

# Bruker Instructions

July 29, 2014

**AV500:** Day queue runs from 8 AM to 6 PM.  
Maximum length of time for any one experiment is 30 minutes.  
Total time for any user is 1 hour.

Night queue runs from 6 PM to 8 AM.  
Maximum length of time for any one experiment AND total time for any user is 3 hours.

**AV400:** Use FACES system to reserve time.

**Use enough solvent** to bring the height of liquid to at least 4 cm. It DOES NOT HELP IN ANY WAY to use less solvent!  
**Do NOT have particles** of any kind floating in the tube.

**Use a pen to label your NMR tube** on the top of the tube, or on the cap. Do NOT attach any kind of label to the upper part of the tube.

**Always report broken NMR tubes to me.** You are responsible for cleaning up glass fragments and spilled chemicals outside the magnet, but I must be informed so I can check that there has been no damage to the probe.

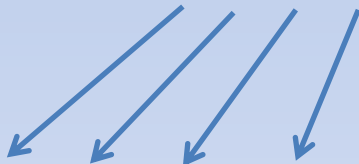
## Data folder structures in Automation

### Bruker

/home/yourname



*name*



"1" "2" "3" "4" ... (experiment number  
or "expno")

### Agilent/Varian

/home/yourname/vnmrsys/data



(Automation  
i.e. New Study)

"*samplename*\_PROTON\_01.fid"  
(folder holds procpa, text, fid)

First experiment run will be saved  
as "1", the second as "2" etc.  
Each of these folders contains the files  
that make up the NMR data.

# To submit experiments use the IconNMR screen

**6. If you want to submit to the night queue click on this box.**

**5. If you want to change parameters click on this box (necessary to update the "Time" field)**

**1. Click here to login or logout**

**2. Select your holder. AV400: Select any available holder**

**3. Click on "Add"**

**4. Fill in Name, change expno if desired, select Solvent, select Experiment, Title**

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	Running	Running	/home	test_sample	1	CDC13	chloroform-d	N 1d_PROTON			00:00:51	morin	14:00 Thu Dec 05 2013
2	Running	Running	/home	test_sample	2	CDC13	chloroform-d	N 1d_C13			00:07:32	morin	14:01 Thu Dec 05 2013
3	Queued	Queued	/home	test_sample	3	CDC13	chloroform-d	N 1d_C13_DEPT1			00:17:40	morin	14:08 Thu Dec 05 2013
4	Available	Available											
5	Available	Available											
6	Available	Available											
7	Available	Available											
8	Available	Available											
9	Available	Available											
10	Available	Available											
11	Available	Available											
12	Available	Available											
13	Available	Available											
14	Available	Available											
15	Available	Available											
16	Available	Available											

**7. To add other Experiments go back to steps 3, 4 and 5, click on the holder then click on "Submit"**

**8. The AV400 will eject the spinner and ask you to replace the tube with your tube**

**9. To start processing double click on a completed entry**

#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig	Remarks
2	2013-12-05 14:06:21	1	test_sample	2	1d_C13		✓	✓					morin	/home/morin		
1	2013-12-05 14:00:53	1	test_sample	1	1d_PROTON	✓	✓	✓	✓	✓	✓	✓	morin	/home/morin		sref: reference peak not found default calibration done

To process data use the TopSpin screen

Click Process to see this screen

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows the 'Process' menu selected, with options like 'Proc. Spectrum', 'Adjust Phase', 'Calib. Axis', 'Pick Peaks', 'Integrate', and 'Advanced'. Below the menu is a toolbar with various icons for file operations and data processing. The central area features a plot of an NMR spectrum with peaks visible. The x-axis is labeled 'ppm' and ranges from 10 to 0. The y-axis is labeled 'Intensity' and ranges from 0 to 14. A file browser on the left shows a directory structure with 'test\_sample' selected. At the bottom, there is a status bar with various system and acquisition parameters.

