

# Flexible and Configurable Tools for the System Administrator

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# Flexible and Configurable Tools for the System Administrator

Administering to a large NMR user group can be a difficult and thankless task. Quite often, there is a broad range of experience levels and needs among the users.

At Agilent we have a number of tools in our software to help the System Administrator manage this task.

# Outline

In this seminar we will learn how to:

- Make Automation work the way **you** want it to - Automation Preferences
- Tailor VnmrJ to meet each of your user's needs - the Persona Manager
- Fully customize your push-button NMR experiments - Study Clones
- Maintain and distribute software customizations with ease - Application Directories
- Maintain and update your system's critical calibrations - Probe Autocalibrations
- Apply VnmrJ's flexible and powerful shimming toolset - ProShim

# Outline

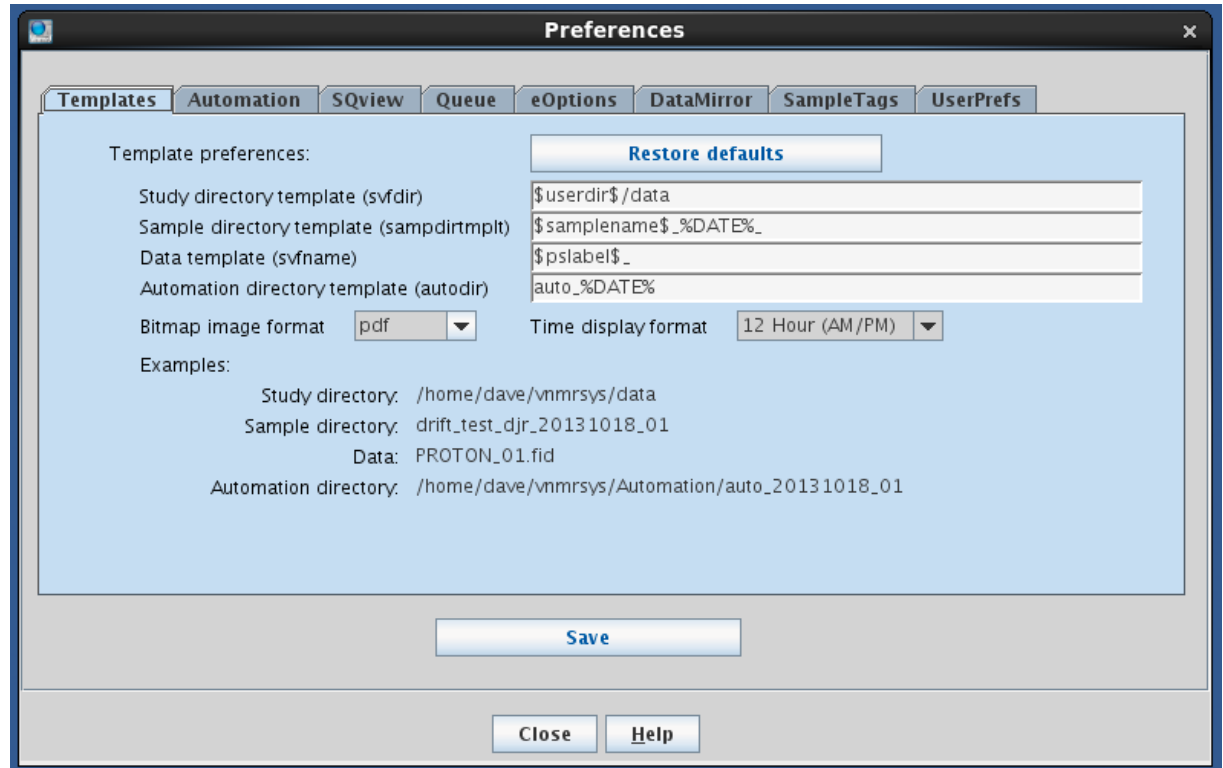
- **Make Automation work the way *you* want it to - Automation Preferences**
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- Fully customize your push-button NMR experiments - Study Clones
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# The Preferences Panels

Have it do what you want, when you want it

The data save templates are critical to the efficient use of the system. They are very flexible and can be used to construct a data archive tree that is constructed automatically.

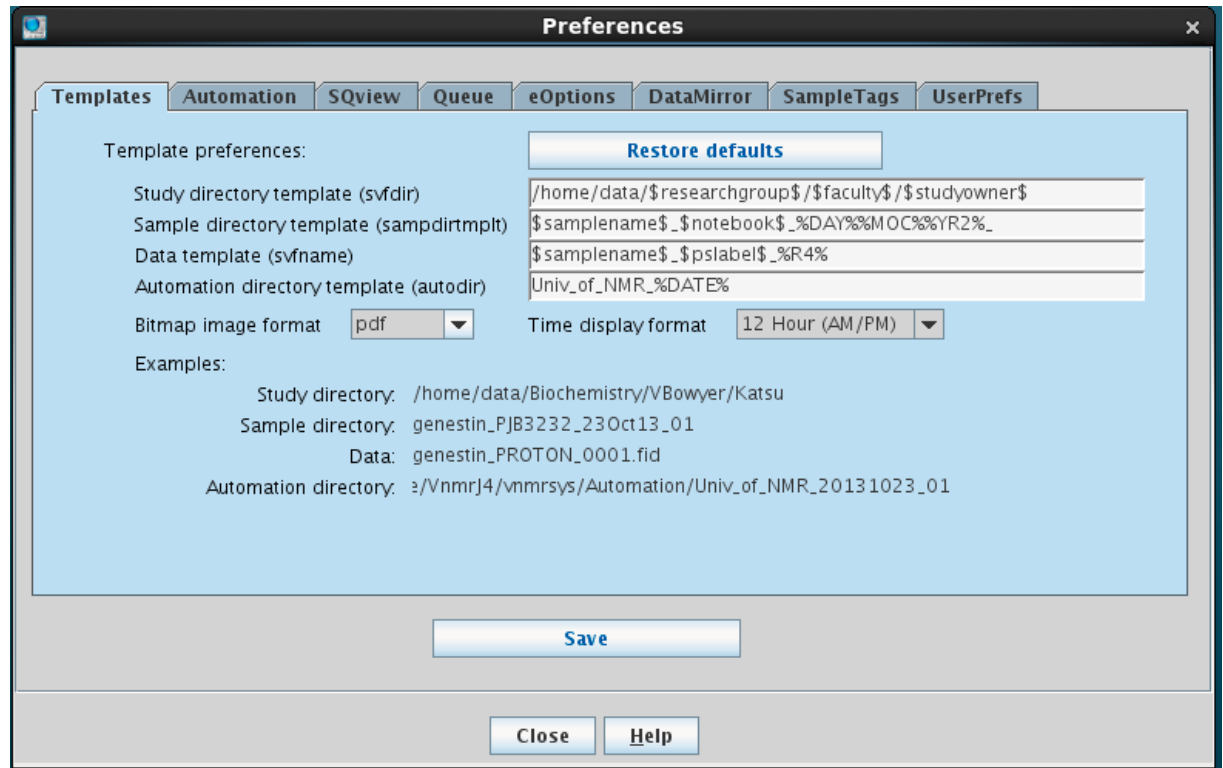
This is the default template. It is valid and does work, but...



# The Preferences Panels

Have it do what you want, when you want it

This is an example of a more useful template. The flexibility is tremendous, meaning your data tree can be easily customized for your particular user's needs.



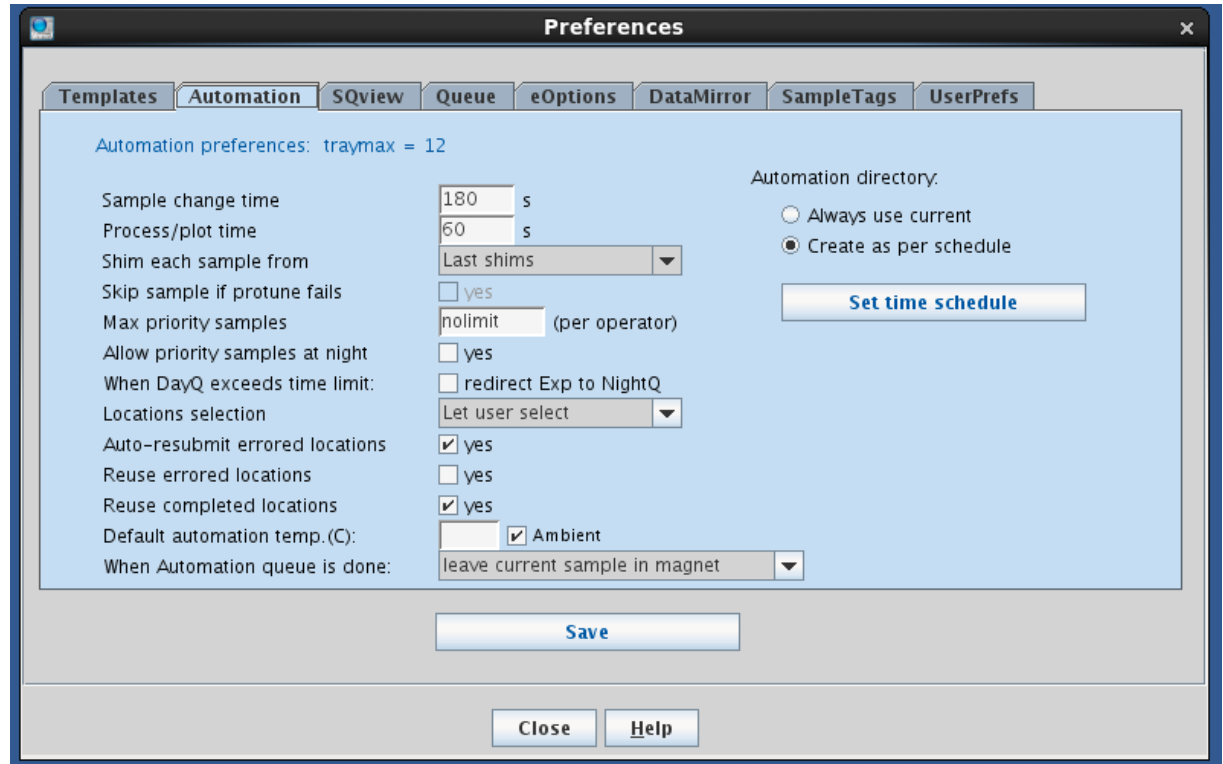
# The Preferences Panels

Have it do what you want, when you want it

The Automation tab contains default values and behaviors that influence exactly how the system operates.

In a multi-user environment, preferences that reset the system for every sample are often a good choice.

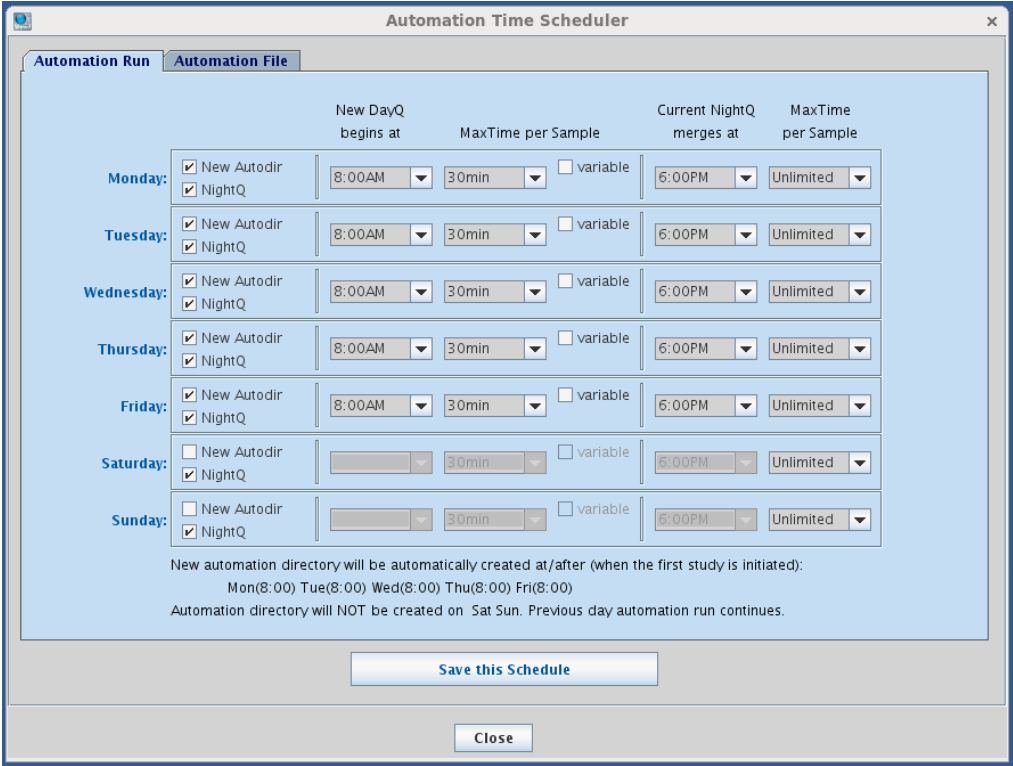
Other preferences are used to control how much freedom users are allowed.



# The Preferences Panels

## Have it do what you want, when you want it

The Time Scheduler is very powerful and allows the account owner to control the robot queue with high resolution.

