Guide for manual acquisition on the user-operated spectrometers

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December 6, 2021

This guide is intended to take you through the basic steps required to acquire spectra manually. The document is formatted as a quick run through followed by discussions of the various points in more detail. This version of the document is illustrated with TopSpin 3, but most of the functions are basically the same in older or newer TopSpin versions, just the TopSpin graphics and where things appear in the menus are slightly different.

Please see the TopSpin help menu for an overview of the TopSpin layout and windows, and the video on the NMR website for tips for sample preparation - some more comments are included in the detailed section in this document.

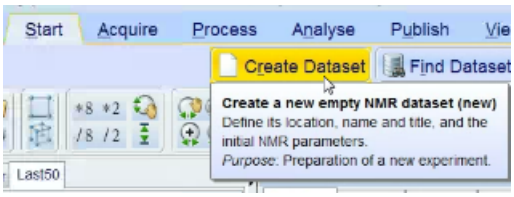


Figure 1: Figures in the margin at the start of each subsection show the relevant flow menu entries

```
rpar proton.std all
```

Figure 2: Below the flow menu is shown example command line commands

Notes on safety

Whilst the spectrometers and TopSpin do have some tools built in to help you to avoid damaging the system, there are plenty of things you can do which will cause problems or damage to the system. Always take care when running experiments manually. The workflow described in this guide is intended to help you to work in a safe way and take advantage of calibrations done by the service personnel to help you get good quality data. Particular things that can cause problems will be noted in this document.

If you are unsure about the effect of modifying any parameters, don't change them! Damage to the systems can be costly to repair and can result in considerable inconvenience to other users.

If you are unsure about anything please get in touch with us - usually during the day we can be found in B28 or elsewhere on the NMR corridor, and if you can't find us you can email us on the nmr@ch.cam.ac.uk address. We do frequently check this out of hours as well. We're always happy to answer questions and it's always safer to check with us if there's anything you are not sure about. Likewise if you think there are any problems with the systems please let us know - we do run a number of regular tests to try to check the ongoing performance of the systems but things can always go wrong and the sooner we know about problems, the sooner we can try to fix them or reduce their impact.

Overview of manual acquisition

HERE WE TAKE YOU THROUGH the basic steps required to perform acquisition of NMR spectra manually. The process can be summarised as:

- Create dataset
- Insert sample
- Choose experiment
- Prepare spectrometer
- Acquire data
- Make new dataset
- Choose new experiment
- Prepare spectrometer
- Acquire data
- ...

The steps required for spectrometer preparation will be different for the first experiment and for subsequent experiments.

TopSpin provides tools to semi-automate many parts of the process, and the predefined experiment parameter sets set up here are designed to minimise the amount of setup you need to do and to help ensure safe operation. Of course in some cases you will need to make changes to the preset parameters and how to do this and what you can reasonably change will be discussed later with examples.

Getting started

You will have a user login on the spectrometer PC, and when you come to the system the previous user should have logged out. Log into the PC and start TopSpin from the icon on the desktop (it is possible that multiple versions will be installed but the current version will always be linked from the desktop).

Once topspin has stared you can usefully open an existing dataset for yours from the browser, as this means that when you come to make a new dataset the parent directory where your own data are stored will already be selected.

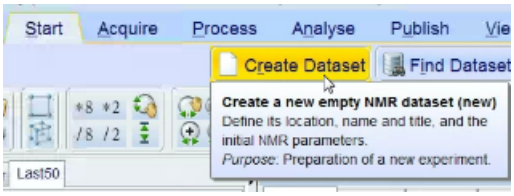
Most of the commands required can be accessed either from the flow menus or by command line commands. If you like typing, remember that if you leave the cursor over a button it will show the corresponding command in brackets.

Figure 3: Move the mouse over a button to show a tool tip with equivalent command line command in brackets.

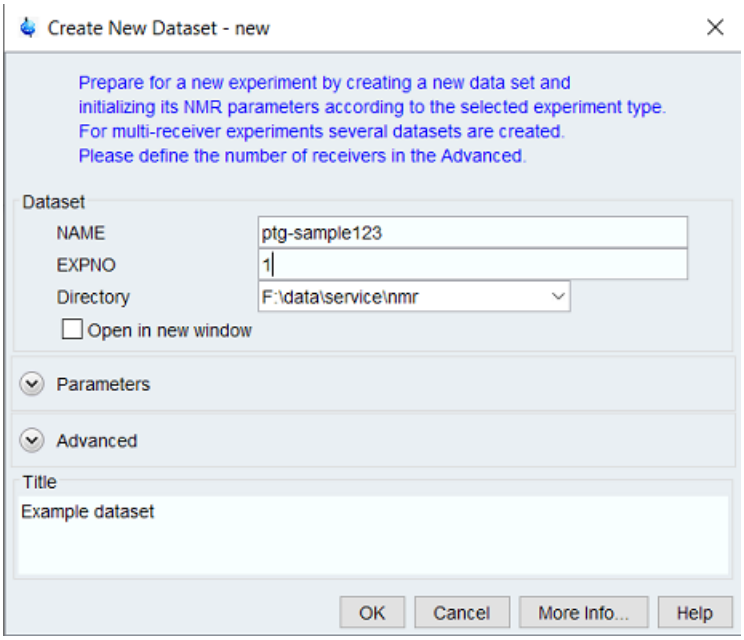
Making a new dataset

Most of what you do in TopSpin requires a dataset to work from - for example the **ATMA** command reads the nuclei set up in the current dataset and tunes the probe accordingly. We can create a new dataset with the command **new** or from the flow menu.

