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.

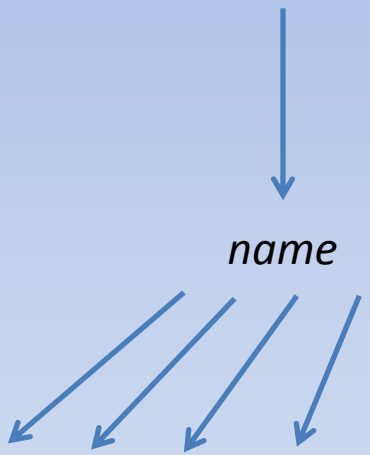
Use a pen to label your NMR tube on the top of the tube, or on the cap. Do NOT attach any kind of label to the upper part of the tube.

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

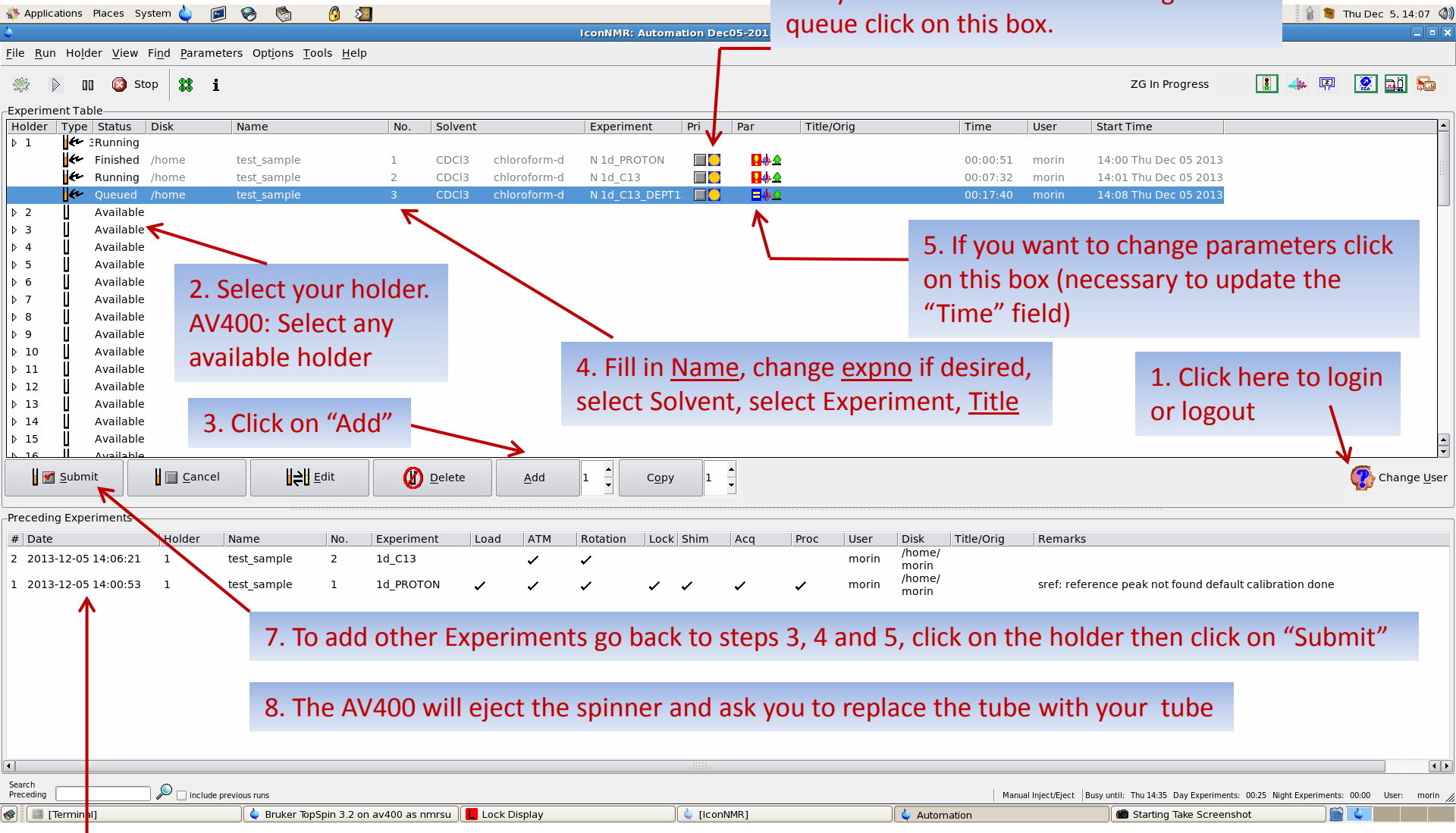
/home/*yourname*/vnmrsys/data

(Automation
i.e. New Study)