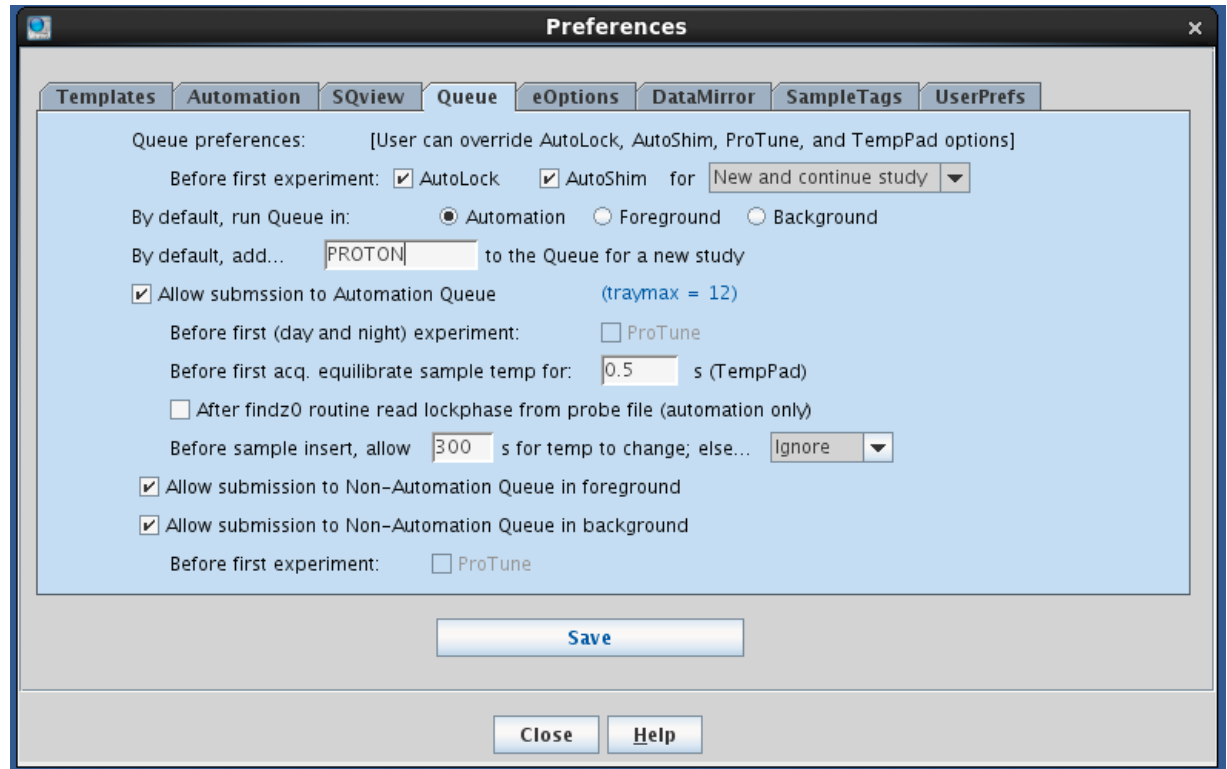


# The Preferences Panels

Have it do what you want, when you want it

The Queue tab contains items that are set as default values for every Study. These values can always be changed by the user when they submit a sample.

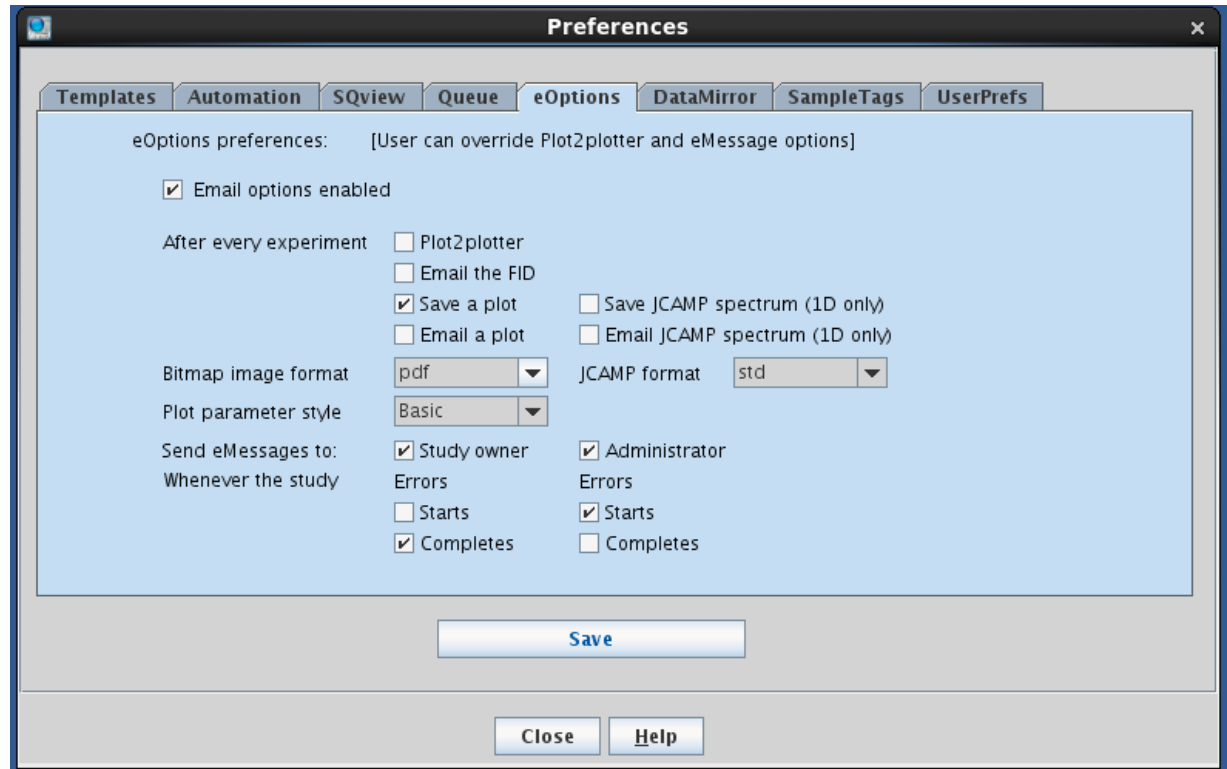
A default experiment saves users from having to select a basic experiment for every sample, and it allows the Express Submit tool to function.



# The Preferences Panels

Have it do what you want, when you want it

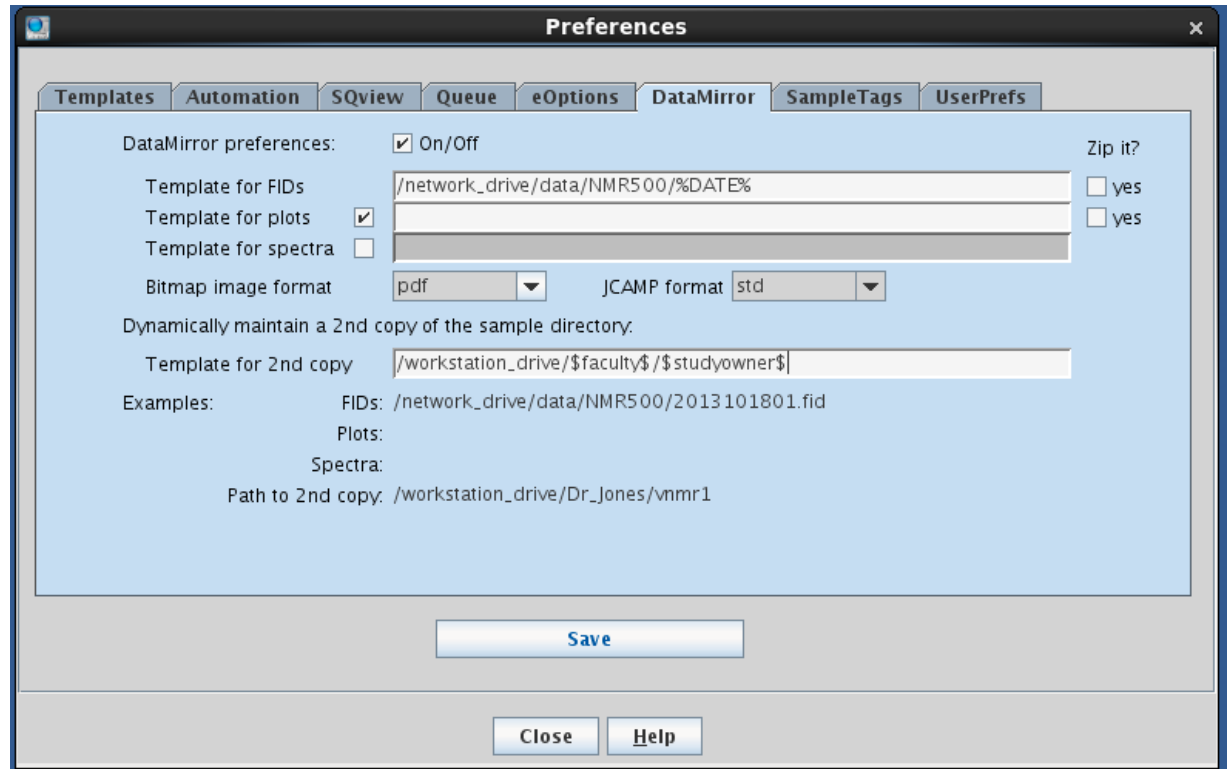
The eOptions tab is exactly that; it sets up the email and the electronic file options.



# The Preferences Panels

Have it do what you want, when you want it

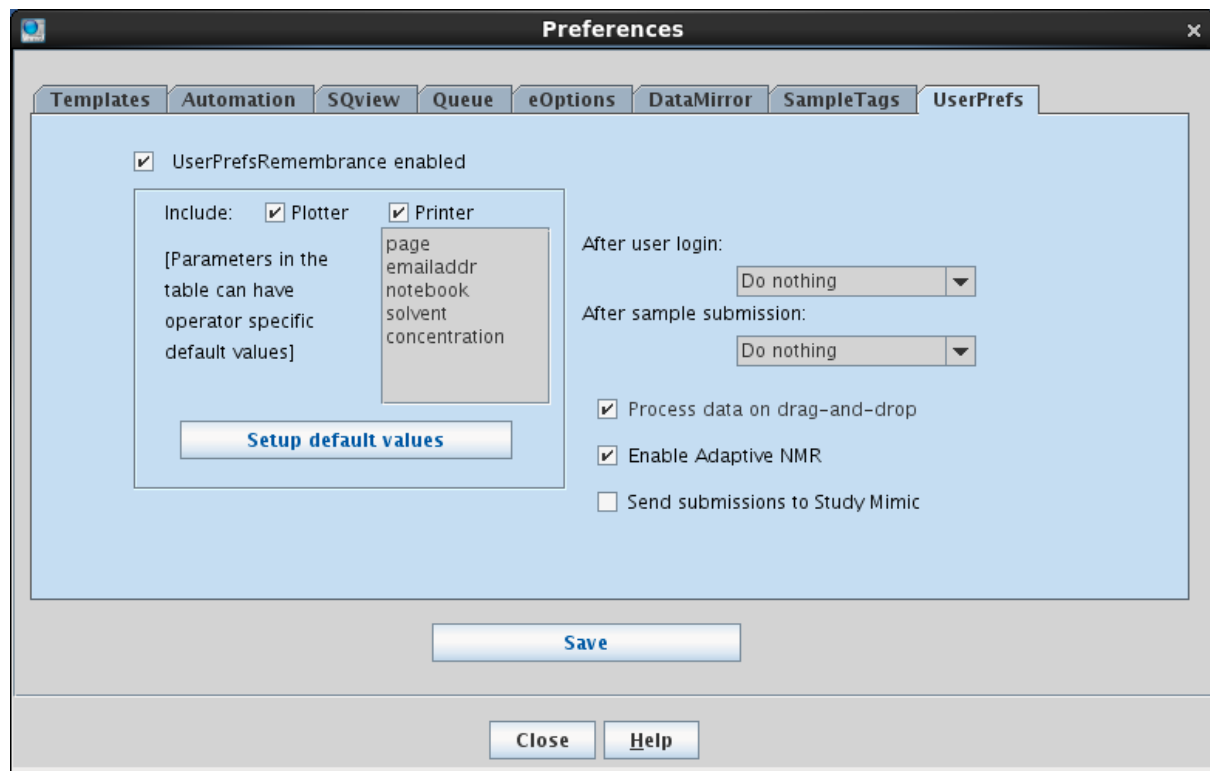
The Data Mirror tab can be used to specify the location of a second copy of the Study directories plus archive versions of plots and spectra.



