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

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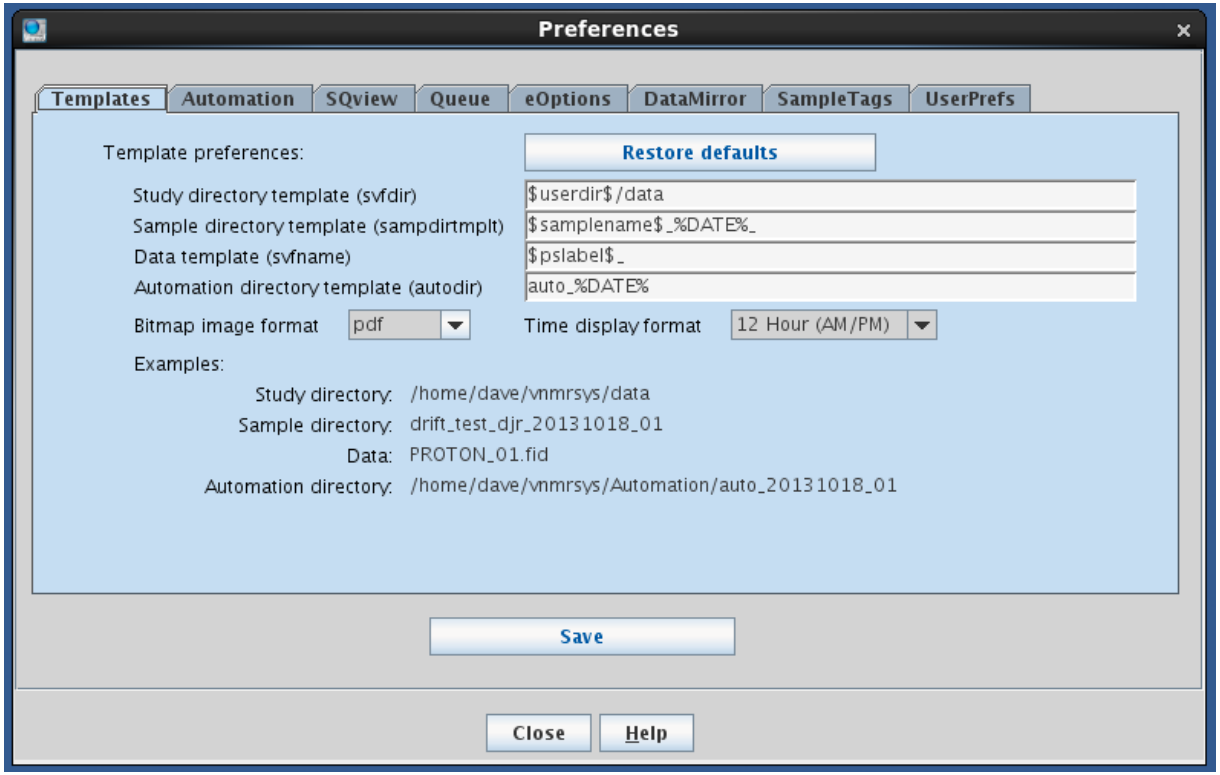
The Preferences Panels

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…



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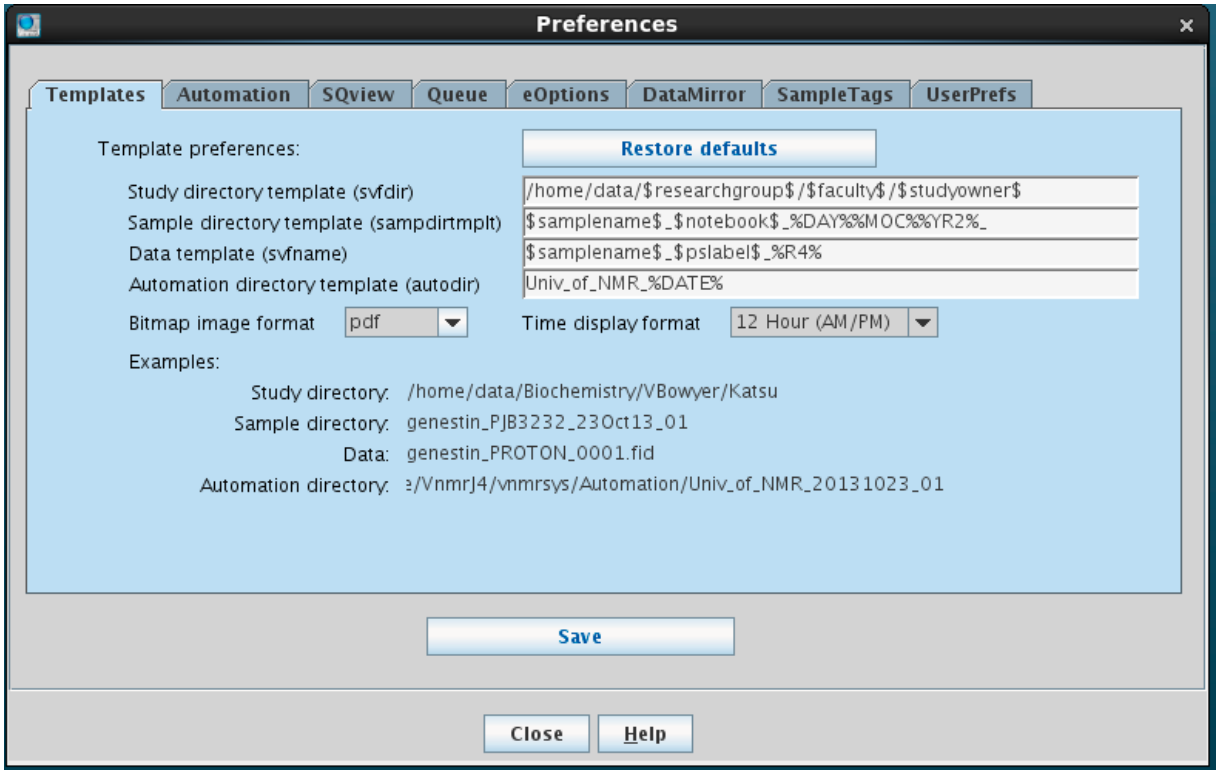
The Preferences Panels

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.



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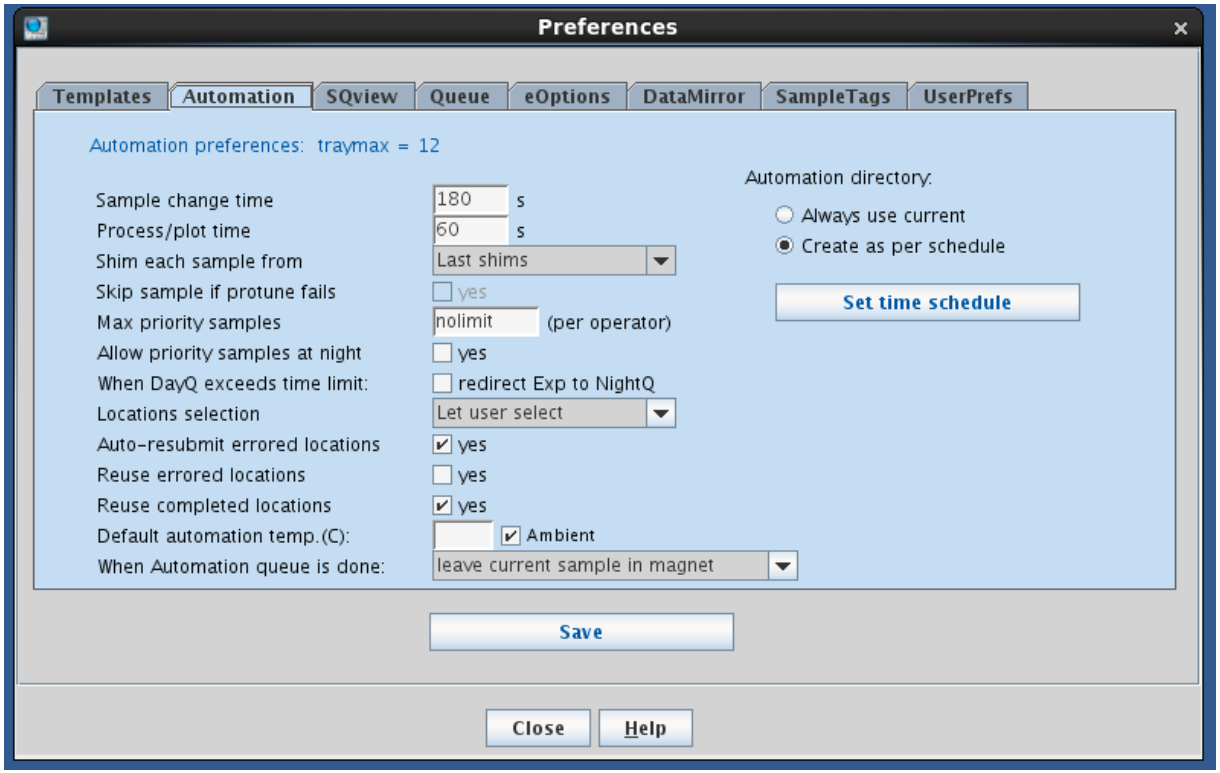
The Preferences Panels

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.



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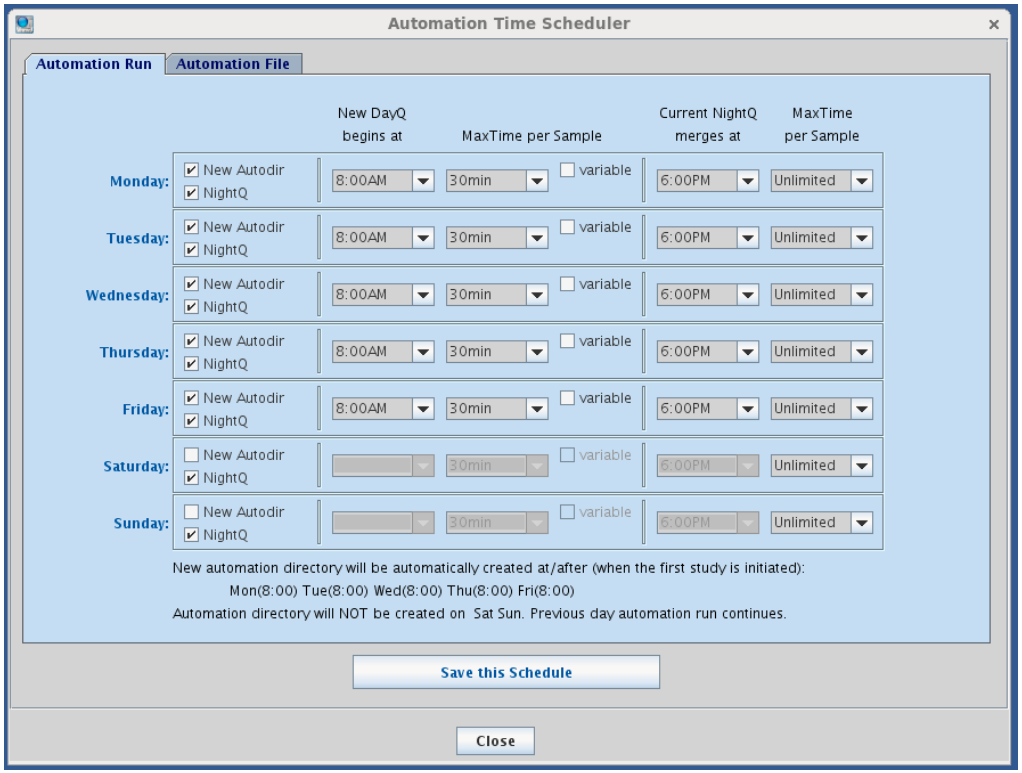
The Preferences Panels

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.



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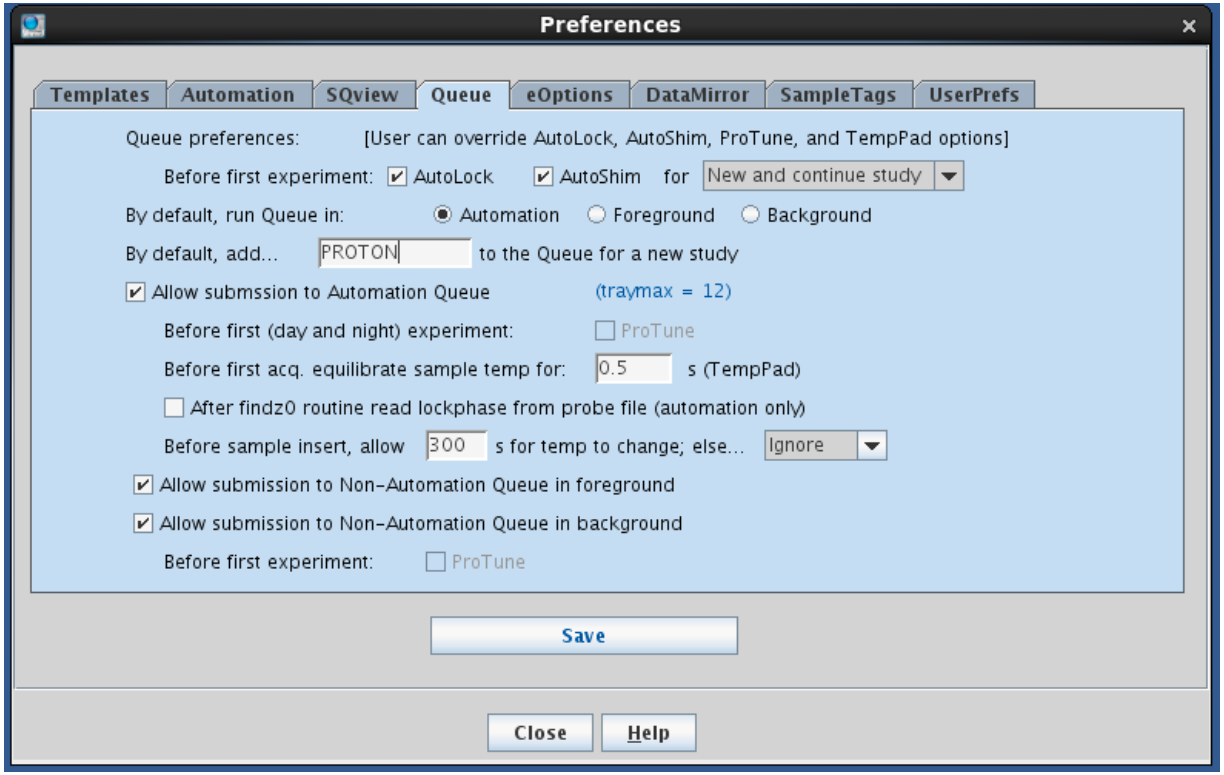
The Preferences Panels

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.