*"samplename*_PROTON_01.fid"
(folder holds procpar, text, fid)

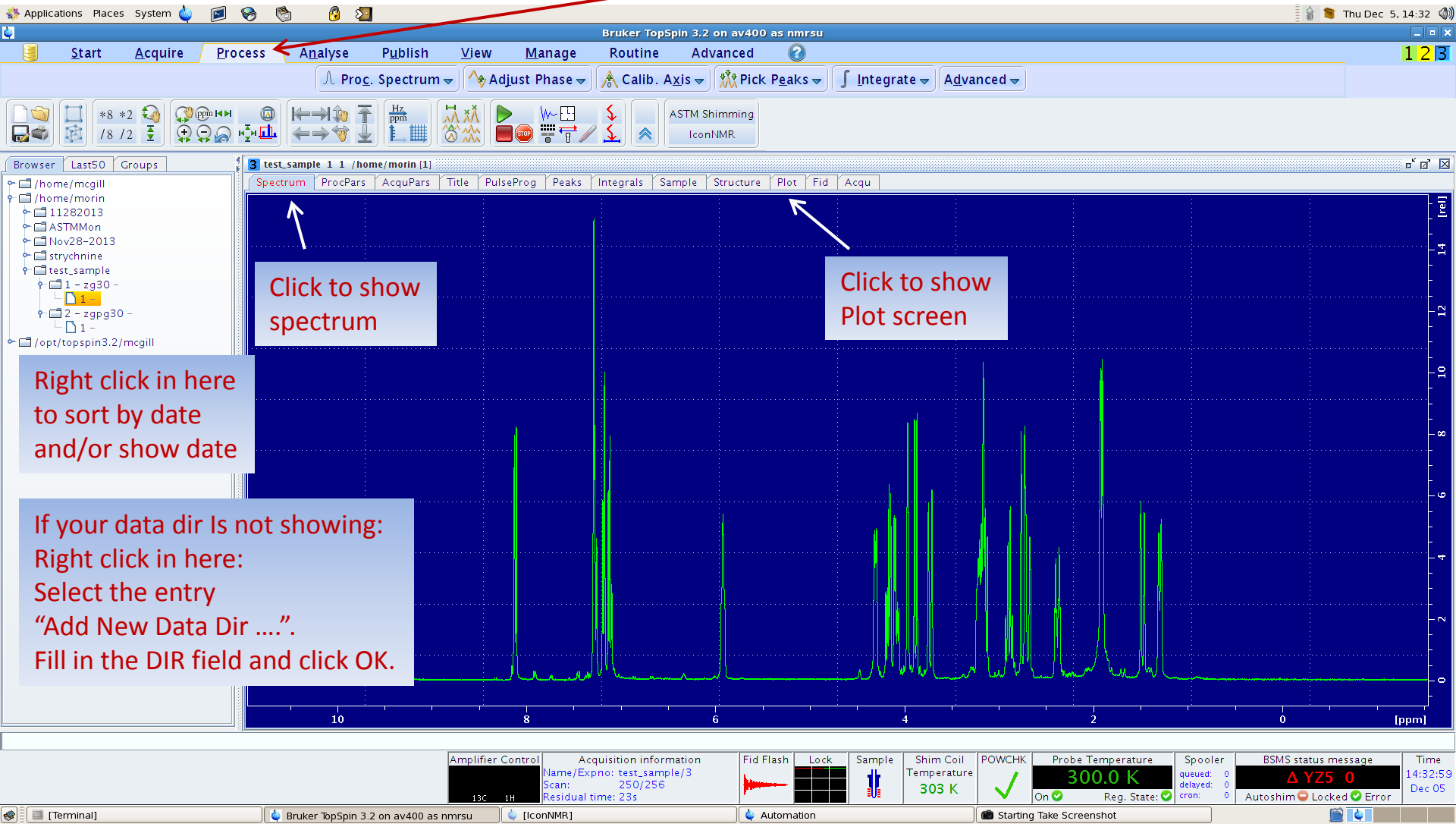
First experiment run will be saved as "1", the second as "2" etc.
Each of these folders contains the files that make up the NMR data.