In the new dataset dialogue, set your dataset name appropriately, for example your initials followed by a sample code. The directory field should be `f:\data\<group>\nmr` where `<group>` is your PI's code (e.g. `rjp` for Phipps group). The expno field can be set to `1` - each acquisition will be in its own separate numbered folder. Click OK to create and open the dataset.

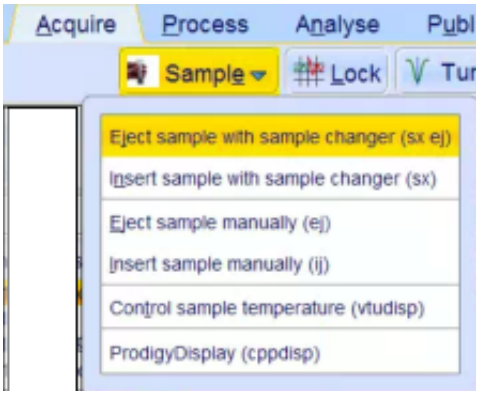


new



Getting your sample into the magnet

First put your sample into the spinner as normal and set the position using the depth gauge. The user-operated spectrometers may or may not have a functioning sample changer. If the system does, you can put the sample in the changer and use the command **sx n** where n is the sample changer position. Otherwise use the **ej** command to turn the lift on, wait for the lift air to be fully on, place your sample, and use the **ij** command to turn off the lift. Never drop a sample into the magnet without the lift air on as this risks sample damage.



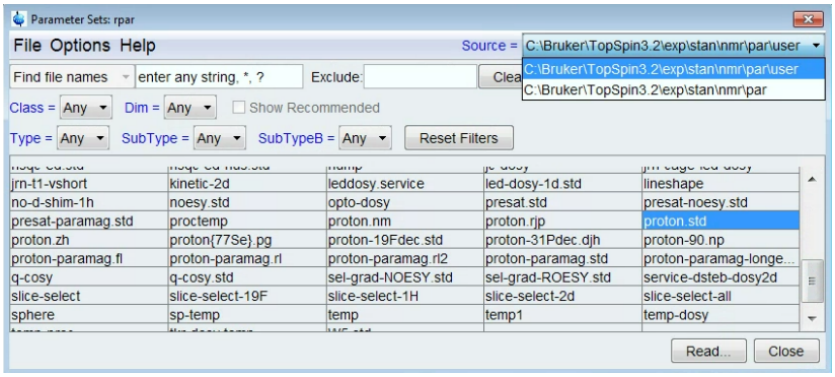
ej

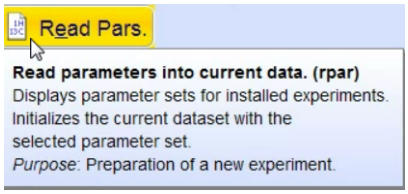
ij

sx <n>

Choosing your first experiment

Before preparing the spectrometer we need to select our first experiment. This is done using the **rpar** command ("read parameters"). **rpar** brings up the parameter selection window:



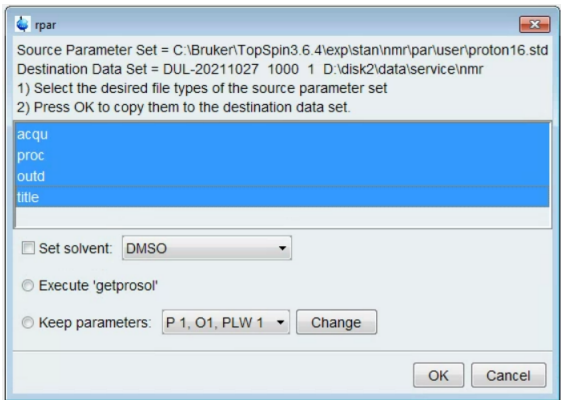


rpar

rpar proton.std all

The service team have created some modified parameter sets, and these are stored in the user subdirectory (or in future in a dedicated directory for service experiments), which can be accessed via the drop-down menu in the top right. We can start by selecting proton.std, and clicking the Read button.