# The Preferences Panels

Have it do what you want, when you want it

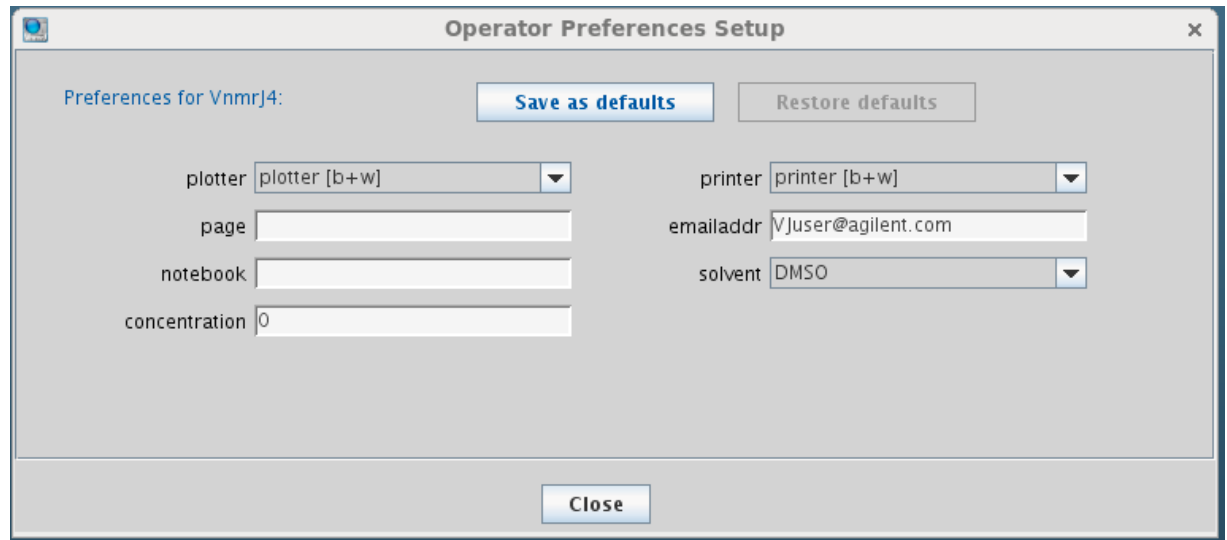
The User Preferences tab controls things like system behavior on log in and log out, plus gives users a place to set default user parameters, such as email address, favorite solvent, and the printer closest to their desk.



# The Preferences Panels

Have it do what you want, when you want it

The User Preferences tab controls things like system behavior on log in and log out, plus gives users a place to set default user parameters, such as email address, favorite solvent, and the printer closest to their desk.



The screenshot shows a dialog box titled "Operator Preferences Setup" with a close button (X) in the top right corner. The main content area is titled "Preferences for Vnmrj4:" and contains two buttons: "Save as defaults" and "Restore defaults". Below these are several input fields:

plotter	plotter [b+w]	printer	printer [b+w]
page		emailaddr	Vjuser@agilent.com
notebook		solvent	DMSO
concentration	0		

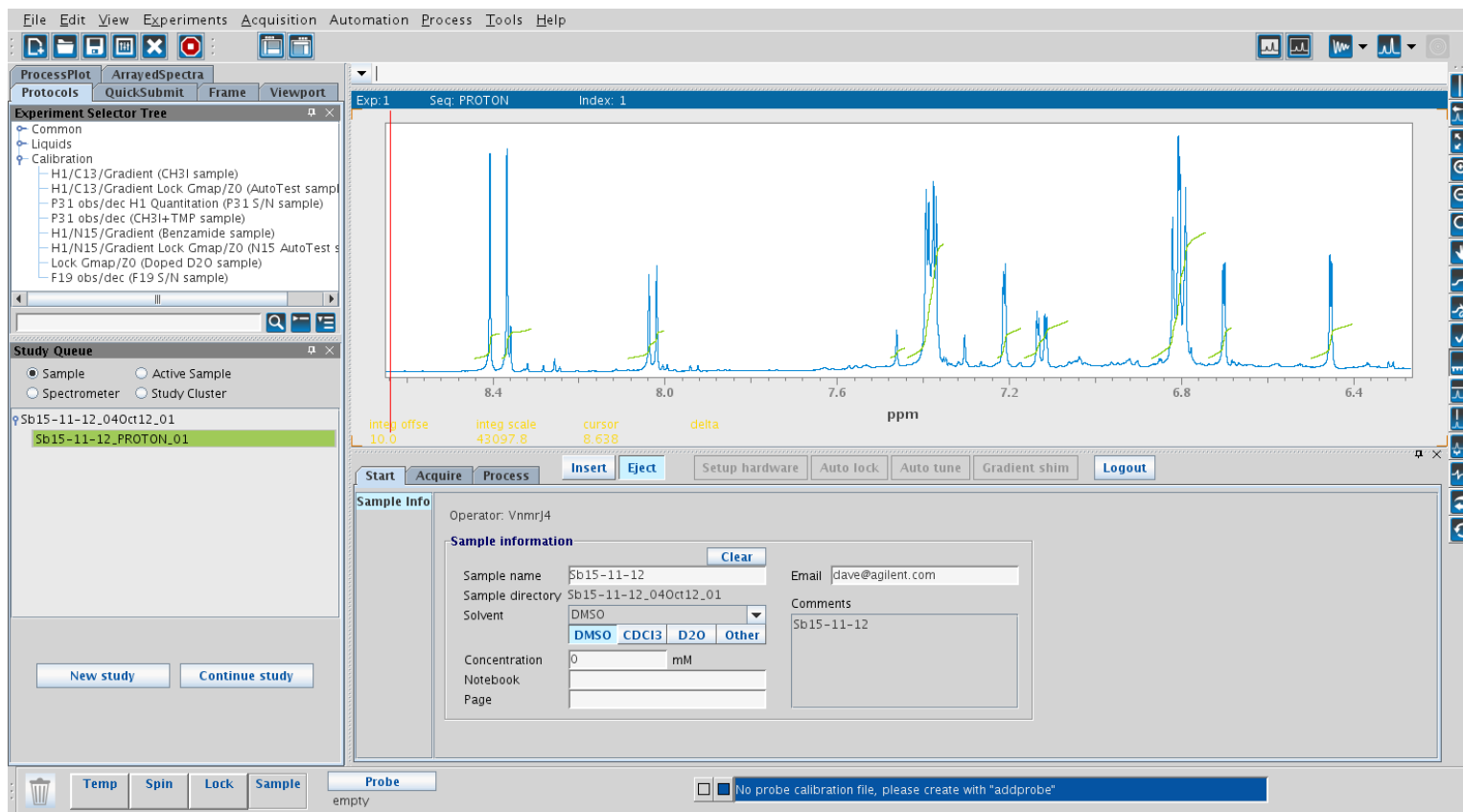
At the bottom center of the dialog box is a "Close" button.

# Outline

:

- Make Automation work the way *you* want it to - Automation Preferences
- **Tailor VnmrJ to meet each of your user's needs - the Persona Manager**
- Fully customize your push-button NMR experiments - Study Clones
- Maintain and distribute software customizations with ease - Application Directories
- Maintain and update your system's critical calibrations - Probe Autocalibrations
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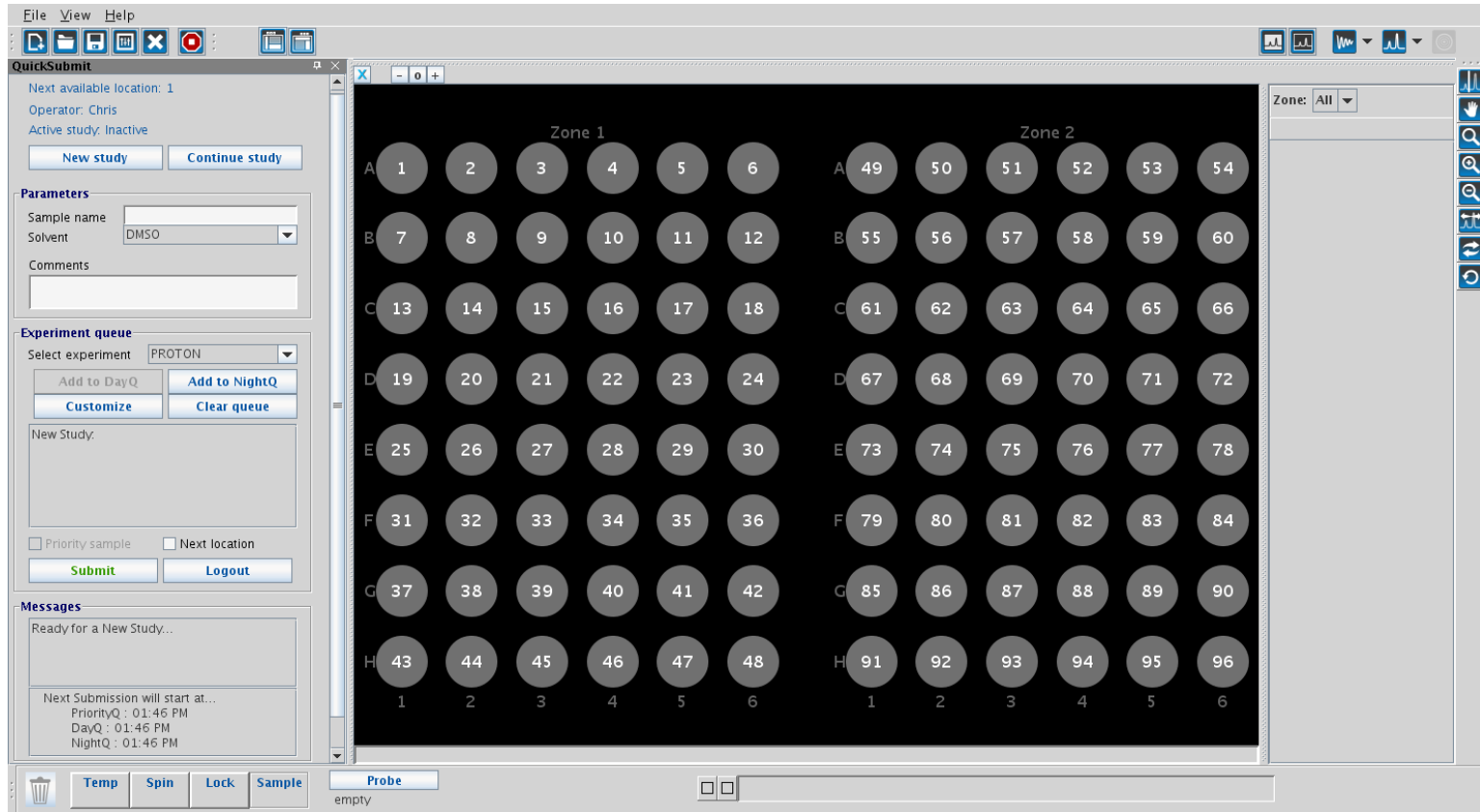
# Persona Manager



The default software interface is very powerful and offers the complete set of tools to the user.

It is also somewhat intimidating when all one wants is a simple proton spectrum.

# Persona Manager

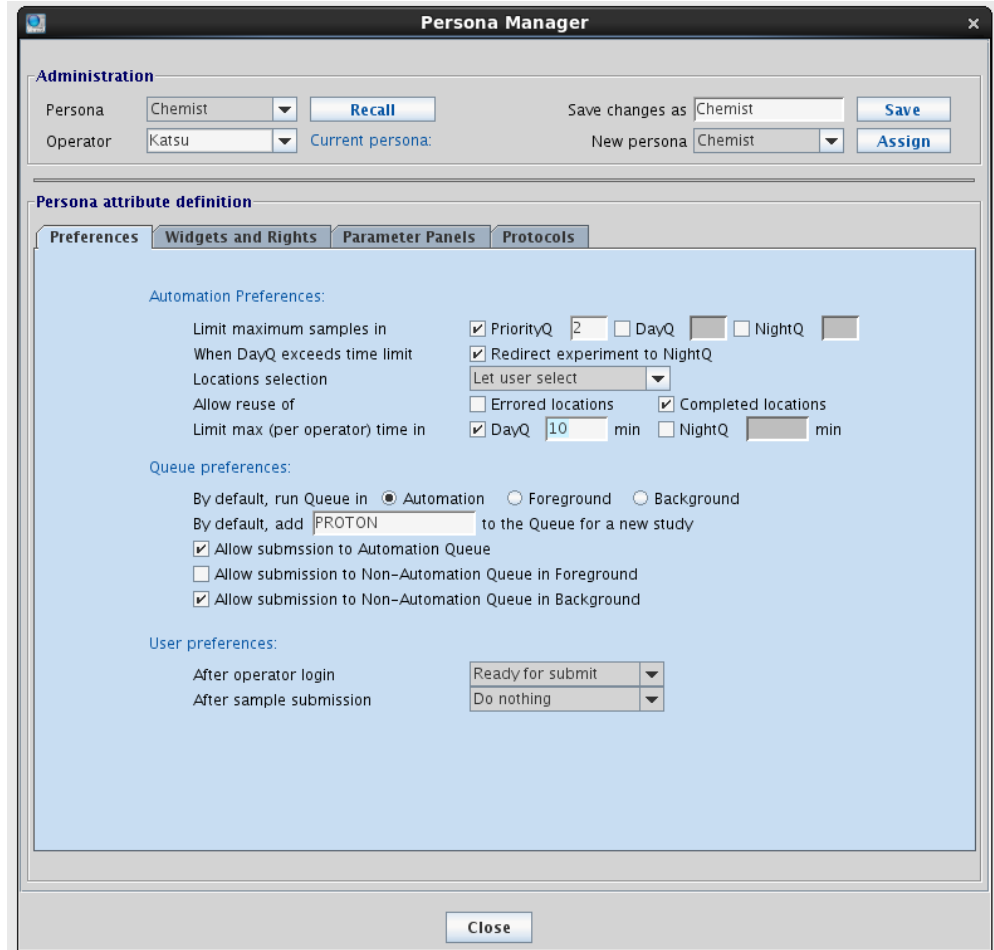


The Persona Manager allows the system to present only those tools any individual user or operator needs, while protecting the system from novice users by hiding operations that they should never perform.