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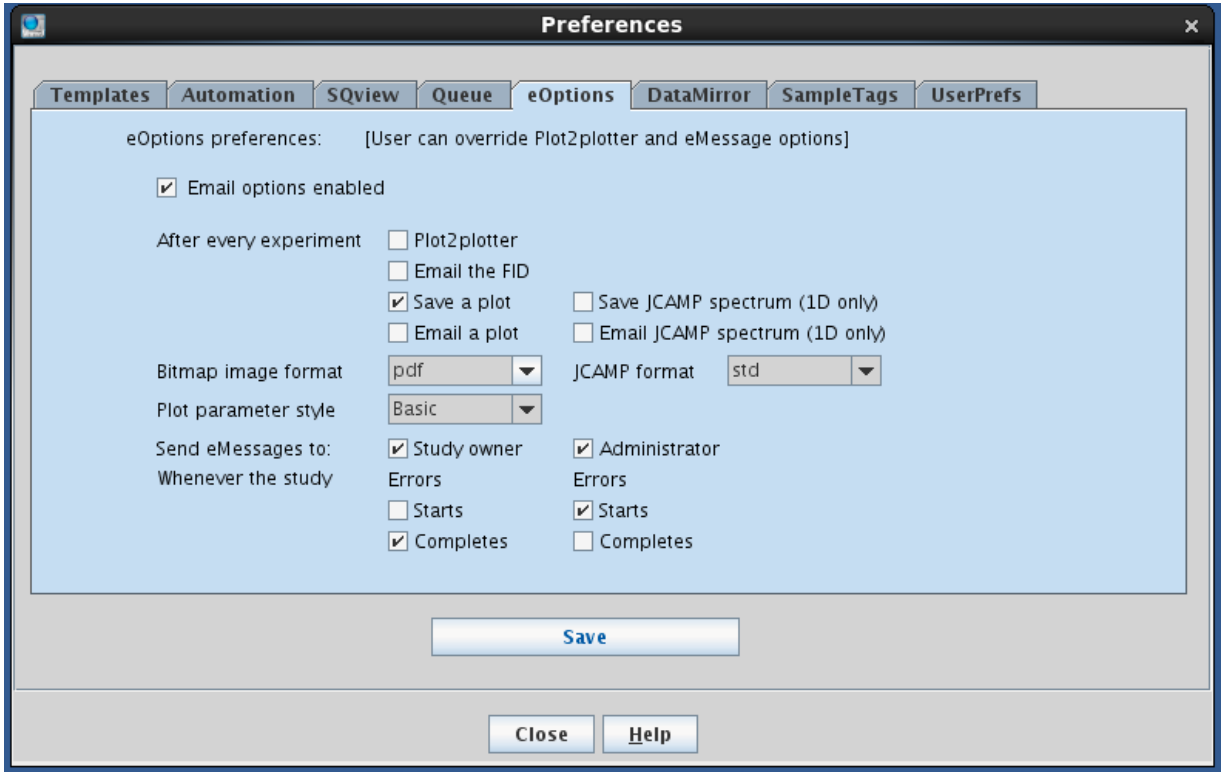
The Preferences Panels

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.



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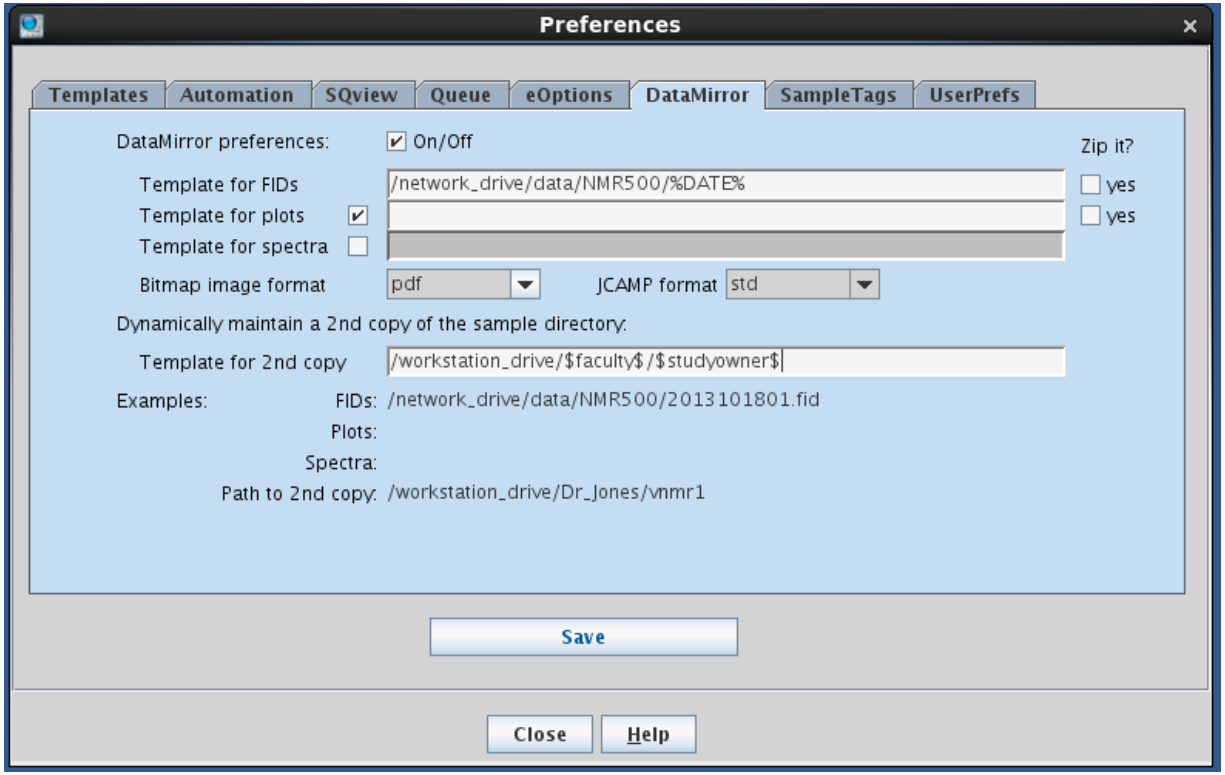
The Preferences Panels

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.



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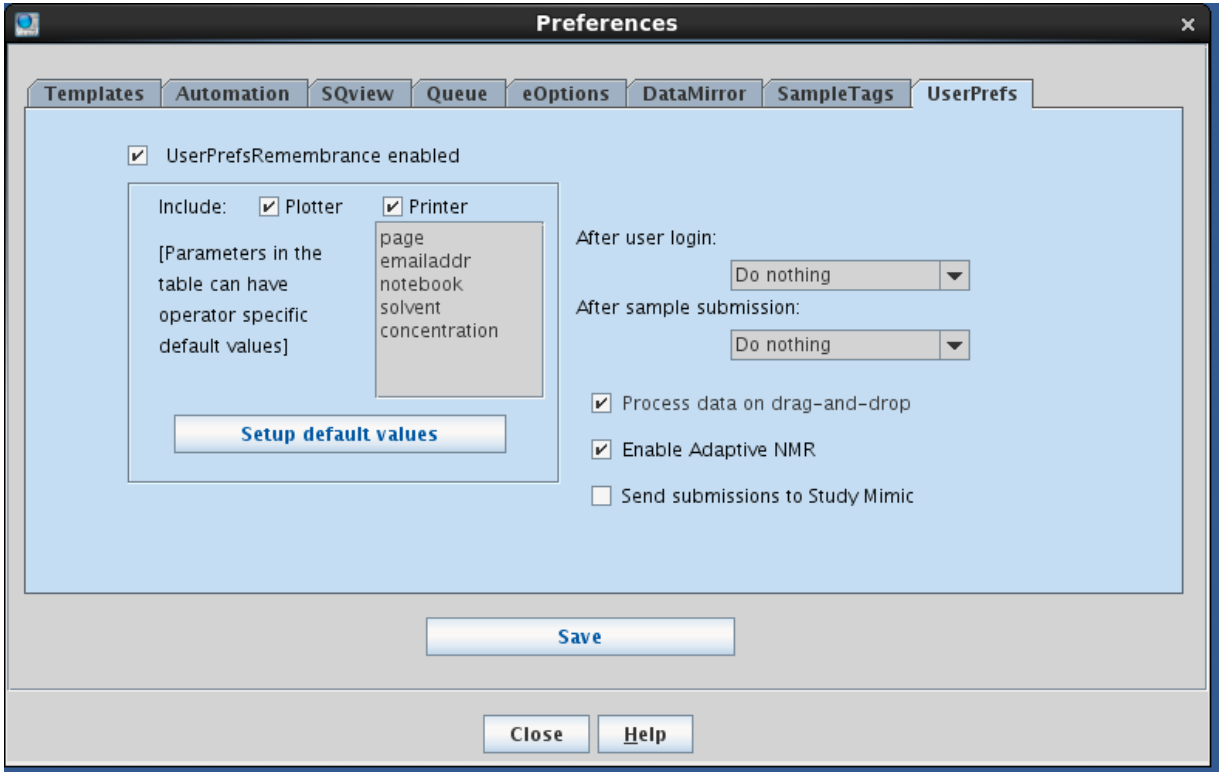
The Preferences Panels

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.



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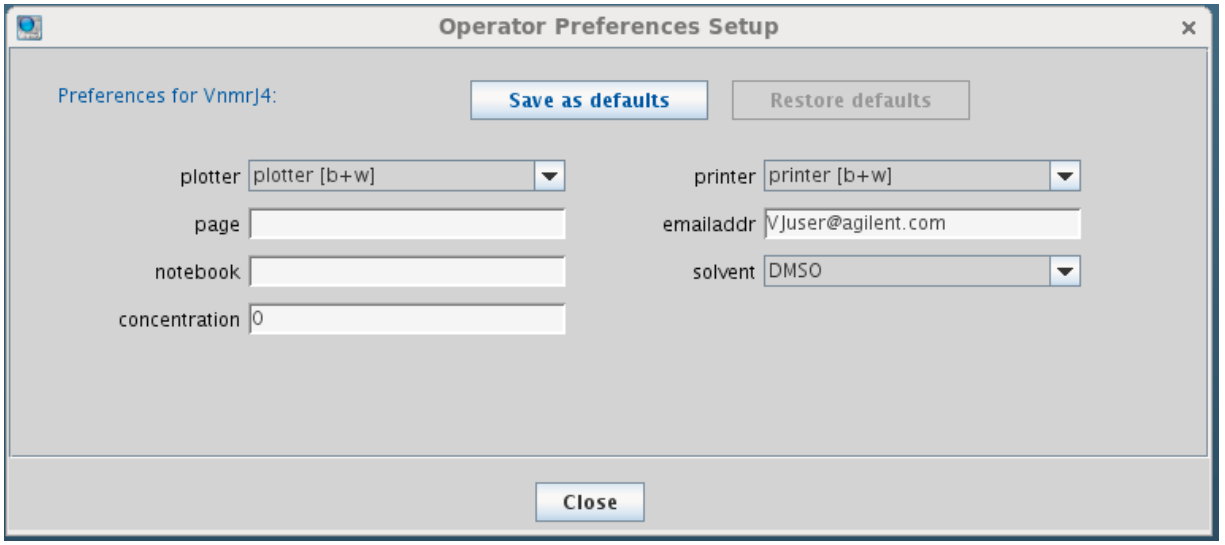

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Outline

:

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- **Tailor VnmrJ to meet each of your user's needs - the Persona Manager**
- Fully customize your push-button NMR experiments - Study Clones
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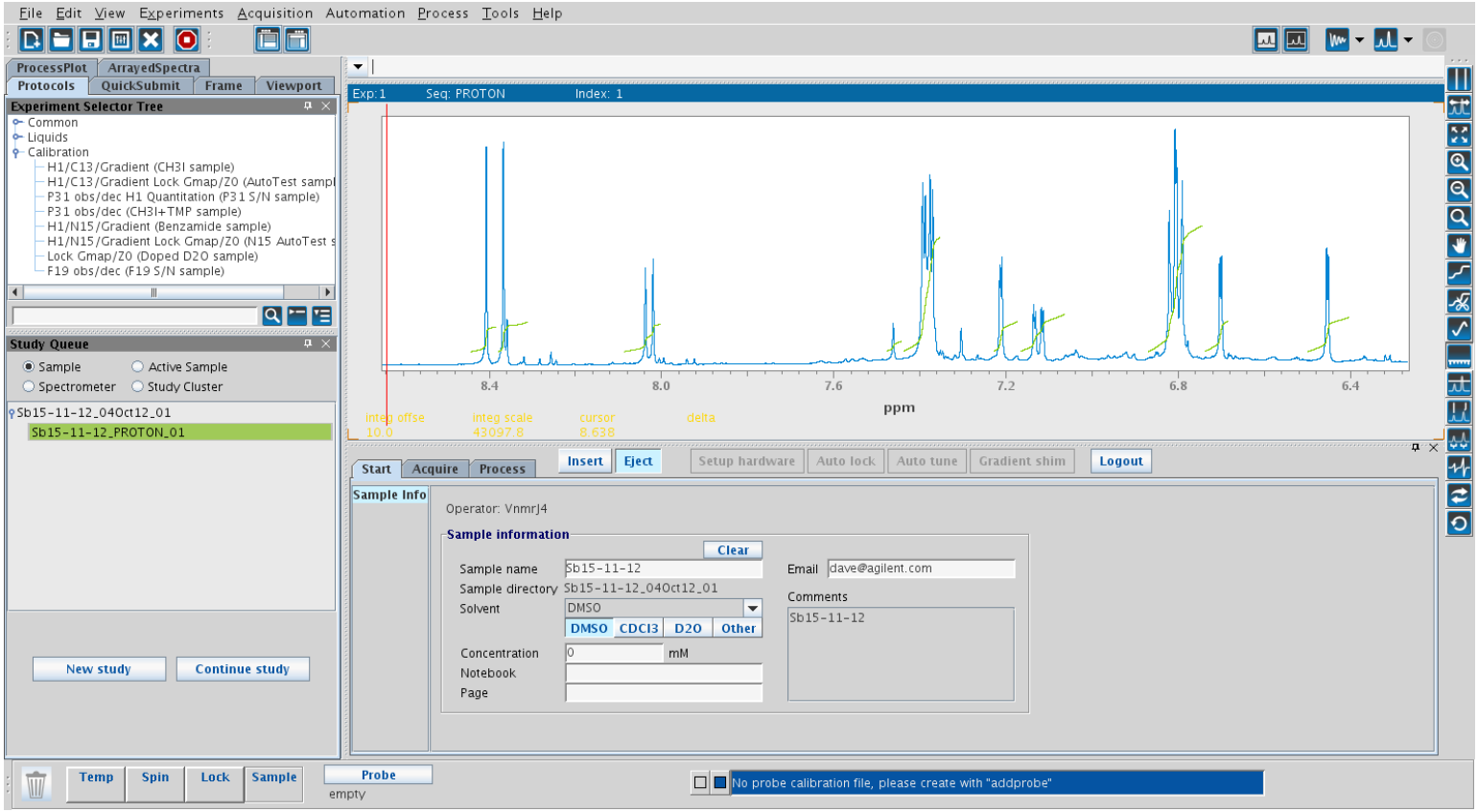
Persona Manager



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.

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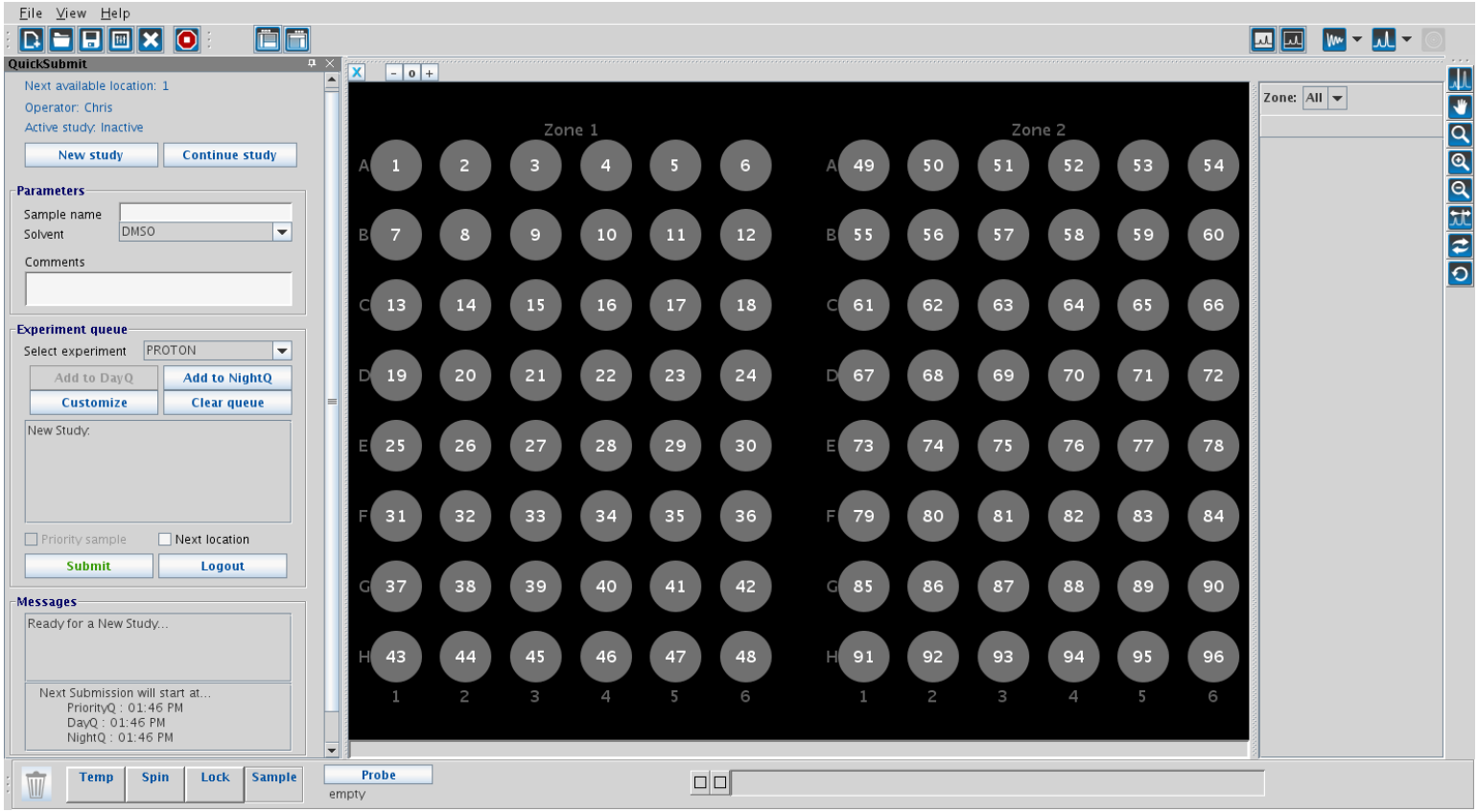
Persona Manager



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.

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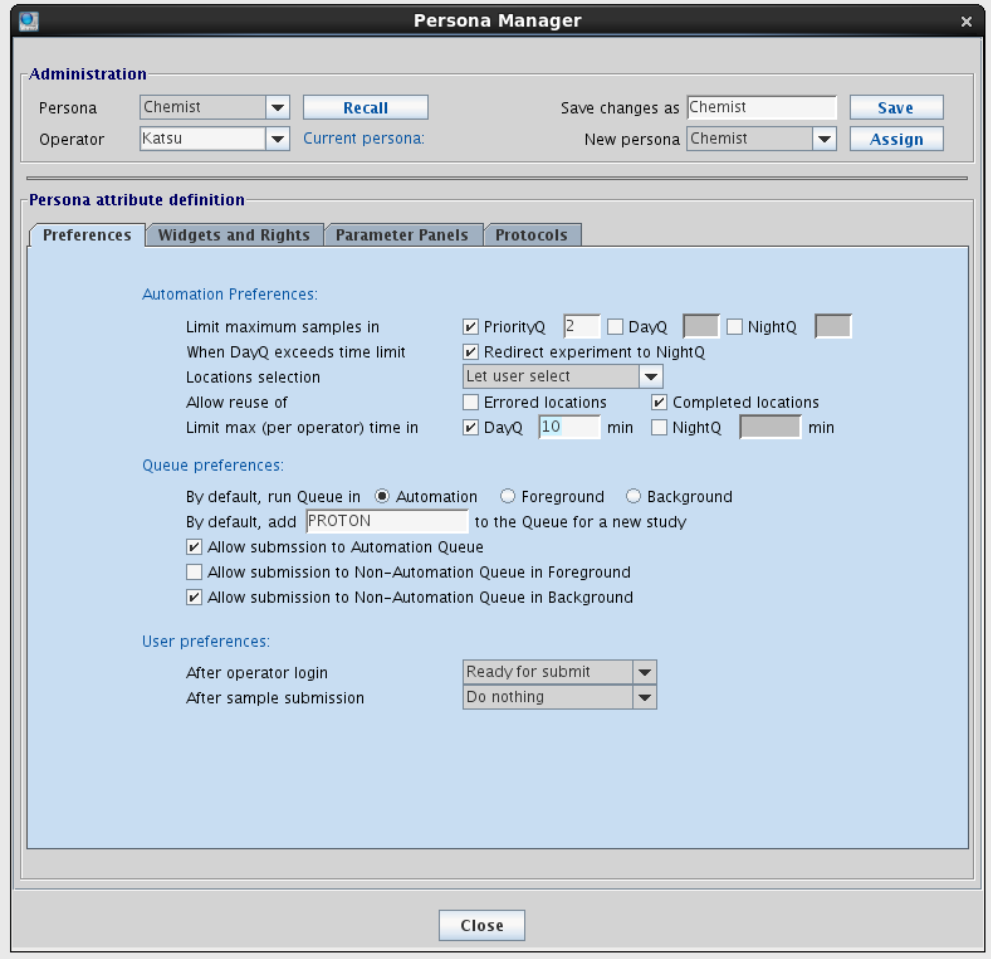
Persona Manager

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.



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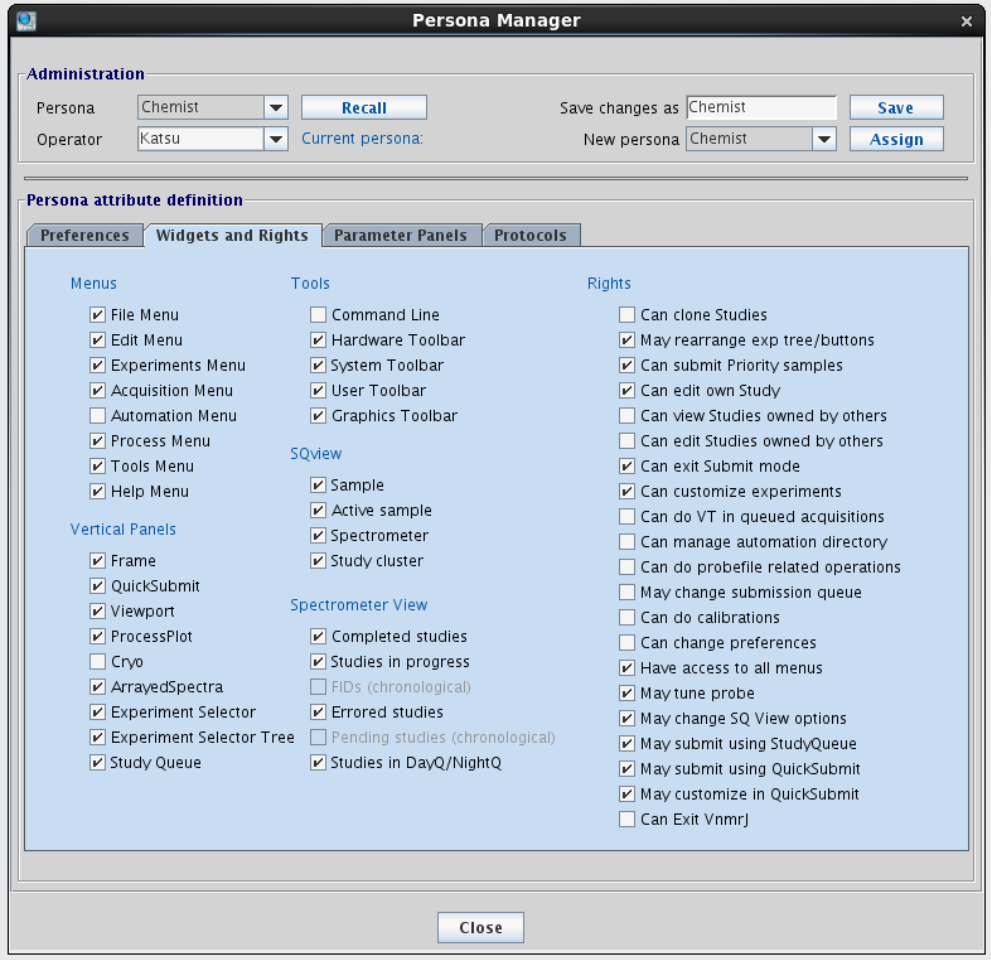
Persona Manager

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.