Click to show spectrum

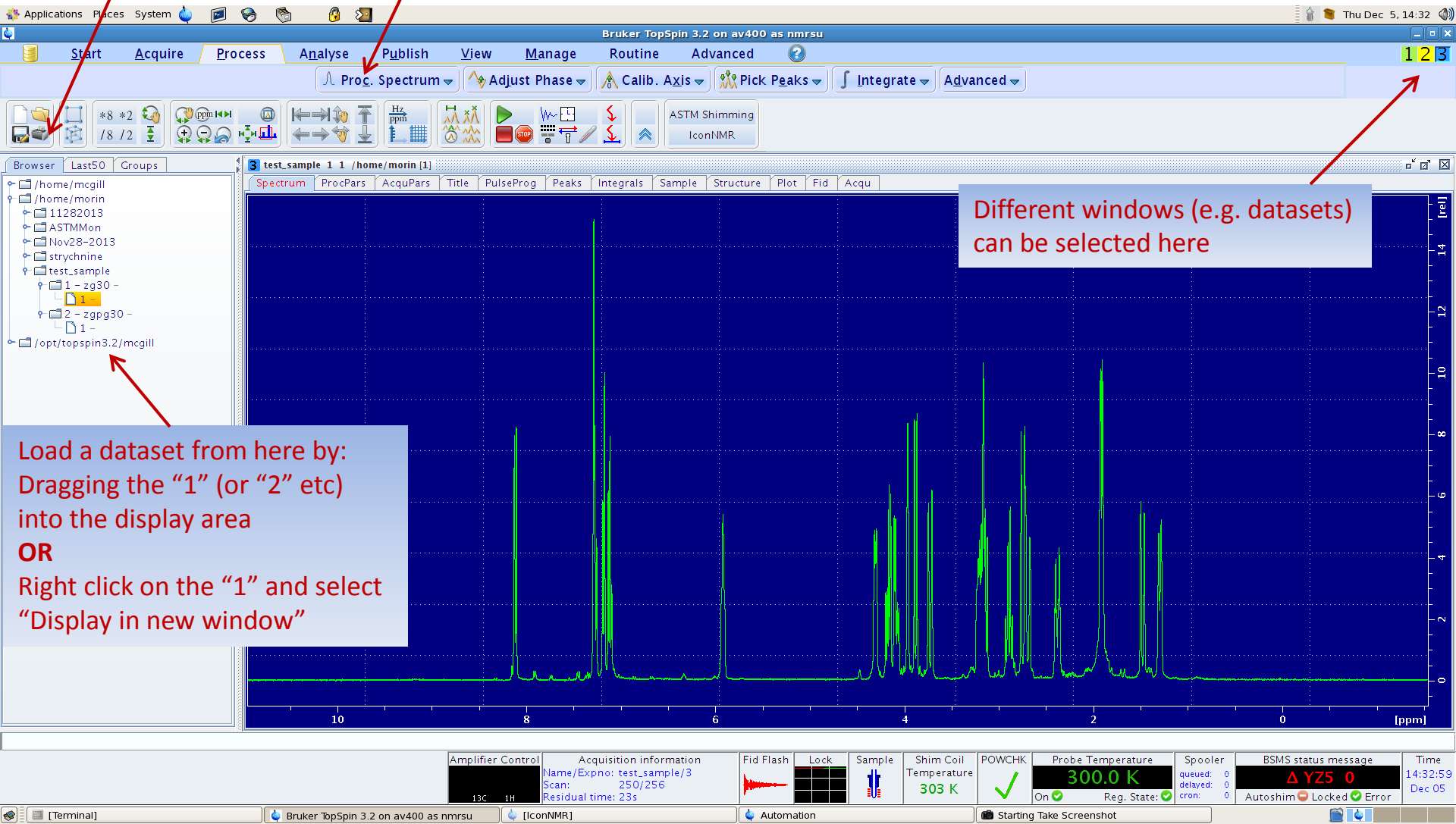
Click to show Plot screen

Right click in here to sort by date and/or show date

If your data dir is not showing: Right click in here: Select the entry "Add New Data Dir ....". Fill in the DIR field and click OK.

Click here to plot

Click here to process the data if need be



Different windows (e.g. datasets) can be selected here

Load a dataset from here by:  
Dragging the "1" (or "2" etc)  
into the display area  
**OR**  
Right click on the "1" and select  
"Display in new window"

Peak picking, click here

The screenshot displays the Bruker TopSpin 3.2 software interface. At the top, the menu bar includes 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', 'Manage', 'Routine', and 'Advanced'. Below the menu bar is a toolbar with various icons for spectrum processing. The main window shows an NMR spectrum with a blue background and green peaks. The x-axis is labeled 'ppm' and ranges from 10 to 0. The y-axis is labeled '[rel]' and ranges from 0 to 14. A toolbar above the spectrum contains icons for peak picking, including a region selection icon, an individual selection icon, a delete icon, and a save icon. Annotations with arrows point to these icons and provide instructions: 'Click on this to pick peaks by defining regions' points to the region selection icon; 'Select this to pick peaks by selecting individually' points to the individual selection icon; 'Select this to delete ALL picked peaks' points to the delete icon; and 'To exit peak picking routine and save' points to the save icon. A status bar at the bottom shows 'zg: acquisition finished', 'no acquisition running', and various system parameters like 'Shim Coil Temperature 304 K' and 'Probe Temperature 300.0 K'. The system tray at the bottom right shows the time '14:33:23 Dec 05' and the date 'Thu Dec 5, 14:32'.

