX Configure Help	
New Users (2 or more) Save User Show all VJ Users Vind.	User Login:
	User Name:
	Home Directory:
vnmr 1	
Create/Delete 2 or more users	VnmrJ Operators:
Input File Path://home/vnmr1/2_users.csv	
✓ Use File for User list input	Interface Type Spectroscopy Imaging
Create      Delete	C de-reinging
	AV
·	Select Directory Disk Space
Add Users Cancel	Look In: 🗋 vnmr1 💌 🖬 🛱 🖬 🔡 🖁
	Desktop
	□ vnmrsys
Data may be saved in the following parent directories. The Label field i presented as the choice to the user in the \"Data save\" pop-up. It cou	
be the same as the directory name or some descriptive text.	
Private Suserdir/data	
K 1	R Batar Directory
Temp Spin Lock	

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.

Reset Operators' I	Password
VnmrJ Operators:	
OK Cancel	Help

#### **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.

-		Modify	Operators			×
Modify Operato	rs 🛛 Delete Operato	nr -				
Operator	Email	Panel Level	Full Name	Show Command	Profile Name	
James	10			no	AllLiquids	
jarrett	10			no	AllLiquids 🔻	=
jfarias	30			Yes	AllImaging	$\mathbf{H}$
mario	30			Y45	BasicLiquids	
nmr 1	30			yes	mybasic	-
		ок Са	ncel 🛛 🖽	Ip	CommonLiquio AllSolids BasicLiquidsSe	

# 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.

Printer configuration - localhost							
<u>File E</u> dit <u>H</u> elp							
New Printer	s Copy Delete Goto Server Refresh						
Server Settings	Settings Policies Access control Printer Options Job Options						
	Settings						
printer1	Description: printer						
	Location:						
	Device URI: hp:/par/HP_LaserJet_6P?device=/dev/parport0	Change					
	Make and Model: HP LaserJet 6P Foomatic/hpijs (recommended)	Change					
	Printer State: Idle						
	State Default Printer						
	Enabled     Make Default Printer						
	Accepting jobs This is the default printer						
	Shared Print Test Page						
	- The least age						
	(B) nevert						
	Revert	<u>Арріу</u>					
Connected to localhost							

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.

🥑 Administrat	ion - CUPS 1.3.7 - Mozilia Firefox	_ <b> </b>
<u>File Edit View History Bookmarks</u> Tools <u>H</u> elp		
💠 💠 🔹 🏟 🙁 🏫 🕑 http://localhost:631/admin	n 🔂 🔹 Google	
🛅 Most Visited 🔻 🦏 Red Hat 💐 Red Hat Magazine 💐 Red H	lat Network 🛛 🤜 Red Hat Support	
C Administration - CUPS 1.3.7 × Red Hat Enterprise L	inux Ve ×	•
Administration Home Administration Class Printers Add Printer (Find New Printers) Manage Printers)	ses Documentation/Help Jobs Printers Server Edit Configuration File View Access Log View Error Log View Prog Log	€
Classes (Add Class) (Manage Classes) Jobs (Manage jobs)	Basic Server Settings:  Show printers shared by other systems  Allow printing from the Internet  Allow remote administration  Use Kerberos authentication (FAQ) Allow users to cancel any job (not just their own) Save debugging information for troubleshooting  Change Settings	
Done		

#### 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.

		VNMR Plotter Configuration
VNMR Device Name	Linux Printer Name	
new_plotter	printer1	drawable area
		Paper Size:         Letter         Width:         215.0         (mm) Height:         279.0         (mm)           Output Format:         POSTSCRIPT         Resolution:         300         (dots per inch)         (dots per inch)           Dicom Printer Host:         Dicom Printer Port:         Dicom Printer Port:         Dicom Printer Port:         Dicom Printer Port:
		Orientation         Paper Margins         Spectrum Area <ul> <li>Portrait</li> <li>L4f (mm)</li> <li>Right (mm)</li> <li>Vernax max (mm)</li> <li>Sector</li> <li>Top (mm)</li> <li>Bottom (mm)</li> <li>14.5</li> <li>14.5</li> <li>14.5</li> <li>Sector</li> <li>No (2maxmax (mm))</li> <li>186.0</li> <li>Sector</li> </ul> <li>Sector</li> <li>Sector</li> <li>Sector</li> <li>Sector</li> <li>Sector</li>
Add new device Delete sele	cted Reset to origin	Reset to default Close Abandon

- 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 <u>ALL</u> changes, click <u>Abandon</u>.

### 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.
- 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.)

<u></u>	applabone4(	00.csb.varianinc.com Co	nfiguration	×
System	Spectrometer 💌	Sample Changer	None	•
Proton Frequency	400 💌	Sample Changer Port	None	•
VT Controller	Present 💌	Shim Set	Varian 28 Shims	•
X Axis Gradient	Not Present	Number of Receivers	1	•
Y Axis Gradient	Not Present 💌	Receiver Configuration	Single Receiver	•
Z Axis Gradient	Performa I 🔹	Lock Frequency	61.3655	-
System Gradient Coil	None	ProTune	Present	<b>_</b>
Number of RF Channels	2	СгуоВау	Not Present	•
PFG board	Present 👻	VT Flow Range	0 to 50	•
		Cryogen Monitor	None	•
RF Channel	1 (Obs) 2 (Dec)			
Synthesizer	Direct Digital II 🖃 Direct D	Digital II 💌		
Maximum Power	63 63			
Type of Linear Amplifier	Full Band 🗾 Full Ban	d 💌		
	O	Cancel <u>H</u> elp		

# 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<sub>2</sub>O 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.
- 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.
- 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 directory.