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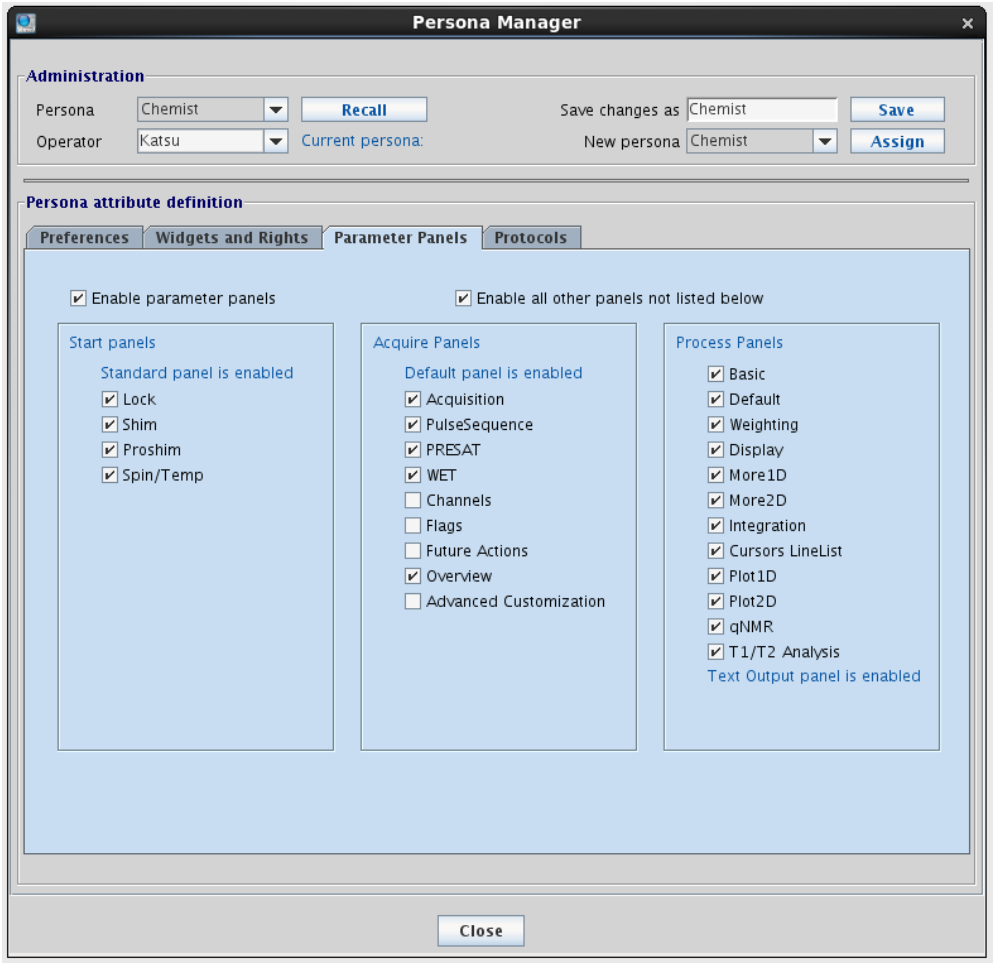
Persona Manager

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.



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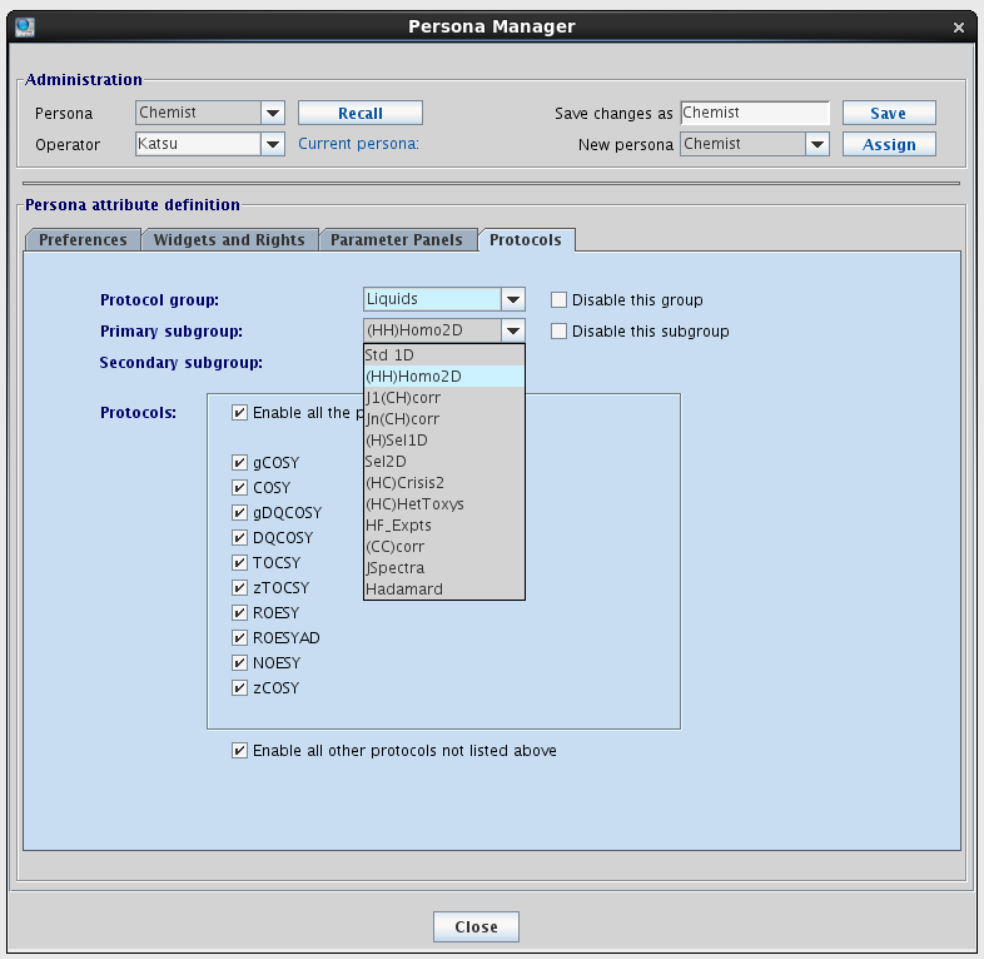
Persona Manager

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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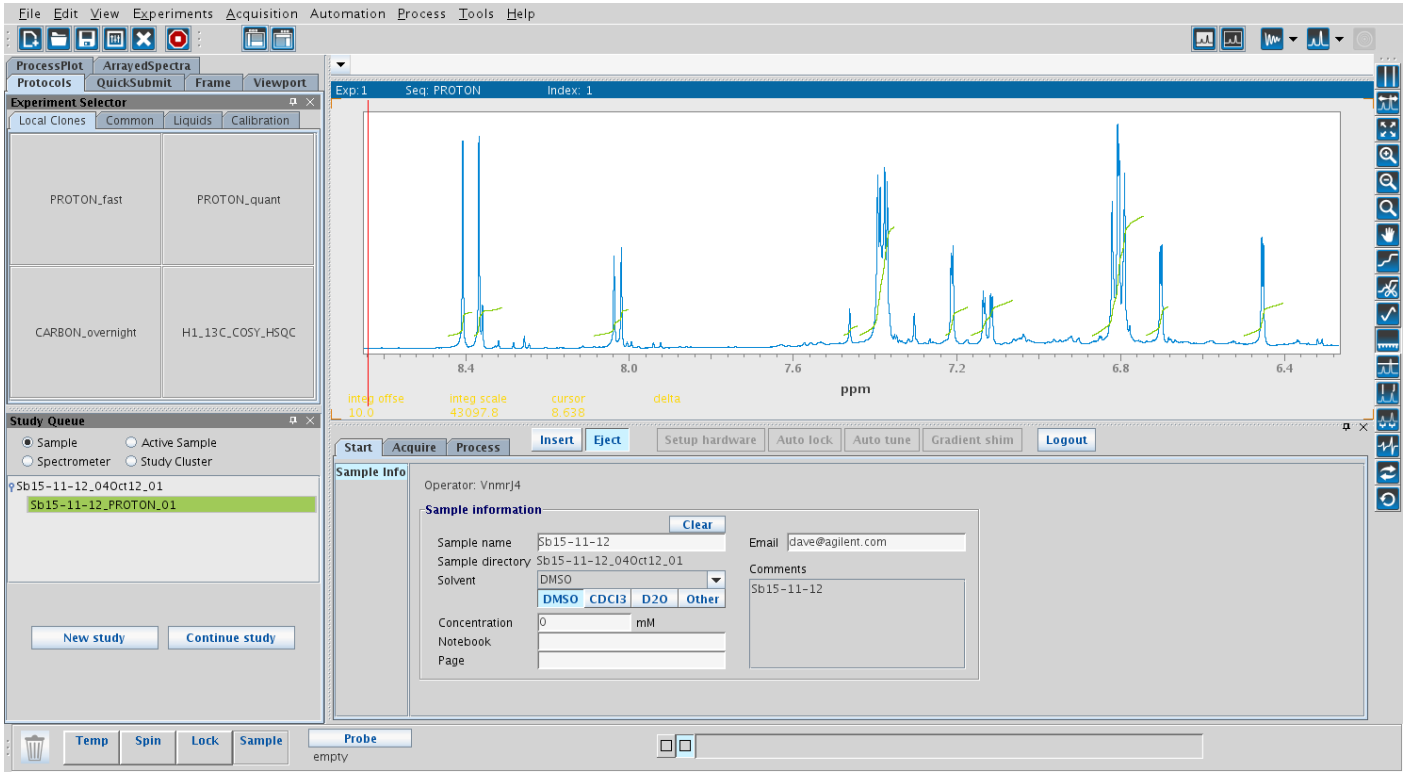
Study Clones

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.

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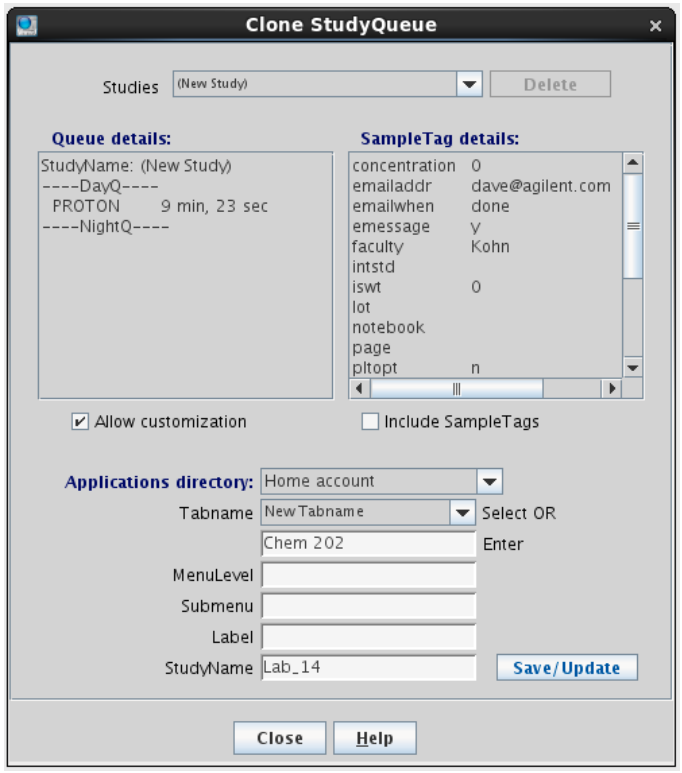
Study Clones

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.

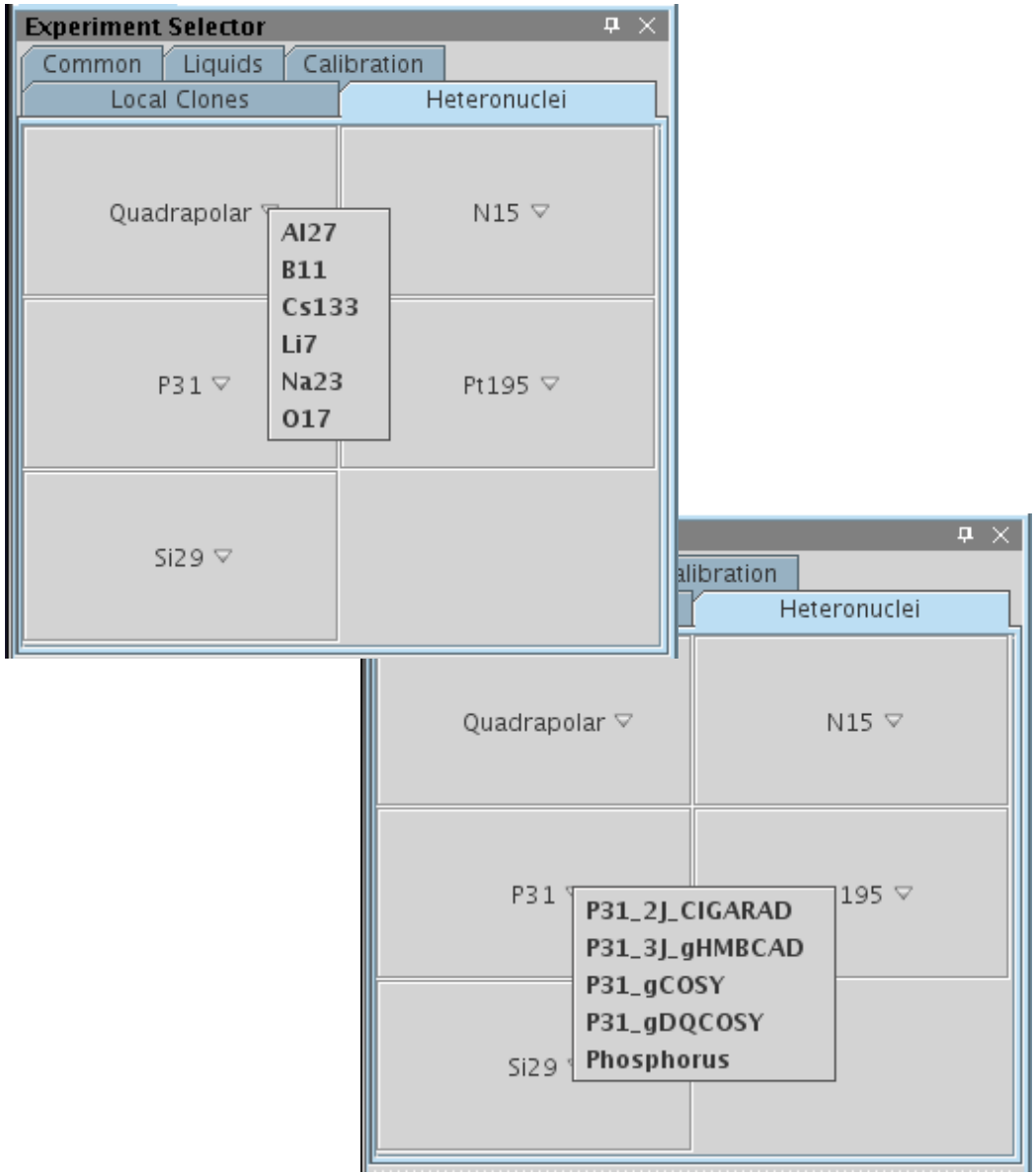
Study Clones can consist of just one experiment, or a collection of experiments, and they can have customized processing and plotting actions associated with them.