Click OK read the parameters (ignore the other options for now!):



If you know the name of the parameter set you want, you can also read the parameters directly from the command line, for example to read the proton.std parameters use:

- **rpar proton.std all**

Read starting shims

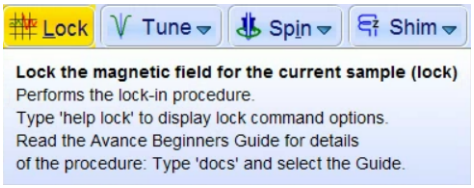
In order to make sure that the field homogeneity is reasonable, we can read in some default shim values. We do this with the command **`rsh`**. Select the relevant shim file and click read - the shim file current should be kept up to date. You can directly read this shim file with the command **`rsh current`**.

`rsh current`

Lock

The lock system serves two functions:

- Setting the total magnetic field so that peaks appear at approximately the exactly expected resonance frequncies
- Keeping the magnetic field exactly constant so that peaks do not move during long experiments



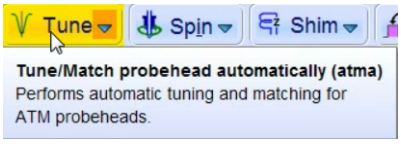
`lock`
`lock cdcl3`

The lock works by measuring the frequency of a reference signal (normally the 2H signal of the solvent) continuously thousands of times per second. The magnetic field is continuously adjusted to keep this frequency very precisely constant. This is necessary because NMR signals are rather sharp. Consider a proton peak with width 0.4 Hz linewidth at 400 MHz - that is a peak width of 1 billionth of the total frequency, so the magnetic field needs to be kept constant to within this level to avoid lineshape distortions. The **`lock`** command brings up the list of available solvents, or you can type e.g.:

- **`lock cdcl3`**

to lock onto chloroform. The lock system sets the frequency of the 2H solvent signal based on the known chemical shift, and if you acquire a spectrum with TMS in the sample it should appear rather close to oppm. As a result, explicitly adding a reference compound is not necessary in general.

Probe tuning



`atma`

The NMR probe is essentially a radio transmitter receiver aerial, which can be tuned so that its resonant frequency matches the NMR frequency. For all probes, the resonance frequency of the probe depends on the solvent used in the current sample, and for broadband probes we can tune to a variety of different nuclei with considerably different resonance frequencies.

In order to get optimal results, we need to optimise the resonance frequency on the current sample, and we need to repeat this if we

change nucleus on the broadband channel. Modern NMR probes have motors attached to the probe which can adjust the resonance frequency automatically under software control. In topspin this is done using the command **atma**.

The **atma** command checks the nuclei set in the current dataset, and tunes the probe for all of them.

Spinning

ro on
ro off

Spinning the sample averages out inhomogeneities in the magnetic field perpendicular to the sample axis. Historically, optimising the offaxis shims was relatively tedious and as a result spinning the sample was considered the norm for 1D experiments. These days maintaining good values for the offaxis shims is much simpler, and spinning is less necessary. Nonetheless it remains the case that sample spinning almost always results in an improved lineshape for 1D spectra.

The disadvantage of spinning is that it can result in the presence of sidebands around peaks, separated by the spinning frequency (usually 20Hz). The sidebands are more noticeable if the offaxis shimming is bad, and are usually strongly present in probes optimised for proton detection.

There are cases where spinning is very much not recommended:

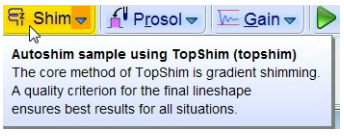
- 2D and selective 1D experiments (for convenience, don't spin if you are going to run selective 1D later)
- Proton experiments on the TCI cryoprobe on Glenlivet
- J-Young tubes (these tend to wobble more creating worse sidebands)

In these cases the artefacts caused by spinning generate more problems than spinning solves. Otherwise it is up to you to decide if it is beneficial!

Note that the optimum shim settings depend on whether you are spinning or not, so if you are going to run 1D experiments spinning you should turn the spinning on before shimming.

The commands **ro on** and **ro off** turn the spinning on and off.

Shimming



topshim ordmax=8 tunea
topshim convcomp tunea

NMR experiments place extremely high demands on the homogeneity of the magnetic field - from example proton signals can be a few tenths of a Hz wide, out of a total magnetic field of hundreds of MHz. As a result ideally we want the magnetic field to be homogeneous to better than 1 part in 10^{10}.

In order to achieve this the magnet has a series of coils which generate distorted magnetic field with shapes related to the spherical harmonic functions, and we can control the current in these coils to compensate for the distortions present. These are known as shim coils after the historical process of using metal shims to move the pole pieces of iron core electromagnets to improve the homogeneity.

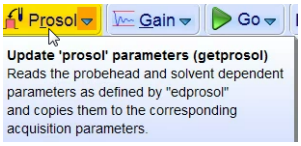
Because of the extreme homogeneity requirements, the differences between different samples (solvent, filling height, even tube differences) mean that we need to optimse the shims for each sample. The most convenient way of doing this is gradient shimming, which uses an imaging technique to measure the magnetic field variations over the sample, and adjust the shim functions to compensate and generate a more homogeneous magnetic field.