Click on this to pick peaks by defining regions

Select this to pick peaks by selecting individually

Select this to delete ALL picked peaks

To exit peak picking routine and save

Integration, click here

The screenshot displays the Bruker TopSpin 3.2 software interface. At the top, the menu bar includes 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', 'Manage', 'Routine', and 'Advanced'. Below the menu bar is a toolbar with icons for 'Proc. Spectrum', 'Adjust Phase', 'Calib. Axis', 'Pick Peaks', 'Integrate', and 'Advanced'. The main window shows an NMR spectrum with a blue background and green peaks. The x-axis is labeled 'ppm' and ranges from 10 to -2. The y-axis is labeled '[rel]' and ranges from -2 to 12. A file browser on the left shows the directory structure: /home/mcgill, /home/morin, 11282013, ASTMMon, Nov28-2013, strychnine, test\_sample, 1 - zg30, 2 - zgpg30, 1 -. The status bar at the bottom contains various system information: Amplifier Control, Acquisition information (no acquisition running), Fid Flash, Lock, Sample, Shim Coil Temperature (304 K), POWCHK (On), Probe Temperature (299.9 K), Spooler (queued: 0, delayed: 0, cron: 0), BSMS status message (YZ5 0), and Time (14:34:05 Dec 05).

Annotations on the screenshot include:

- An orange box at the top with the text "Integration, click here" and a red arrow pointing to the 'Integrate' button in the toolbar.
- A blue box on the left with the text "Click on this to integrate (by dragging mouse from left to right)" with an arrow pointing to the 'Integrate' icon in the toolbar.
- A blue box in the center with the text "Select this to delete ALL integrations" with an arrow pointing to the 'Delete All Integrations' icon in the toolbar.
- A blue box on the right with the text "To exit integration routine and save" with an arrow pointing to the 'Save' icon in the toolbar.
- A blue box at the bottom with the text "Calibrate the integrals by putting cursor on one, right clicking and selecting 'Calibrate Current Integral'" with an arrow pointing to the 'Calibrate Current Integral' icon in the toolbar.

Plotting, click here

The screenshot shows the Bruker TopSpin 3.2 software interface. The main window displays a 1H NMR spectrum of morin. The x-axis is labeled 'ppm' and ranges from 5.0 to 0.0. The spectrum shows several peaks, with a prominent one at approximately 1.0 ppm. The interface includes a menu bar at the top with options like 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', 'Manage', 'Routine', and 'Advanced'. A toolbar below the menu bar contains various icons for file operations and data processing. On the left side, there is a 'Browser' pane showing a file tree structure. In the center-left, there is a 'Limits' section with buttons for 'Limits', 'Expand', and 'Display'. The 'Plot' button in the top menu is circled in red. The 'Limits' button in the toolbar is also circled in red. The status bar at the bottom shows 'no acquisition running' and '300.0 K'.

Obtain a plot by clicking here

If the plot does not have the same expansion as the spectrum click here ("Apply user limits ...")