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

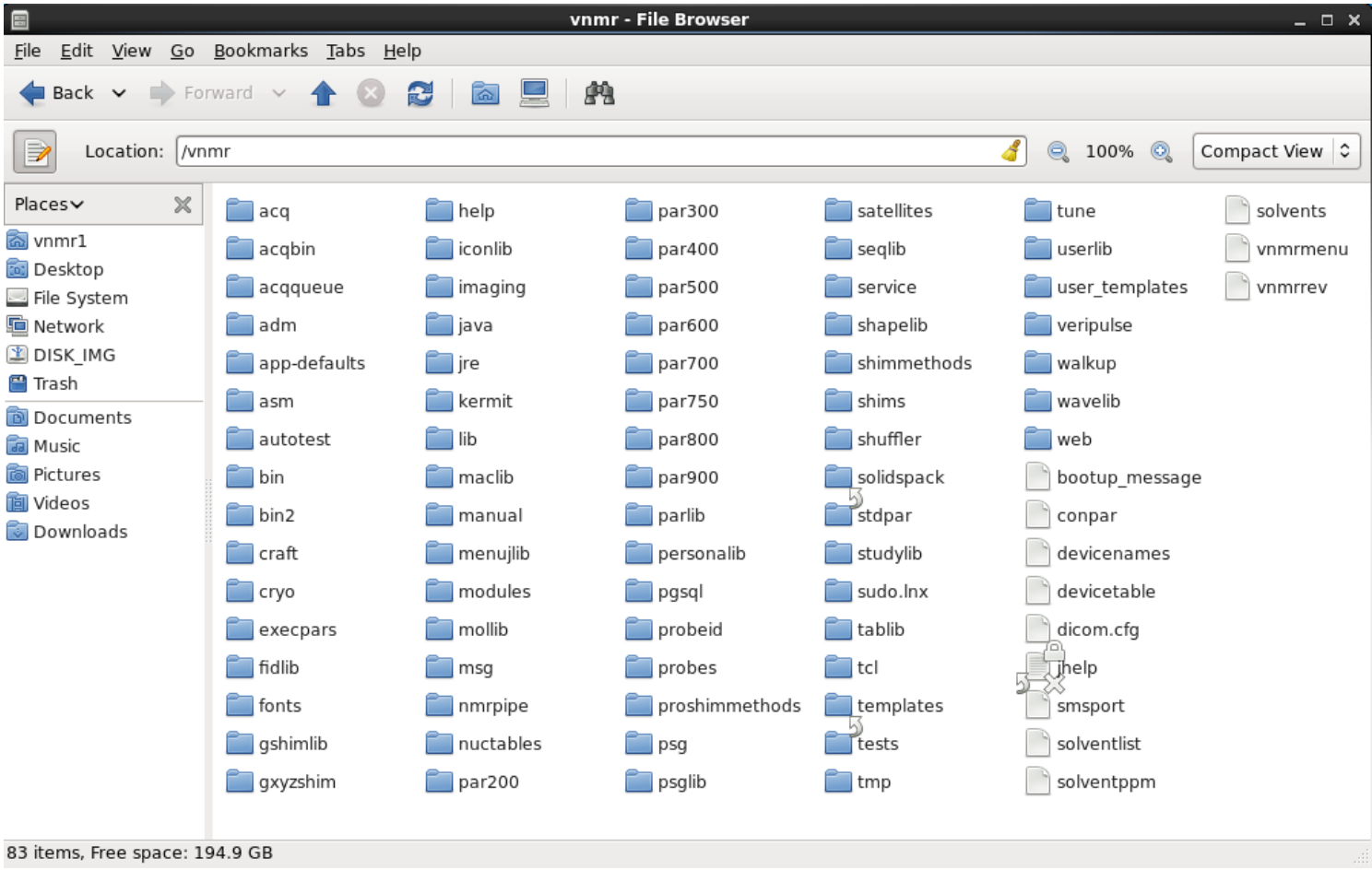
Maintain and distribute software customizations with ease

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

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

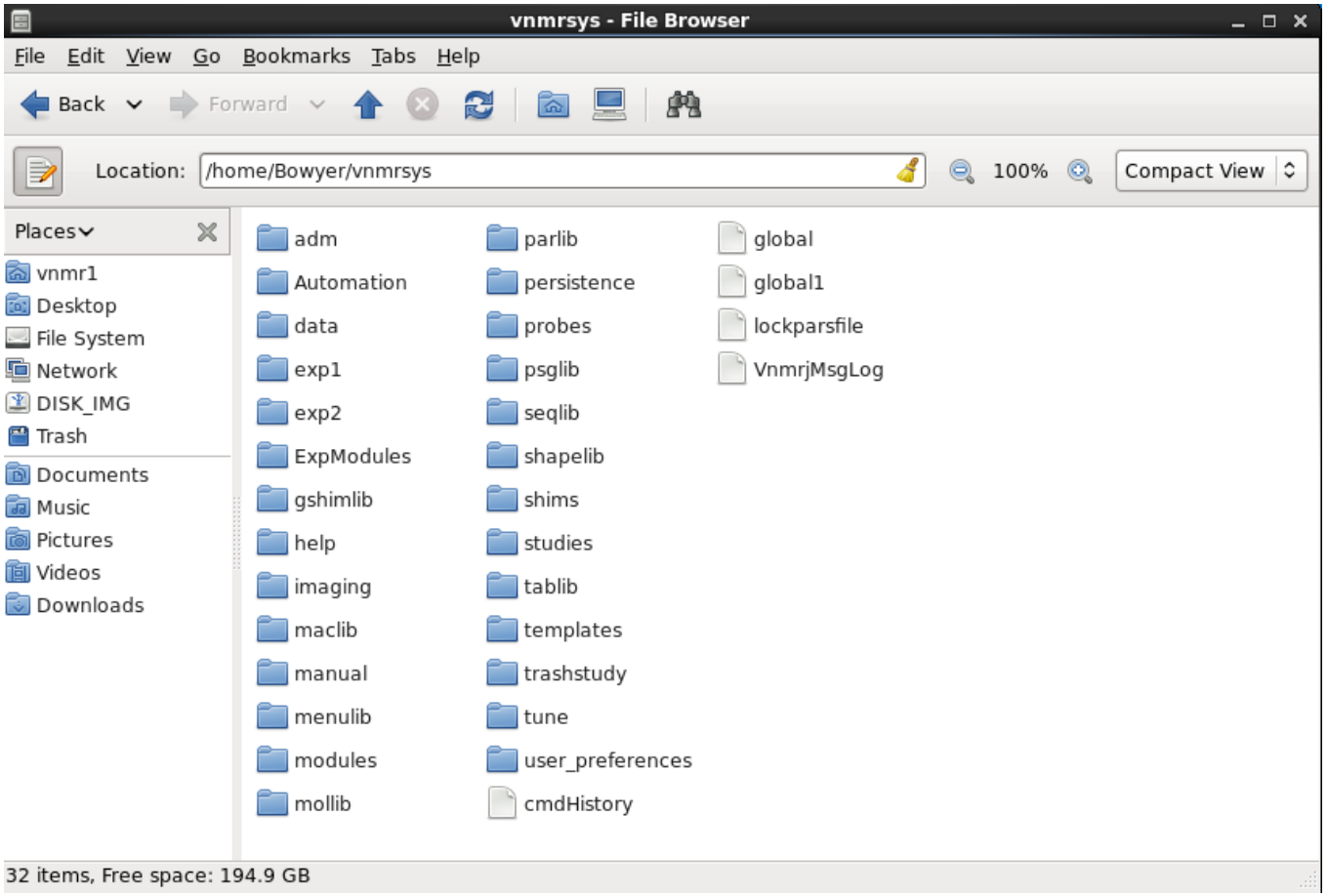
System Application Directory

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



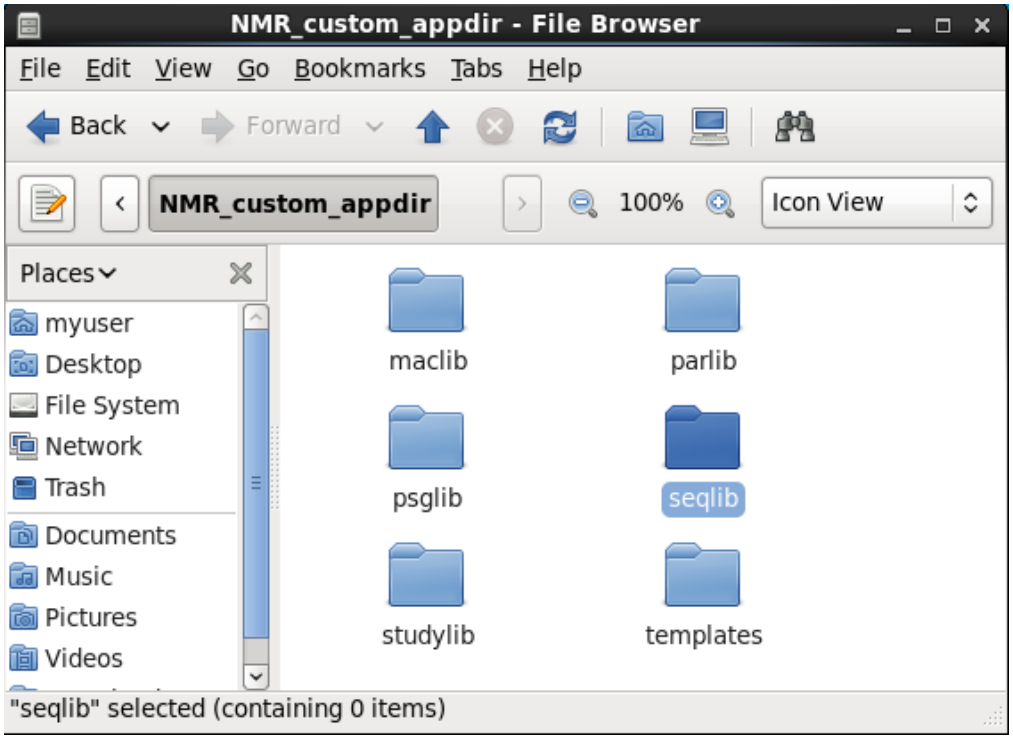
Application Directory Searching

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

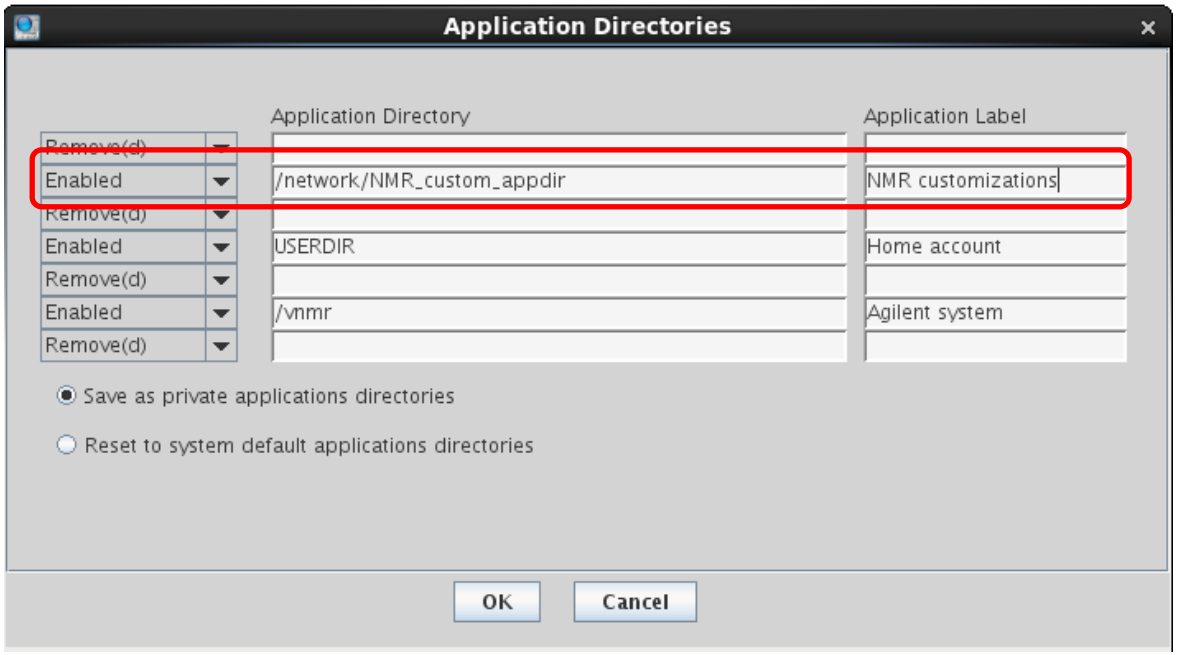
Suppose we had a collection of files (e.g. pulse sequences, setup macros, and so on) that we would like to be made available on one or more NMR systems

