KJM 5280

V

NMR processing everywhere
with Windows Remote Desktop
and TopSpin 3.5
at
nmr-server.uio.no

Windows Server 2012

Version 1.4

© F. Rise May 2018

Nmr-server.uio.no is the final destination for all NMR data generated at the University of Oslo NMR Center. Our entire eight nmr instrument PCs copy data to nmr-server.uio.no/nmr every 30 minutes or so. You use **nmr-server.uio.no** to grab data from (drag and drop or copy and paste between two desktops), and process the data with MestreNova or TopSpin on your own PC or Macintosh. You can also process your NMR data with the software TopSpin 3.5 on **nmr-server.uio.no** from anywhere**.** There are 21 Topspin licenses on the server. They all can be in use at the same time.
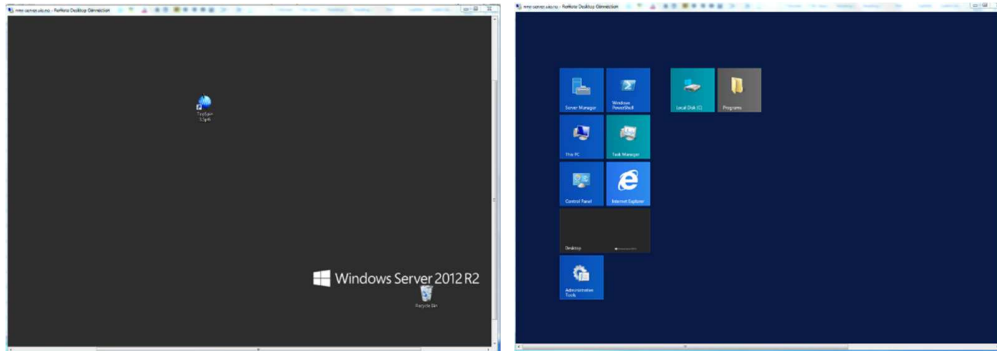
On a Windows 7 PC when you are connected to a uio.no network, you will navigate to Start, All Programs, Accessories, Remote Desktop Connection (RDC). Double click on RDC.
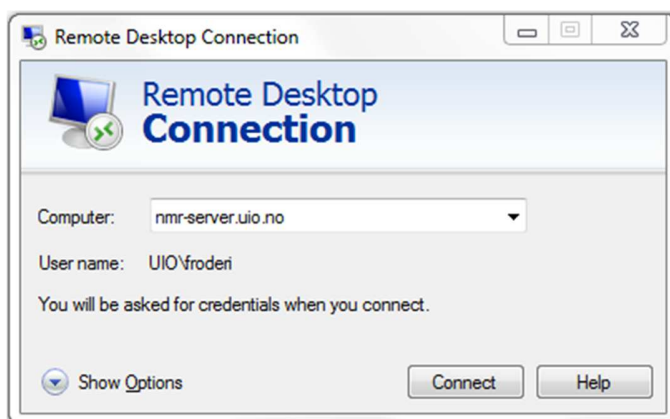
Type nmr-server.uio.no.
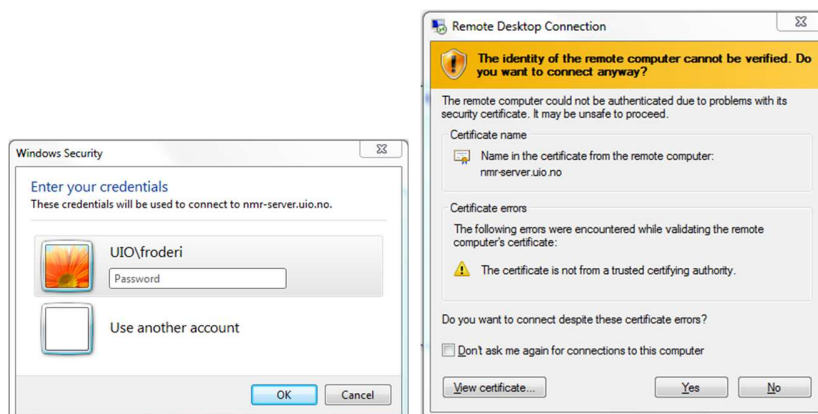
Type your password and ignore the warning coming up. Click on yes.

For people used to Windows 7 a "strange" Windows 2012 desktop comes up. If unfamiliar, you will struggle a bit. Locate the TopSpin program icon somewhere on the desktop. If you are unlucky, you get the desktop shown in the right and you have to find a way to switch to the left appearance.

We are now doing a huge departure in this document and going back to step one. If you want to connect to nmr-server.uio.no and process your nmr-data, while you are at home or travelling you have to make a so-called connection file before connecting.

Use a browser and connect to: http://www.uio.no/tjenester/it/nett/utenfra/rdp/index.html

Choose between Windows or Mac.

For Windows: https://www.uio.no/tjenester/it/nett/utenfra/rdp/windows/



Regretfully this is in Norwegian only ☹

(Kontormaskin is confusing here since we are not connecting to an office PC at all.) You are asked if you want to open or save the file. It is suggested to "save as" so you save to a location you know about. Saving to desktop is usually the safest option if you want to find the connection file again.

The connection file can luckily also be used to connect when you are the University of Oslo.
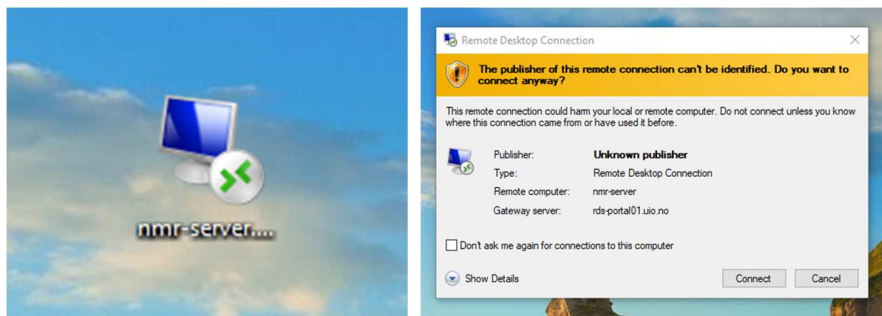
Double click on the nmr-server.uio.no RDC connection symbol you have made earlier and wisely placed on your Windows or Macintosh desktop. Ignore the warning that pops up, click on connect.
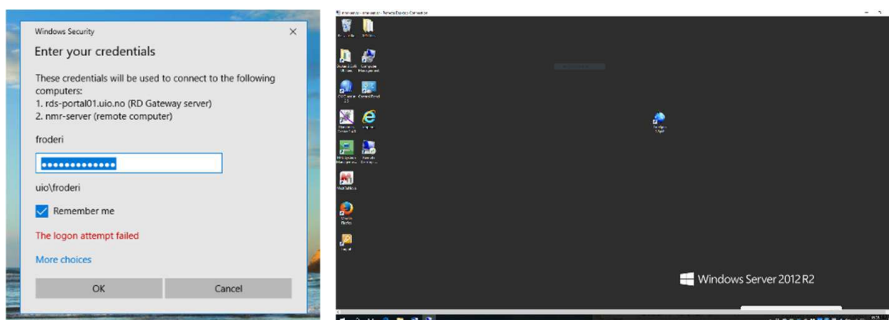
Do as shown and click on OK. Suddenly another desktop comes on top of your own pc desktop. If you are lucky, it looks like this. It might look different since Windows 2012 looks a bit like

Windows 10 and the screen might be filled with useless tiles or squares and you have to fight a bit to find the TopSpin 3.5 icon/program.

Please continue on Page 11. The next pages will show you how this is performed if you use a Macintosh. Use a browser and connect to:
http://www.uio.no/tjenester/it/nett/utenfra/rdp/index.html

Click on Mac


Click on "installer den fra App Store" and it does not install directly, we are still in the Windows world with all its unnecessary and extra steps. ☹ Click on View in Mac app store.
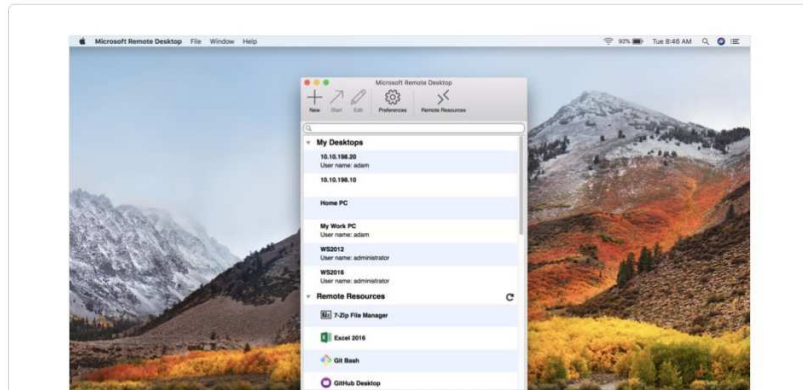
Finally, the place to install from appears. Click on Open and install the program. Every Macintosh user understand how this is done.
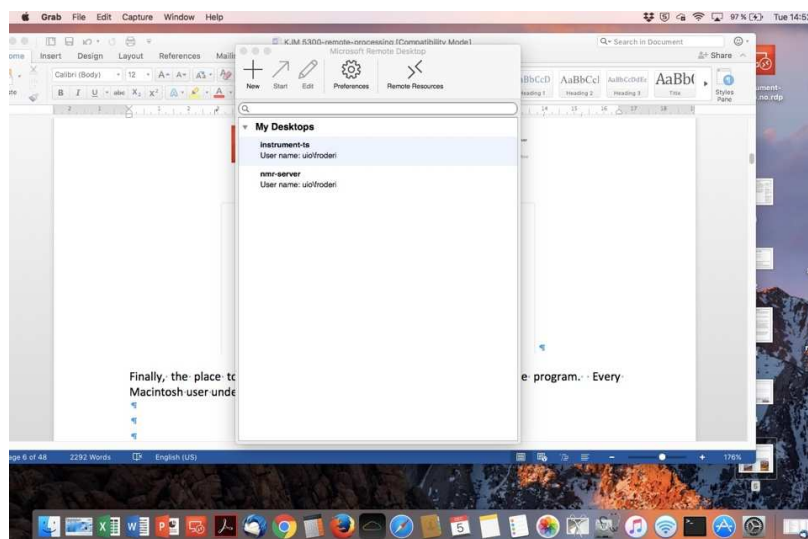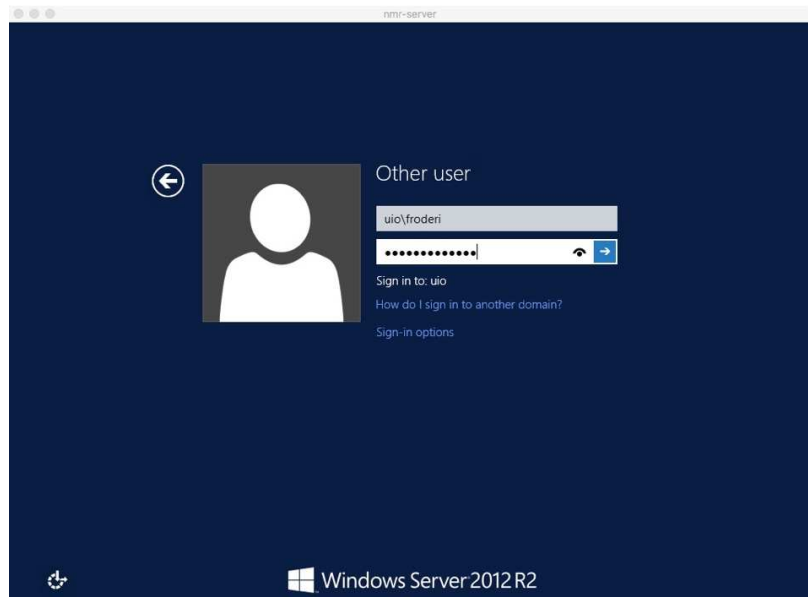

Clicking on the Microsoft Remote Desktop icon in the dock (number 6 from left) brings up the two installed Connection files (on the "authors" Mac). Here nmr-server.uio.no is selected.
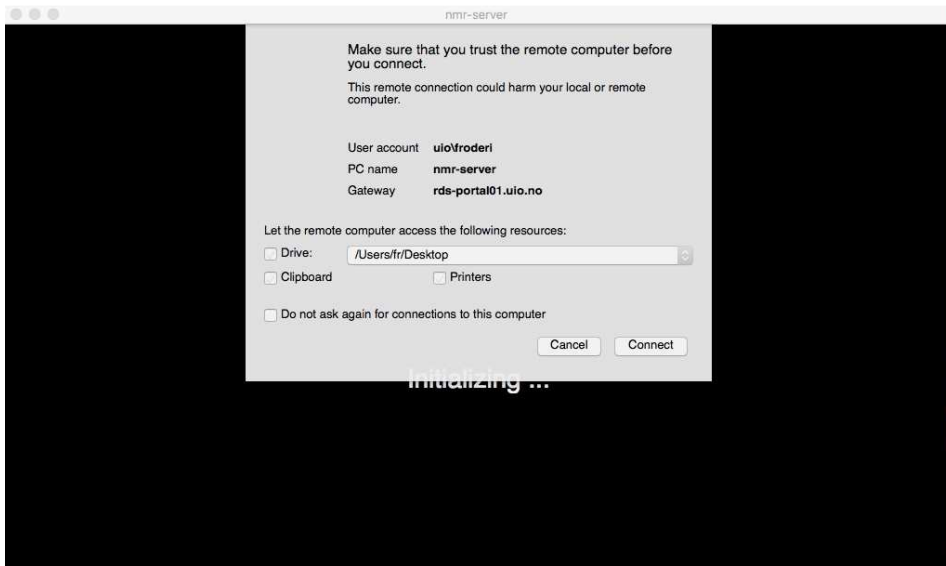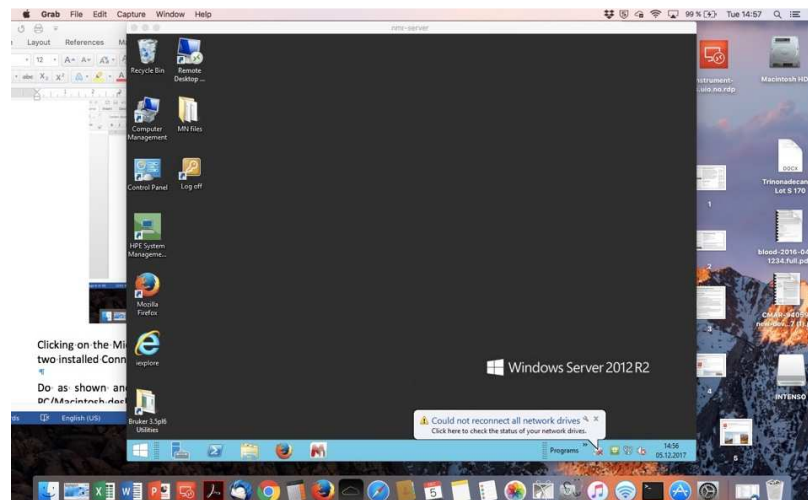
You then have to select "Let the remote computer access the following resources" as /Users/Desktop. Then click on Connect.
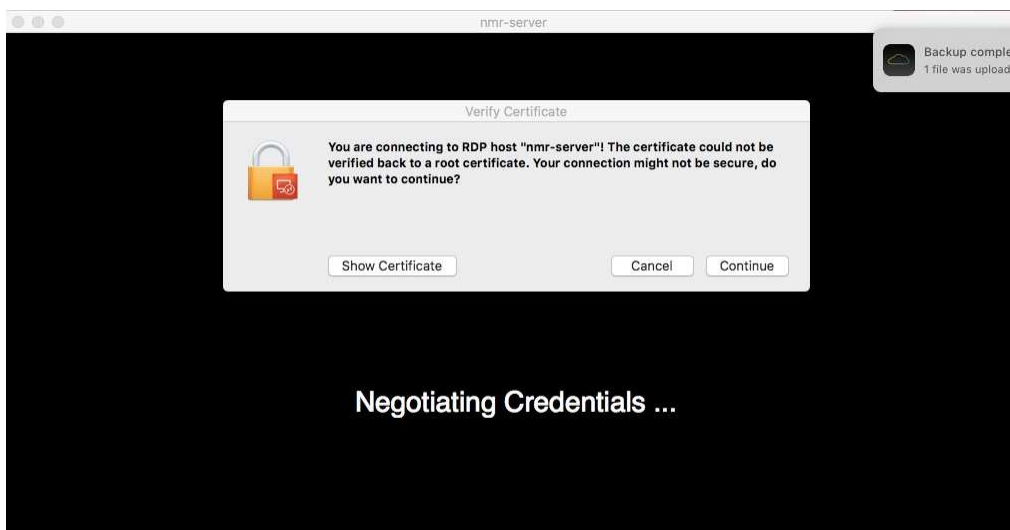
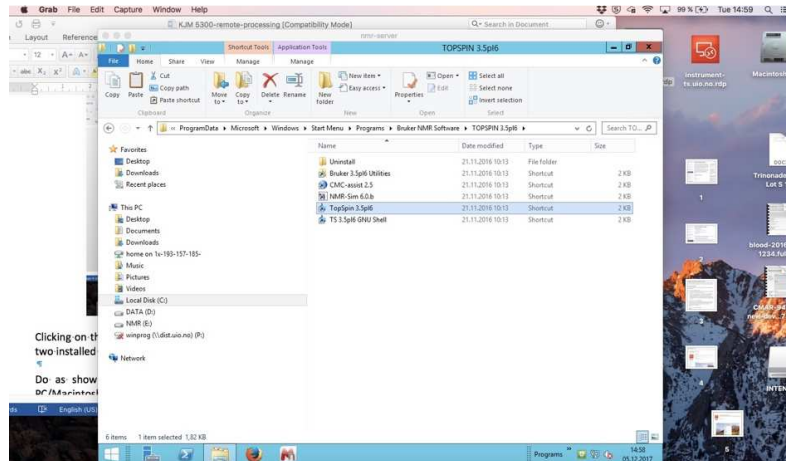Warning comes up. Ignore it and click on Continue.
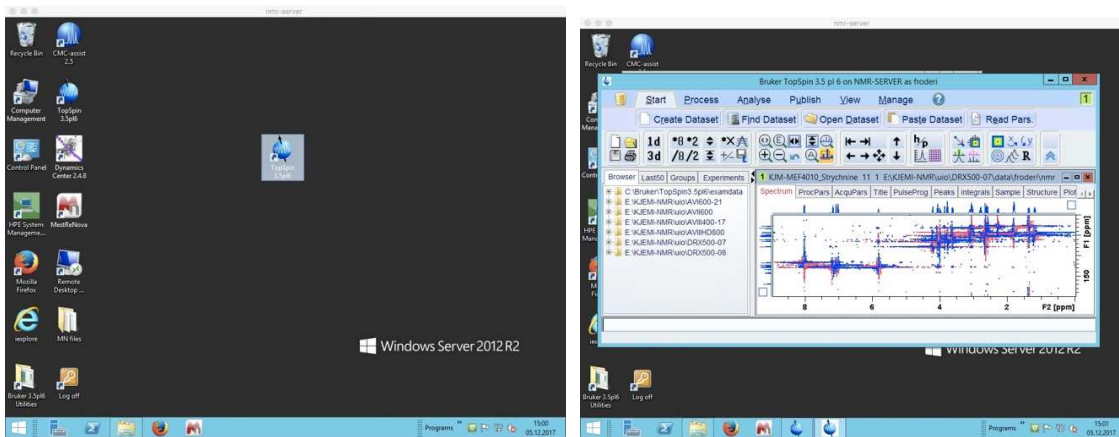
Fill in. Click on the arrow.