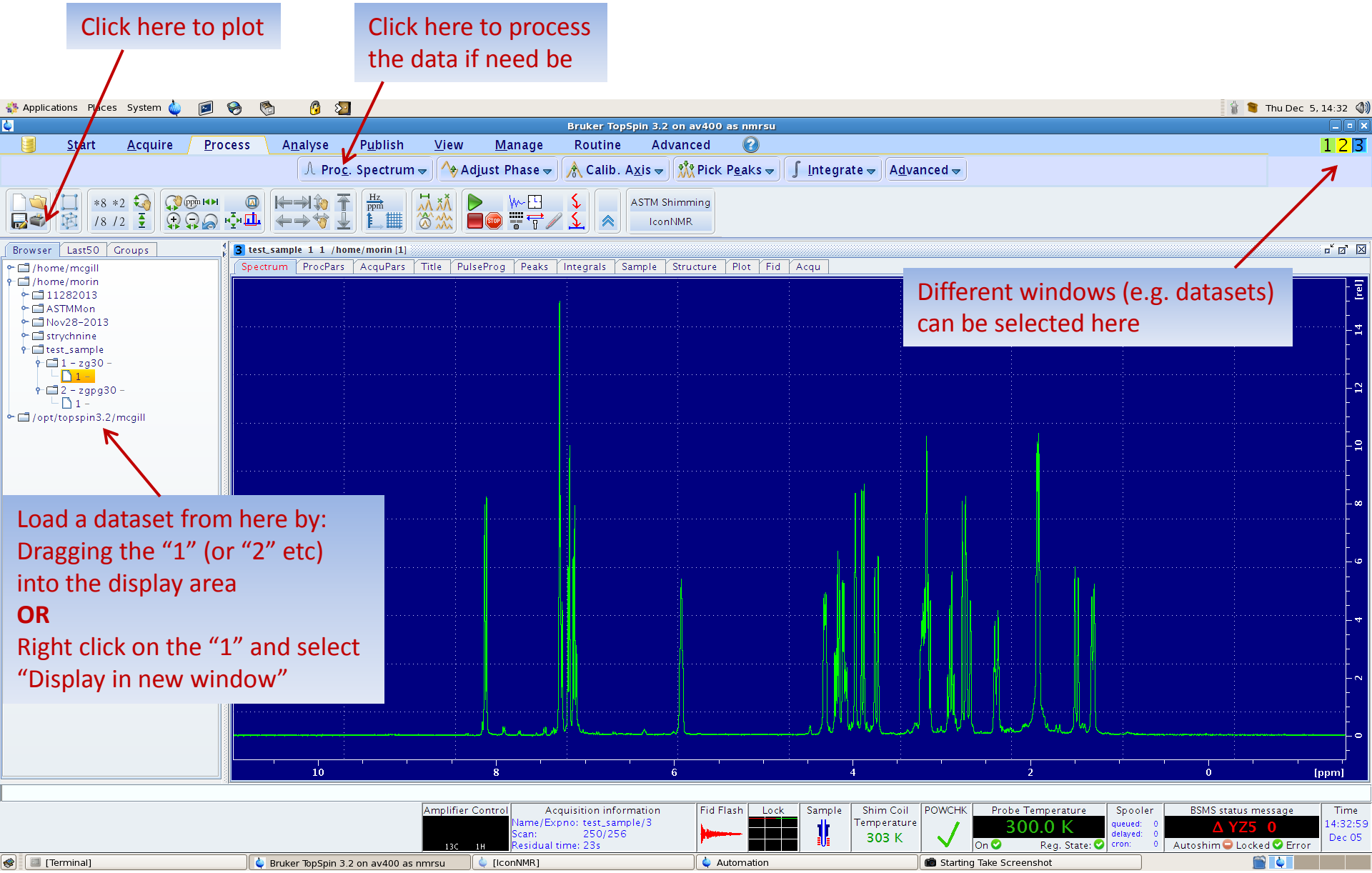
To submit experiments use the IconNMR screen