Can use scroll button to increase or decrease vertical scale before plotting



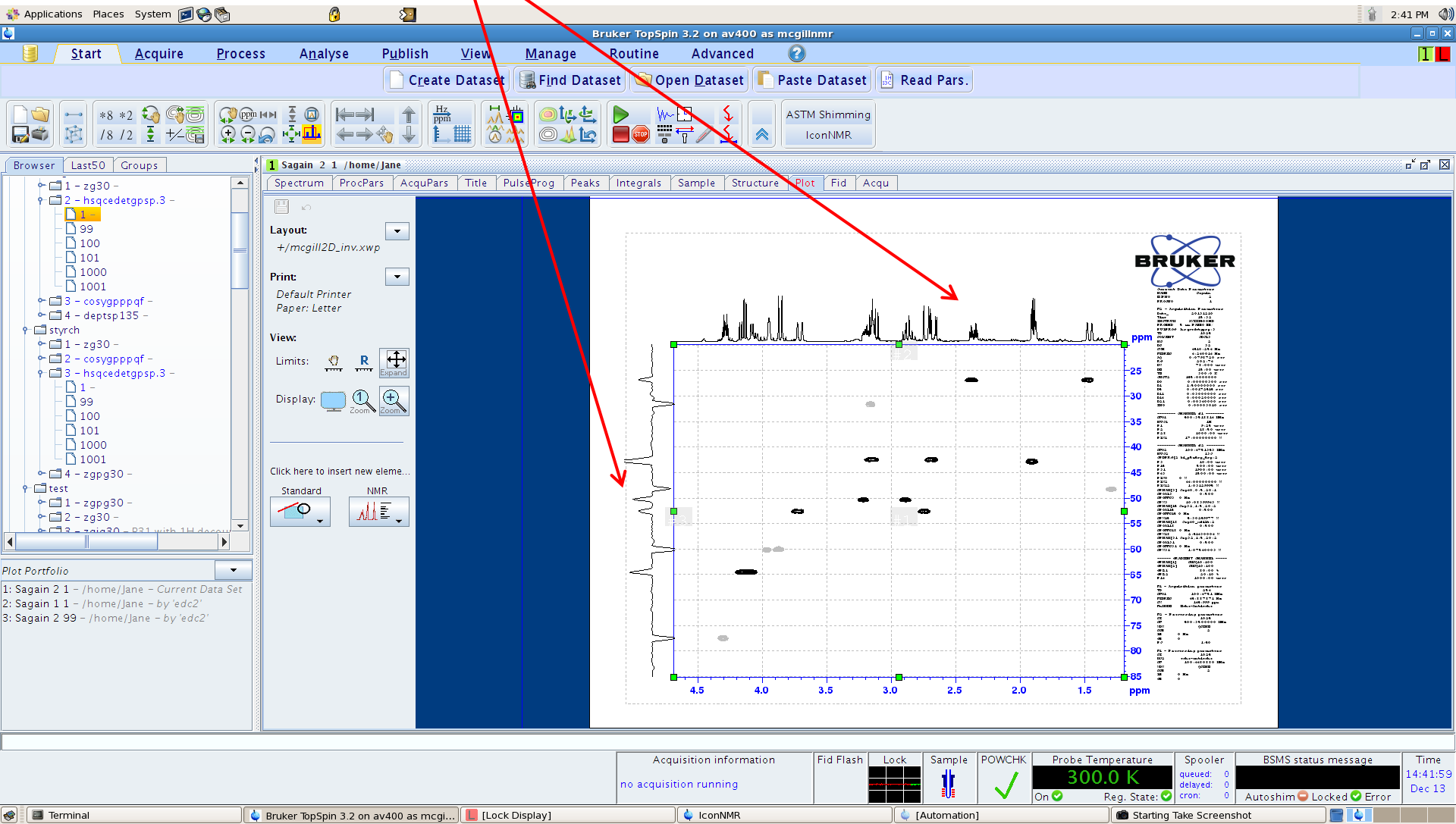
The scroll button changes vertical scale of the 1D spectrum if this box is selected. Deselect to change the vertical scale of the 2D spectrum.

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows a 2D NMR spectrum with a 1D projection at the top. The x-axis is labeled 'F2 [ppm]' and ranges from 8 to 2. The y-axis is labeled 'F1 [ppm]' and ranges from 120 to 0. The spectrum shows several peaks in the 1D projection and a 2D contour plot below it. A red arrow points from the top text box to a small green square in the top right corner of the spectrum plot area. Another red arrow points from the same text box to a small green square in the bottom left corner of the spectrum plot area. A third red arrow points from a text box to the left side of the spectrum plot area. A fourth red arrow points from a text box to the bottom left corner of the spectrum plot area. The interface includes a menu bar (Start, Acquire, Process, Analyse, Publish, View, Manage, Routine, Advanced), a toolbar with various icons, and a browser window on the left showing a file tree. The status bar at the bottom displays acquisition information, including 'no acquisition running', 'Probe Temperature 300.0 K', and 'BSMS status message'.

Right click to insert 1D spectrum instead of the projection by selecting External Projection

Right click here to move baseline to center

Clicking in these regions will allow you to change the vertical scale of the 1D spectra



# Use the "IconNMR: auto Online Controls" window to monitor the acquisition

Click here to see your spectrum during the acquisition

Click here to halt the acquisition And save your data

Automation In Progress

Current Experiment Info

Holder No: 2

Name: strychnine

No.: 1

Time Remaining: 26 Min 28 Sec

Current Expt : N 1d\_C13 512 scan

View

Lock

FID Spectrum

Controls

Halt Autoplot

Stop Automation Search

Stop Automation

Amplifier Control Acquisition information Fid Flash Lock Sample Shim Coil Temperature POWCHK Probe Temperature Spoofers BSMS status message Time

1% TH Name/Expt: strychnine/1 Scan: 7/512 Residual time: 26m29s

302 K 296.2 K

On Reg. State: Auto Shim Locked Error

10:01:37 Feb 11