The current gradient shimming tool in topspin is **`topshim`**. This has some reasonable built in intelligence, and is optimised for different solvents. It was however developed before the more modern probes on Glengrant/Aberlour, and it can be affected by convection in the sample (only a significant issue on the cryoprobes on Glenlivet and in the future Arran), so just running **`topshim`** will usually not give the best results. The recommended shimming commands are:

- **`topshim ordmax=8 tunea`** for Auchtentoshan / Glengrant
- **`topshim convcomp tunea`** for organic solvents on Glenlivet / Arran

If you are running with sample spinning the **`tunea`** option (which adjust the low order offaxis shims with reference to the lock signal) can be omitted, but if you leave it in it should skip that step if the sample is spinning).

Reading in probe calibrations



`getprosol`

NMR experiments involve (sequences of) pulses, and to work optimally the lengths and amplitudes of the pulse must be calibrated to rotate the magnetization of the sample through well defined angles. Values for the pulses used in a given experiment are stored in parameter sets in principle (although the power levels in Bruker default parameter sets are set to zero for safety reasons), but in order to simplofy keeping track of the calibrations we store them separately from the parameter sets, so that they can be easily updated, and we read the calibrated numbers into a dataset after reading a parameter set.

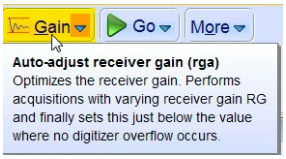
The use of a separate table of pulse calibrations also simplifies working with different probes on the same instrument - for example the cryoprobes require much less power than the room temperature probes, and can be easily damaged by excessive power. Forcing the

power levels to be read from the probe specific table prevents the case where a parameter set is loaded with powers appropriate for a room temperature probe, and then executed on a cryoprobe.

The table containing these numbers is called the ***prosol*** table (for ***probe*** and ***solvent*** dependent parameters, although with automatic tuning the solvent dependence is largely historical). The command to read in the calibrations relevant for a given experiment is:

- **getprosol**

Receiver gain adjustment



rga

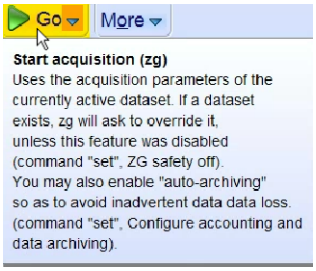
NMR spectrometers have a comparatively high dynamic range (compared for example to mass spectrometers), but the dynamic range present in NMR spectra can be extremely high. For example a tube of pure water is 110M in protons, but we can see signal from concentrations as low as easily 100μM in a single scan (six orders of magnitude dynamic range) and we might want to see even smaller signals.

The time domain signal in NMR is detected using an analogue-to-digital converter, and these have finite amplitude resolution. If a signal is too intense it will be clipped, drastically distorting the FID and ruining the data. On the other hand if the signal is too weak, it may be smaller than the lowest amplitude level of the digitiser and not be detected. Although NMR spectrometers have improved vastly in this respect it is still necessary (for proton detected expreiments at least) to scale the FID signal so that it fits into the range of the digitiser without being too weak.

This is done by amplifying the analogue signal before digitisation, by a parameter called the receiver gain, denoted ***rg***. This can be optimised for the current experiment by the command:

- **rga**

Running the first experiment



zg

Now we are ready to actually acquire some data. When acquiring data, topspin first zeroes any existing data in the dataset, then acquires new data and stores it once the experiment has finished. The command to do this is **zg** (zero and go).

This will acquire data according to the current parameters and tehn transfer the data to disk once the experiment completes, at which point you can process the data. We'll see that you can also process as the experiment is acquiring.

Subsequent experiments

ONCE WE HAVE ACQUIRED OUR FIRST EXPERIMENT we can continue with subsequent experiments on the same sample. Of course many of the setup steps have already been done and do not need to be repeated (sample insertion, shimming), but others will need to be done again for new experiments (reading new parameters, setting spinning, perhaps ATMA).

The first action in order to run a new experiment is to create a new dataset. We could use the **new** command as before, but the simplest option is to simply move to the next experiment number, which is done with the command **iexpno**. On the systems here this has even been shortened by a macro so you can just use the command **i**.

The **iexpno** command simply copies the existing parameters from the current dataset to the next experiment number assuming it doesn't already exist, and opens the new dataset. If the next experiment number already exists, it just opens it without modifying any parameters.

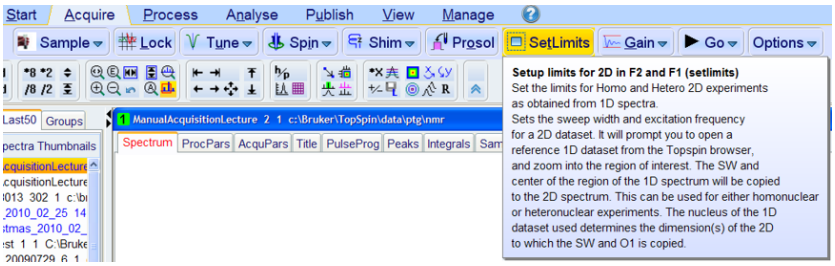
Once you have created a new dataset, you can choose your experiment and go through the relevant setup steps:

- Read experiment parameters with **rpar**
- Tune the probe with **atma**
- Set the spinning appropriately with command **ro on** or **ro off**
- Read in probe calibrations with **getprosol**
- Set any required parameters - **ns** etc.
- Adjust receiver gain with **rga**
- Acquire with **zg**

The atma step can be skipped for experiments just using protons, or if the X-nucleus has not been changed since the probe was last tuned. For example, if you ran tuned the probe to run a 1D proton, then you want to run a COSY, you don't need to repeat **atma**. Likewise if you have just tuned the probe for a 1D carbon, and you want to run a carbon HSQC, you don't need to repeat. However if you are not sure what X-nucleus the probe is tuned to, it's always safer to repeat **atma**. Note also that in general the probe can only be tuned to one X-nucleus at a time - so if you run a ^{19}F experiment, then a ^{13}C, and then you want to run a ^{19}F experiment again, you have to redo **atma**.

2D experiments

Most of the same considerations apply for 2D experiments as for 1D. The main differences are that you always want to run non-spinning, because otherwise you will get visible artefacts in the 2D spectra, and that you might want to optimise the spectral width and centre frequency, particularly of the indirect dimension. For homonuclear correlation experiments like COSY / NOESY this is easily done using the **`setlimits`** tool:



To use this, after reading the parameters for your 2D experiment, type **`setlimits`** or select from the Acquire flow menu.It will prompt you for what to do - *Do not click to close the popup window!* Open a 1D proton spectrum of your sample form the dat browser, zoom in on teh required region, and *then* click OK to close the dialogue box and set the frequencies.

For heteronuclear experiments, it might make sense to change the spectral width for the indirect dimension (not the direct dimension, as this will change the acquisition time of the FID which can cause problems in experiments with decoupling). You can set the parameter **`o2p`** to the ppm value in the middle of the X-nucleus range, and the parameter **`1 sw`** to a bit larger than the range of chemical shifts (10% larger, for example). You can see the parameters of the indirect dimension with the command **`eda`** or in the AcquPars tab of the dataset window click the A button to show all the parameters if it is only showing the relevant parameters list.

As an example, if you want to run a ^{1}H-^{31}P HMBC, and your 1D ^{31}P spectrum has peaks over a range from +50 to -100 ppm, you could set **`o2p`** to -25, and **`1 sw`** to 150.

Note that for the ^{1}H-^{13}C HSQC experiments, the experiment requires the carbon centre frequency to have a certain value, in order to implement compensation for the variety of J-couplings typically present. So you should not change the **`o2p`** value in this case.

Note also that the standard COSY experiments we use here, use what is called a double-quantum filter, which suppresses singlet peaks in order to make the spectrum look nicer. However, this means

that the **rga** command doesn't work. The default **rg** value in the standard COSY parameter sets should be OK in general, or you can change it to the value from a proton expeiment on the same sample.

While you are acquiring

```
tr
tr 2
halt
halt 2
stop
```

For longer experiments, there are a number of things you might want to do while the data is acquiring. You might want to check if you can see any signal at all, or if the signal to noise ratio is good enough that you can stop the experiment.

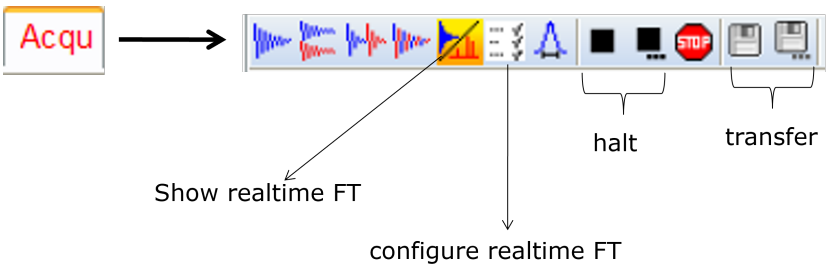
For full processing options, the **tr** command copies the data to disk (normally this is only done at the end of the experiment for 1D spectra), so you can process as normal. For a quick look, in the Acqu tab of the dataset you can show a real-time FT of the FID. You can't easily phase this, so it will usually look not phased, but may be enough to see if you have any signal or not.

For 2D (or higher) experiments, the data is written to disk at the end of each row, so the **tr** command is not needed. You can just process directly (e.g. **xfb** or the "proc spectrum" button in the process flowbar).

The **halt** command transfers any acquired data to disk (or finishes the current increment, for 2D experiments), and then stops the experiment. The **stop** command immediately stops the experiment without saving any data. It also suspends the spooler to avoid any other queued experiments running.

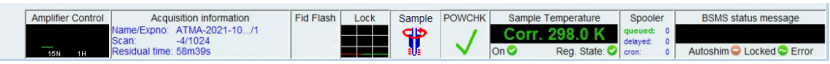
The **halt** and **tr** commands can take a number as an argument - this forces the command to be executed only after the next multiple of that number of scans. For some experiments in order to get good data you need to run a multiple of some number of scans to correcly suppres artefact signals - for example in selective 1D experiment you always need a multiple of 2 scans, so you could use the command **tr 2**. The required number of scans is indicated in the pulse program and shows up in the relevant parameters list.