# Persona Manager

Giving every user only the tools that they need.

Each Persona can have a set of customized preferences, making default behaviors specific to individual users.

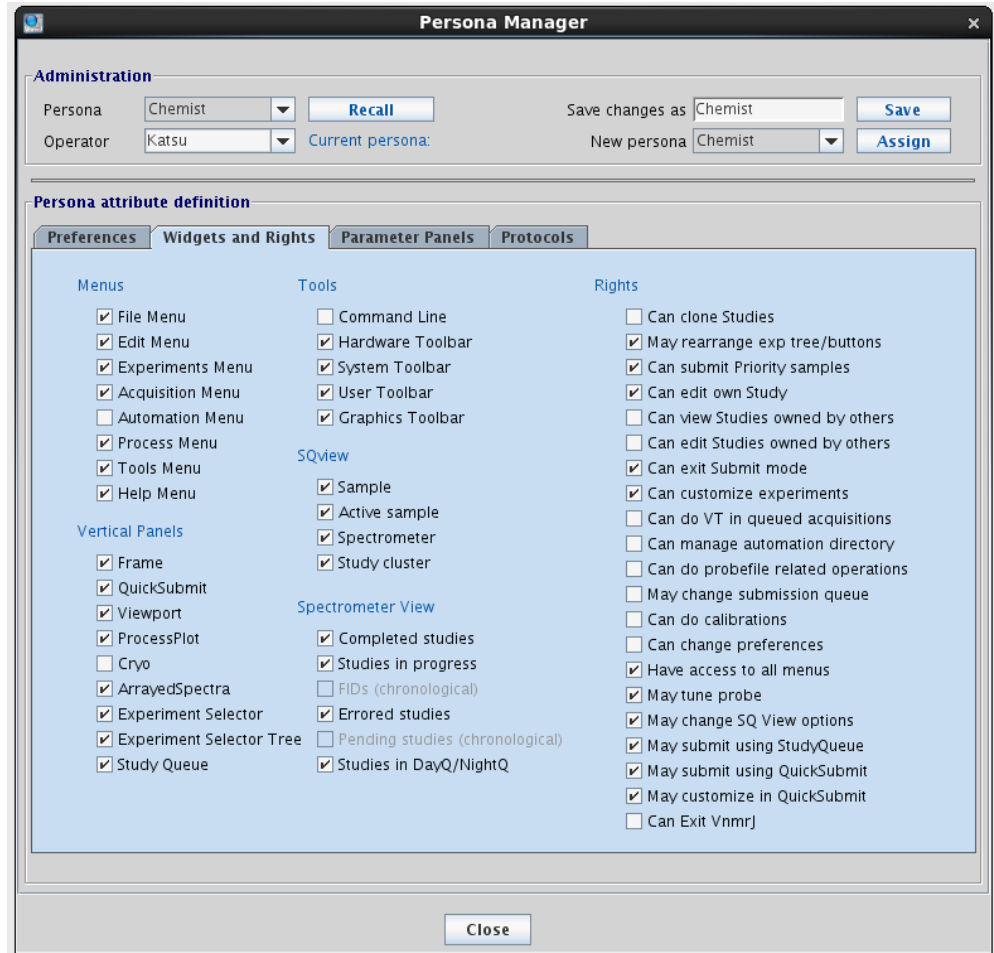


# Persona Manager

Giving every user only the tools that they need.

Each Persona can have a set of widgets and rights, allowing specific tools and actions to be either displayed or hidden.

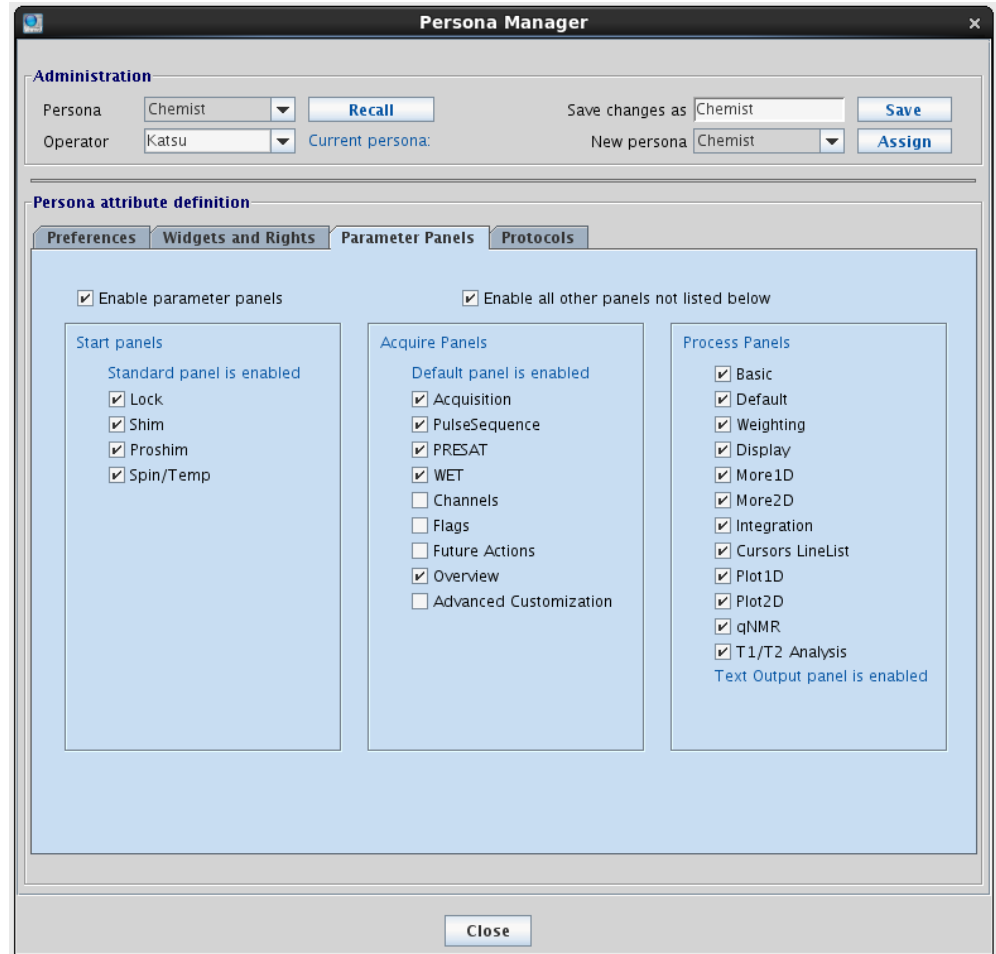
There is a high level of granularity for these actions.



# Persona Manager

Giving every user only the tools that they need.

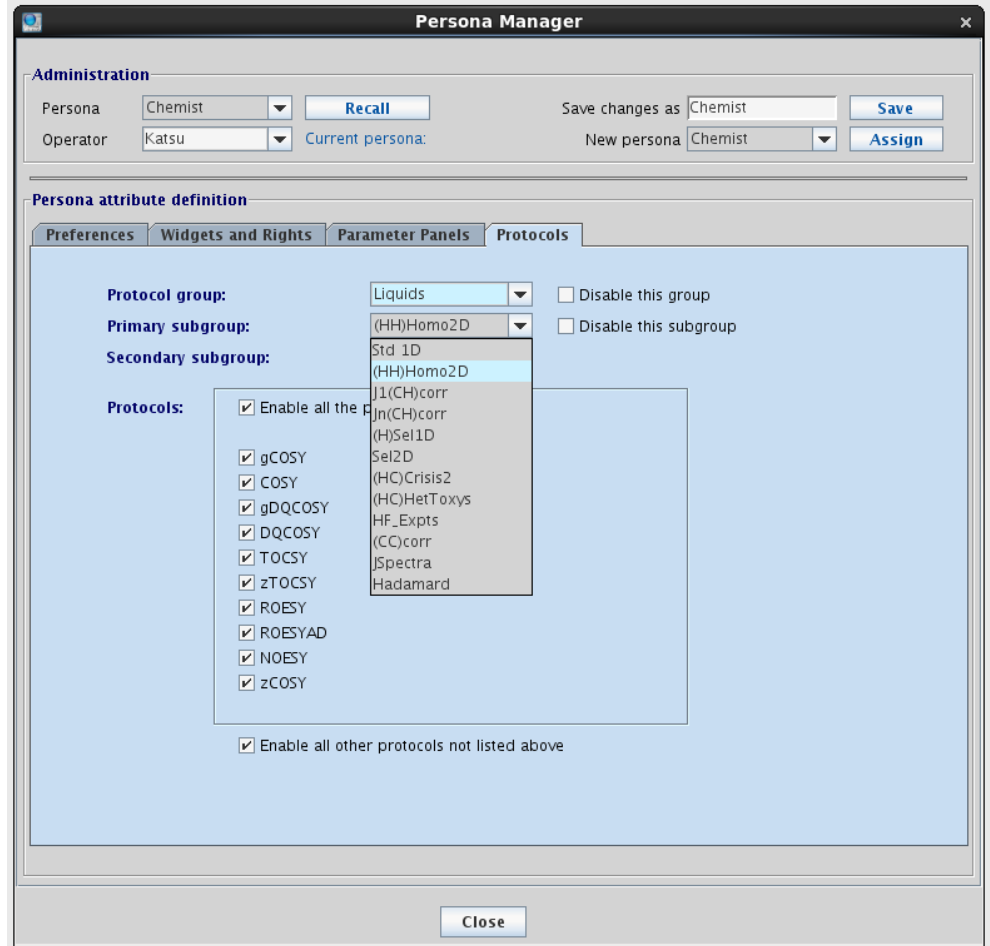
Each Persona can have a set of allowed and forbidden panels, greatly simplifying the interface while preventing novice users from typing in poor parameter choices.



# Persona Manager

Giving every user only the tools that they need.

While VnmrJ comes with several hundred pulse sequence choices, not every users really needs to run them all. Persona Manager can control the Experiment Selector by enabling and disabling protocols, both individually and by groups and families.

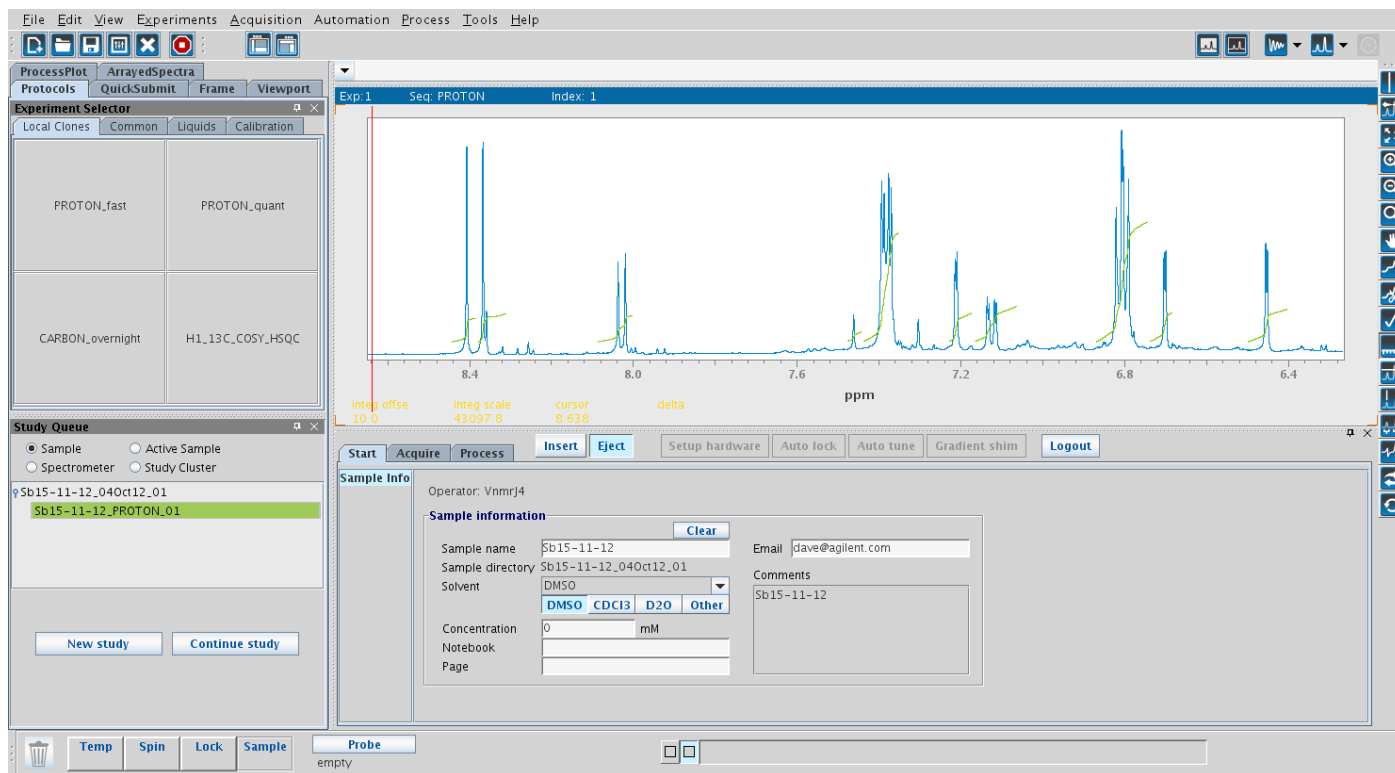


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# Study Clones

A button for every occasion



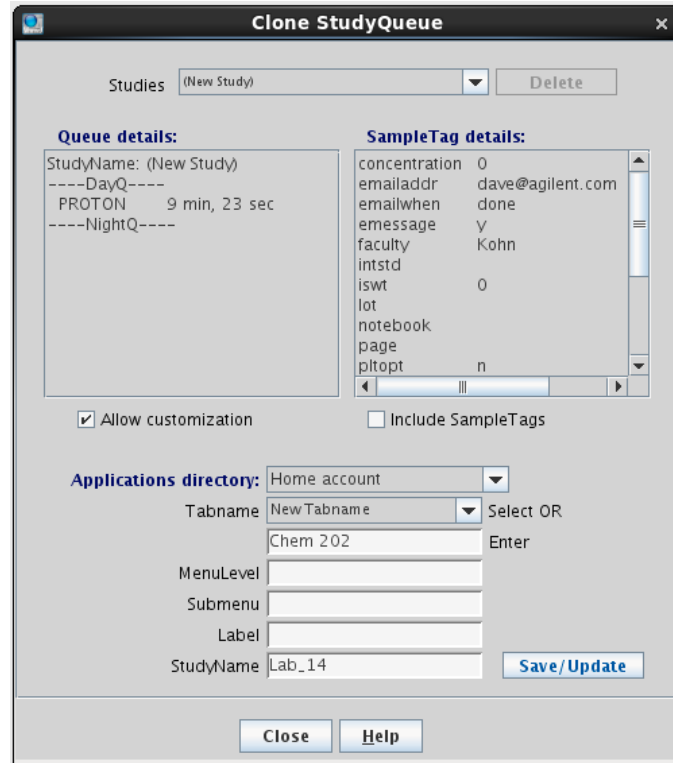
Study Clones allow a simple, fast way to customize the Experiment Selector to contain the experiments you want with exactly the parameters and behaviors you want.