And up it comes, the somewhat unpleasant Windows Server 2012-R2 desktop on the cute Macintosh desktop. And the TopSpin icon is of course missing and we have to dig into the Windows world to find it.
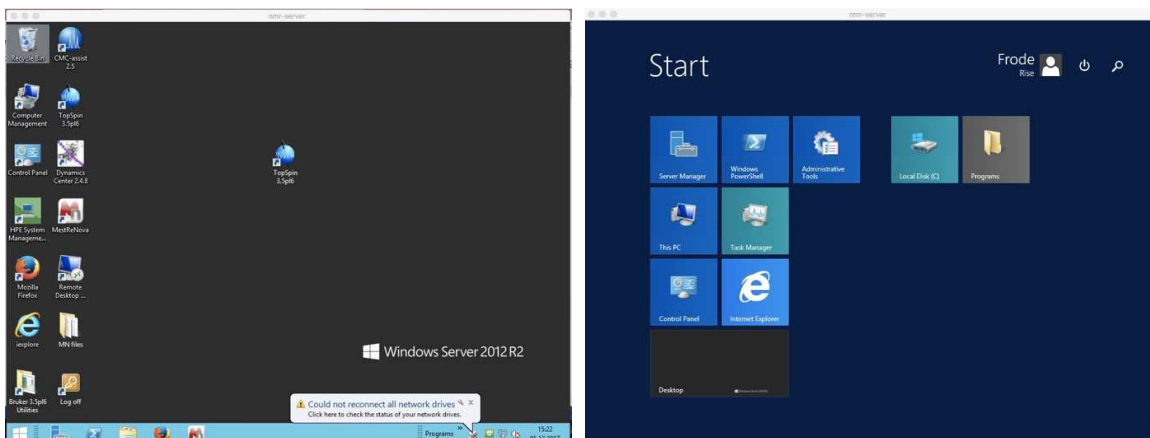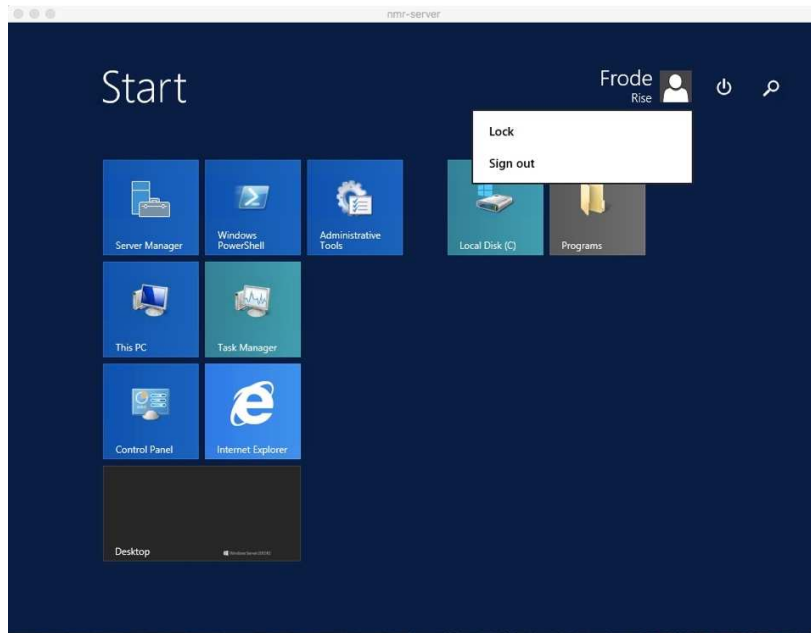
After poking around a bit, the program is found. Copy.

Past it. And click on it to start the program. Remember to exit the Topspin program.


Exit Windows by clicking on the windows symbol in lower left corner. Then Click on the user name up to the right.

Then select Sign out to exiting the Windows 2012 server properly. The rest of the instructions are made in a double Windows world using a Windows 10 PC to connect to the Windows 2012 server. Move on to next page.

Back were we left off many pages ago. Before using TopSpin, it might be wise to familiarize yourself with the disk and file structure of the server.
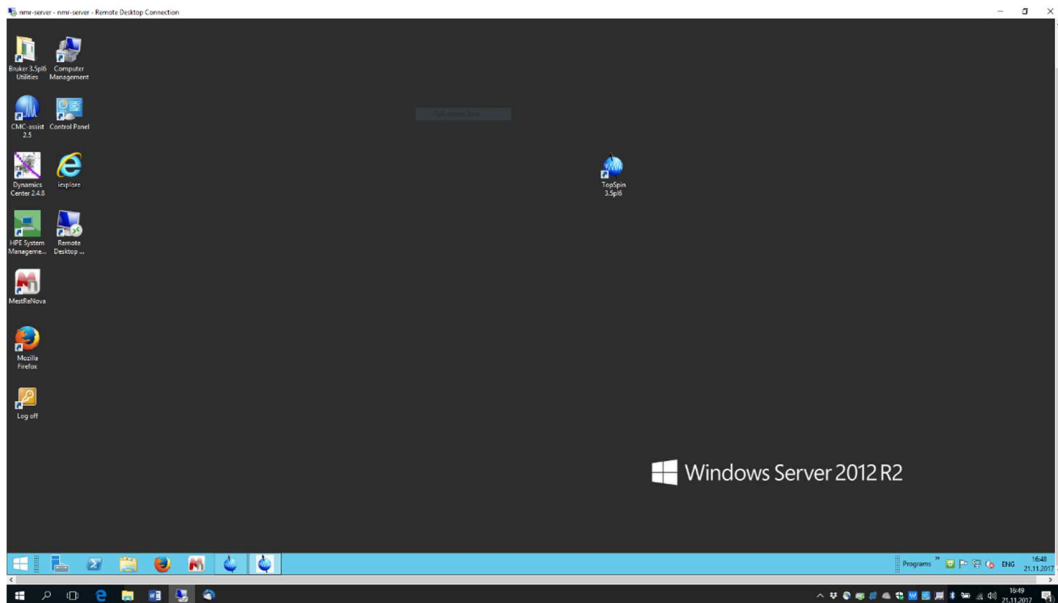

Move the desktop up so you have two Windows symbols in lower left corner, one for the server and one for your own Windows 7 or 10 PC – if you are on a PC. Click on the upper ⊞ of the two.
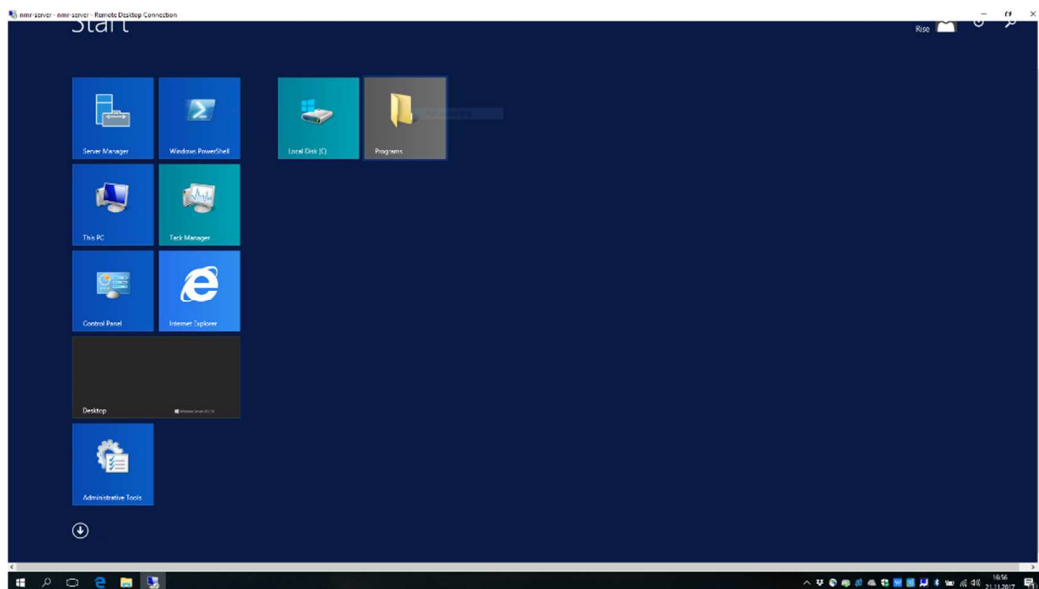

Click on Local Disk C and a more useful appearance opens up.
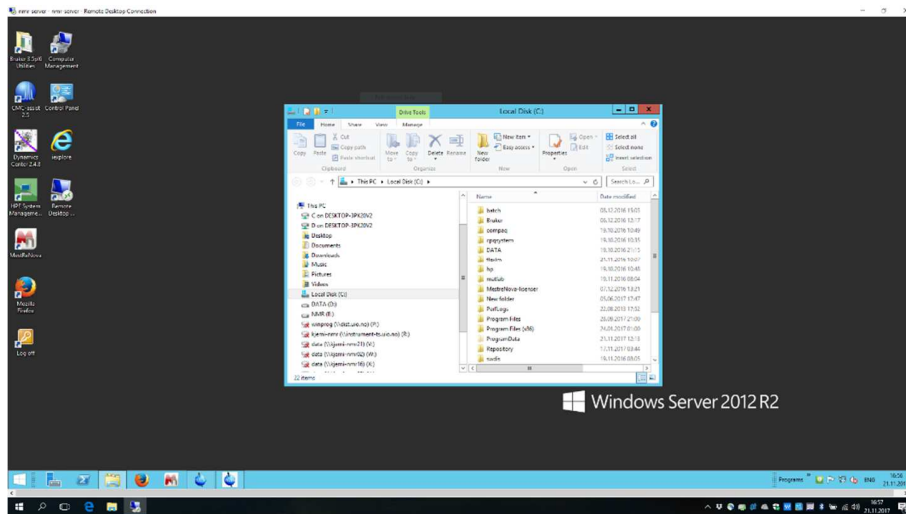
Here we see that nmr-server.uio.no is having three locations (disks) C, D and E. NMR data is located in D and E. In the D drive, there is mostly located vintage NMR data. As said before new nmr-data is coming into E once every night from instrument-ts.uio.no.
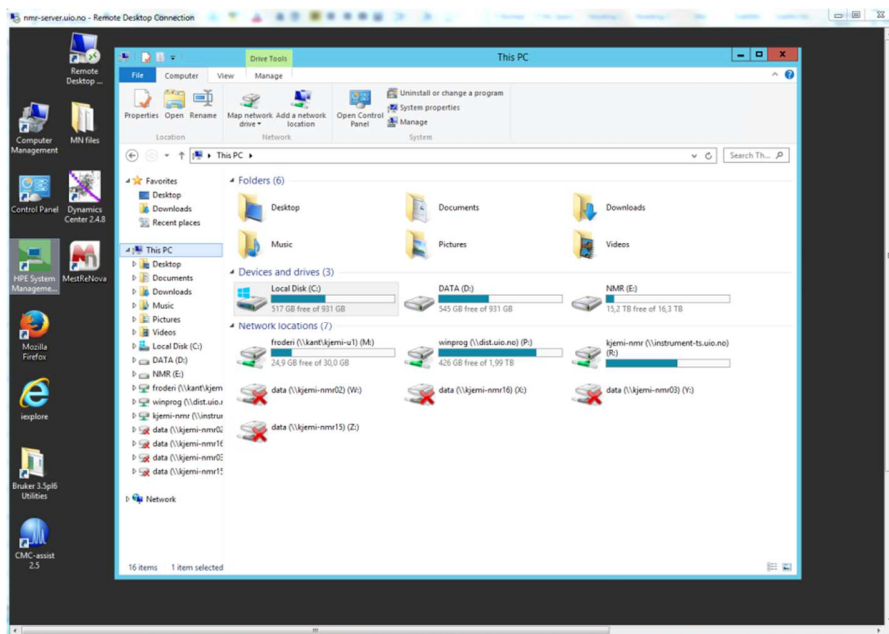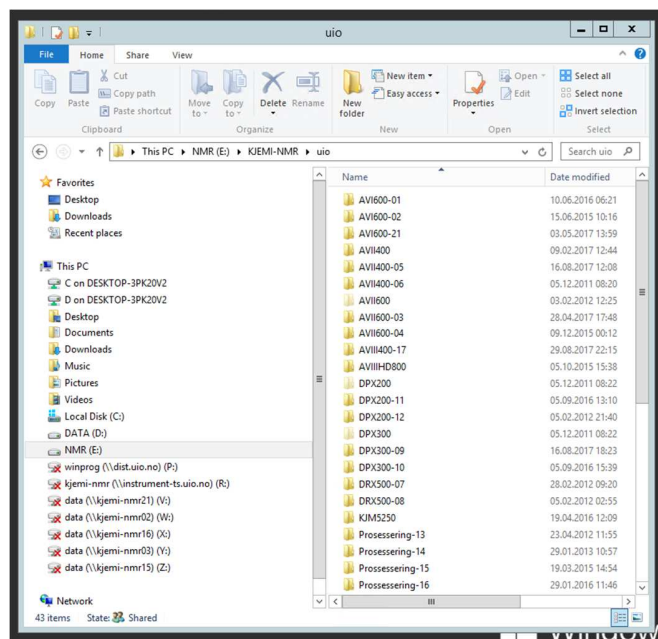

Another view of the Server setup is seen here. The intelligent student might realize from this screen shot how to manually get "today´s" nmr-data over to nmr-server.uio.no?
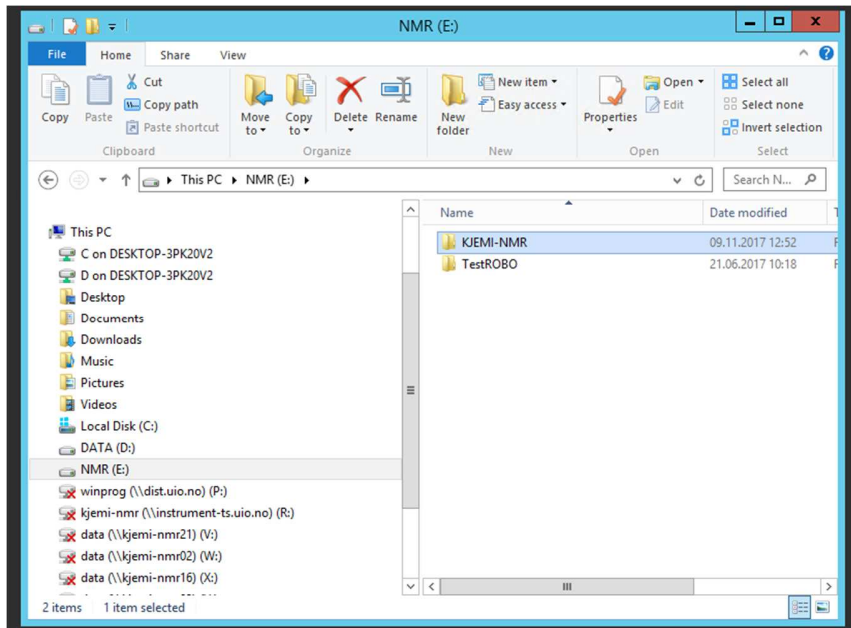
We are now on a tour to see where the data from the different NMR spectrometers are located on the server. Click on E and then on KJEMI-NMR
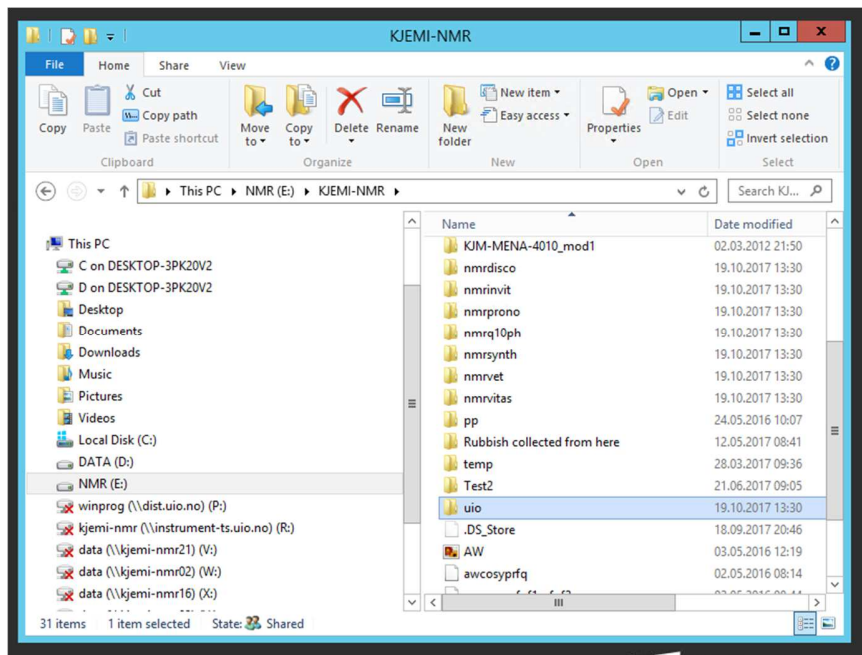