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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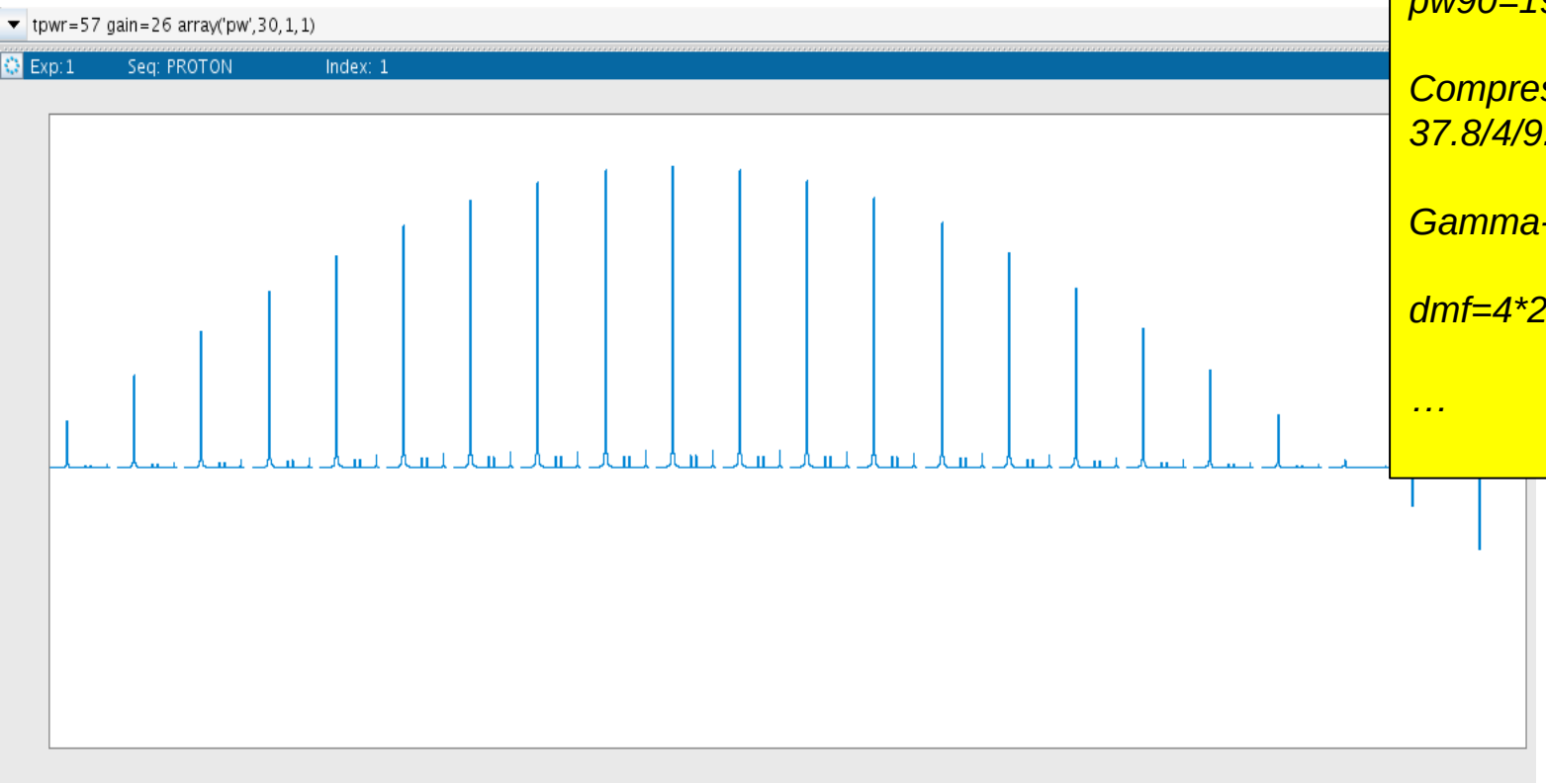
Manual Probe Calibrations

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

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



pw90=19.2/2 = 9.6 us

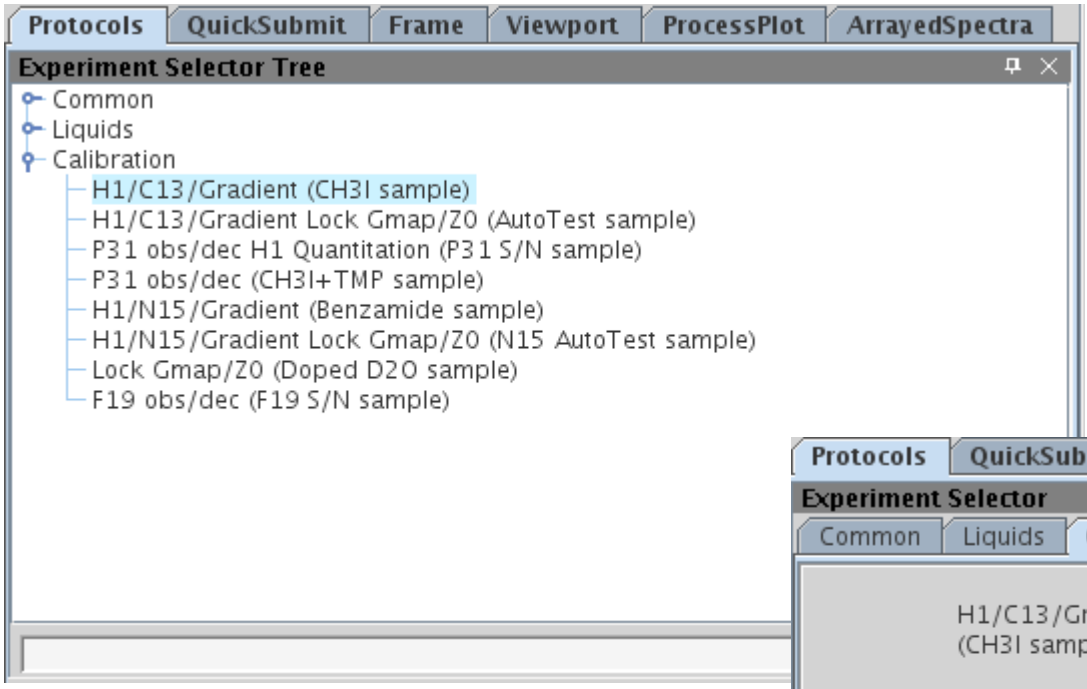
Compression factor = 37.8/4/9.2 = 1.03

Gamma-H2 = 2304 Hz

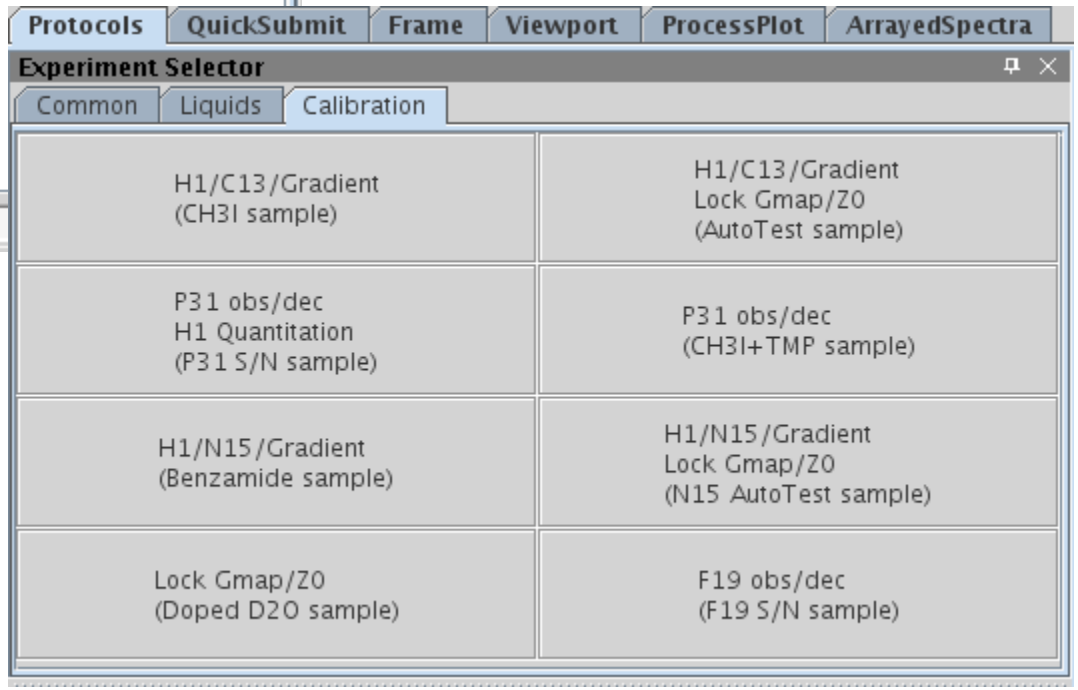
*dmf=4*2304 = 9360 Hz*

…

VnmrJ Autocalibrations

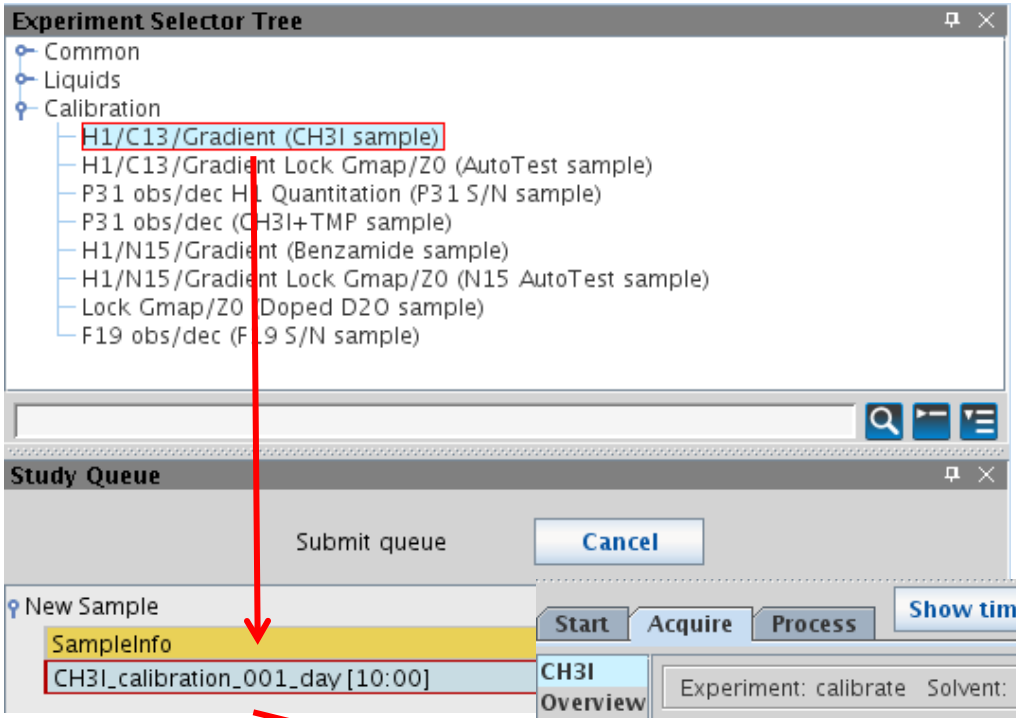


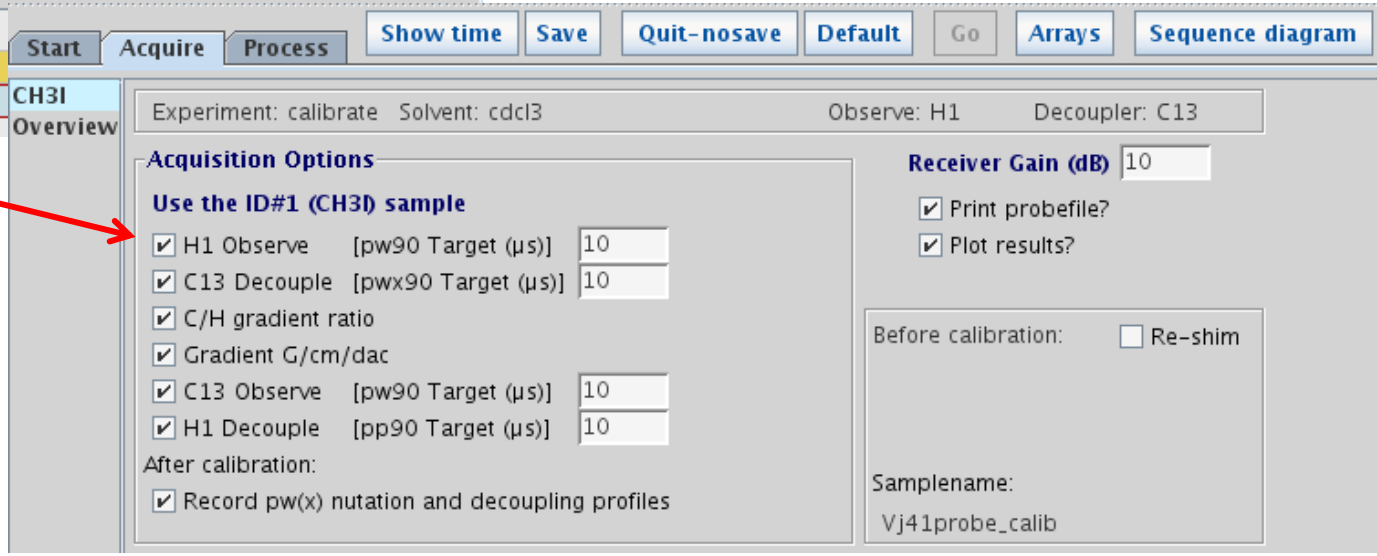
Autocalibrations from Experiment Selector (Tree).