- 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 **Ik** 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**

<b>P</b>		Preferences			×
Email enabled	🕑 Enable En	nail Options			
Templates Automation	SQview Queue	eOptions	DataMirror	SampleTags	UserPrefs
Template Preference	es:	Re	store to defau	ilts	
Study Director	y Template (svfdir):	/home/vnmr1/vr	mrsys/data/\$stu	dyowner\$	
Sample Directory Temp	late (sampdirtmplt):	<pre>\$notebook\$_\$pa</pre>	ge\$%R0%		_
Data 1 Automation Directory	Template (svfname):	spsiabels_ssam auto_%DATE%	olename\$_%R3%		_
Ritman image format:	pdf	Time dis	play format: 12F	four (AM /PM)	-
Examples:					
Study Dire	ectory: /home/vnmr:	L/vnmrsys/data/v	mmr1		
Sample Dire	actory: 213_5				
Automation Dire	Data: PROTON_Eth	/indanone_001.f	d		
Automation Dire	2001y. auto_201102	10_01			
		Save			
	Edit <u>U</u> ndo	Close	Abandon		

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: Spslabel\$), 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 <<u>notebook>\_<page></u>, 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 <<u>pslabel>\_<samplename></u> with a three digit revision after it. Several other samples templates are shown below:

			P	references			
	Email enabled	🗹 Er	nable Ema	il Options			
Templat	Automation	SQview	Queue	eOptions	DataMirro	r SampleTags	UserPrefs
	Template Preferen	ces:		Re	store to de	faults	
	Study Direct	ory Template	(svfdir): //	iome/vnmr1/vr	mrsys/data/\$	studyowner\$	_
	Sample Directory Tem	plate (sampo	lirtmplt): Bo	ok_\$notebook	\$_Page_\$page	\$%R0%	_
	Data Automation Director	v Template (s v Template (	autodir): au	ito_%DATE%	piename\$_%K	576	_
	Bitmap image forma	t: pdf	-	Time dis	play format:	L2Hour (AM/PM)	-
	Examples:						
	Study Di	rectory: /ho	me/vnmr1/	vnmrsys/data/v	/nmr1		
	Sample Di	Data: PRC	K_213_Page	2_5 ndanone 001 f	id		
	Automation Di	rectory: auto	2011021	6_01			
					-		
Save							
		Edit	<u>U</u> ndo	Close	Abandon		

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

		Pr	eferences			×		
Email enabled 🗹 Enable Email Options								
Templates Automation	SQview	Queue	eOptions	DataMirro	or SampleTags	UserPrefs		
Template Prefere	nces:	a dan Katinga Ub	Re	store to de	faults	_		
Sample Directory Ter	nplate (samp)	dirtmplt): Bo	ok_\$notebook	S_%DAY%%MO	C%%YR%%R0%	_		
Dat	a Template (s	vfname): \$p	slabel\$_\$sam	plename\$_%R	3%	_		
Automation Directo	ory Template	(autodir): au	to_%DATE%					
Bitmap image form	at: pdf	-	Time dis	play format:	12Hour (AM/PM)	•		
Examples:								
Study D	irectory. /ho	me/vnmr1/\	mmrsys/data/v	/nmr1				
Sample D	Deter BOC	K_213_16Fe	b2011	La .				
Automation	Data: FRG	o 20110216	5 01	iu -				
Automation E	mectory, aut	0_20110210	/_01					
		ş	Save					
	Edit	<u>U</u> ndo	Close	Abandon				

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

Preferences							
Email enabled 🕑 Enable Email Options							
Templates	Automation	SQview	Queue	eOptions	DataMirror	SampleTags	UserPrefs
Template Preferences: Restore to defaults							
Study Directory Template (svfdir): //home/vnmr1/vnmrsys/data/\$studyowner\$/%DATE%							
Sample Directory Template (sampdirtmplt): \$notebook\$_\$page\$%R0%							
Data Template (svfname): \$pslabel\$_\$samplename\$_%R3%							
А	utomation Director	y Template	(autodir): a	uto_%DATE%			
Bi	tmap image format	pdf		<ul> <li>Time dis</li> </ul>	play format: 121	Hour (AM/PM)	<b>•</b>
Examples:							
Study Directory: /home/vnmr1/vnmrsys/data/vnmr1/20110216							
Sample Directory. 213_5							
Automation Directory auto 20110216 01							
Save							
Edit Undo Close Abandon							

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.

Start Acqu	ire Process Setup Hardware ClearSampleInfo	Show Time Stop			
Standard Lock Shim Proshim Spin/Temp	Spinner: liquids Regulate Speed 20 Current Off Spin Off	Control spinner from this panel only Abort after spinner error Warn after spinner error Ignore spinner error			
	Temperature       Regulate Temp       25       Current       Off       Temp Off       VT Air Flow:       10       I / min       VT Air Off	Control temperature from this panel only Abort after temperature error Warn after temperature error Ignore temperature error Reset Pneumatic Router Reset VT Controller			

## VnmrJ 3 QuickStart Guide

**Administrator Tools** 

#### For more information

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