These commands can be accessed from the Acqu tab ot the dataset window:



Status bar

The acquisition status bar can show you lots of things that are going on with the spectrometer. You can change what's visible, but the below would be fairly typical choices. Richt-click on the blnk area to the left of the staus bar (or under the command line if the status bar is not visible), to change settings or turn on or off.



These show:

- Amplifier control: this shows an indication of the pulse power being applied as green bars. If the probe is not properly tuned, much of this power will be reflected back to the amplifier, and this is shown by red bars. If you see red and green bars of similar intensity, stop the experiment and check with us.
- Acquisition information: This shows the currently acquiring dataset, the scan counter (and increment counter for 2D), and the residual time. Double click this section to open the currently acquiring dataset.
- Fid flash: This just indicates that some acquisition is happening. It doesn't flash in time with anything.
- Lock: this shows a small copy of the lock display. Double click to open the main lock display window.
- Sample: This shows whethere there is a sample in the magnet and if it's spinning. The example here shows a sample spinning, if not spinning the red arrow will be absent. If there is no sample there will either be a hand or question mark.
- POWCHK: this shows if the powercheck tool is active or not. This limits (only!) the maximum power applied on a given nucleus in an experiment. It is critically important for the cryoprobe systems as exceeding the allowed peak power can easily damage the probe. For room temperature probes it will not stop the most common source of damage which is excessive decoupling, but with standard parameter sets and the prosol table decoupling parameters should always end up set to sensible values.
- Sample Temperature: this shows the current sample temperature. For the newer systems it looks like this and will be green if the current probe temperature is at the set value, blue if it's lower

than the set value, and red if higher. If it says corr before the temperature that means some correction has been applied and the temperature will be fairly accurate, at least around room temp.

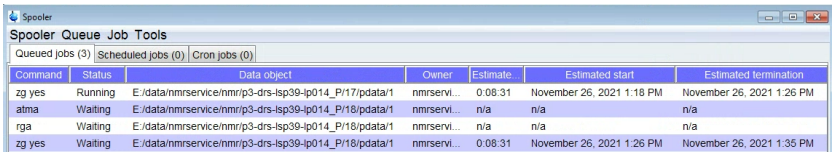
- Spooler. The command spooler shows queued commands. More details below.
- BSMS status message: Shows whetehr the system is locked and if autoshim is active. Here the lock is pending and autoshim is off.

Spooler

The command spooler is a useful way to queue up acquisition commands. For example, if you want to run an experiment, and you haven't yet tuned the probe, you need to do **`atma rga`** and **`zg`**. Normally you would have to wait for each command to finish before executing the next, but with automatic command spooling on you can type them immediately, and they will be queued up and will run in sequence.

You can also queue multiple experiments - after executing **`zg`** you can make a new dataset, read parameters etc., and do **`atma rga`** and **`zg`** in the new dataset.

Double clicking in the spooler section of the status bar opens the list of currently spooled commands:



For each command it shows the command, the status (running, queued), the associated dataset, the duration (if known), and the expected start and end times. The start and end times don't account for queued jobs which have an unknown duration.

If you realise you have made a mistake when spooling commands, like forgetting to add **`atma`**, you can right-click on entries in the spooler to delete them, and then add the correct desired sequence of commands.

Note also the commands are executed on a dataset, exactly as it is at the time the spooler runs the command, not at the time you type the command. So if you realise you forgot to change the number of scans before queueing an experiment, for example, you can go back to the dataset before it starts and change ***`ns`***, and it will run with the new value.

Going into more detail

IN THIS PART WE GO INTO MORE DETAIL about the steps outlined above. We will go through more of the options for various commands, and a bit more theoretical background.

Sample preparation

In addition to the general guidance in the training video, some additional comments may be useful to help you get the best spectral quality.

- Use pure, *dry*, (deuterated) solvent.
- Use the right amount of sample: Don't be tempted to use less than 40 mm filling depth (about 550 µL).
- Make sure your sample dissolves!

Using dry solvent makes it easier to see exchangeable protons. If the solvent is quite dry and the sample concentration not too high, you can often even see correlations to exchangeable protons in COSY / HMBC experiments which can be useful for assignment. The HSQC experiment will confirm which protons are not bonded to carbons. Remember that most solvents are hygroscopic so take care if storing bottles for extended periods. Chloroform bottles should be stored in the dark to prevent phosgene formation, and storing over activated 4Å molecular sieves helps to remove water.

If the sample volume is too small, it will be difficult or impossible to shim the sample well, and the gain from increased concentration will be cancelled out by the spreading out of the signal. The intensity of NMR signals is essentially proportional to concentration, so having much more solvent than needed (i.e. reduced concentration) will reduce your S:N ratio, which may be important for low sensitivity experiments e.g. carbon or HMBC.