Then you click on uio

However, there are several entries for most of the NMR spectrometers? AVI600-01, AVI600-02 and AVI600-21 for instance. What you see might change over time since there is a gradual change of PCs at the UiO Nmr Center. AVI-600-01 was the Windows XP PC running AVI600 for many years. AVI600-02 was made as a backup and is still in room Ø 332 – as a processing only PC. AVI600-21 is now (May 2018) the PC running the AVI600 NMR spectrometer. You will not get the whole history for all the instrument- PC combinations here, but only the list of the currently used PCs so you will be able to locate your data: AVI600-21, AVII400-05, AVIII600-04, AVIII400-17, AVIIHD800, DPX200-11, DPX300-09 and DRX500-0X.
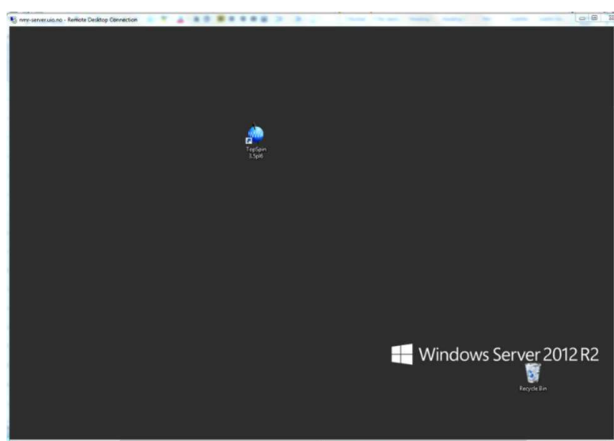

Now we want to connect the disk partitions containing your NMR data inside TopSpin. Click on the TopSpin Icon to start the program.
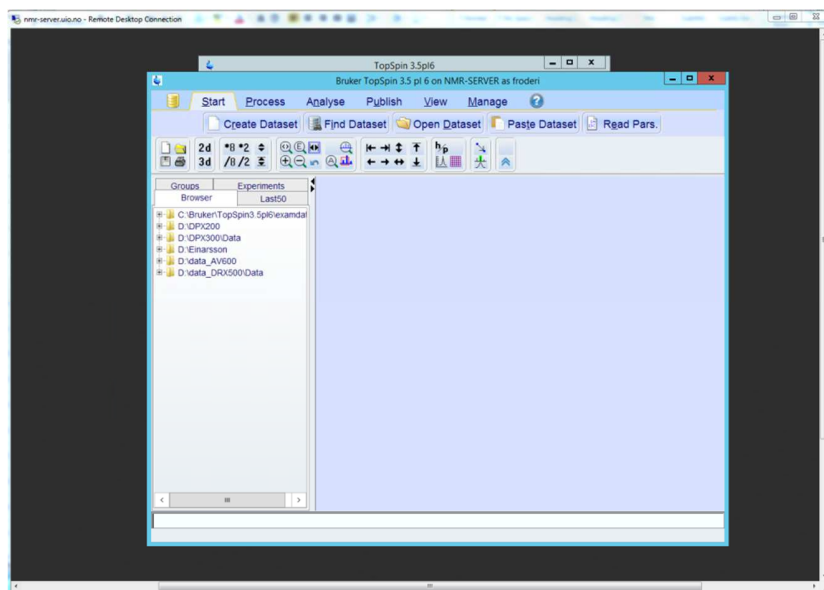
Here you see a bunch of disk partitions containing old or vintage NMR data from the time the current NMR instruments were controlled by SGI Linux computers, on the left-hand side of TopSpin interface. (Since it is hard to operate NMR instruments forever with obsolete Windows XP PCs investigations into switching back to Linux from Windows, e.g. Cent OS 7 computers.) Right click in the left pane. Navigate to folders you need. Nevertheless, there is a chaotic file system on this computer.
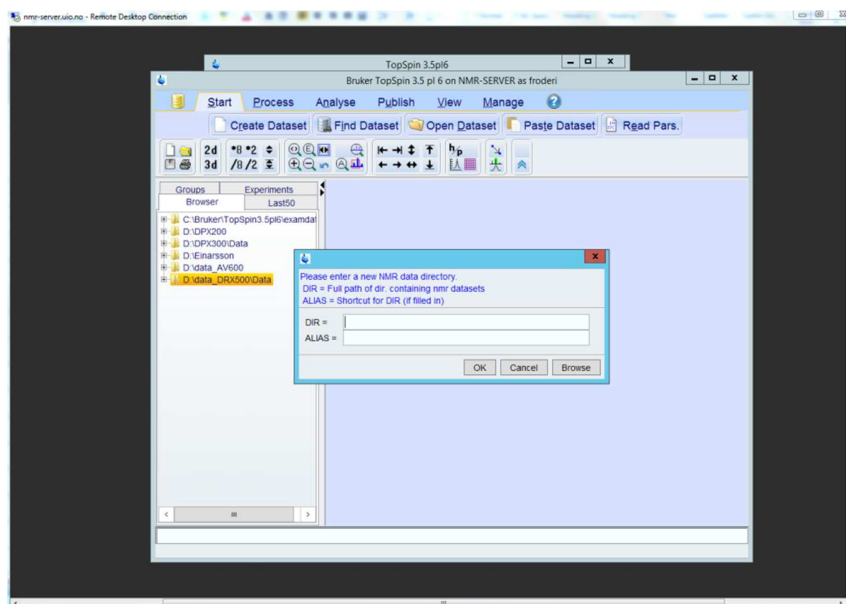
Observe the pop op window, click on Browse and navigate through the disk systems until you find a useful location.
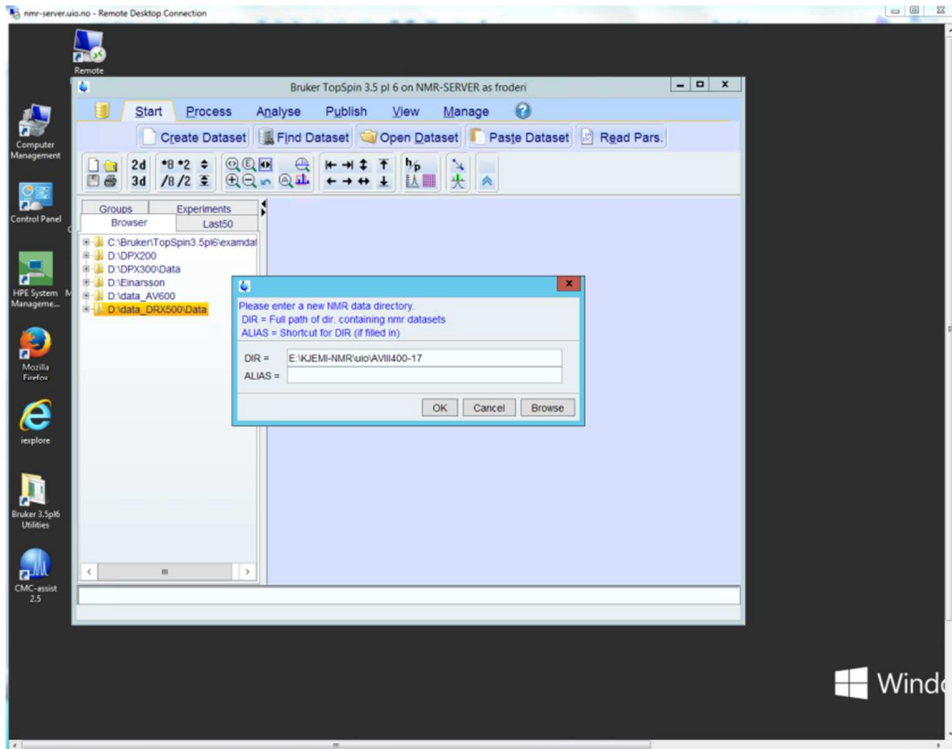
For instance, the newest 400 MHz instrument! Click on OK
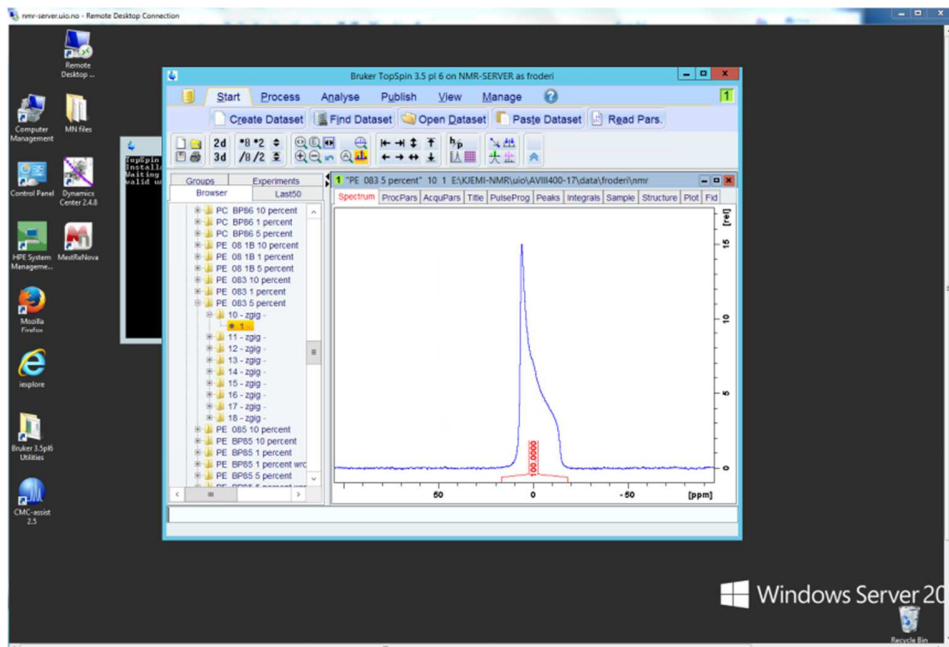
You can now navigate to a dataset in your location for the backup data for the AVIIIHD400 NMR instrument. You open it by clicking on the correct folder or file in the experiment, you might click and open sever layers before the spectrum or the unprocessed data appears in the main window.

Alternatively, you choose to drag and drop into the main window. In the spectrum above and below you see a ^{31}P semi solid NMR experiment.
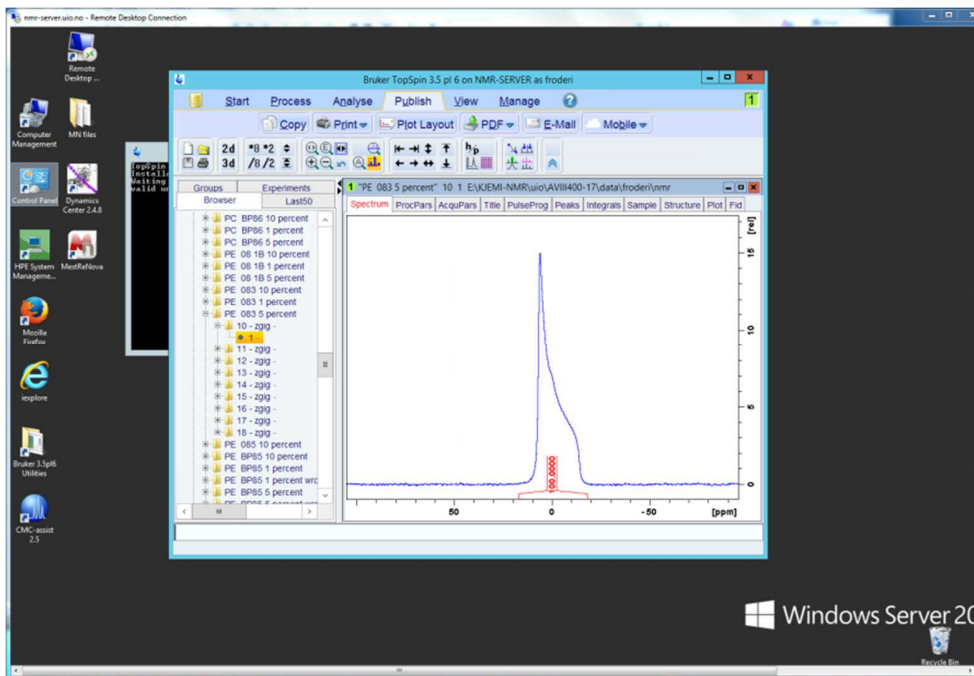

Click on Publish and locate the Copy button. Use it. In addition, paste the spectrum in a word document you already have open on your own PC. Great being able to copy a spectrum from TopSpin located on the nmr-server.uio.no desktop to Microsoft Word on another desktop. ☺
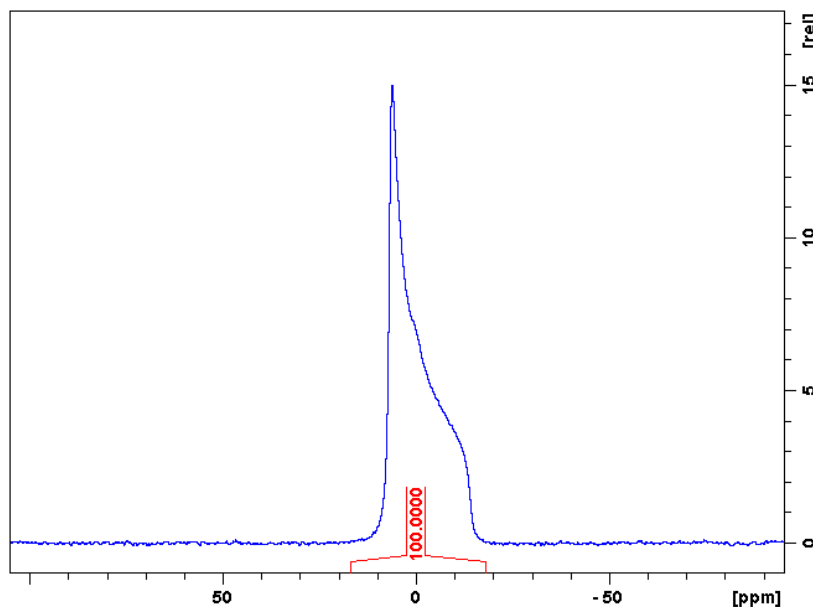