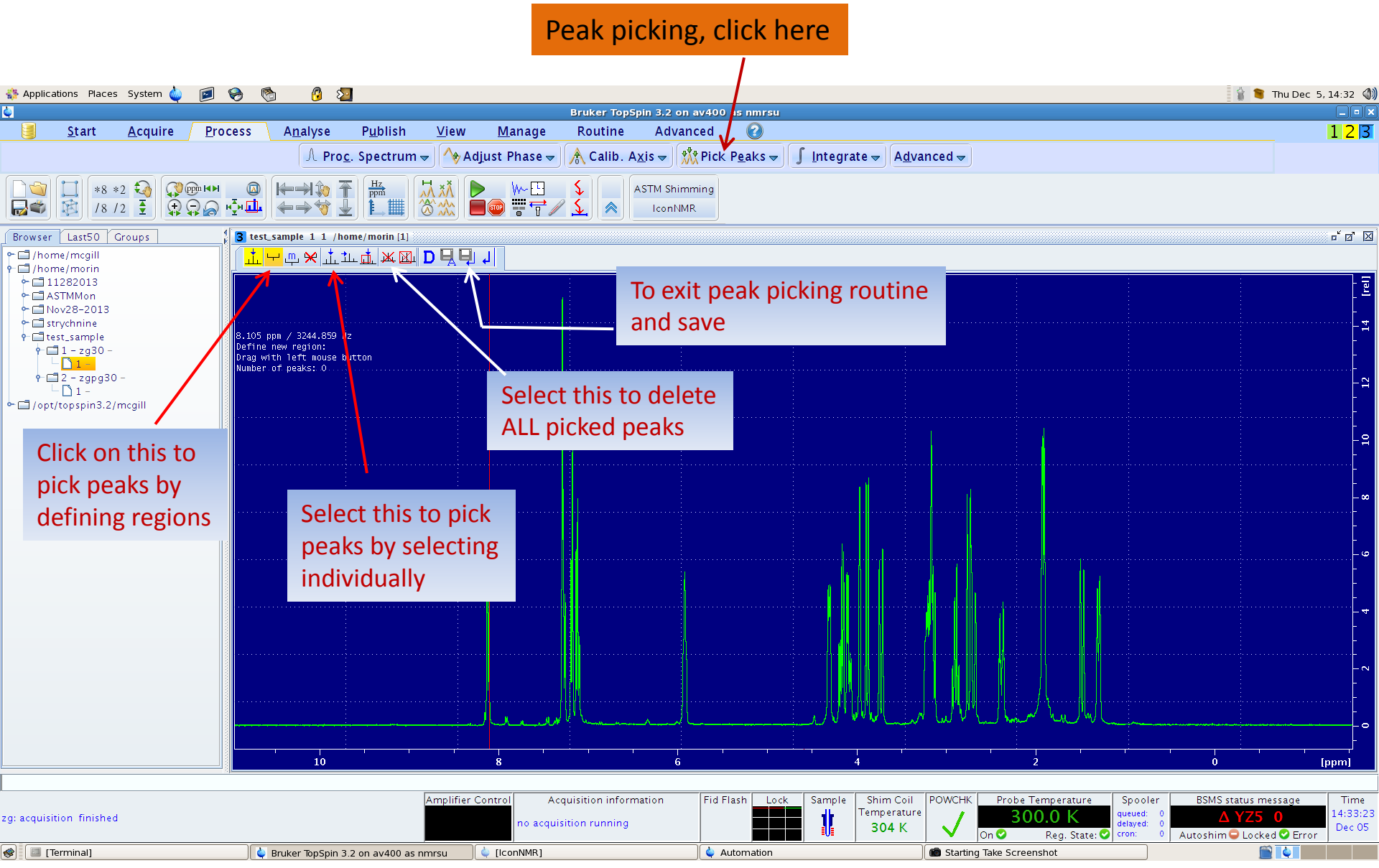


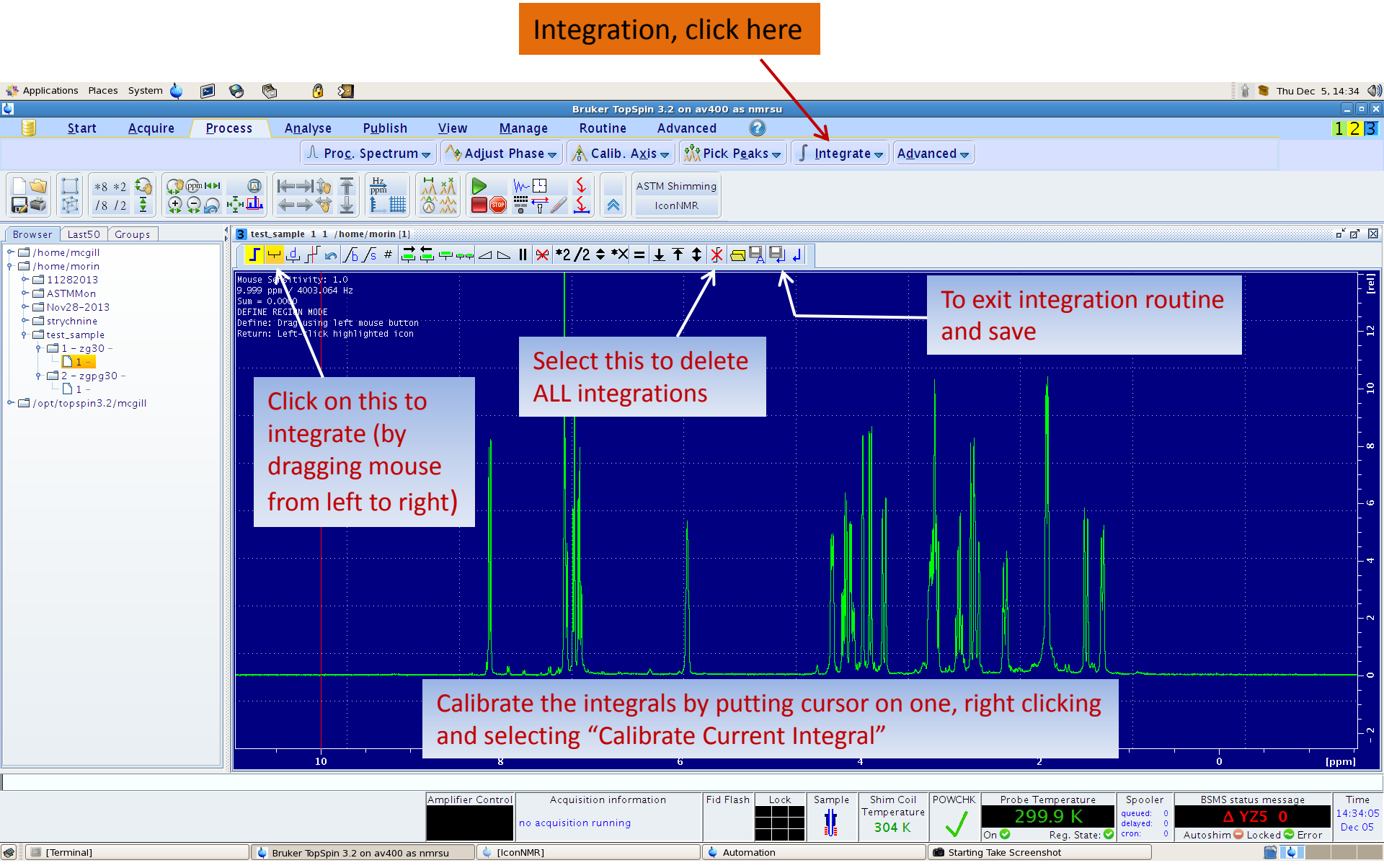
To process data use the TopSpin screen

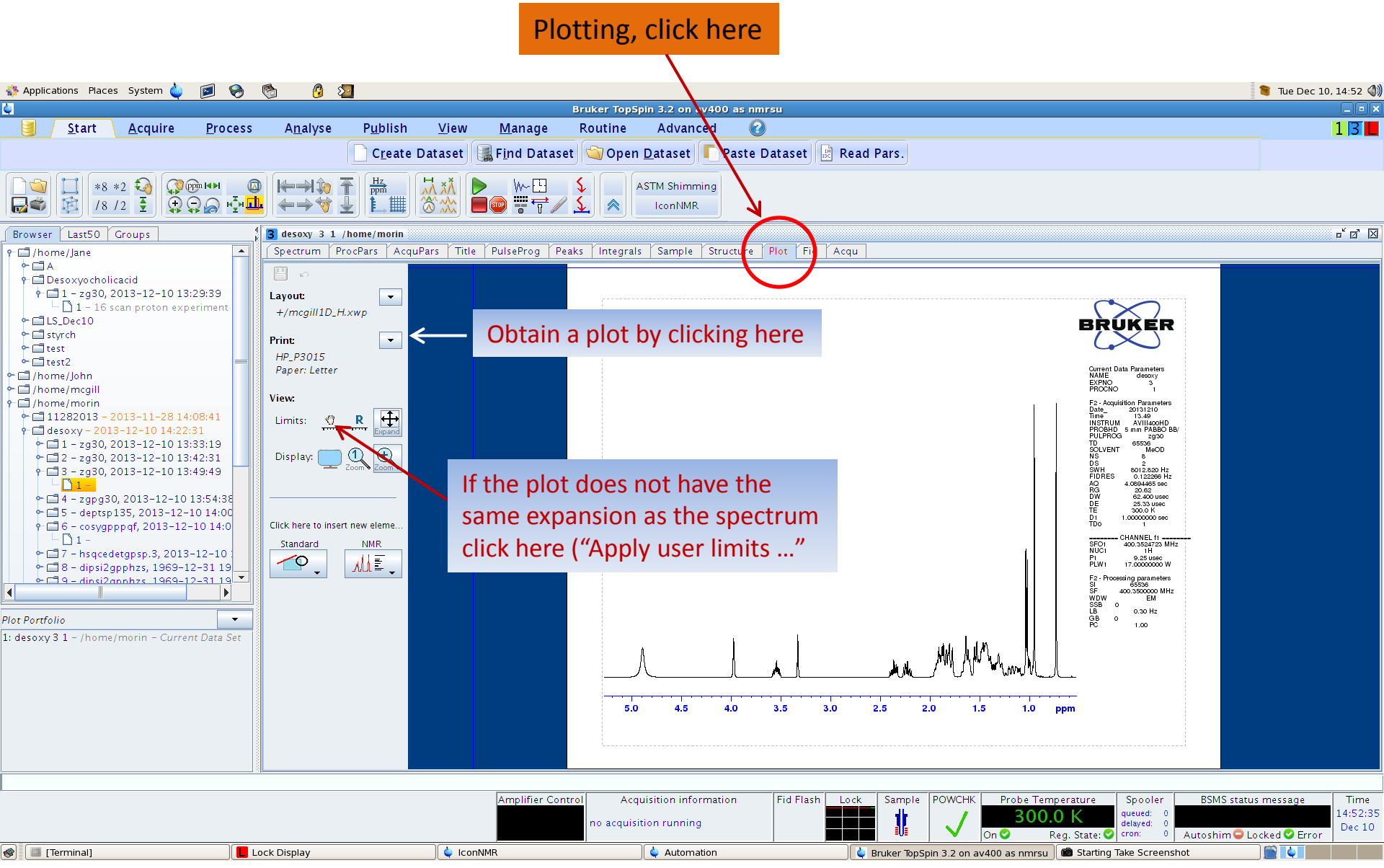
Click Process to see this screen




Click here to plot
Click here to process the data if need be
Bruker TopSpin 3.2 on av400 as nmrsu
Start
Acquire
Process
Analyse
Publish
View
Manage
Routine
Advanced
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
ASTM Shimming
IconNMR
Browser
Last50
Groups
/home/mcgill
/home/morin
11282013
ASTMMon
Nov28-2013
strychnine
test_sample
1 - zg30 -
1 -
2 - zgpg30 -
1 -
/opt/topspin3.2/mcgill
test_sample 1 1 /home/morin [1]
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
Acqu
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"
10
8
6
4
2
0
[ppm]
Amplifier Control
Acquisition information
Name/Expno: test_sample/3
Scan: 250/256
Residual time: 23s
Fid Flash
Lock
Sample
Shim Coil Temperature
303 K
POWCHK
Probe Temperature
300.0 K
On
Reg. State:
Spooler
queued: 0
delayed: 0
cron: 0
BSMS status message
Δ YZ5 0
Autoshim
Locked
Error
Time
14:32:59
Dec 05
[Terminal]
Bruker TopSpin 3.2 on av400 as nmrsu
[IconNMR]
Automation
Starting Take Screenshot