Undissolved solid material in the sample can affect the shimming substantially. If you find your sample is not sufficiently soluble you can always add more solvent, but you must make sure that the sample is well mixed - Concentration gradients in the sample will lead to the solvent signal looking well shimmed but your sample signals not. Consider preparing the sample in a small vial, where it's easy to mix the sample well and check for solubility, and transferring from there to the NMR tube. If there is a lot of suspended material, you can filter through a plug of glass (not cotton) wool tightly packed into a Pasteur pipette. If you have transfered your solution to the

tube and realise there is not enough sample, add a little more solvent and shake the sample well to ensure good mixing.

Remember that the signal to noise ratio in NMR experiments is proportional to the square root of the number of scans, so if sensitivity is the limiting factor in your experiments, doubling the amount of sample means the experiment only takes ¼ of the time. If you have very limited amounts of sample, come and talk to us about the best way to proceed , before making up the sample. Very high sample concentrations can also cause problems with broadening of signals in proton spectra, so don't feel the need to add hundreds of mg of sample just because it's available. For samples of reasonable molecular weight with no complications a few tens of mg will be sufficient even for carbon spectra.

Sample tubes

Try to avoid damaging tubes - ones the tubes are damaged there is an increased risk of samples breaking when they are inserted into the probe. In particular for samples submitted to the service you must use undamaged tubes of 7 inch minimum length, as shorter or damaged tubes cannot be picked up by the sample changer on the service instrument. Any scratches on the tube in the region of the sample can affect shimming, so avoid using scratched tubes for important samples.

Tubes should be dry - don't use an oven for this, as the tubes can warp, blowing dry nitrogen is preferred. The tubes should ideally be stored completely flat or basically upright, to prevent warping. If tubes are not completely straight, this can cause spinning problems.

Finally it is good practice to wipe the outside of the tube after putting it in the spinner, to prevent dirt getting into the probe.

Sample temperature

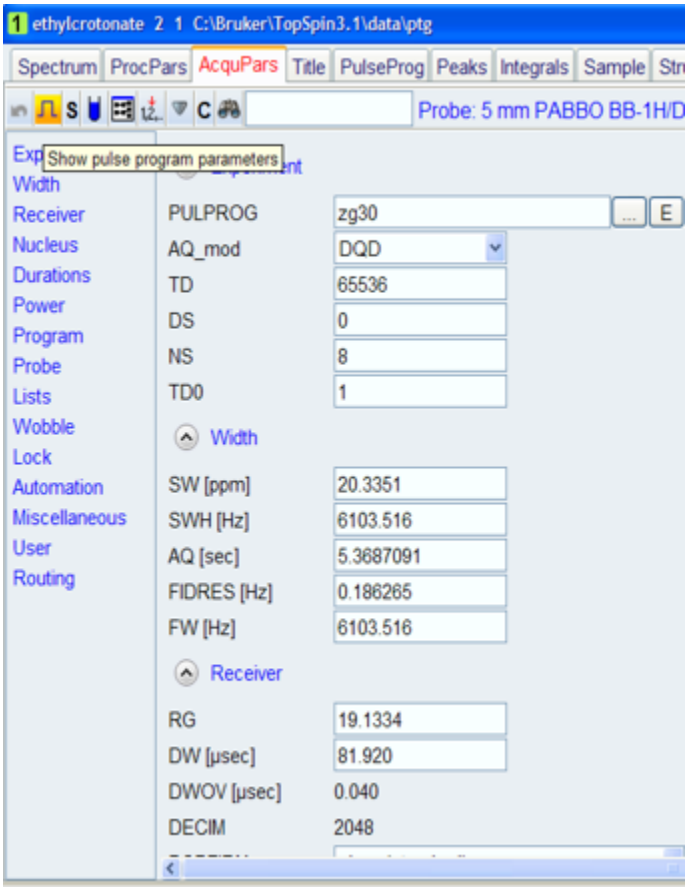
Because work at temperatures other than ambient requires special spinners and other considerations, this will be documented elsewhere. See the service if you need work at high or low temperatures. To give you an idea of what can be done, Glengrant is in principle capable of temperatures from $-40\,^{\circ}\mathrm{C}$ to at least $120\,^{\circ}\mathrm{C}$ without too much trouble, and even lower temperatures with a nitrogen evaporator (this involves substantially more work and time).

The temperature should be set to 298 K and this will show up in the spooler. Some change will happen when you insert the sample, but if the indicated sample temperature is significantly different from this before you insert the sample or doesn't stabilise after a few minutes please contact us immediately.