What it looks like when pasted.
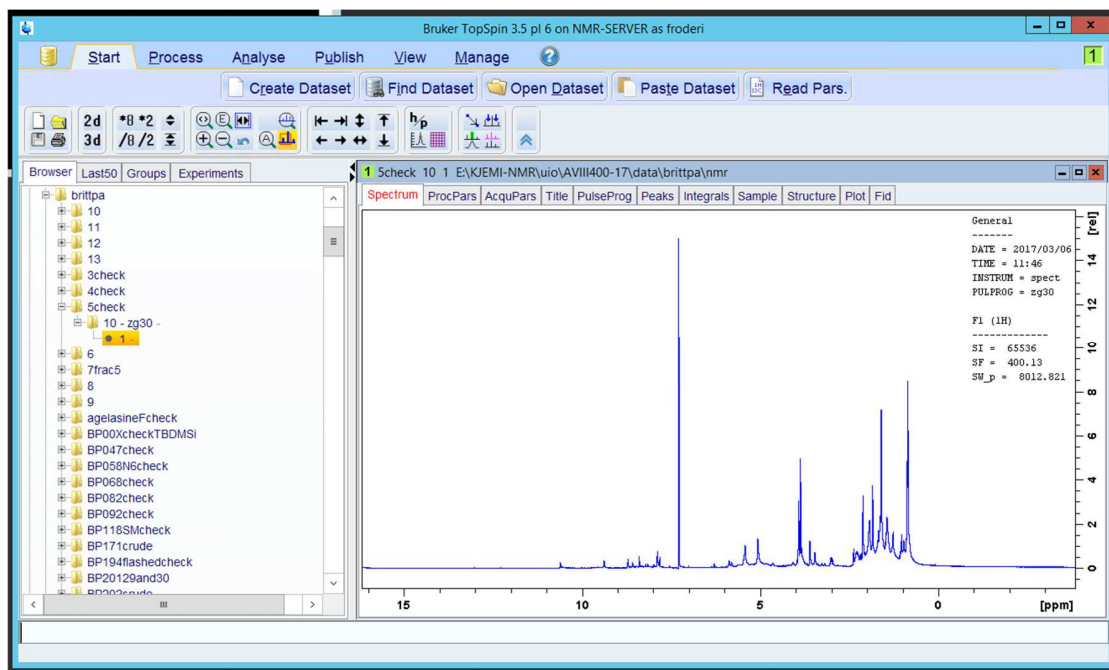
Your user account exists only at locations where you earlier on the original NMR acquisition PC have performed an experiment or more. Your user account is missing at all other locations on the server. When you want to use a place to process data at you might create yourself there if you start from someone else´s spectrum. Open a spectrum (above). Type edc or new in the command line and the following window pops up (below). Change the experiment NAME and locate the user name, brittpa in this example.
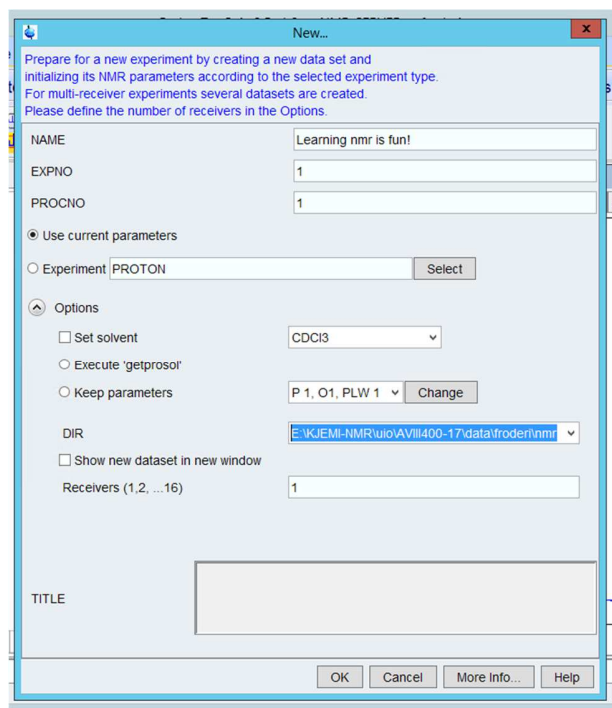
Then you change the user to yourself. Beware not to remove any **** in the process and click OK to make a place on the system for yourself
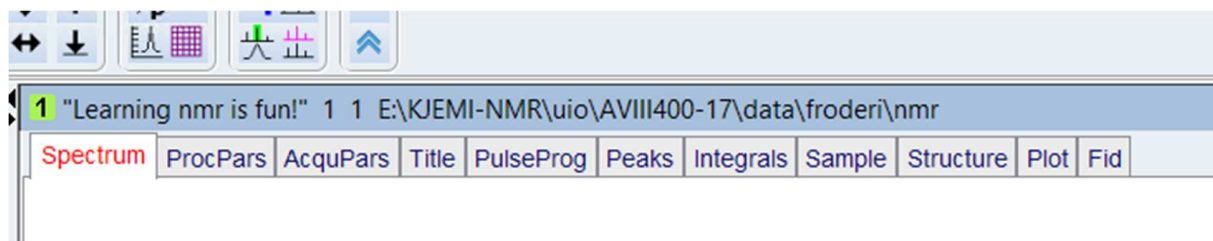
In one of the top lines of the program, the experiment name is changed. Moreover, somewhat miraculously the file structure is made at the same time.
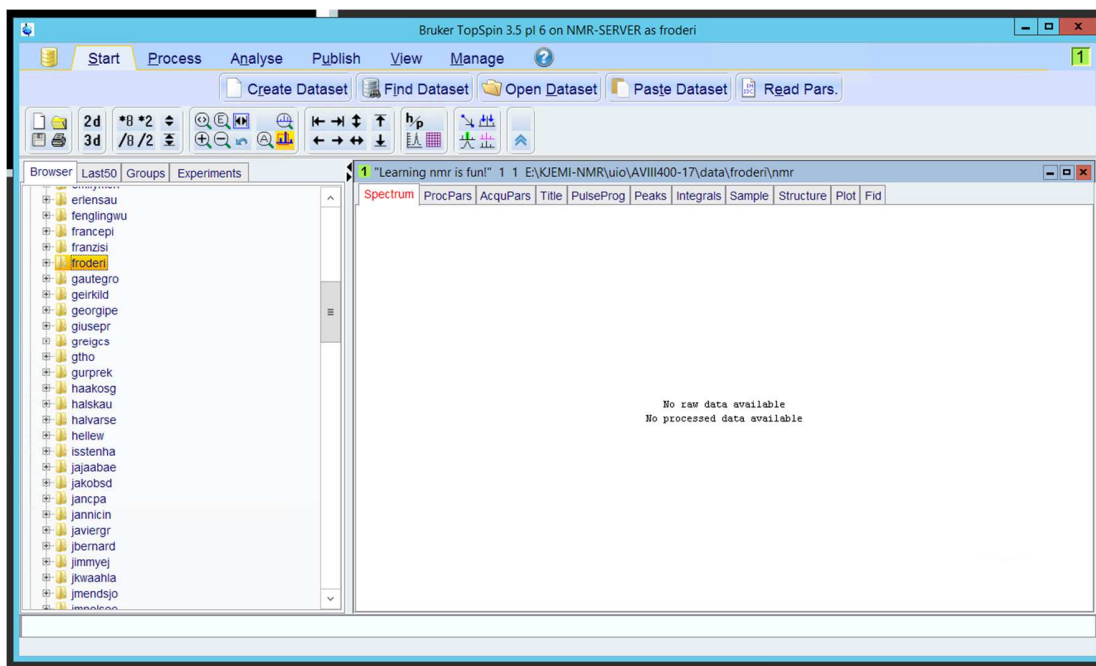
The next task is to copy the training NMR data set you used when you learned to use TopSpin 1.3 into your newly created location.
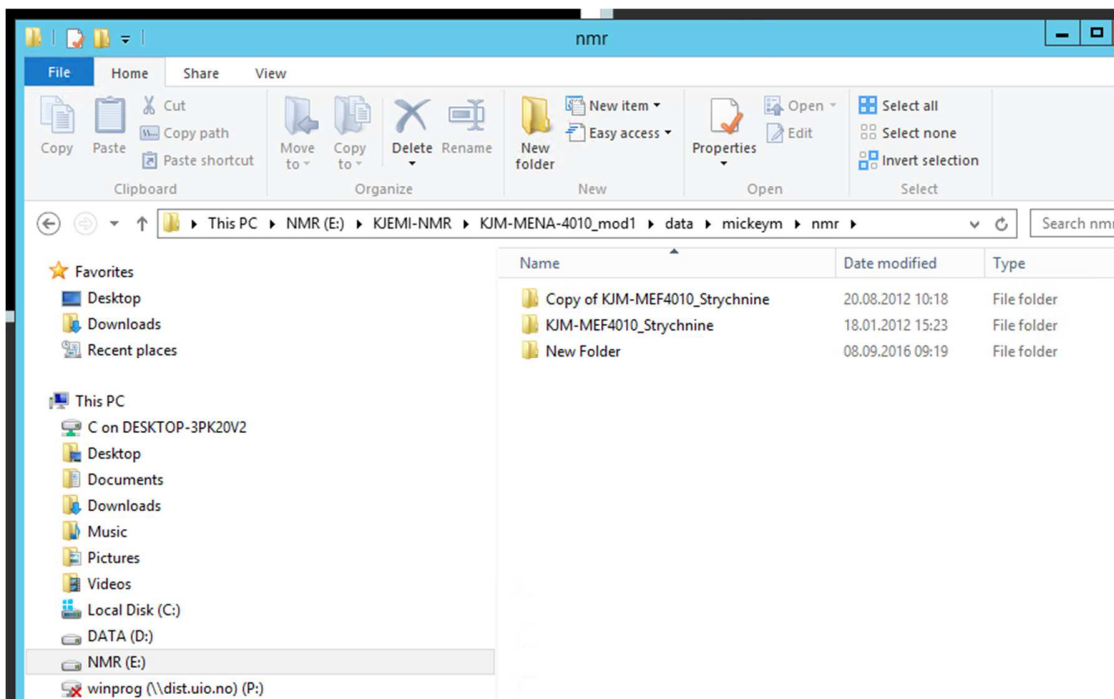

Observe the location of the Mickey Mouse folder and find it yourself.
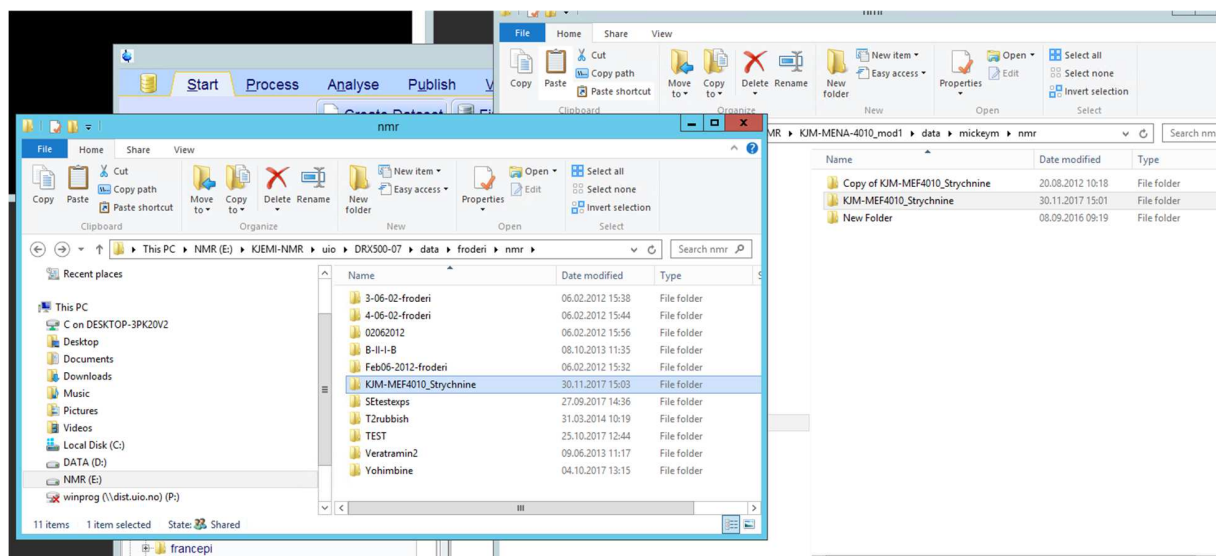
Have the source and the destination open at the same time, please copy, and **paste** the folder into the destination. If you drag and drop the folder, it will be removed from its place and you are the last person doing this operation.
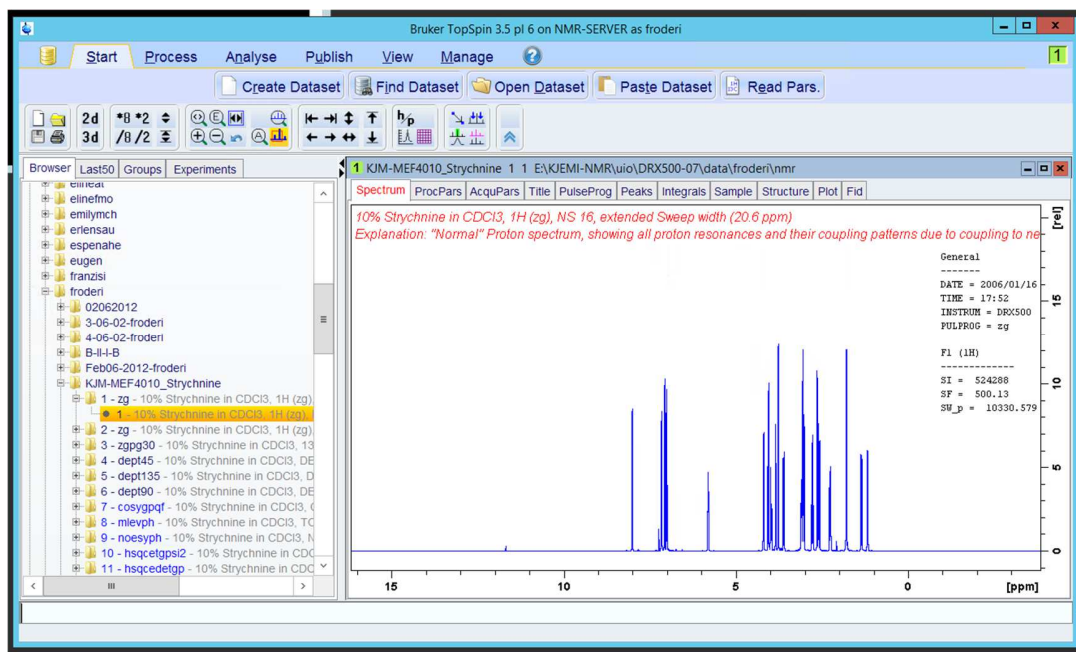
Time to start familiarizing yourself with the program and processing NMR data.
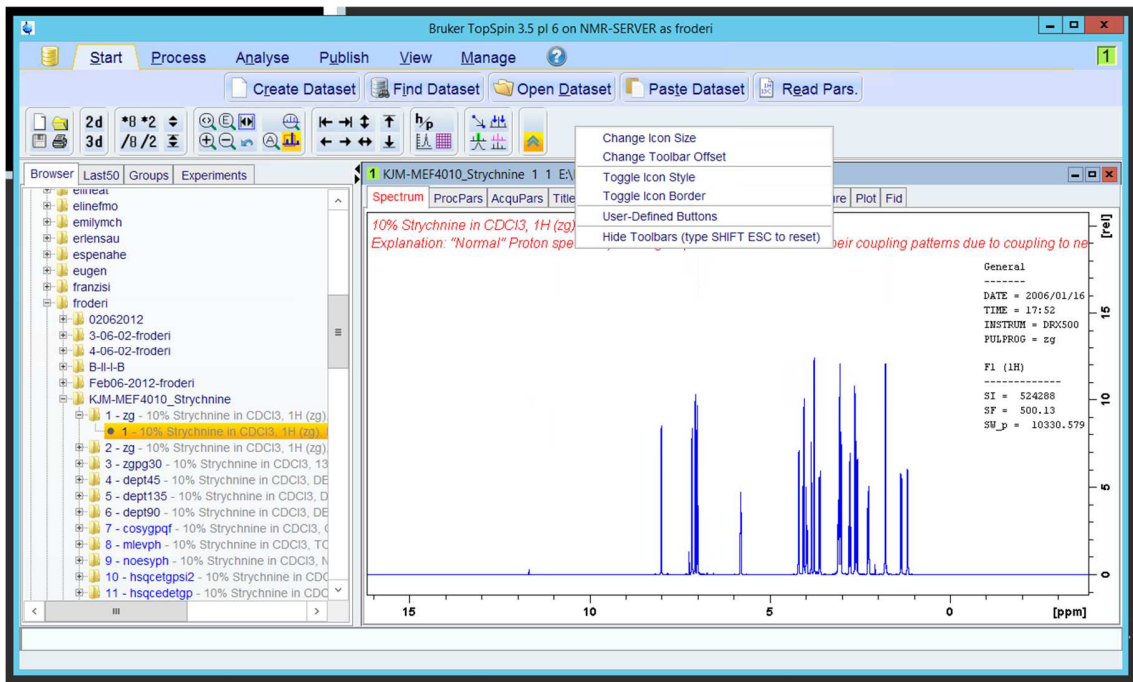
Click on the empty place to the right of the two lines of the smaller click on symbols (3rd and 4th lines in the program) and test out the options coming up. Test for instance Toggle Icon Style and observe the result.
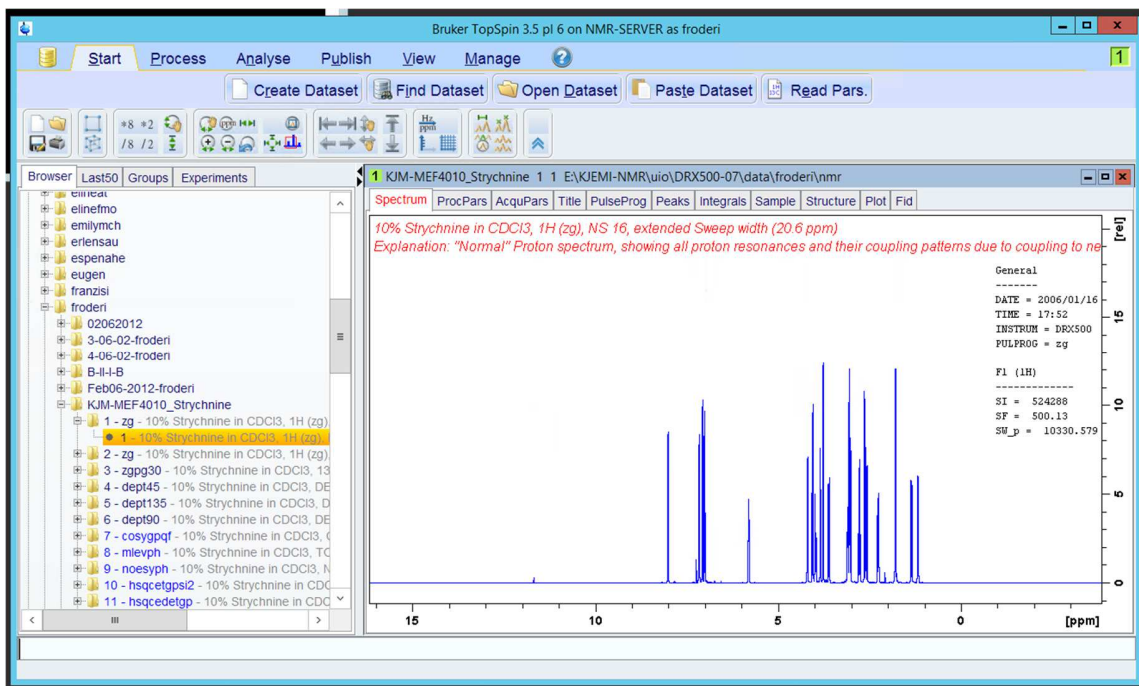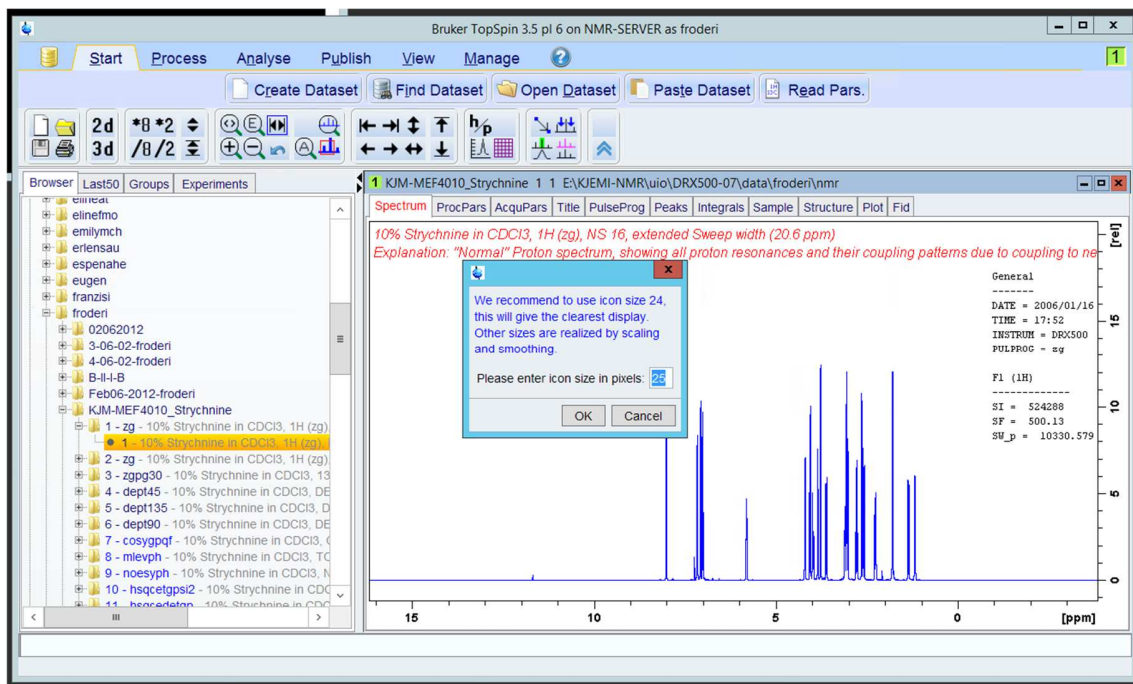
People initially trained with TopSpin 1.3 usually change back to the old-fashioned appearance. Change the Icon Size if they are too large or small for you.
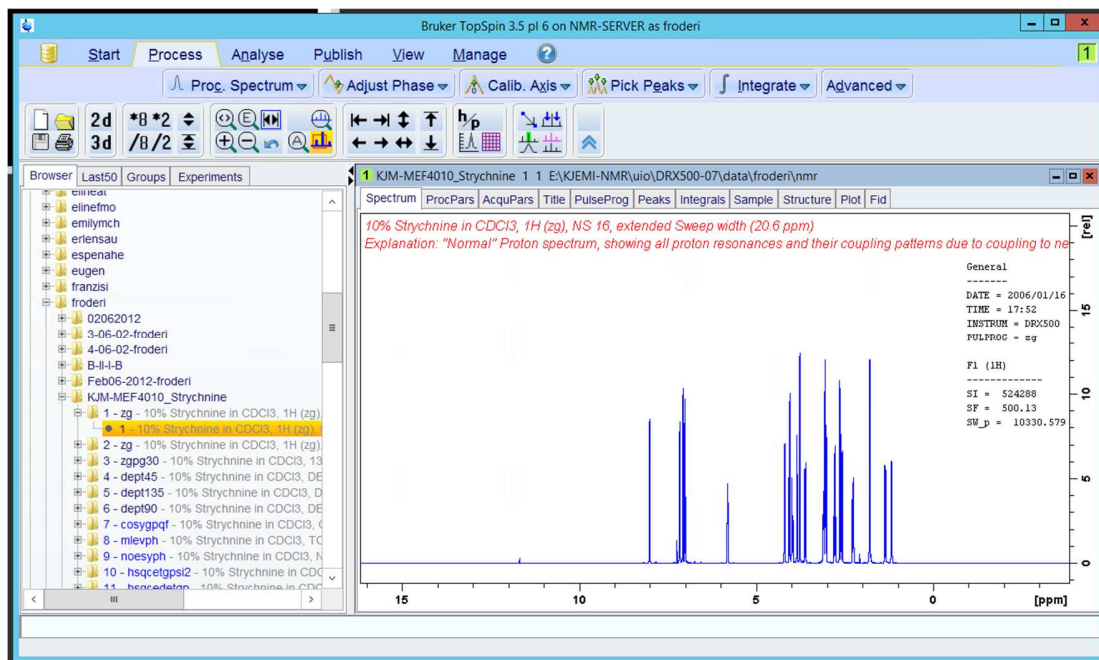
Observe the main clickable symbols Start, Process, Analyze, Publish, View, Manage and **?**. Test them and observe what shows up in line two. By clicking on the symbols in line 2 you again get different options available for you.