# Study Clones

A button for every occasion

The Study Clone popup allows you to create exactly what you want in a study, then name it something that anyone can recognize and use.

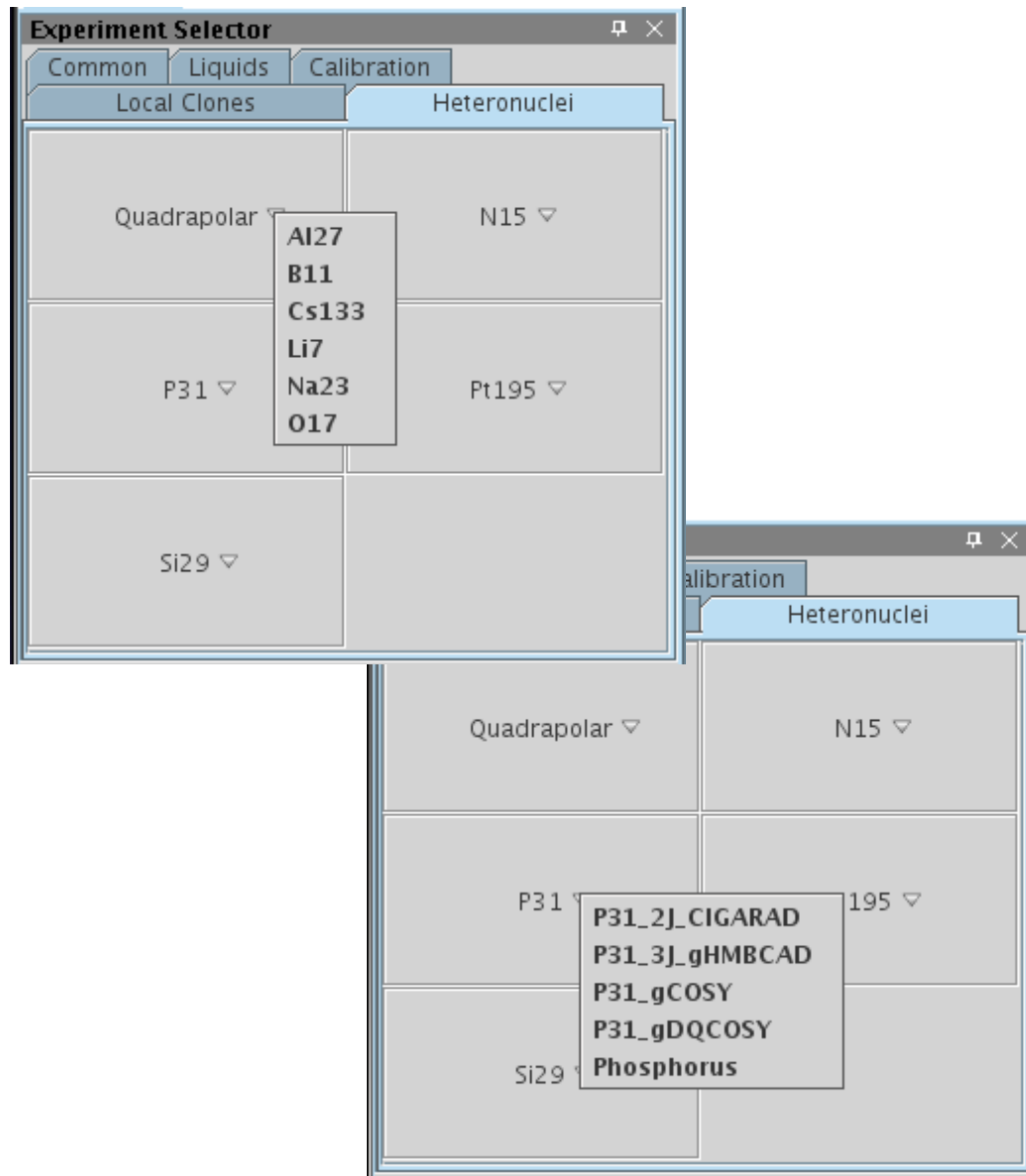
Study Clones can consist of just one experiment, or a collection of experiments, and they can have customized processing and plotting actions associated with them.



# Study Clones

A button for every occasion

These clones were created by an administrator at a university to satisfy demand from the user base.



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# Application Directories

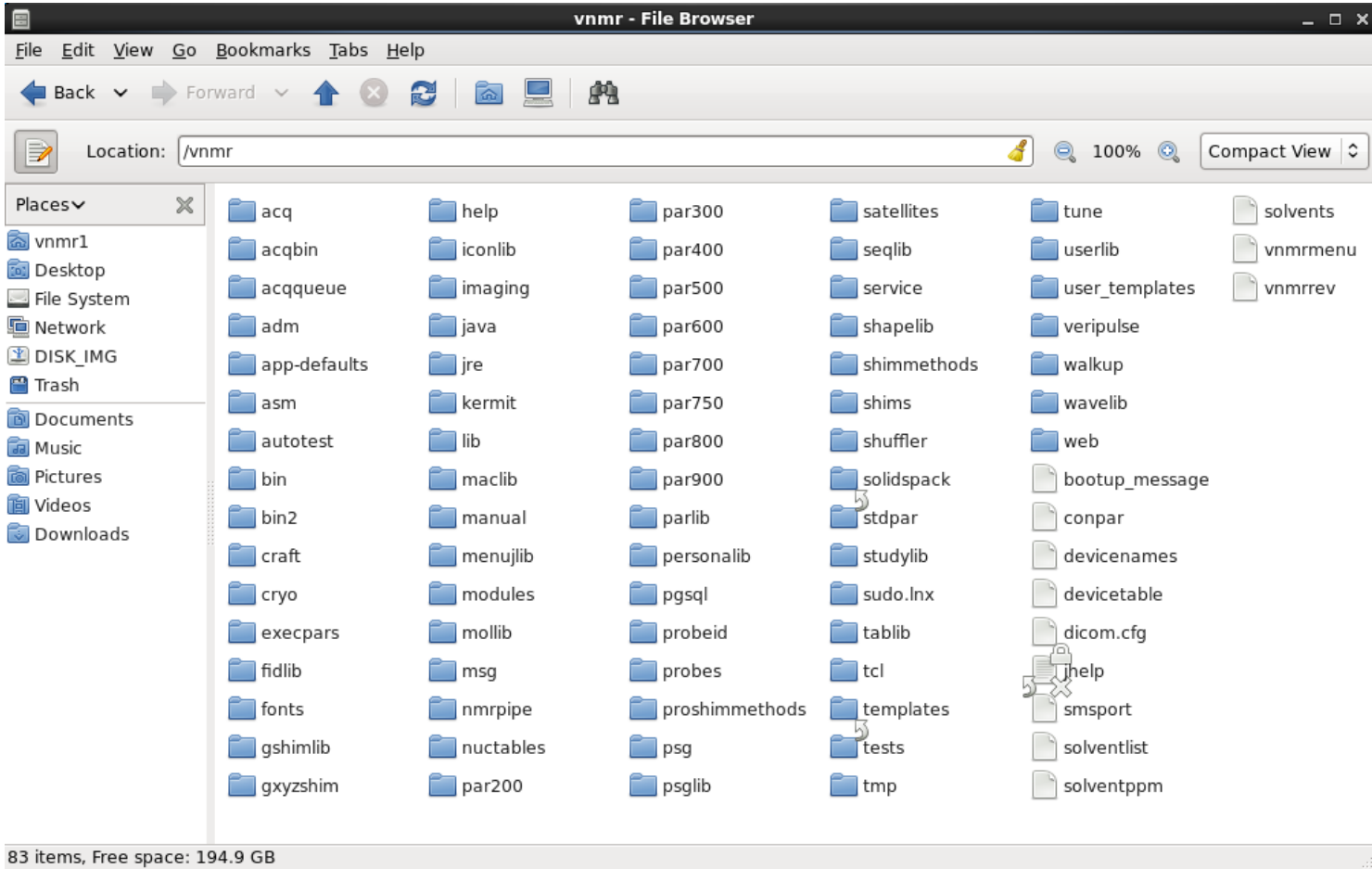
Maintain and distribute software customizations with ease

What exactly is an “Application Directory” (appdir)?

A folder that contains files that “stuff” like parameters, pulse sequences, probe files that VnmrJ can use