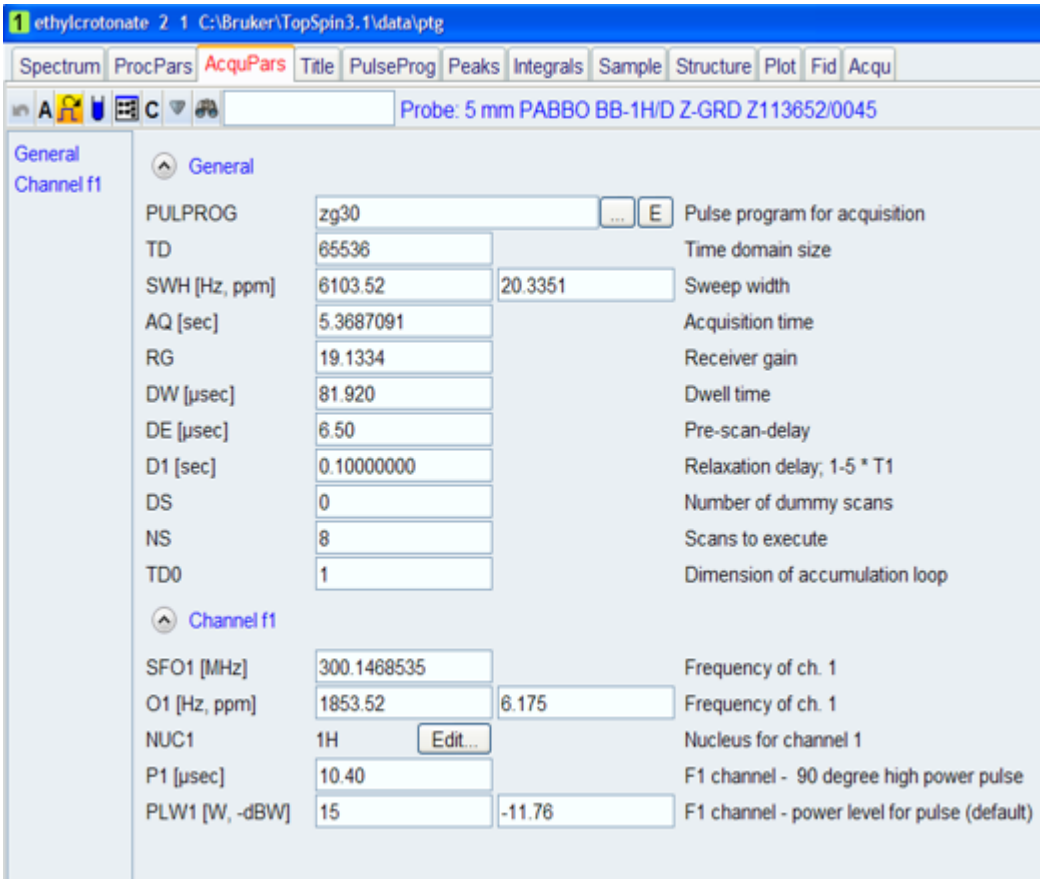
Modifying experimental parameters

eda
ased

The standard .std parameter sets will work well in most cases, but sometimes you will want to modify parameters. It is important to understand what parameters you can reasonably modify safely! Always check with the NMR team if you are unsure. To view the parameters of an experiment, after reading the parameters with **rpar**, you can click on the AcquPars tab in the dataset window. This will show either a long list of all parameters, which can be forced with the command **eda**:

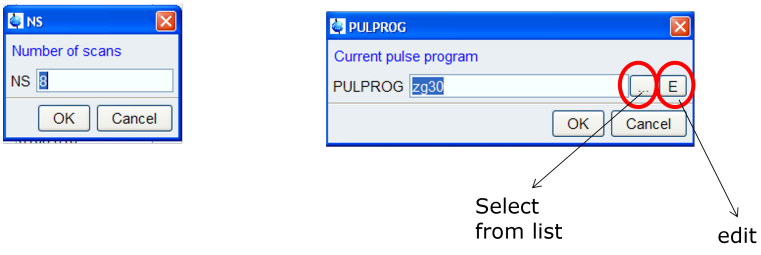


or a short list of experiment-relevant parameters, which can be forced with the command **ased**:



Usually most of the parameters you care about will show up in **ased**, the exception is the parameters for the indirect dimension of 2D experiments which are only visible in **eda**. You can click on entries in the list on the left side to go to a particular section of the parameters, e.g. eda clicking "nucleus" will take you to the section where the different nuclei used in the experiment are defined.

You can modify parameters in a number of ways, as well as entering values in the **eda** or **ased** displays. You can type the parameter name to open a dialogue box, for example ***ns*** or ***pulprog***:



For parameters that take a file as input (***pulprog***, or **vdlist** for exam-

ple) you can enter the name in the dialogue box directly, or select from a list of available files, and you can edit the current file (but you should only do this for example for lists that you have created).

You can also type the parameter name and value directly on the command line, for example:

```
ns 8
```

to set the number of scans to 8.

Note that parameter changes are immediately saved! If you want to make sure what parmaeters were used when an old dataset was acquired, you can view the "status" parameters - these are a copy of the parmaeters made when the experiment is run. They can be viewed in the **eda** display by clicking the S button at the top of the dataset window.

Parameter details

The relevant parameters list is divided into a sections:

More about shimming

TopSpin dataset structure

Receiver gain effects