The rest of this document will follow the outline of document IV used in KJM 5300 "Processing of nmr spectra with emphasis on TOCSY, NOESY and HSQC". However, the continuation from here will be less verbose and depend more on pictures.
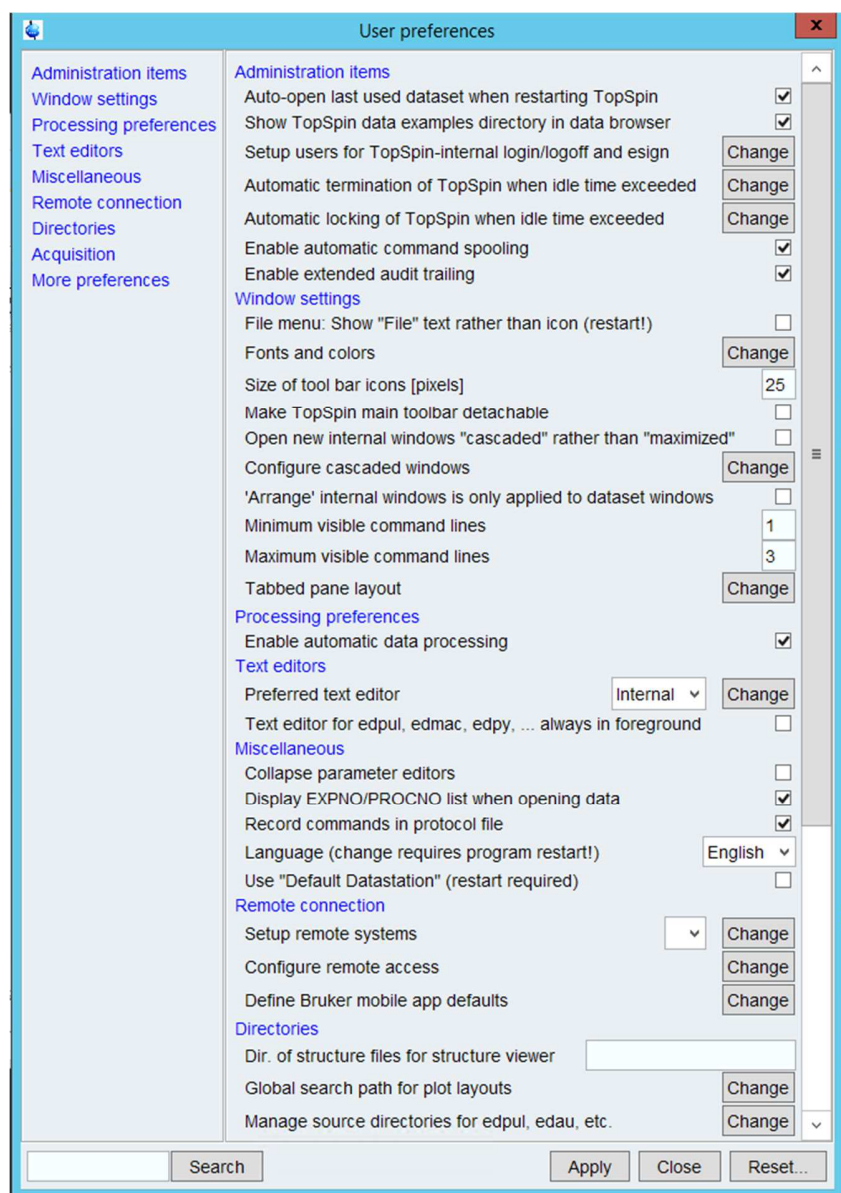
Remember Manage and thereafter Preferences to change many settings in the program.
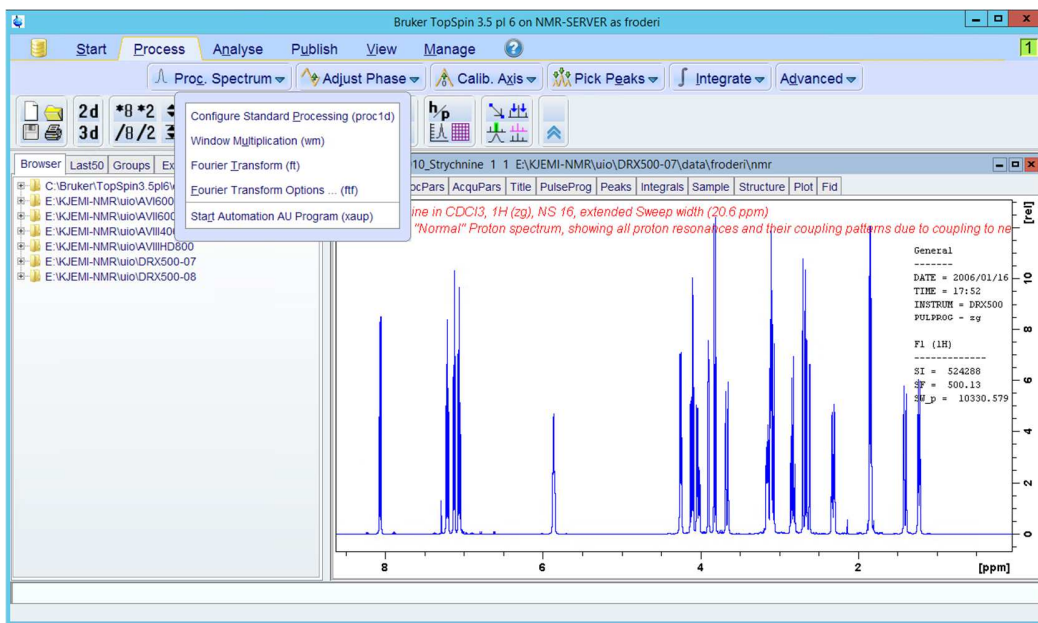
In the Process pane, you find the new commands proc1d and xaup that can be useful newcomers to use instead of efp or ft. Instead of using efp, apk and abs try out xaup and proc1d!
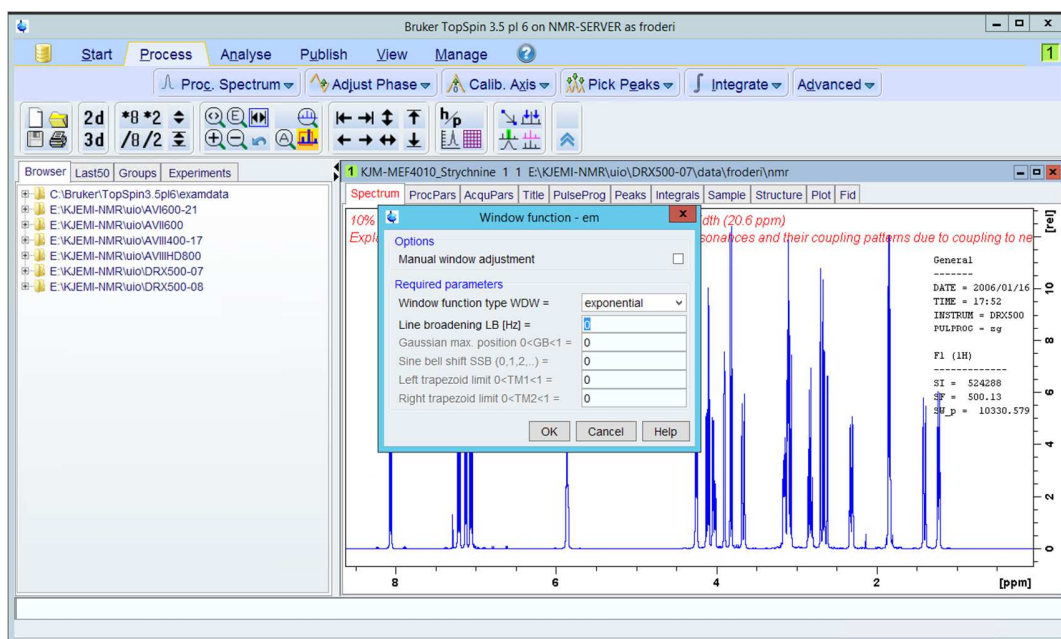
Under wm, you can set various line broadenings in Hz – for instance 1 or 0.3. The window function can also be changed from exponential to another one. Try them out.
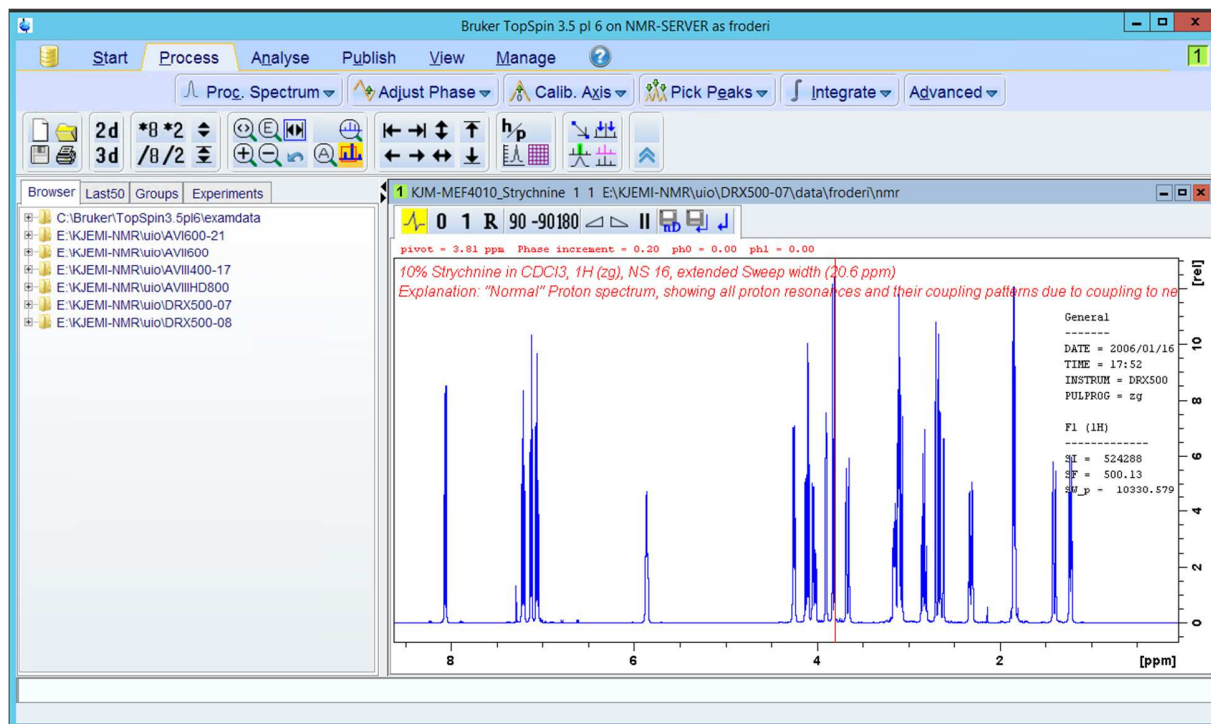
The Adjust phase pane brings up the usual 0 and 1 – zero and first order phasing options.
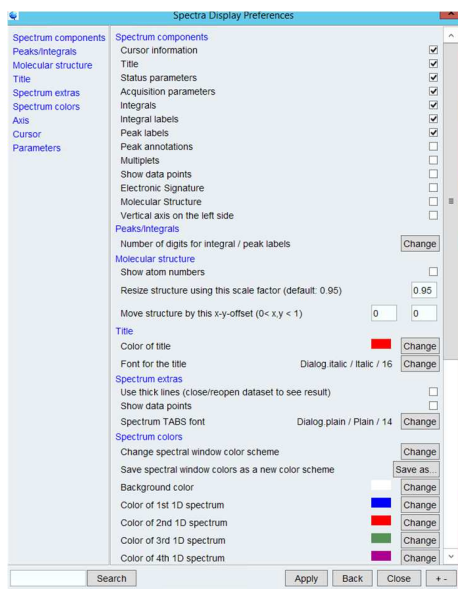