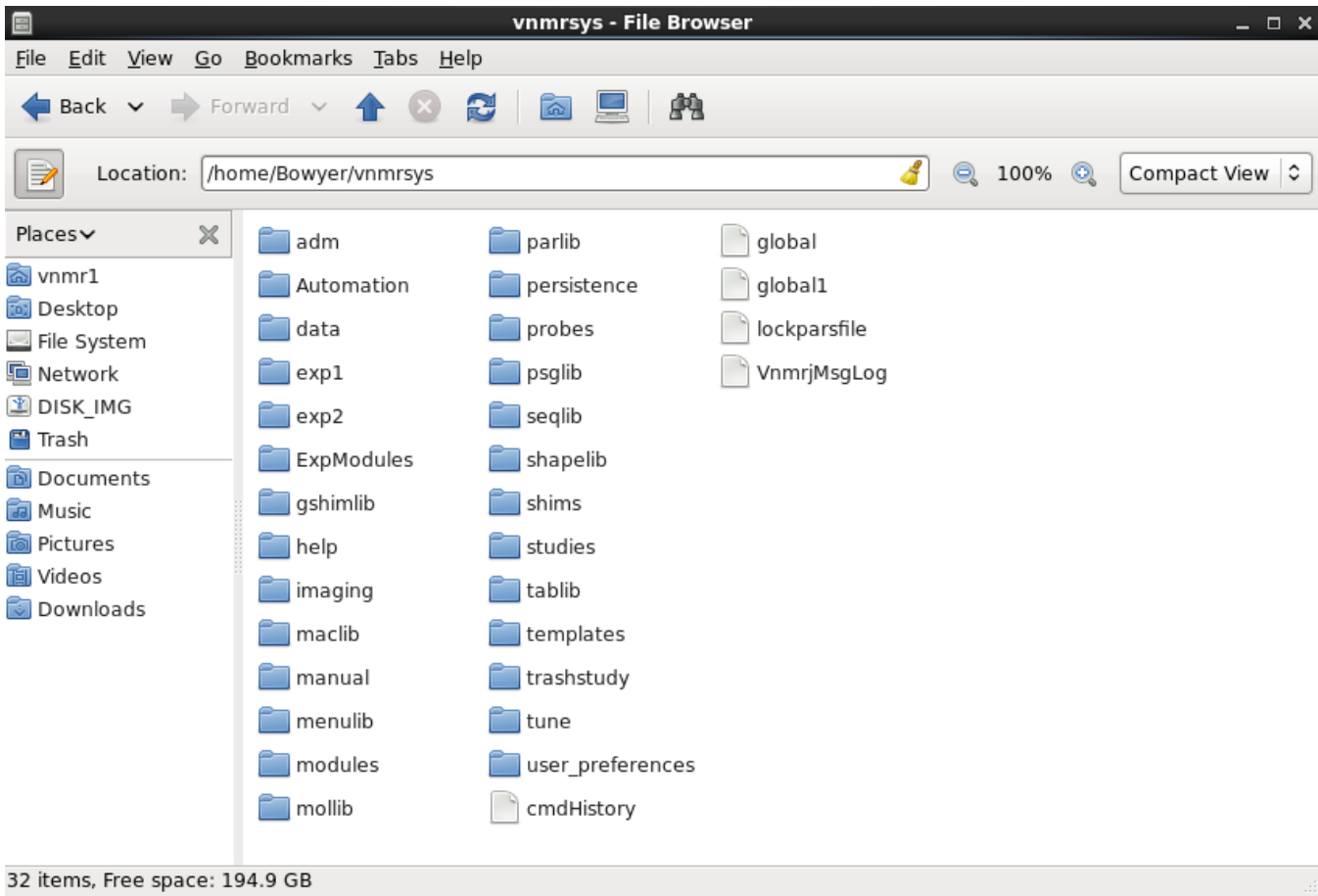
# System Application Directory

VnmrJ installed into a folder linked to by /vnmr



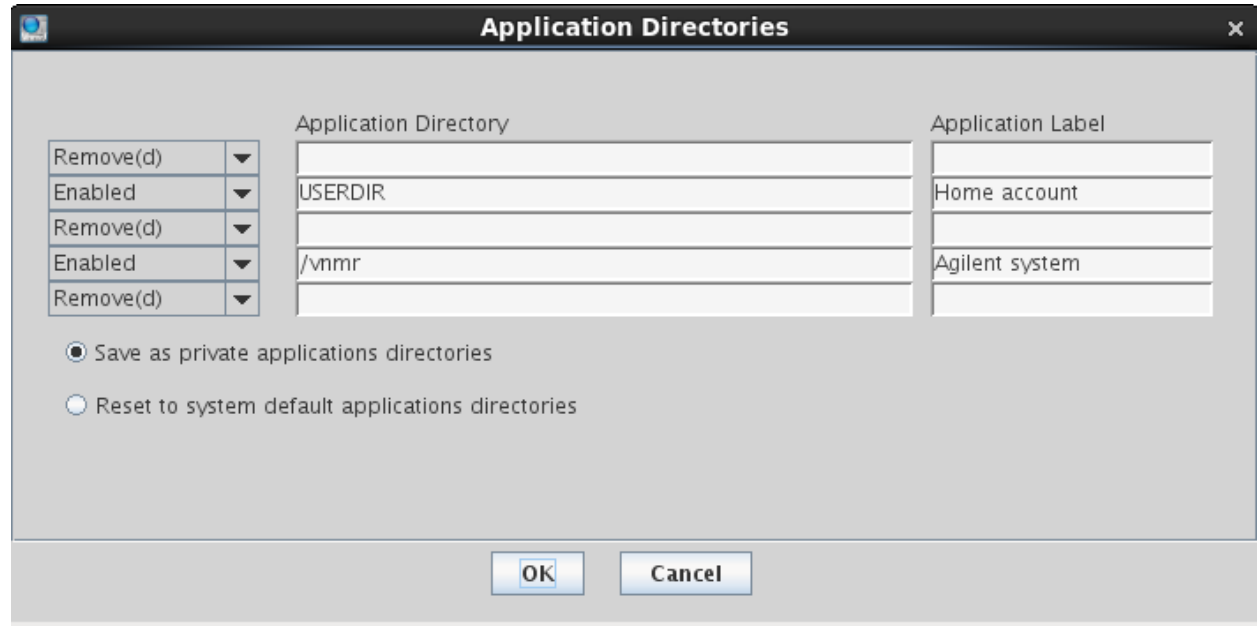
# vnmrsys Application Directory (USERDIR)

The home directory of each user account MUST contain a vnmrsys directory



# Application Directory Searching

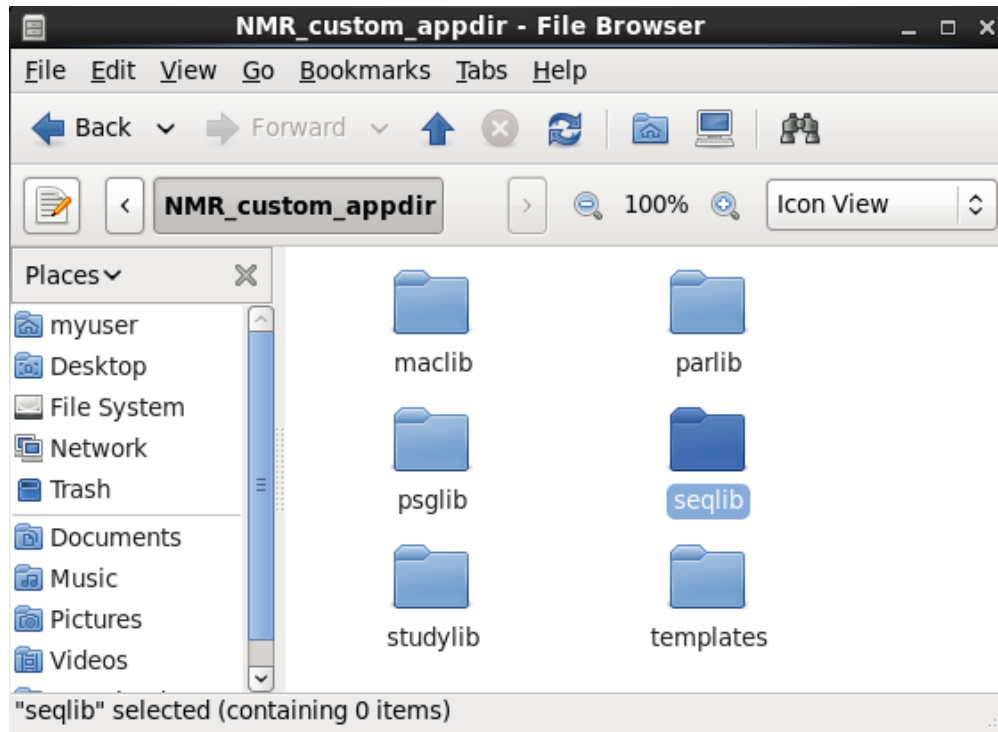
Whenever a “file” request is executed, such as a call to a macro, VnmrJ searches through the list of Application Directories to find a “match”. The first “file” that matches is the one that’s used.



# Adding an Application Directory

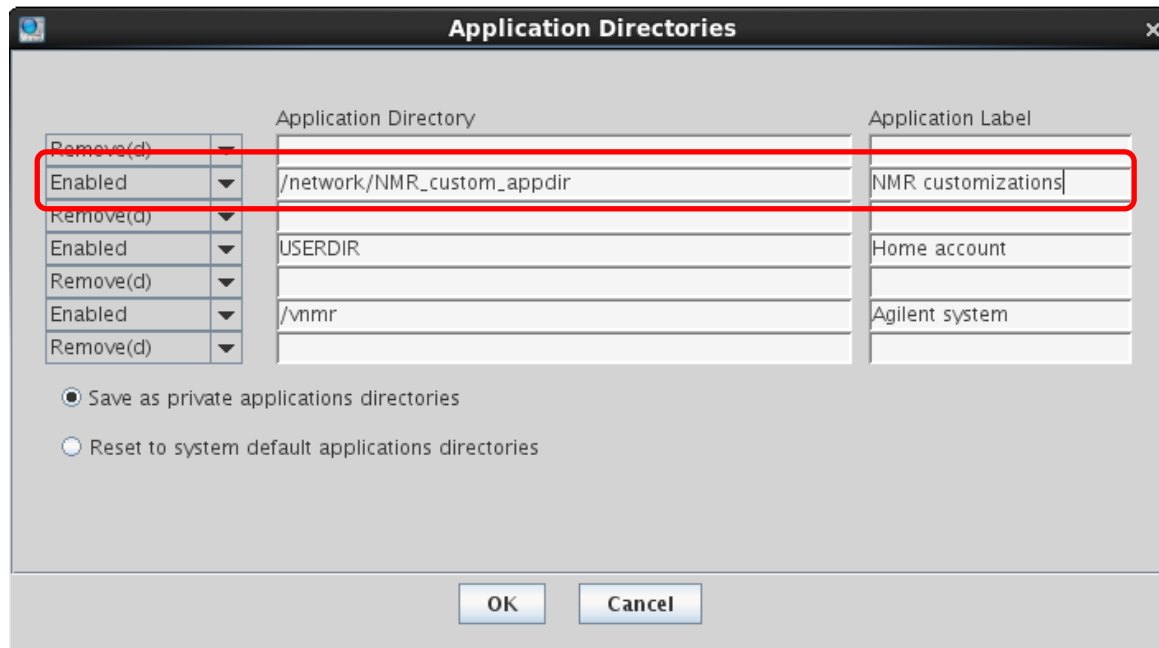
Suppose we had a collection of files (e.g. pulse sequences, setup macros, and so on) that we would like to be made available on one or more NMR systems

Simply place the files in appropriate folder according to VnmrJ “rules” (e.g. macros in a folder called maclib)



# Adding an Application Directory

Now “link in” the folder to VnmrJ in the “Application Directories” popup window



Putting Application Directory folder on a network drive means a centralized set of customizations can be accessed and used by several instruments – easier to maintain 😊

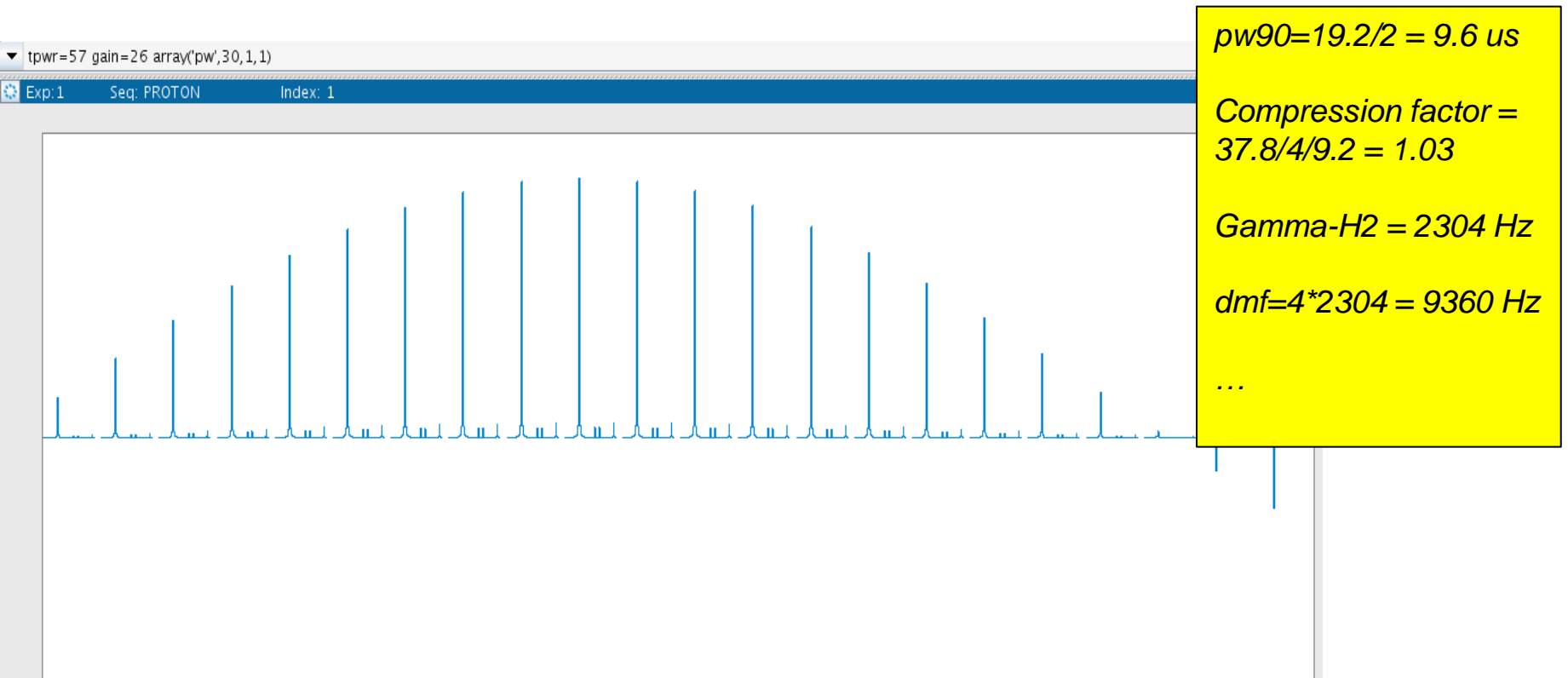
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# Manual Probe Calibrations

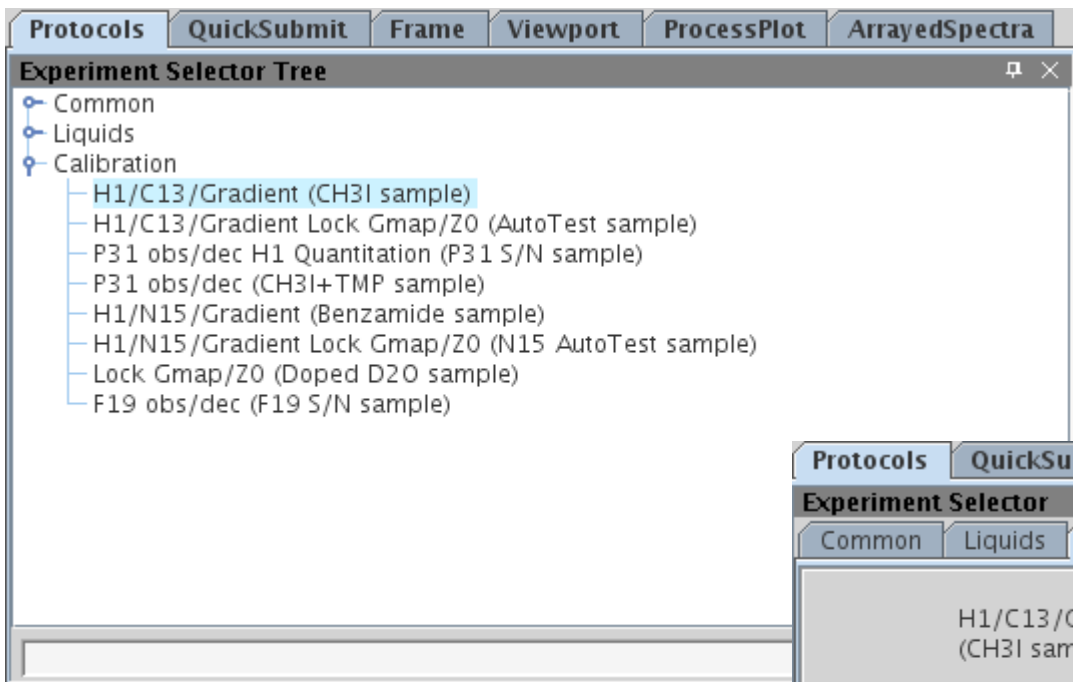
Setting up and iterating parameter values, interpreting and calculating results “by hand”

Requires detailed “spectroscopist-level” knowledge of NMR and VnmrJ



# VnmrJ Autocalibrations

Autocalibrations from Experiment Selector (Tree).