Standard samples shown in parentheses

Autocalibrations in the Study Queue

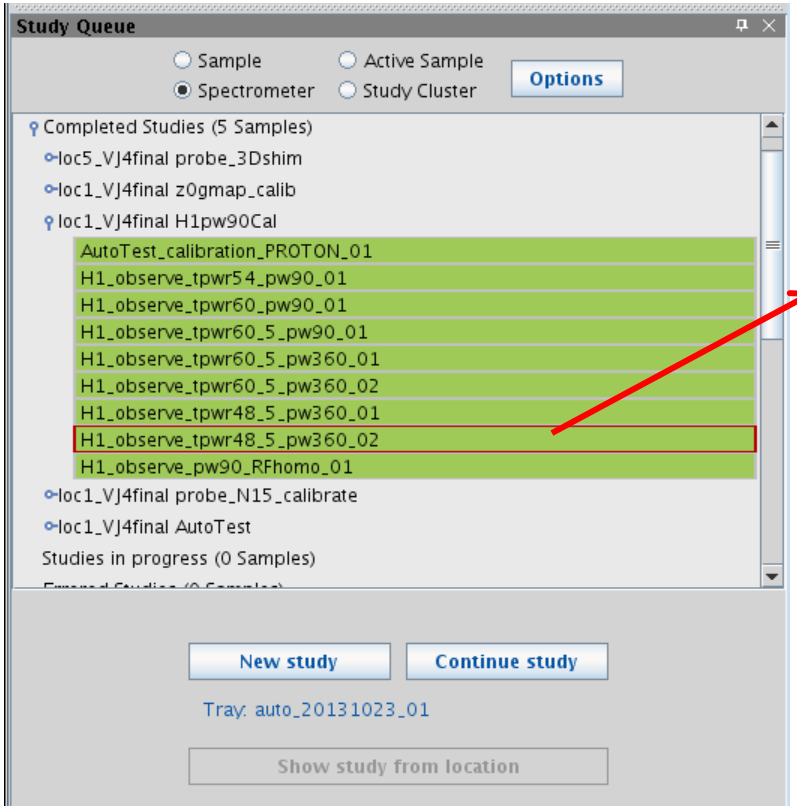


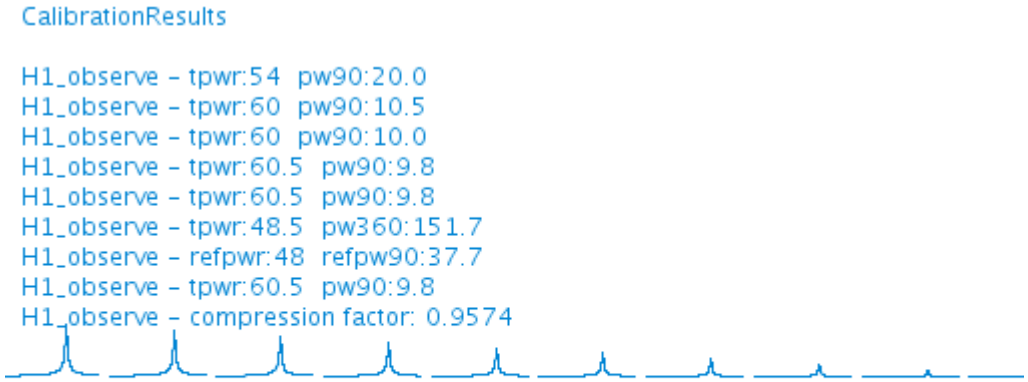


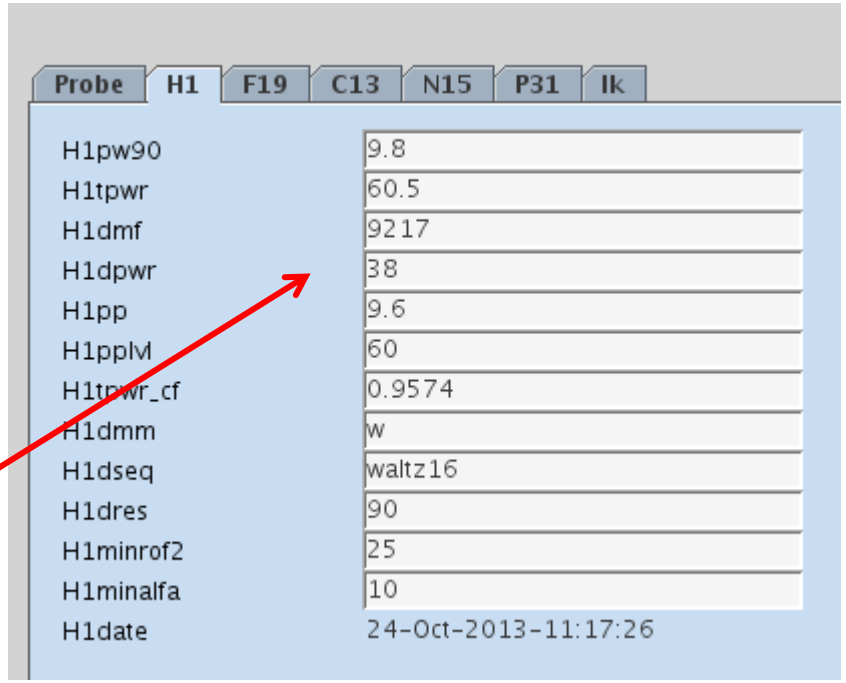
Drag calibration into Study Queue, then select specific calibrations and set targets

Locking, tuning and shimming done automatically

Autocalibrations in the Study Queue







Probe file is automatically updated

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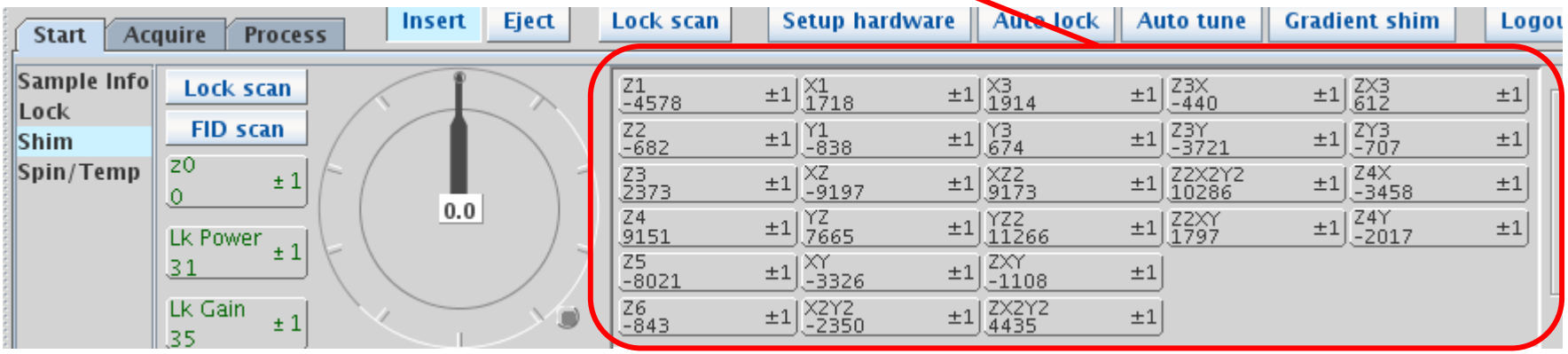
What is Shimming?

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!



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 Shimming Toolset

"Mix-and-Match" different shimming methods, including:

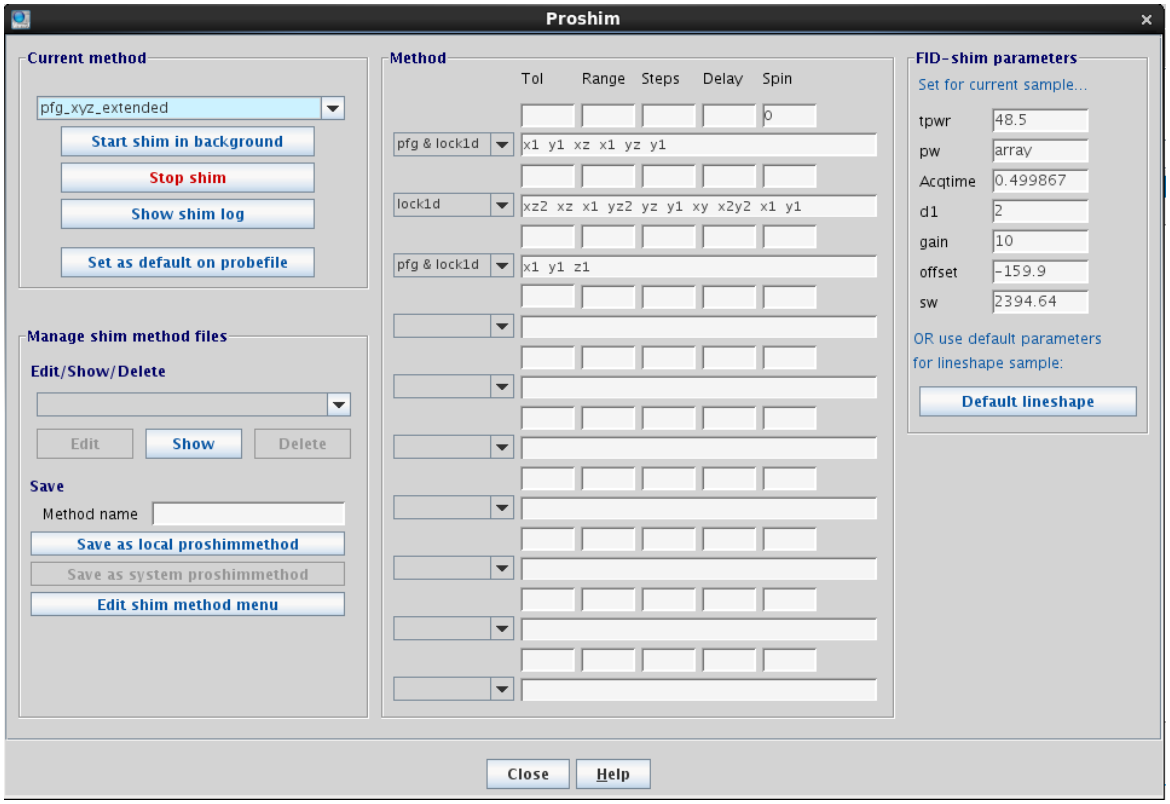
- Full 3D gradient shimming
- 1D gradient shimming (PFG, homospoil, convection compensated)
- FID shimming
- Lock shimming
- Spectrum shimming

Choose and tailor shimming 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.