The writer found it useful to bring up Spectra display settings from inside of User preferences found under Manage and Preferences.
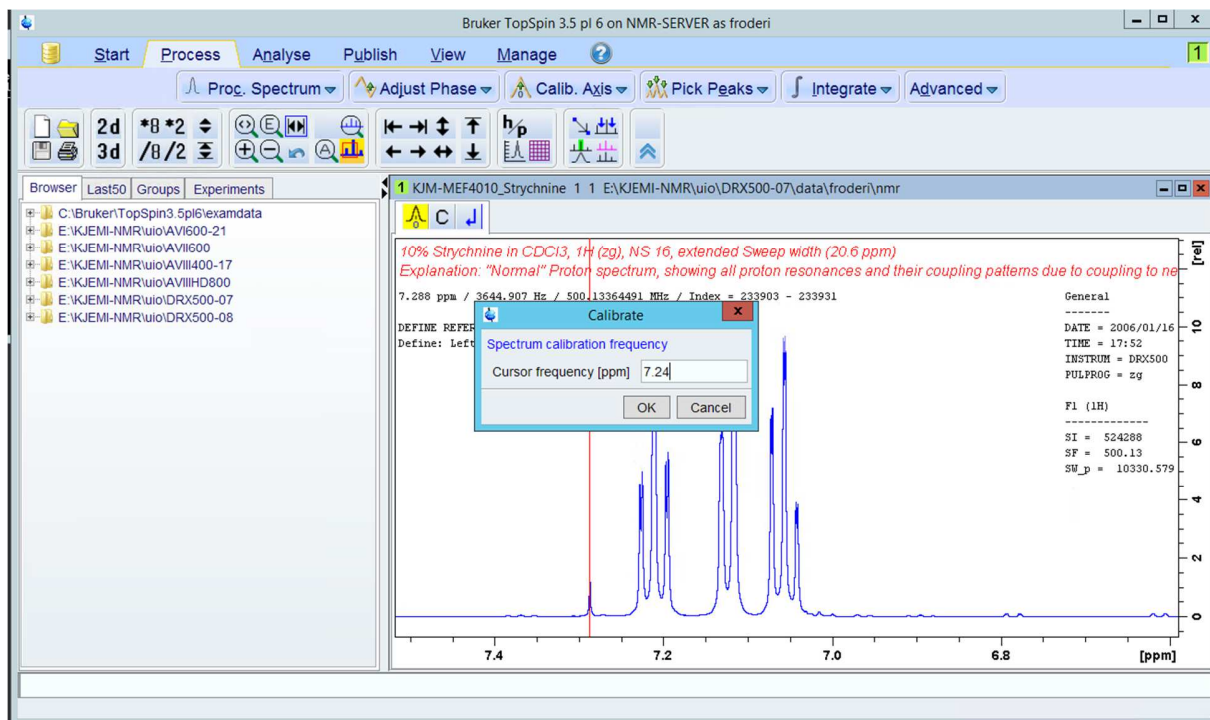
Calibration is done under Calib Axis.
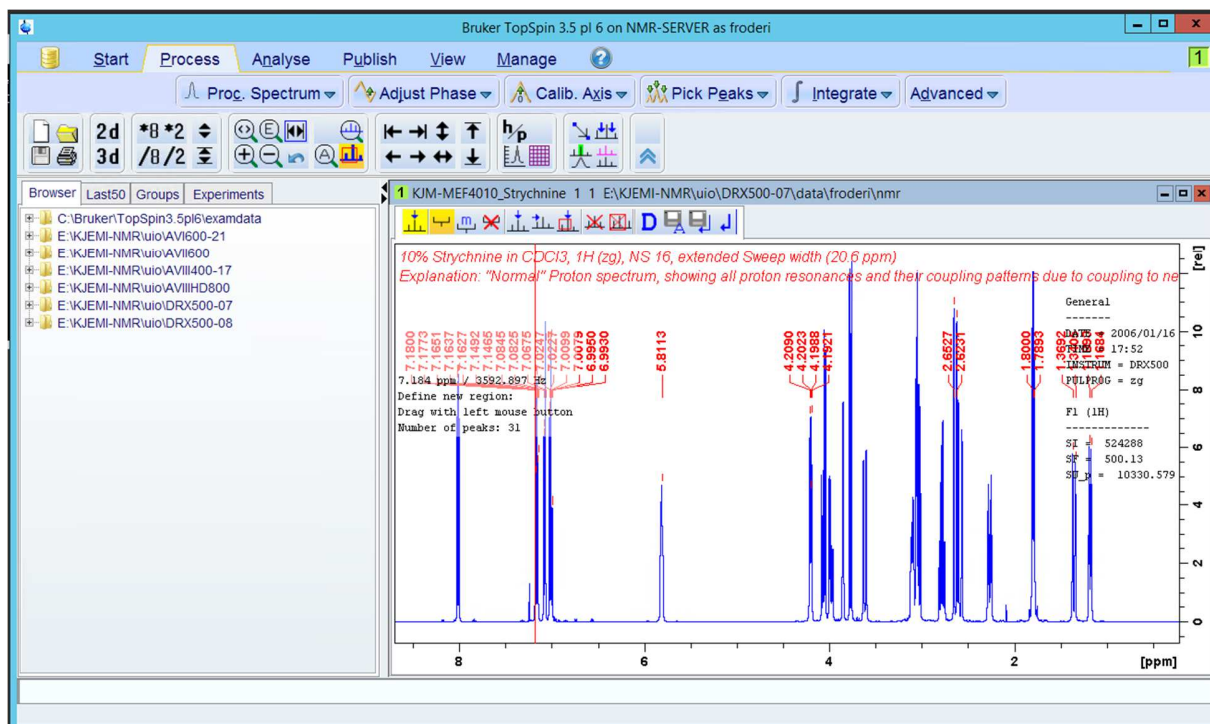
Pick Peaks and Integrate is doing the usual stuff, but not identical to what happens inside TopSpin 1.3. Fool around and try out as much as possible.
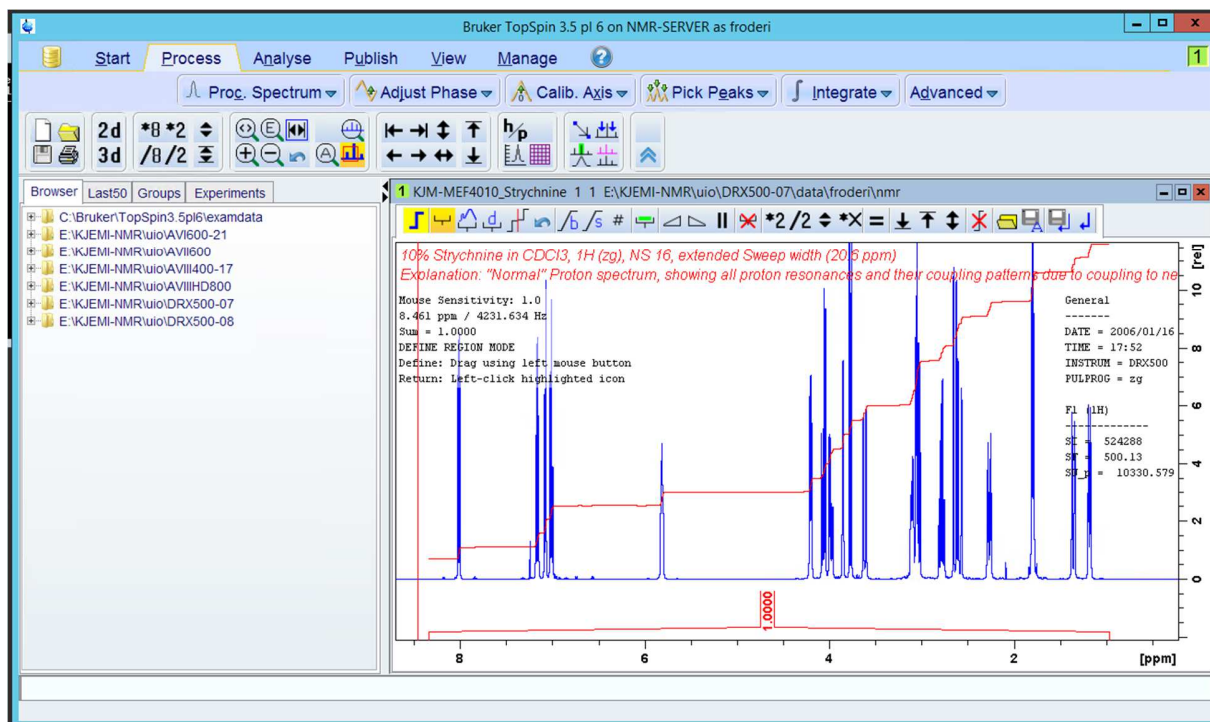
Do not forget to integrate the whole spectrum, use the Bias, and Slop buttons with the mouse to make the integral flat. After flattening remove it (remember how?) and integrate again.
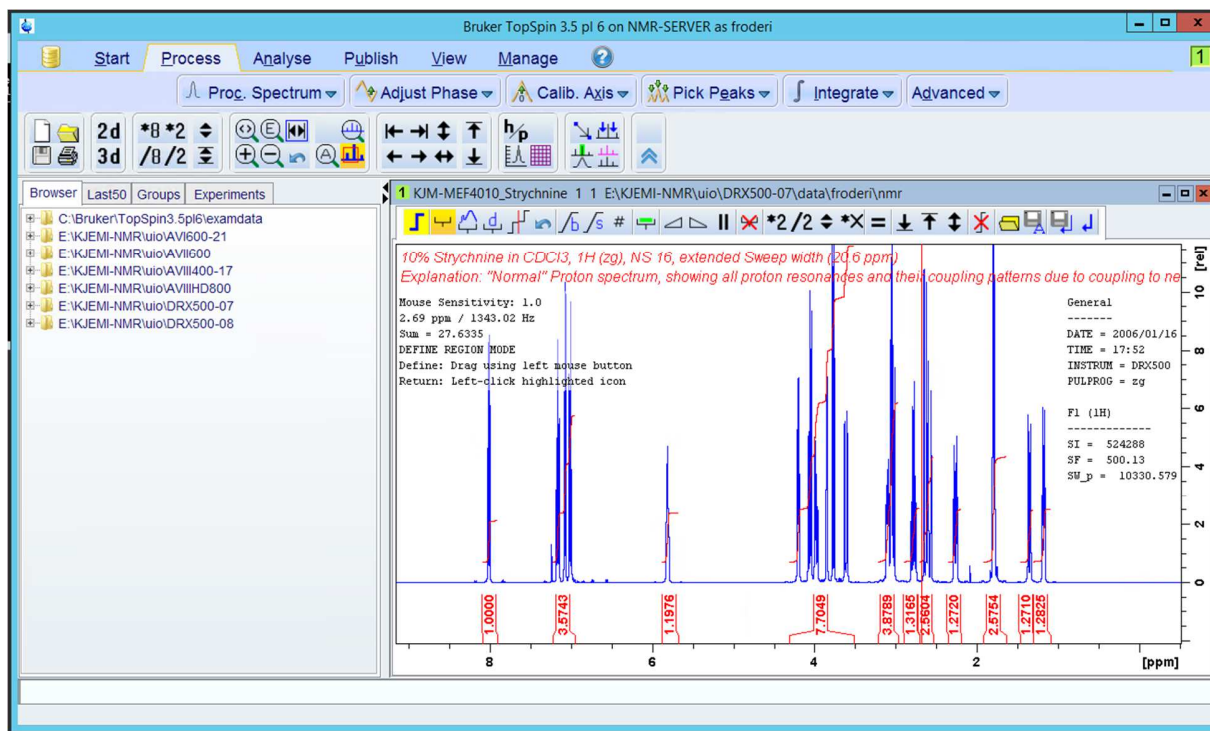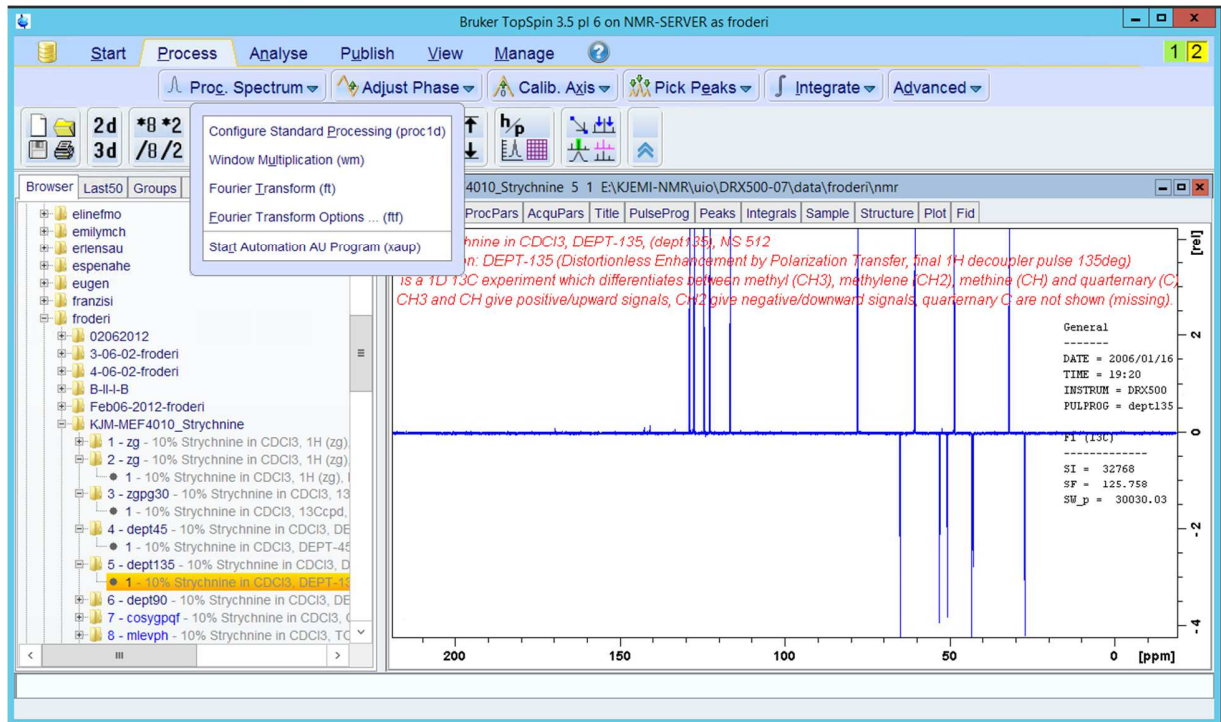
Either proc1d or xaup was great in processing DEPT spectra, or did both do it well in your case?
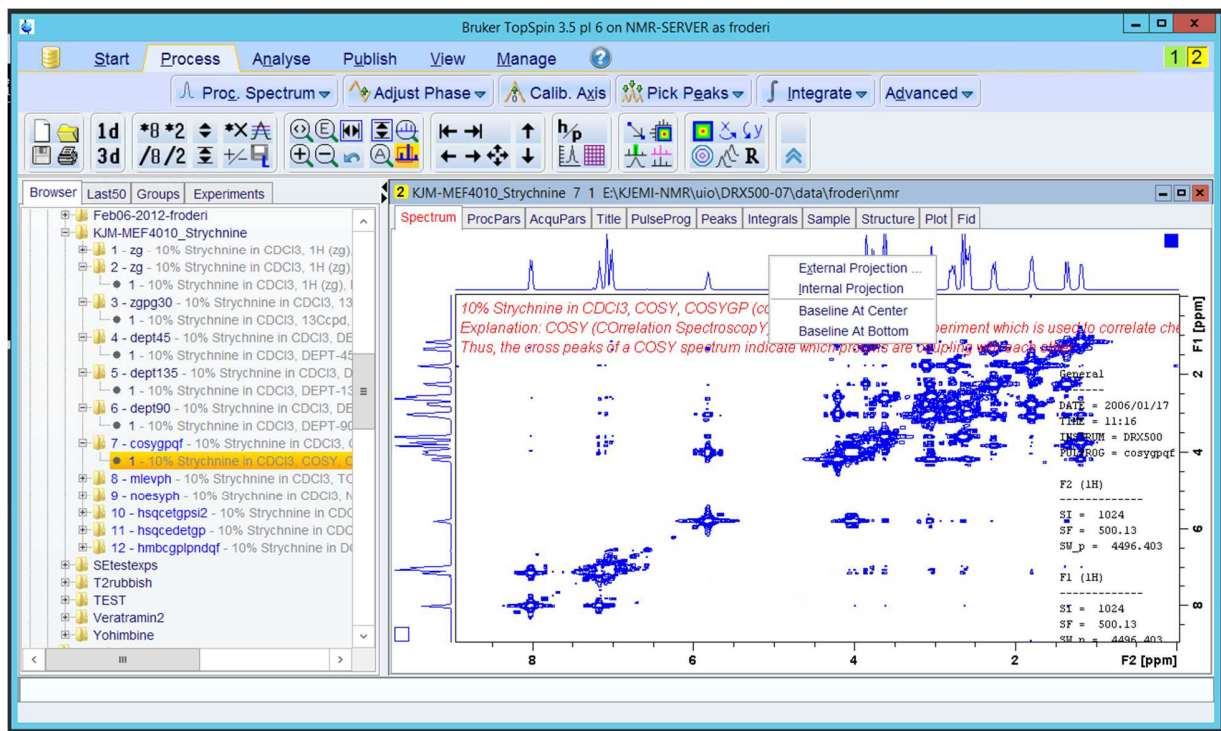
Xfb, ab1, abs2 and sym gave a good COSY.
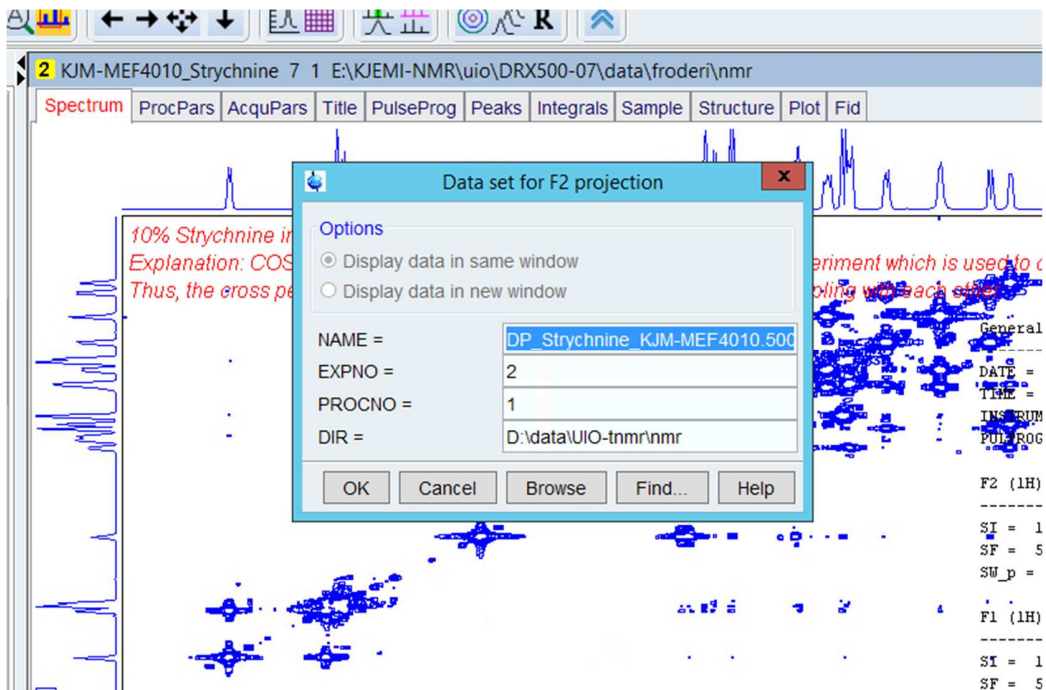