Common	Liquids	Calibration
H1/C13/Gradient (CH3I sample)	H1/C13/Gradient Lock Gmap/Z0 (AutoTest sample)	
P31 obs/dec H1 Quantitation (P31 S/N sample)	P31 obs/dec (CH3I+TMP sample)	
H1/N15/Gradient (Benzamide sample)	H1/N15/Gradient Lock Gmap/Z0 (N15 AutoTest sample)	
Lock Gmap/Z0 (Doped D2O sample)	F19 obs/dec (F19 S/N sample)	

Standard samples shown in parentheses

# Autocalibrations in the Study Queue

Drag calibration into Study Queue, then select specific calibrations and set targets

Locking, tuning and shimming done automatically

The screenshot displays the Agilent software interface for setting up an experiment. The **Experiment Selector Tree** on the left shows a hierarchy: Common > Liquids > Calibration. Under Calibration, the item **H1/C13/Gradient (CH3I sample)** is highlighted with a red box. A red arrow points from this item down to the **Study Queue** window. In the Study Queue, the item **CH3I\_calibration\_001\_day [10:00]** is highlighted with a red box. Another red arrow points from this item to the **CH31 Overview** panel. The CH31 Overview panel shows the following configuration:

- Experiment: calibrate Solvent: cdc13 Observe: H1 Decoupler: C13
- Acquisition Options**
  - Use the ID#1 (CH3) sample**
  - H1 Observe [pw90 Target (μs)] 10
  - C13 Decouple [pwx90 Target (μs)] 10
  - C/H gradient ratio
  - Gradient G/cm/dac
  - C13 Observe [pw90 Target (μs)] 10
  - H1 Decouple [pp90 Target (μs)] 10
- After calibration:
  - Record pw(x) nutation and decoupling profiles
- Receiver Gain (dB)** 10
  - Print probefile?
  - Plot results?
- Before calibration:  Re-shim
- Samplename: Vj41probe\_calib

# Autocalibrations in the Study Queue

Study Queue

Sample     Active Sample  
 Spectrometer     Study Cluster    Options

Completed Studies (5 Samples)

- loc5\_VJ4final probe\_3Dshim
- loc1\_VJ4final z0gmap\_calib
- loc1\_VJ4final H1pw90Cal
  - AutoTest\_calibration\_PROTON\_01
  - H1\_observe\_tpwr54\_pw90\_01
  - H1\_observe\_tpwr60\_pw90\_01
  - H1\_observe\_tpwr60\_5\_pw90\_01
  - H1\_observe\_tpwr60\_5\_pw360\_01
  - H1\_observe\_tpwr60\_5\_pw360\_02
  - H1\_observe\_tpwr48\_5\_pw360\_01
  - H1\_observe\_tpwr48\_5\_pw360\_02**
  - H1\_observe\_pw90\_RFhomo\_01
- loc1\_VJ4final probe\_N15\_calibrate
- loc1\_VJ4final AutoTest

Studies in progress (0 Samples)

Tray: auto\_20131023\_01

New study    Continue study

Show study from location

## CalibrationResults

H1\_observe - tpwr:54 pw90:20.0  
 H1\_observe - tpwr:60 pw90:10.5  
 H1\_observe - tpwr:60 pw90:10.0  
 H1\_observe - tpwr:60.5 pw90:9.8  
 H1\_observe - tpwr:60.5 pw90:9.8  
 H1\_observe - tpwr:48.5 pw360:151.7  
 H1\_observe - refpwr:48 refpw90:37.7  
 H1\_observe - tpwr:60.5 pw90:9.8  
 H1\_observe - compression factor: 0.9574



Probe	H1	F19	C13	N15	P31	Ik
H1pw90				9.8		
H1tpwr				60.5		
H1dmf				9217		
H1dpwr				38		
H1pp				9.6		
H1ppM				60		
H1tpwr_cf				0.9574		
H1dmm				w		
H1dseq				waltz16		
H1dres				90		
H1minrof2				25		
H1minalfa				10		
H1date						24-Oct-2013-11:17:26

Probe file is automatically updated

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# What is Shimming?

Adjustments to the static magnetic ( $B_0$ ) field to make it as homogeneous (“flat”) as possible (of the order of a few ppb).

Typical modern NMR system has more than 20 individual shim currents to optimize

Shimming by hand can be tedious, time consuming, and very difficult (if not impossible) to do!

The screenshot shows the software interface for an NMR system. The top menu bar includes: Start, Acquire, Process, Insert, Eject, Lock scan, Setup hardware, Auto lock, Auto tune, Gradient shim, and Logout. On the left, there are sections for Sample Info, Lock, Shim, and Spin/Temp. The Shim section is active, showing a dial set to 0.0 and several parameters: z0 (0), Lk Power (31), and Lk Gain (35). A red circle highlights a table of shim parameters:

Z1	-4578	±1	X1	1718	±1	X3	1914	±1	Z3X	-440	±1	ZX3	612	±1
Z2	-682	±1	Y1	-838	±1	Y3	674	±1	Z3Y	-3721	±1	ZY3	-707	±1
Z3	2373	±1	XZ	-9197	±1	XZ2	9173	±1	Z2XZ	10286	±1	Z4X	-3458	±1
Z4	9151	±1	YZ	7665	±1	Y2Z	11266	±1	Z2XY	1797	±1	Z4Y	-2017	±1
Z5	-8021	±1	XY	-3326	±1	ZXY	-1108	±1						
Z6	-843	±1	X2Y2	-2350	±1	ZX2Y2	4435	±1						

# When, What and How to Shim?

Installation: a new NMR system or probe requires optimization of all the RT shims “from scratch”

- Requires full 3D gradient mapping and adjustment of shims

Maintenance: periodic touch-up of shims to ensure optimum performance (reference “lineshape” spectrum may be recorded to verify quality of shimming).

- Usually less extensive adjustments needed than during installation, but can still be time consuming

“Sample-to-sample”: adjustment of a subset of shims for each sample prior to data collection

- May just require adjustment of “axial” (Z) shims. 1D gradient shimming is often most rapid and robust method, but other methods may be applicable

# ProShim – A Complete Shimmiing Toolset

“Mix-and-Match” different shimmiing methods, including:

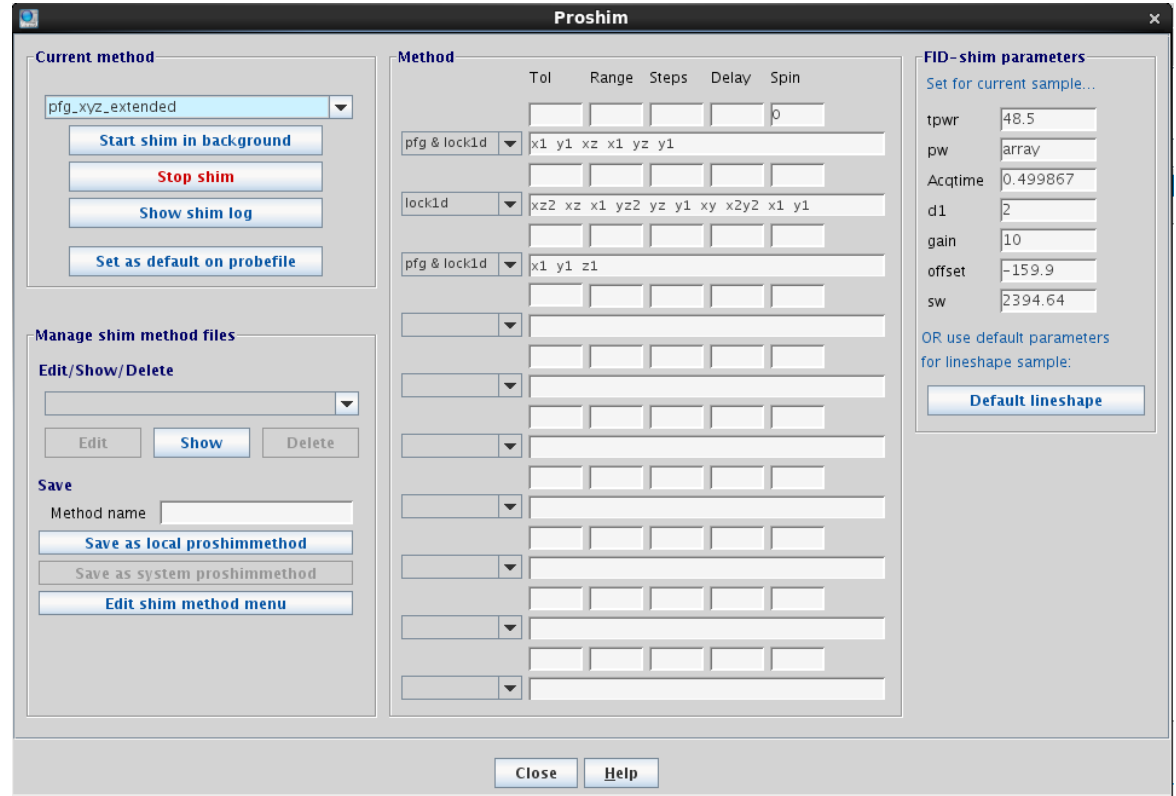
- Full 3D gradient shimmiing
- 1D gradient shimmiing (PFG, homospoil, convection compensated)
- FID shimmiing
- Lock shimmiing
- Spectrum shimmiing

Choose and tailor shimmiing method(s) to suit sample/application

How are shim methods created and combined....?

# ProShim Method Editor

The Shim Editor manages the ProShim methods and allows you to build the method you want, using the tools you want, in the order that you want them to run.