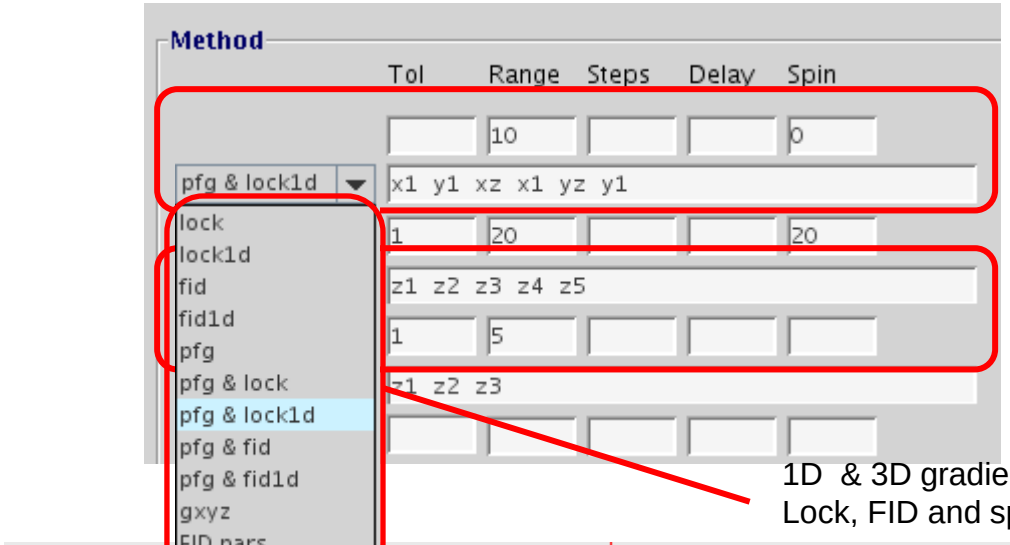


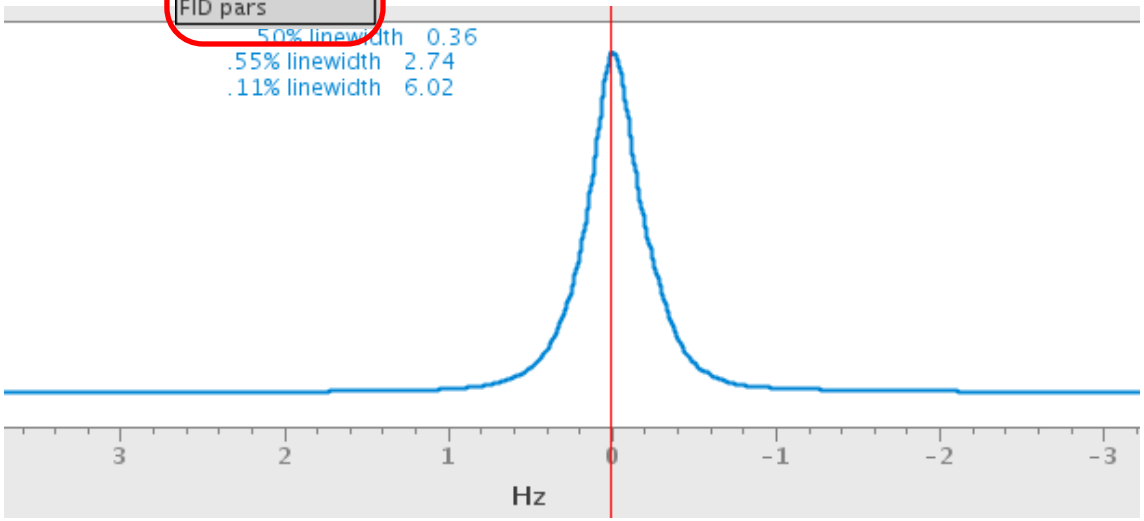
ProShim Method Editor

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

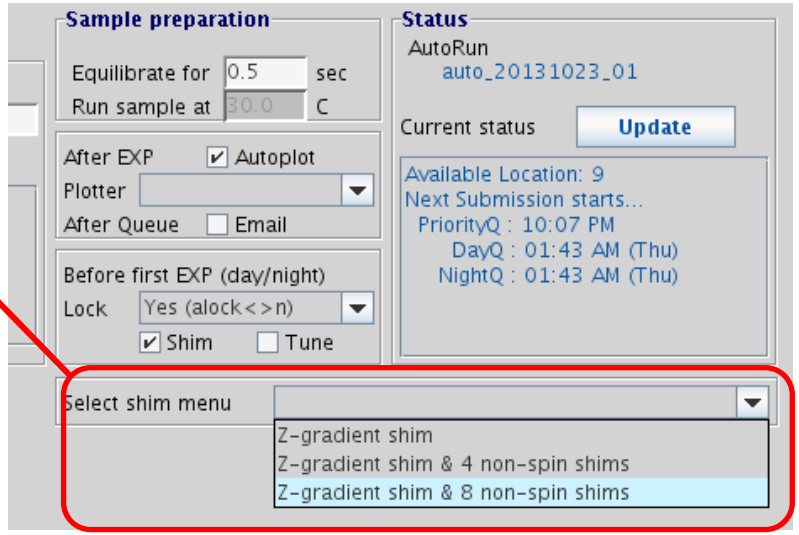
“fid” shimming uses the FID area, but can also use specific peak height or linewidth from the spectrum





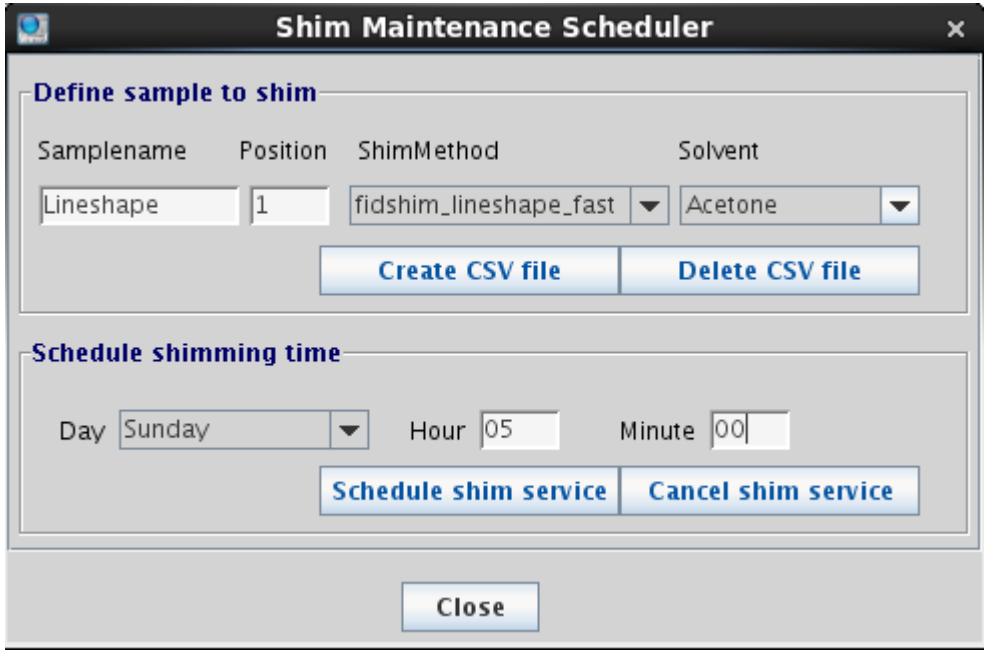
ProShim Shim Menu Editor

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



ProShim Scheduler

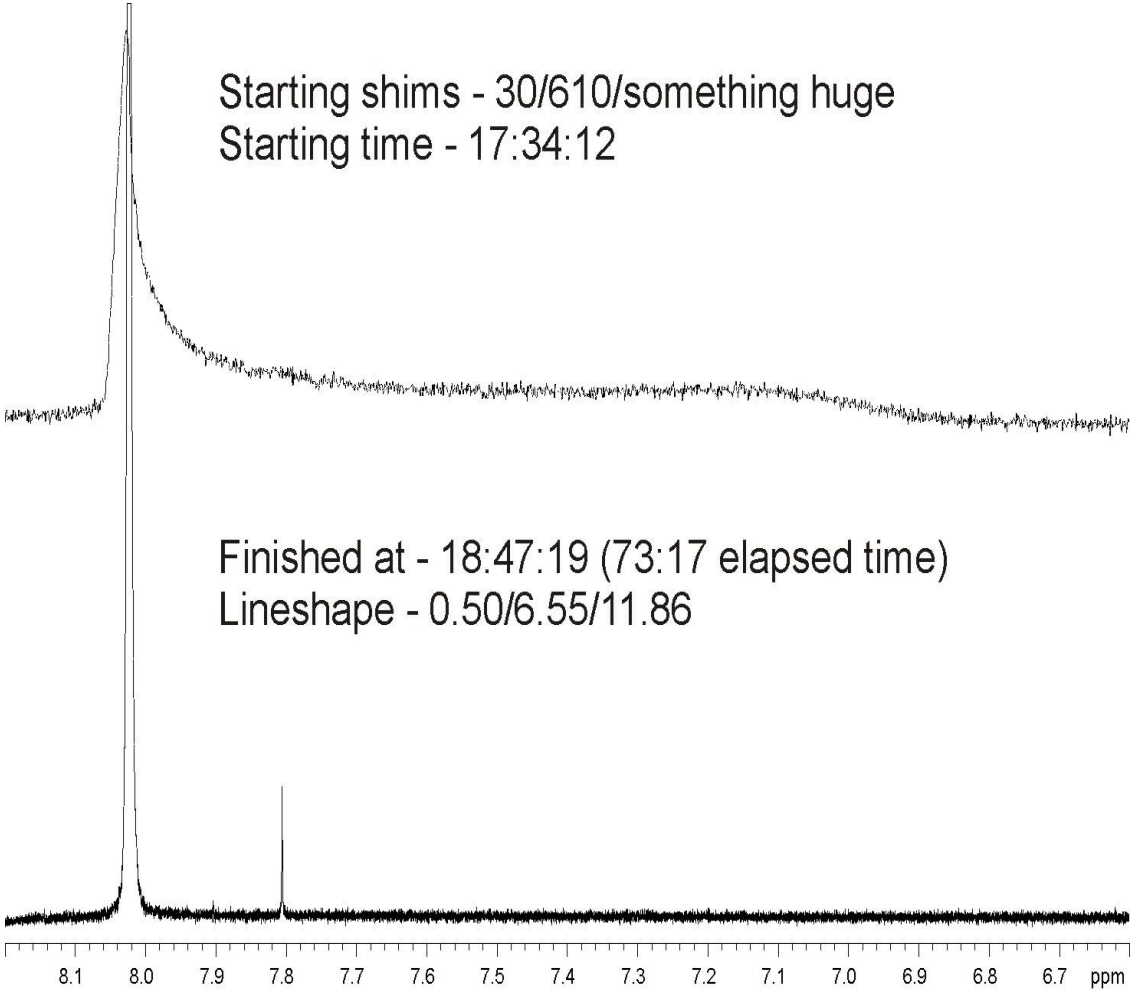
The final piece of the ProShim puzzle is a tool that allows you to schedule routine maintenance shimming to occur automatically.



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:

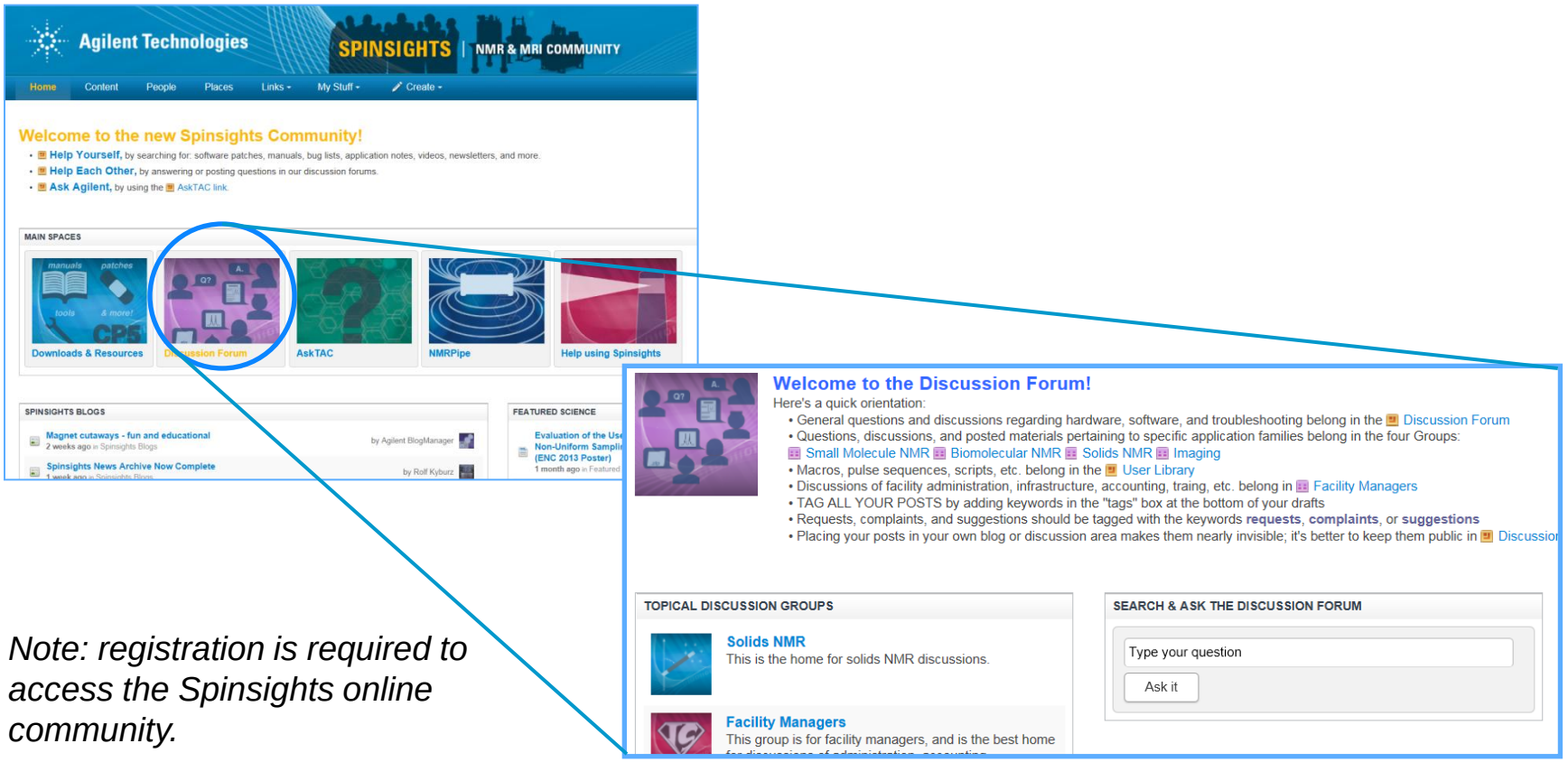
Ron Crouch
Krish Krishnamurthy
Dan Iverson
Software Team

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.



Note: registration is required to access the Spinsights online community.