Adding external 1D spectra on the sides of the 2D is still a painful experience. Both the experiment Name and the Directory are simply wrong and must be corrected completely. Alternatively, use the Browse to find the 1D.
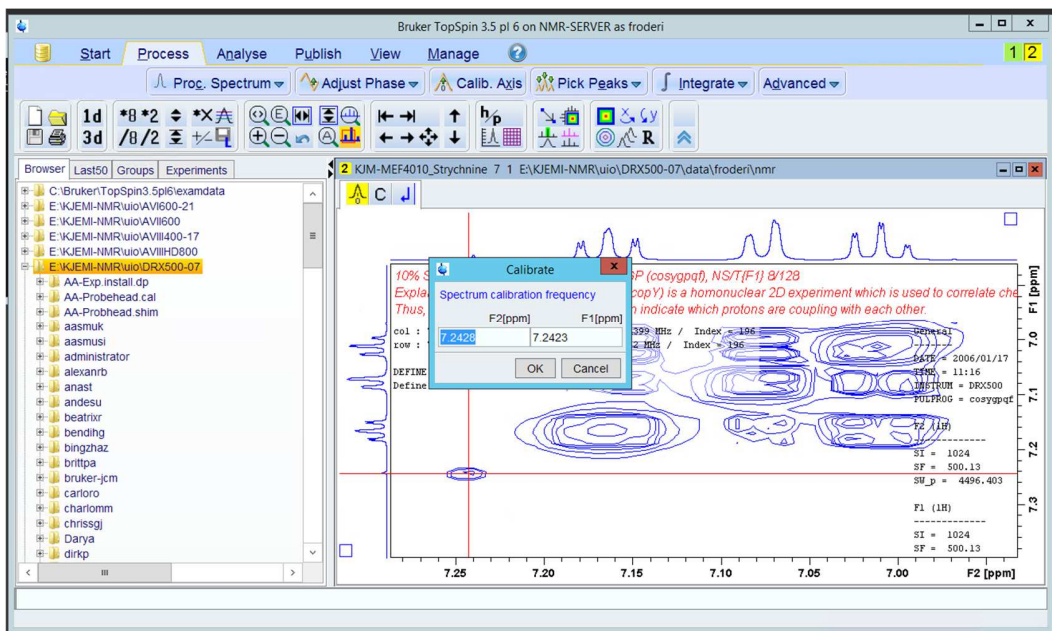
Caleb axis works nicely.
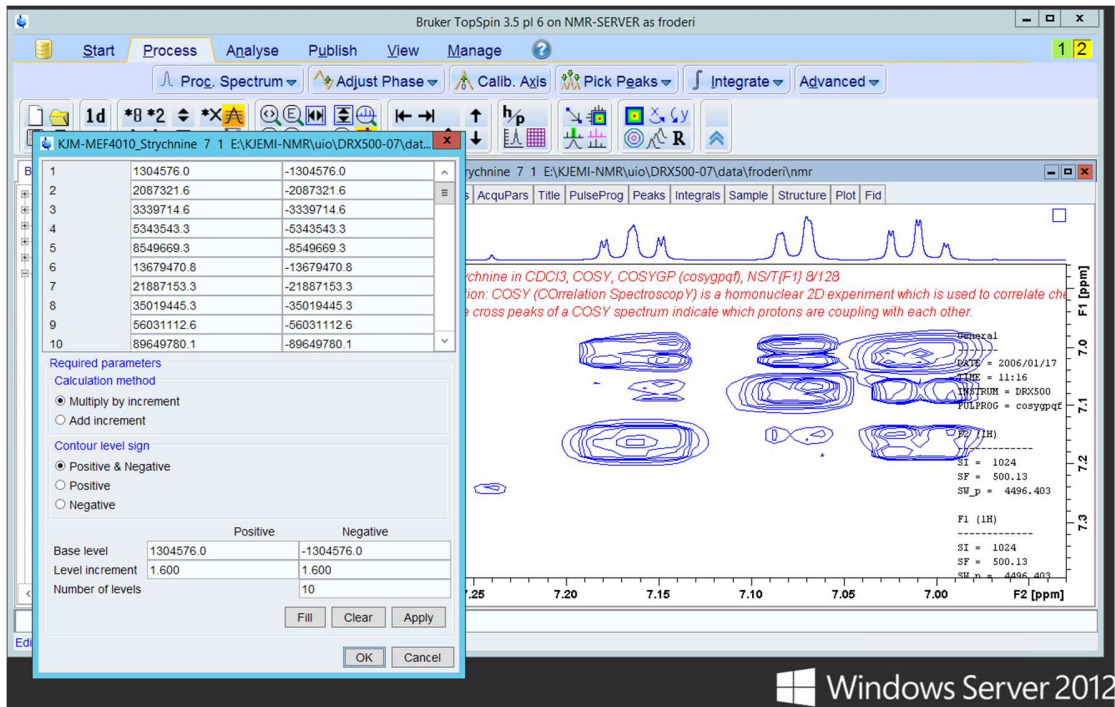
Adding more contours in "the map" are done by clicking on the 8th symbol in the upper line, e.g. the A with the four horizontal lines and then changing Level increment and Number of levels followed by Fill, Apply and OK.
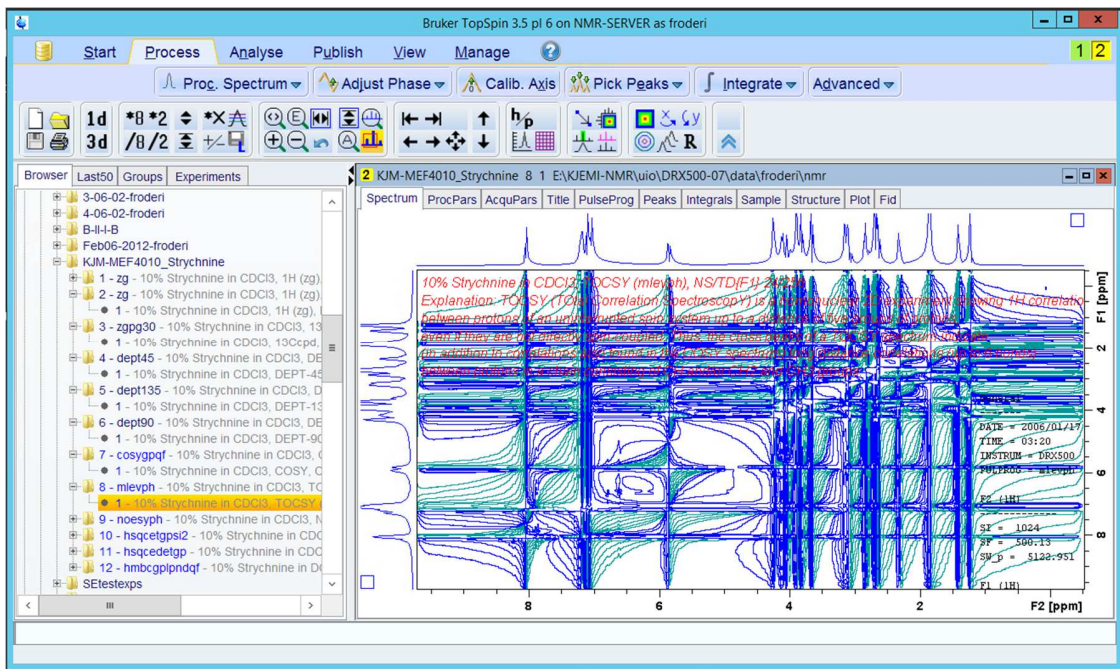
Please open the TOCSY dataset (mlev). Xfb if it is not Fourier transformed yet.
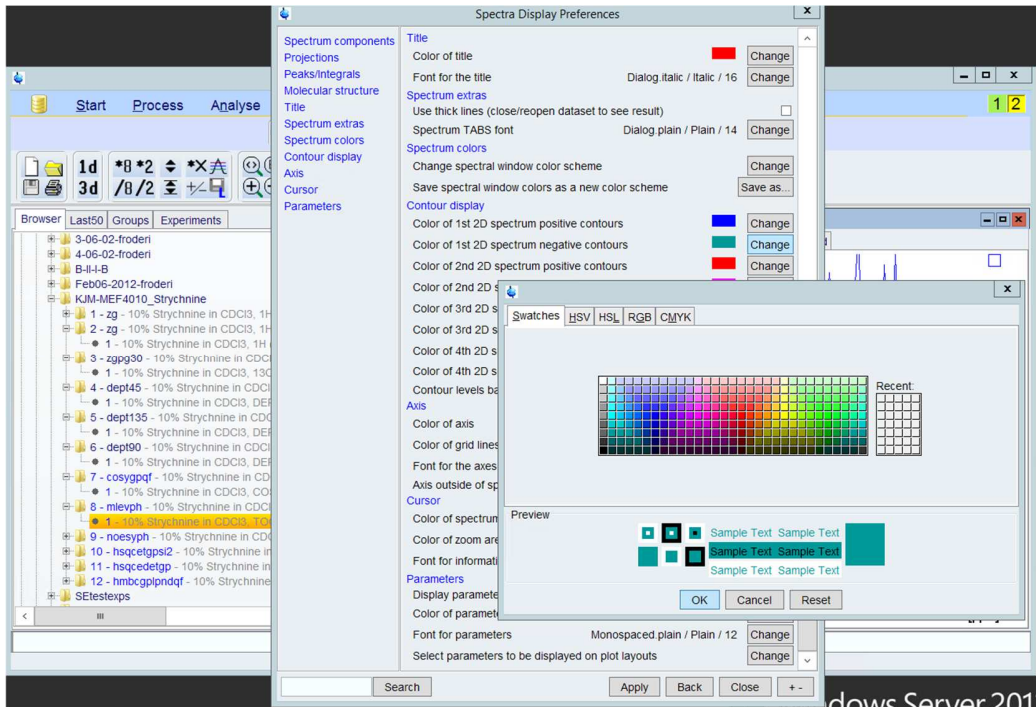
Use Manage, Preferences and Spectra Display Preferences to get the ugly green color away from the spectrum.
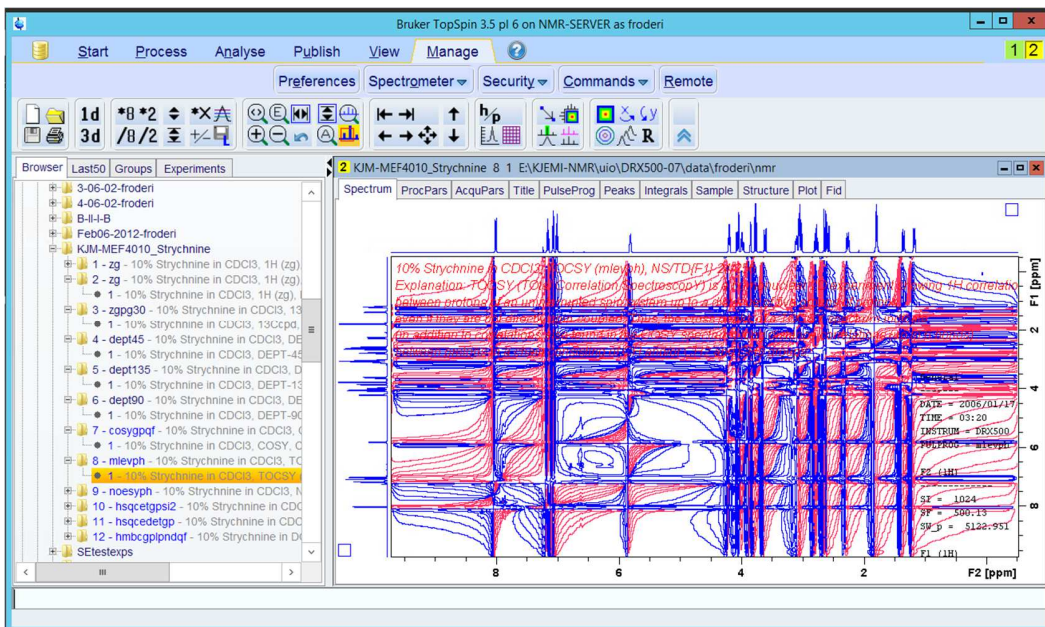
Insert the previously calibrated 1D ^{1}H NMR spectrum on both sides. You ought to remember from the TopSpin 1.3 how to do this.