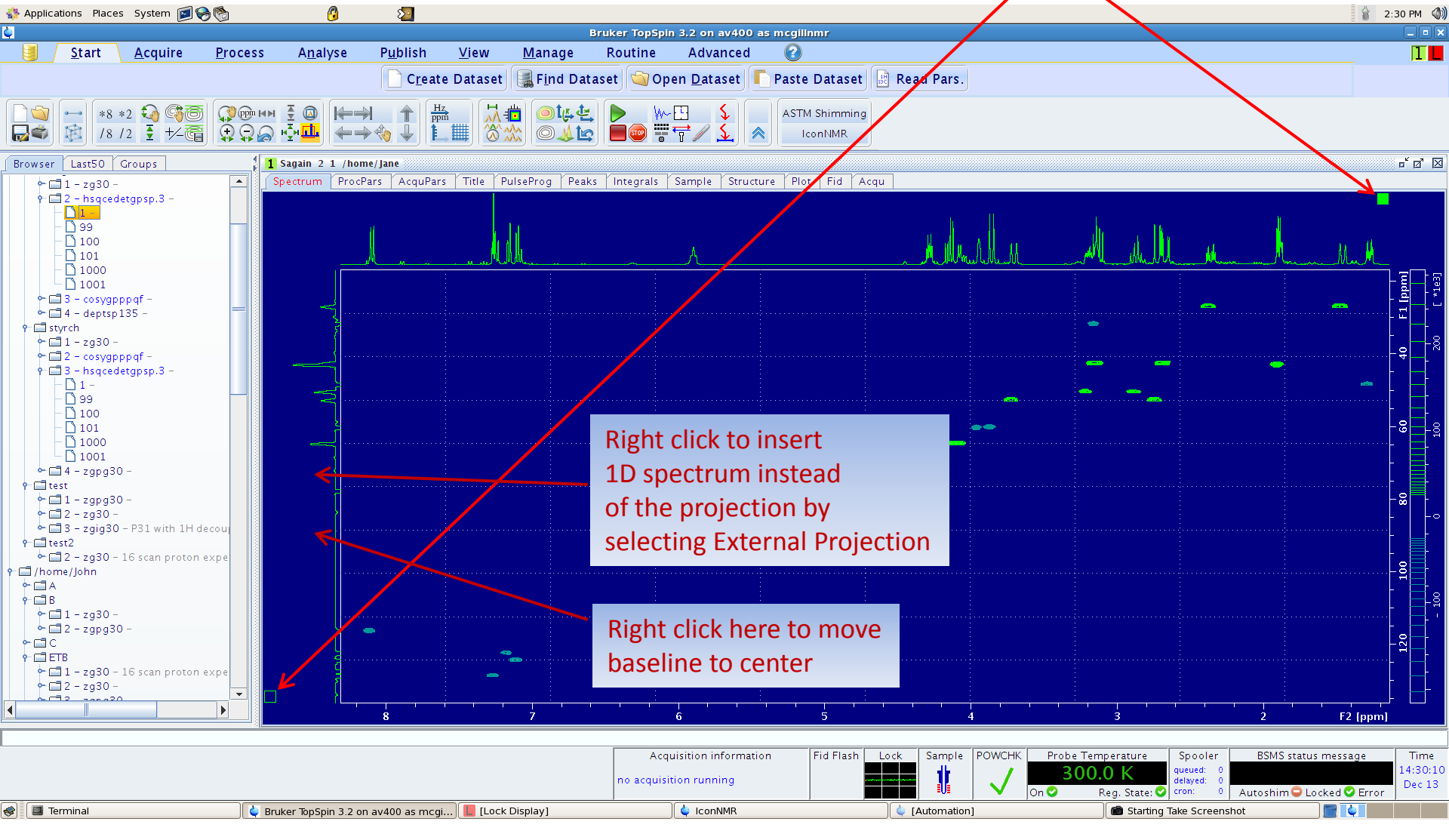

Peak picking, click here
Bruker TopSpin 3.2 on av400 as nmrsu
Start
Acquire
Process
Analyse
Publish
View
Manage
Routine
Advanced
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
ASTM Shimming
IconNMR
Browser
Last50
Groups
/home/mcgill
/home/morin
11282013
ASTMMon
Nov28-2013
strychnine
test_sample
1 - zg30 -
1 -
2 - zgpg30 -
1 -
/opt/topspin3.2/mcgill
test_sample 1 1 /home/morin [1]
8.105 ppm / 3244.859 Hz
Define new region:
Drag with left mouse button
Number of peaks: 0
To exit peak picking routine and save
Select this to delete ALL picked peaks
Click on this to pick peaks by defining regions
Select this to pick peaks by selecting individually
10
8
6
4
2
0
[ppm]
zg: acquisition finished
Amplifier Control
Acquisition information
no acquisition running
Fid Flash
Lock
Sample
Shim Coil Temperature
304 K
POWCHK
Probe Temperature
300.0 K
On
Reg. State:
Spooler
queued: 0
delayed: 0
cron: 0
BSMS status message
Δ YZ5 0
Autoshim
Locked
Error
Time
14:33:23
Dec 05
[Terminal]
Bruker TopSpin 3.2 on av400 as nmrsu
[IconNMR]
Automation
Starting Take Screenshot


Integration, click here
Bruker TopSpin 3.2 on av400 as nmrsu
Start
Acquire
Process
Analyse
Publish
View
Manage
Routine
Advanced
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
ASTM Shimming
IconNMR
Browser
Last50
Groups
/home/mcgill
/home/morin
11282013
ASTMMon
Nov28-2013
strychnine
test_sample
1 - zg30 -
2 - zgpg30 -
/opt/topspin3.2/mcgill
test_sample 1 1 /home/morin [1]
Mouse Sensitivity: 1.0
Sum = 0.0000
DEFINE REGION MODE
Define: Drag using left mouse button
Return: Left-click highlighted icon
Click on this to integrate (by dragging mouse from left to right)
Select this to delete ALL integrations
To exit integration routine and save
Calibrate the integrals by putting cursor on one, right clicking and selecting “Calibrate Current Integral”
[ppm]
Amplifier Control
Acquisition information
no acquisition running
Fid Flash
Lock
Sample
Shim Coil Temperature
304 K
POWCHK
Probe Temperature
299.9 K
Spooler
BSMS status message
Time
14:34:05
Dec 05
[Terminal]
Bruker TopSpin 3.2 on av400 as nmrsu
[IconNMR]
Automation
Starting Take Screenshot