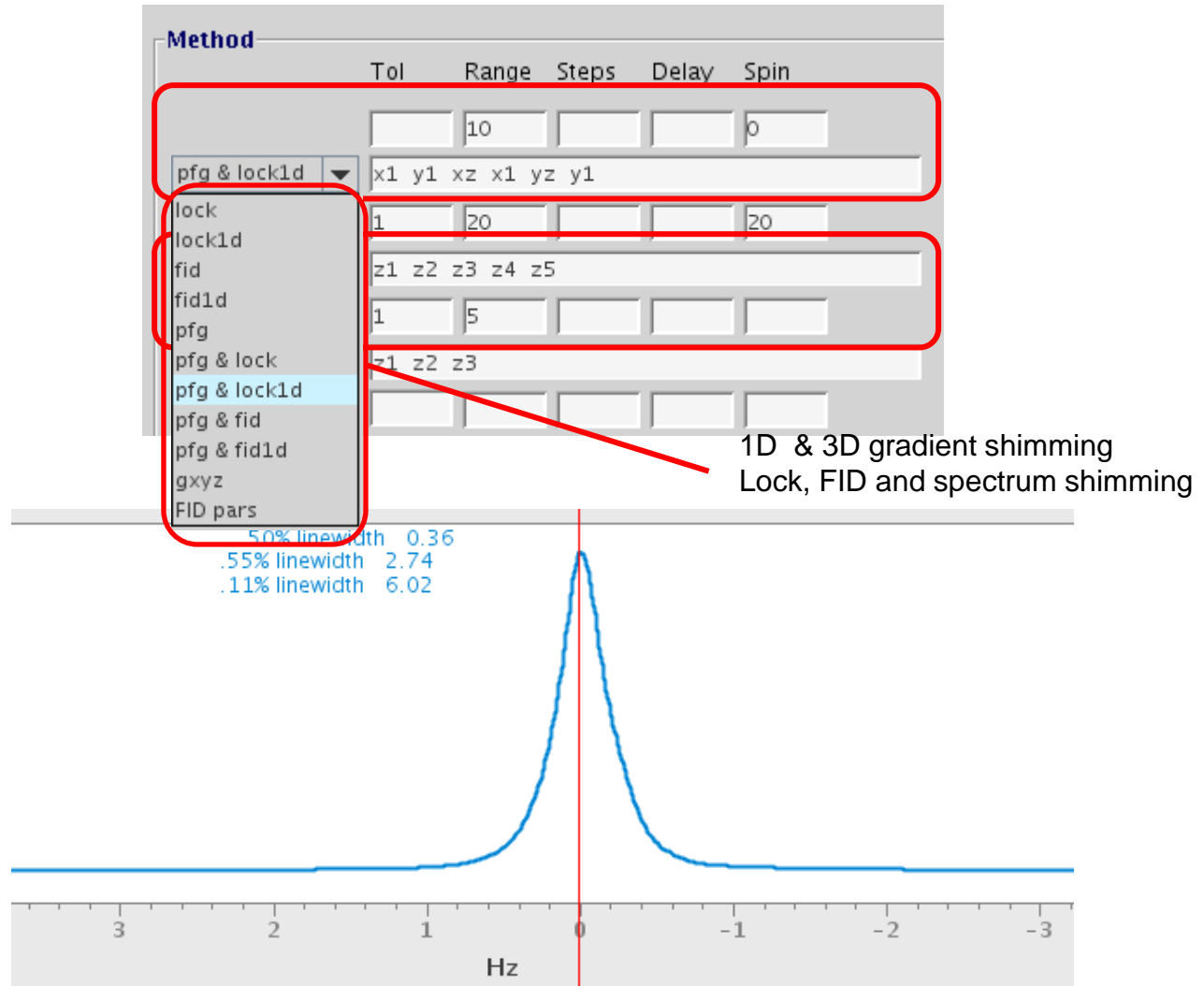


# ProShim Method Editor

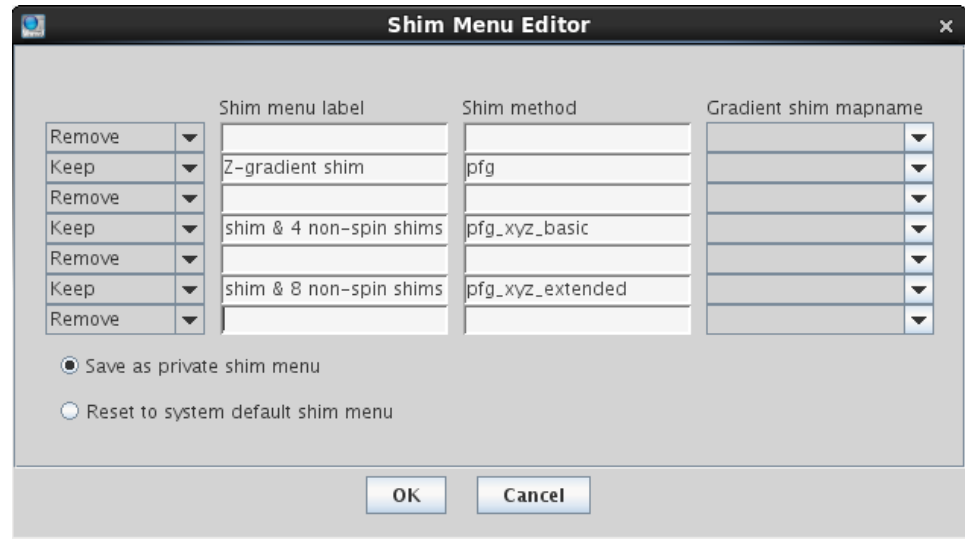
Which shims to adjust and how are entered into each row in the Method Editor

Each row is a separate shimming “stage”, characterized by the method and shims adjusted

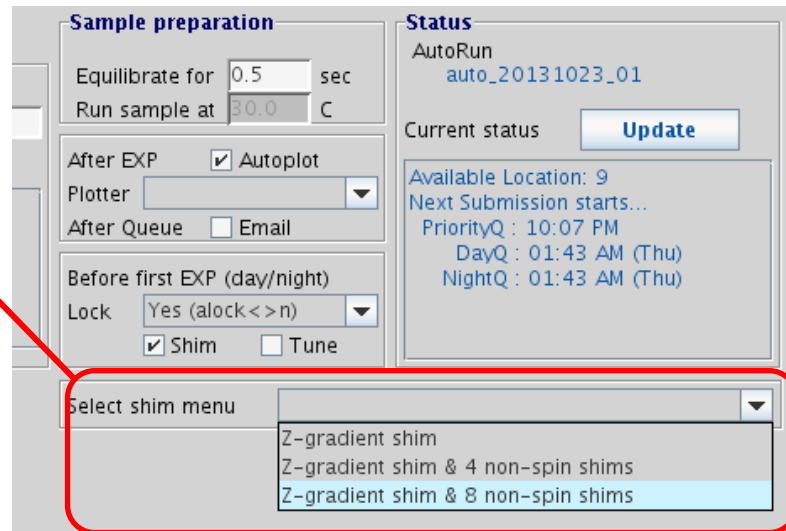
“fid” shimming uses the FID area, but can also use specific peak height or linewidth from the spectrum



# ProShim Shim Menu Editor

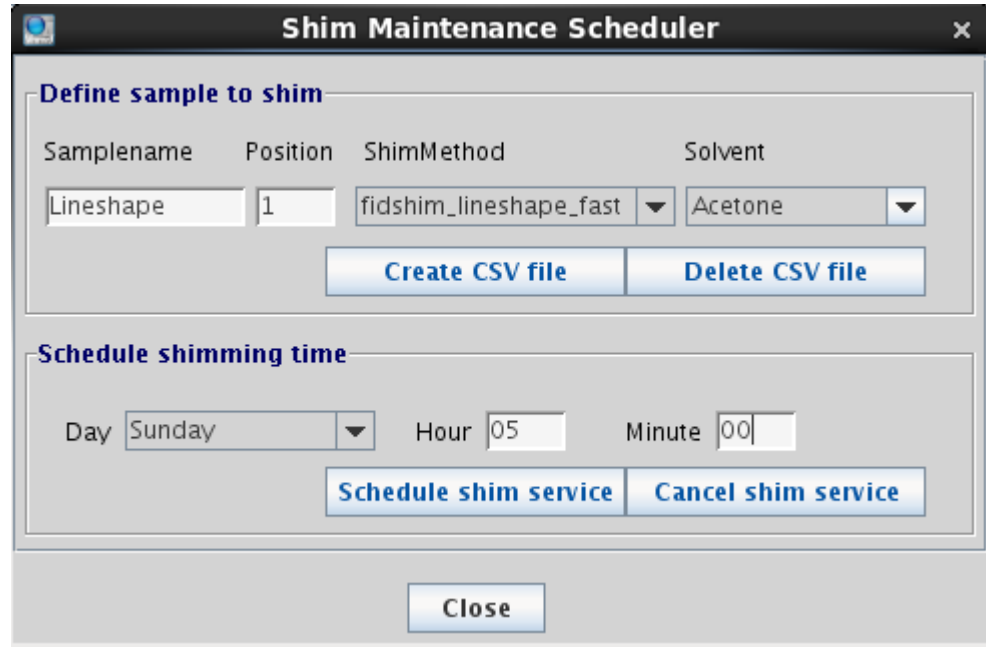


Once the methods are created, the Shim Menu Editor allows you to add them to the menu for use in Automation.



# ProShim Scheduler

The final piece of the ProShim puzzle is a tool that allows you to schedule routine maintenance shimming to occur automatically.



The screenshot shows a software window titled "Shim Maintenance Scheduler". It is divided into two main sections: "Define sample to shim" and "Schedule shimming time".

**Define sample to shim**

Samplename	Position	ShimMethod	Solvent
Lineshape	1	fidshim_lineshape_fast	Acetone

Buttons: **Create CSV file**, **Delete CSV file**

**Schedule shimming time**

Day: Sunday, Hour: 05, Minute: 00

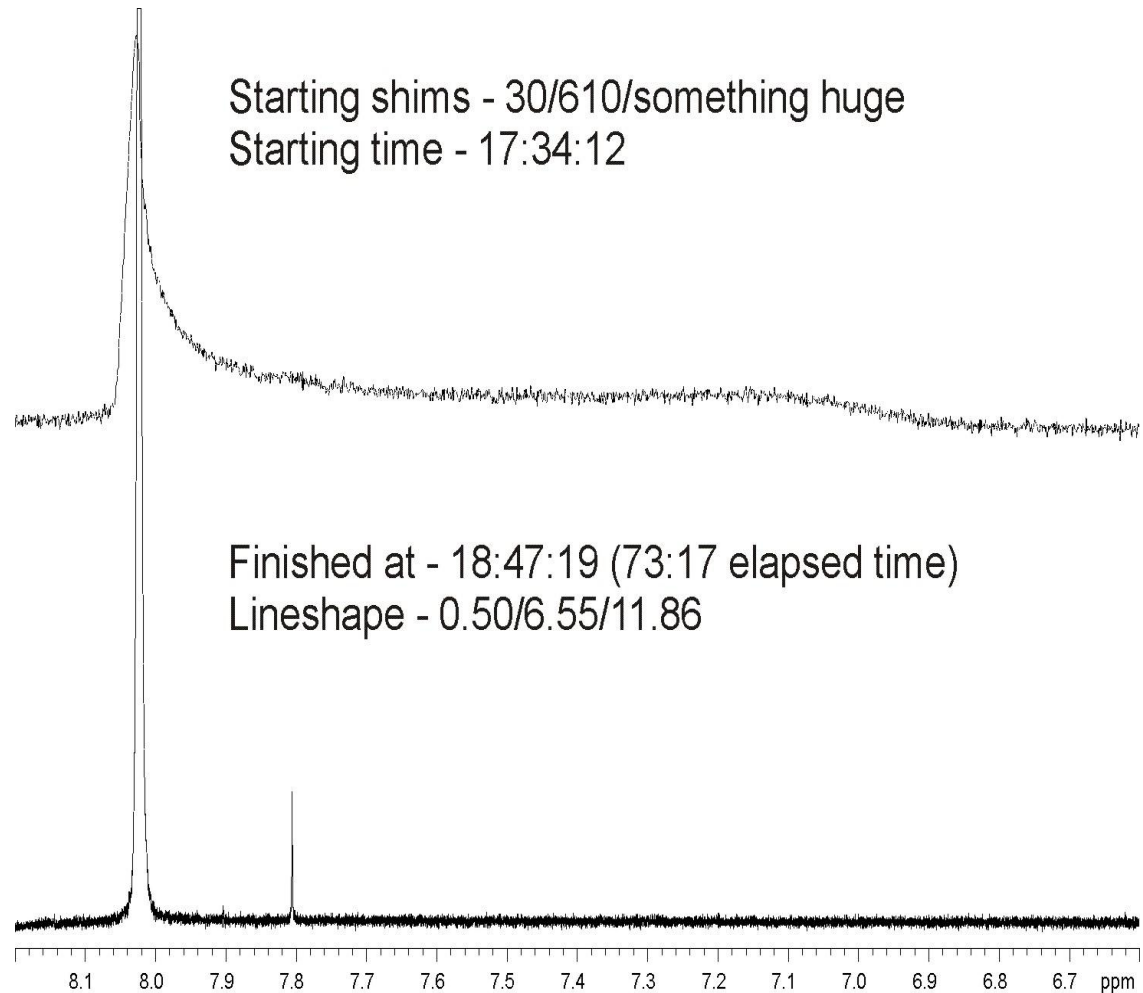
Buttons: **Schedule shim service**, **Cancel shim service**

Bottom button: **Close**

# ProShim

ProShim works even when the starting shims are very poor.

The result can be quite extraordinary.



# Conclusions

- Automation Preferences
- Persona Manager
- Study Clones
- Application Directories
- Probe Autocalibrations
- ProShim

**VnmrJ provides the tools you need to manage your systems, control your users, and maintain a high level of spectral quality.**

# Thank You!



Acknowledgements:

Ron Crouch  
Krish Krishnamurthy  
Dan Iverson  
Software Team



**Agilent Technologies**

# Questions?

## Q&A now and later

Additional questions can be asked on our Spinsights NMR & MRI Community at <https://spinsights.chem.agilent.com>.

Agilent Technologies  
SPIN SIGHTS | NMR & MRI COMMUNITY

Home Content People Places Links - My Stuff - Create -

Welcome to the new Spinsights Community!

- 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.

MAIN SPACES

Downloads & Resources Discussion Forum AskTAC NMRPipe Help using Spinsights

SPIN SIGHTS BLOGS

FEATURED SCIENCE

Welcome to the Discussion Forum!

Here's a quick orientation:

- General questions and discussions regarding hardware, software, and troubleshooting belong in the Discussion Forum
- Questions, discussions, and posted materials pertaining to specific application families belong in the four Groups:
  - Small Molecule NMR
  - Biomolecular NMR
  - Solids NMR
  - Imaging
- Macros, pulse sequences, scripts, etc. belong in the User Library
- Discussions of facility administration, infrastructure, accounting, training, etc. belong in Facility Managers
- TAG ALL YOUR POSTS by adding keywords in the "tags" box at the bottom of your drafts
- Requests, complaints, and suggestions should be tagged with the keywords requests, complaints, or suggestions
- Placing your posts in your own blog or discussion area makes them nearly invisible; it's better to keep them public in Discussion Forum

TOPICAL DISCUSSION GROUPS

Solids NMR  
This is the home for solids NMR discussions.

Facility Managers  
This group is for facility managers, and is the best home for discussions of administration, accounting, training, etc.

SEARCH & ASK THE DISCUSSION FORUM

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