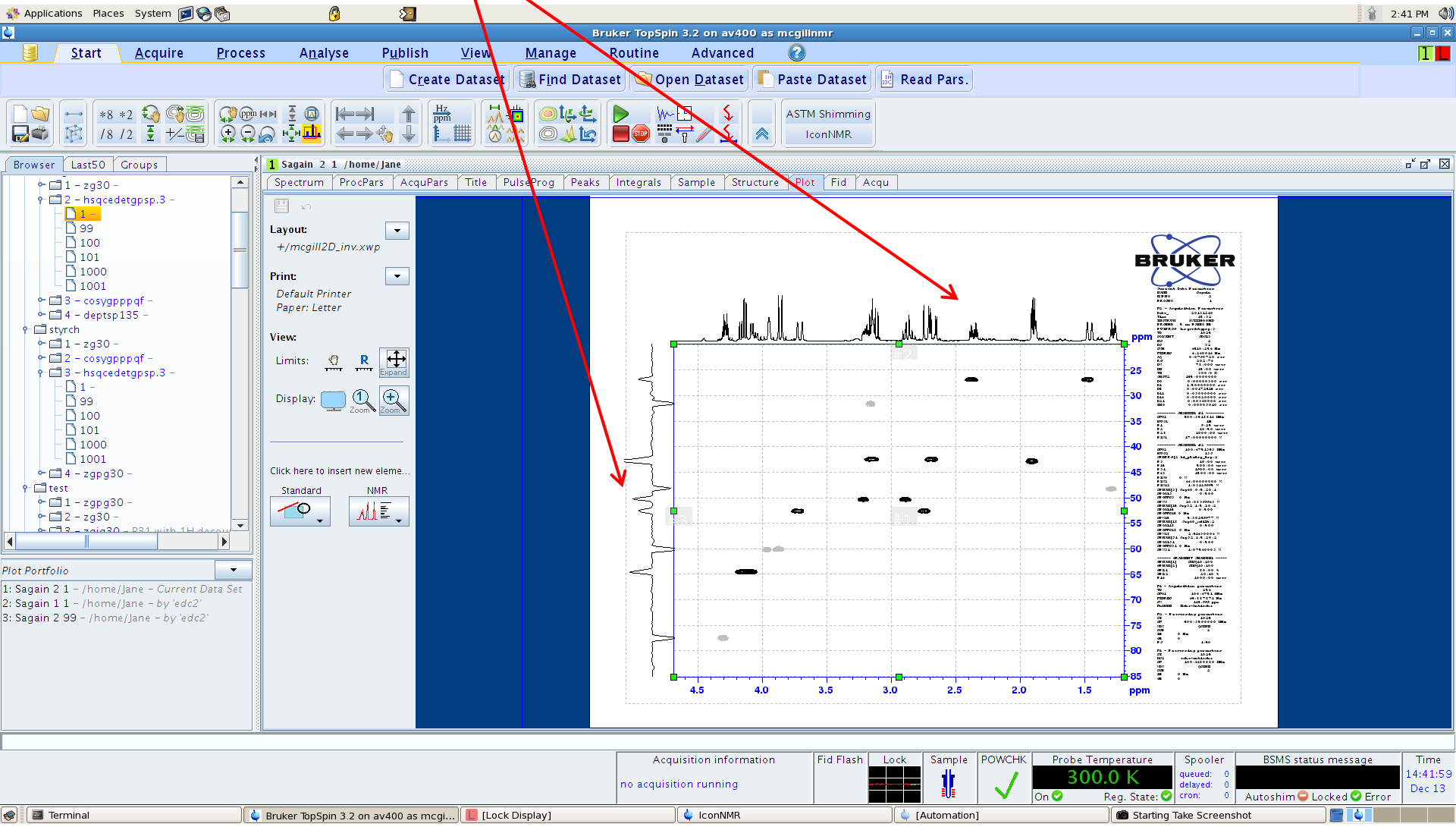


Can use scroll button to increase or decrease vertical scale before plotting

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.



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