rsr 1 or rser 1

sinm
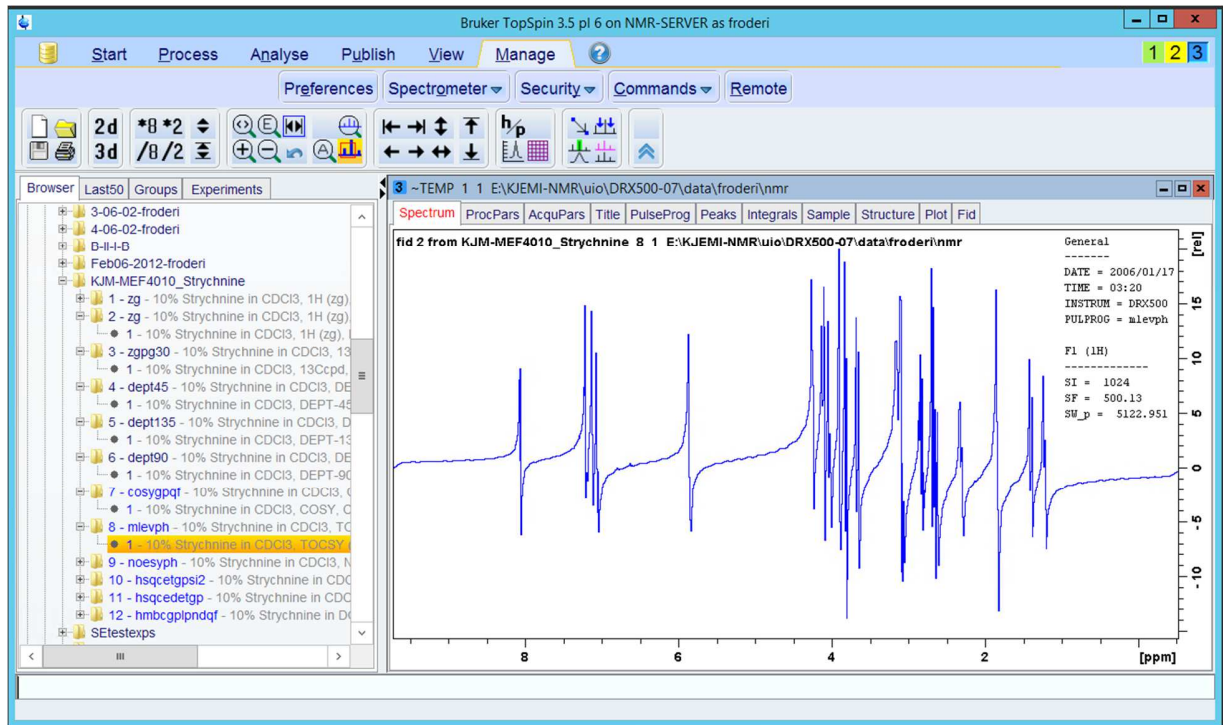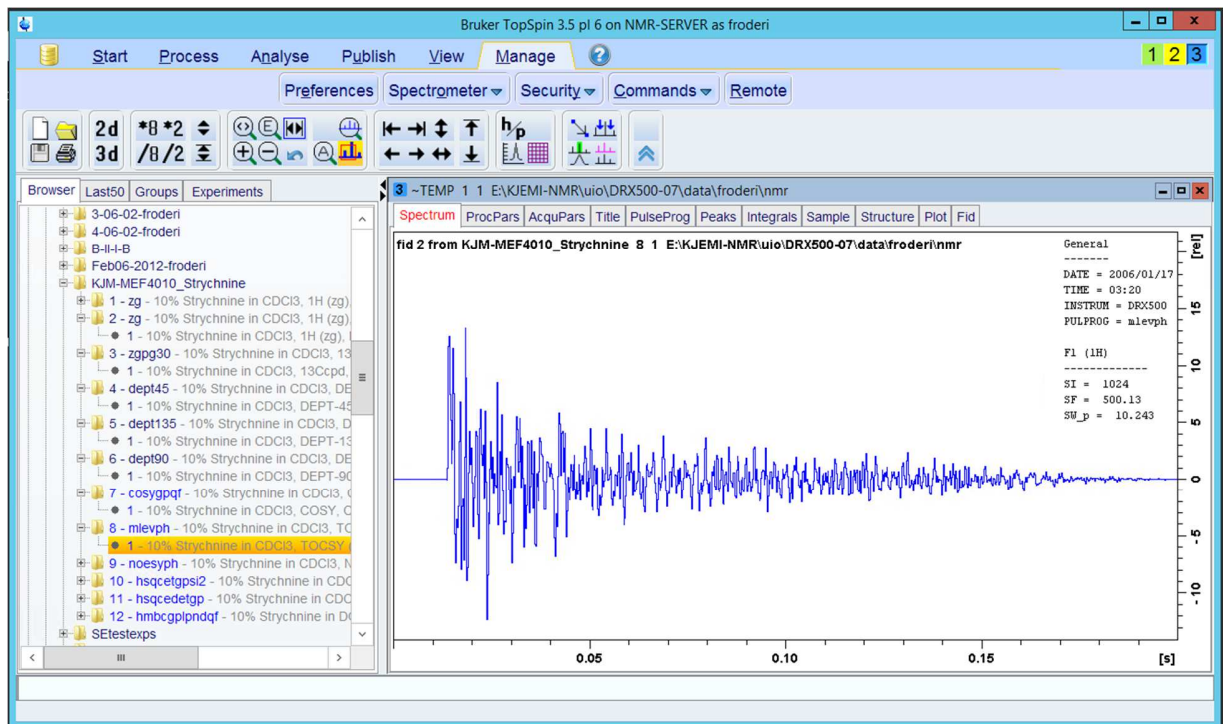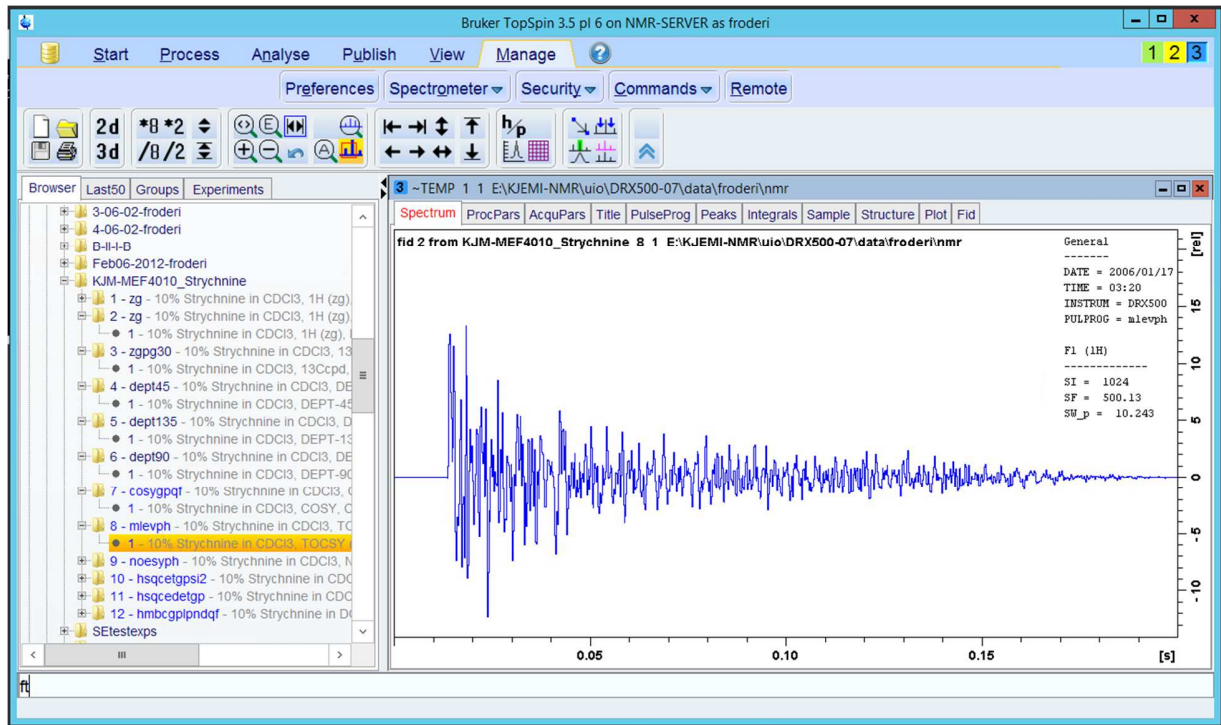
ft
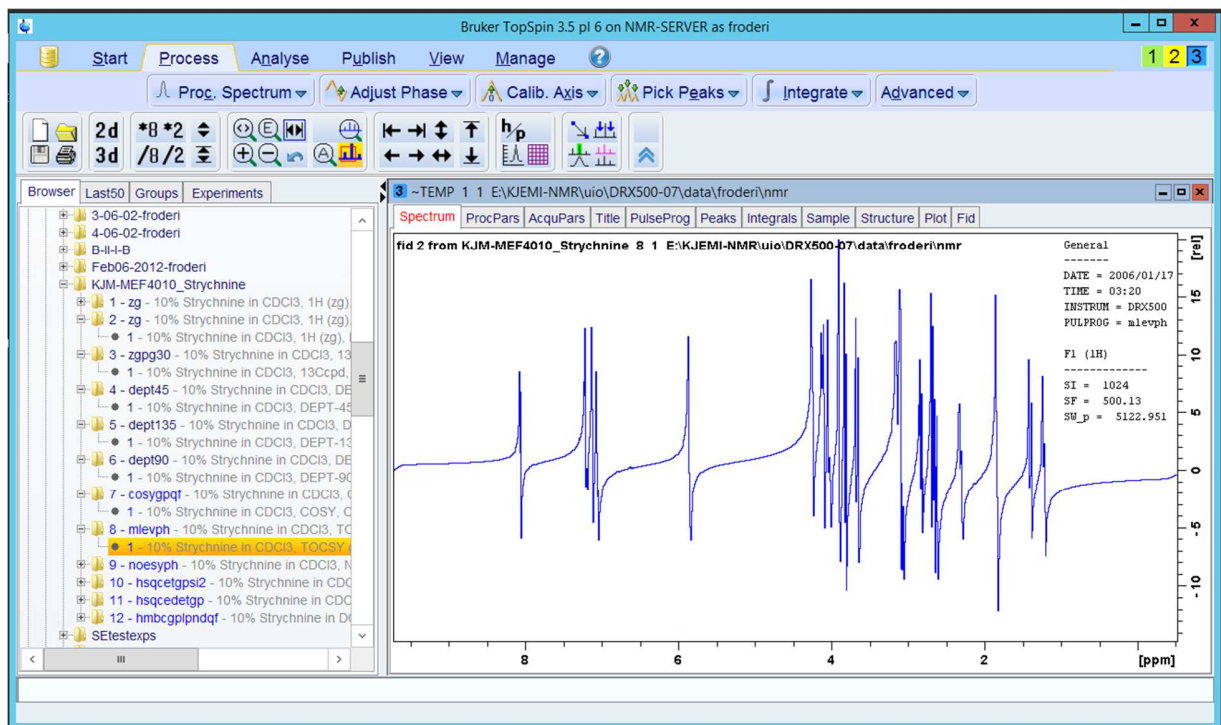
Click on process and then Adjust Phase (left and right side of Adjust Phase give different options, explore them.
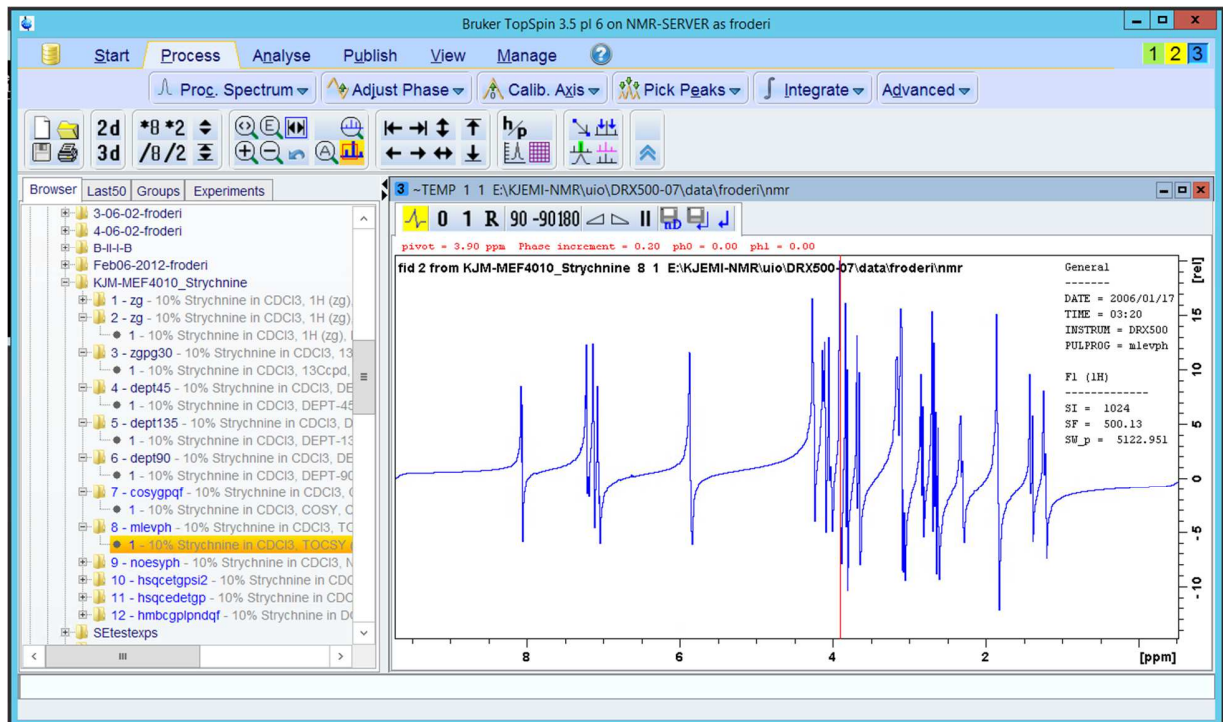
Select the option that give you manual phasing.
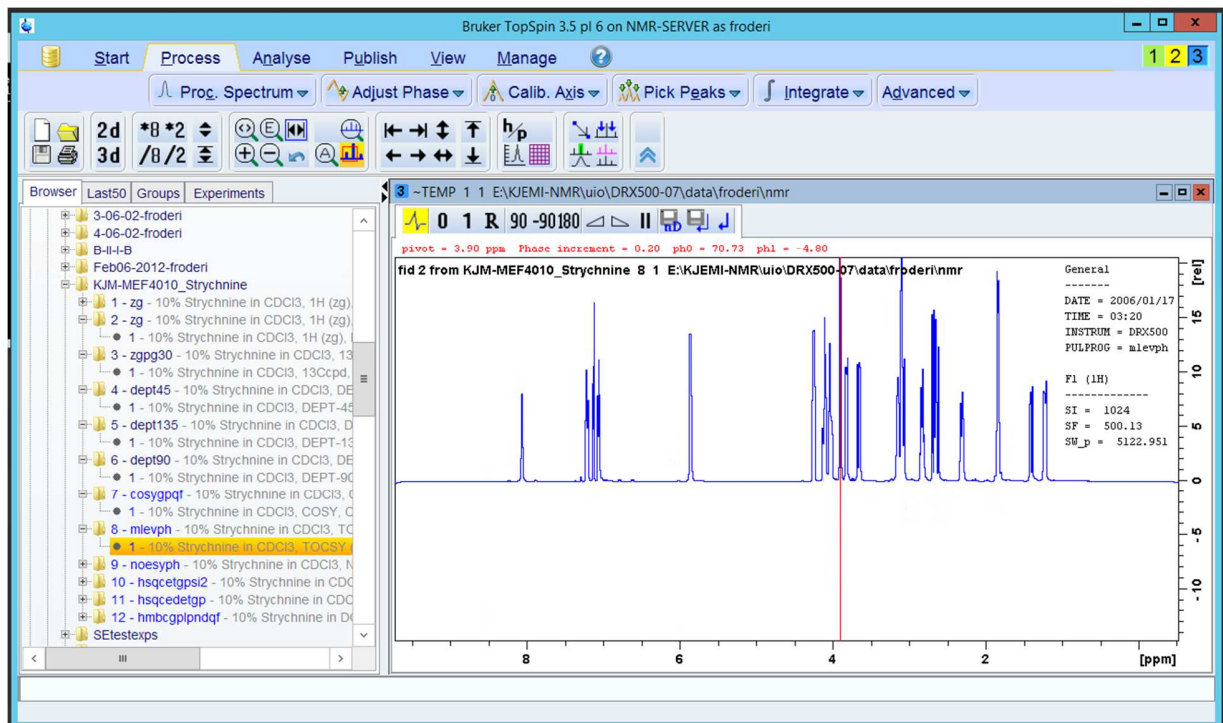
Do the phasing with "0" and "1" if "0" does not do the trick alone, with mouse. Save with nD
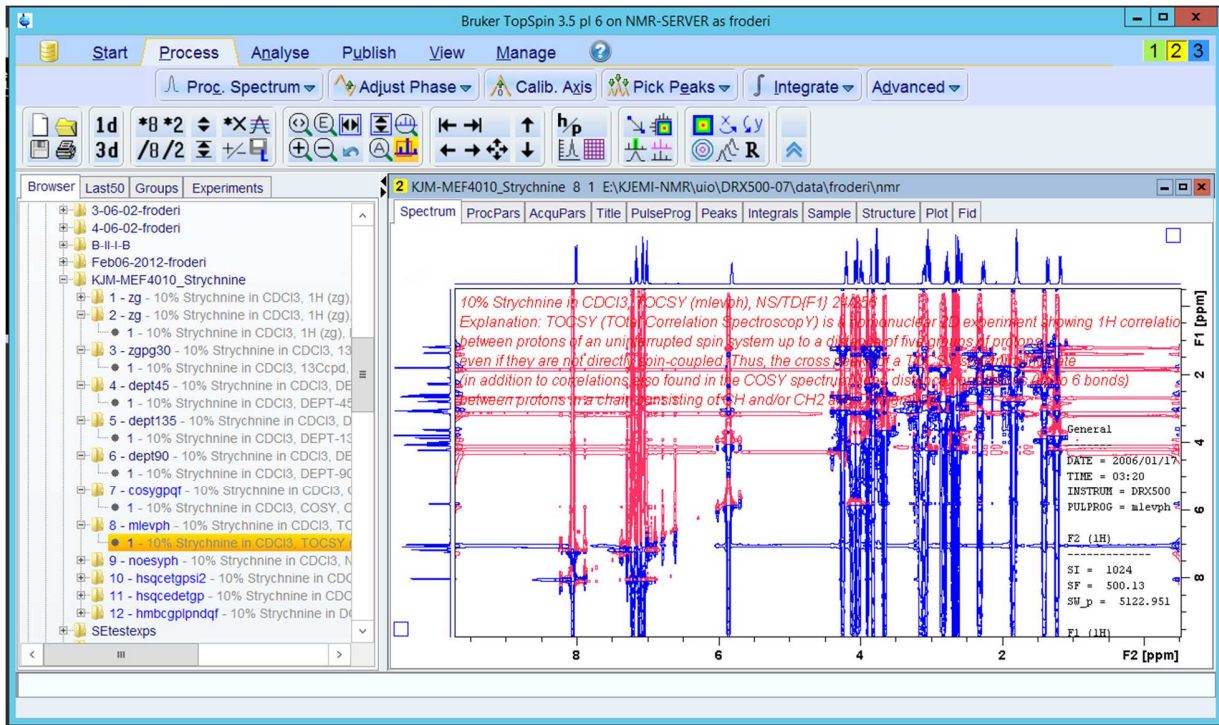
Xfb and see observe the improvement horizontally.
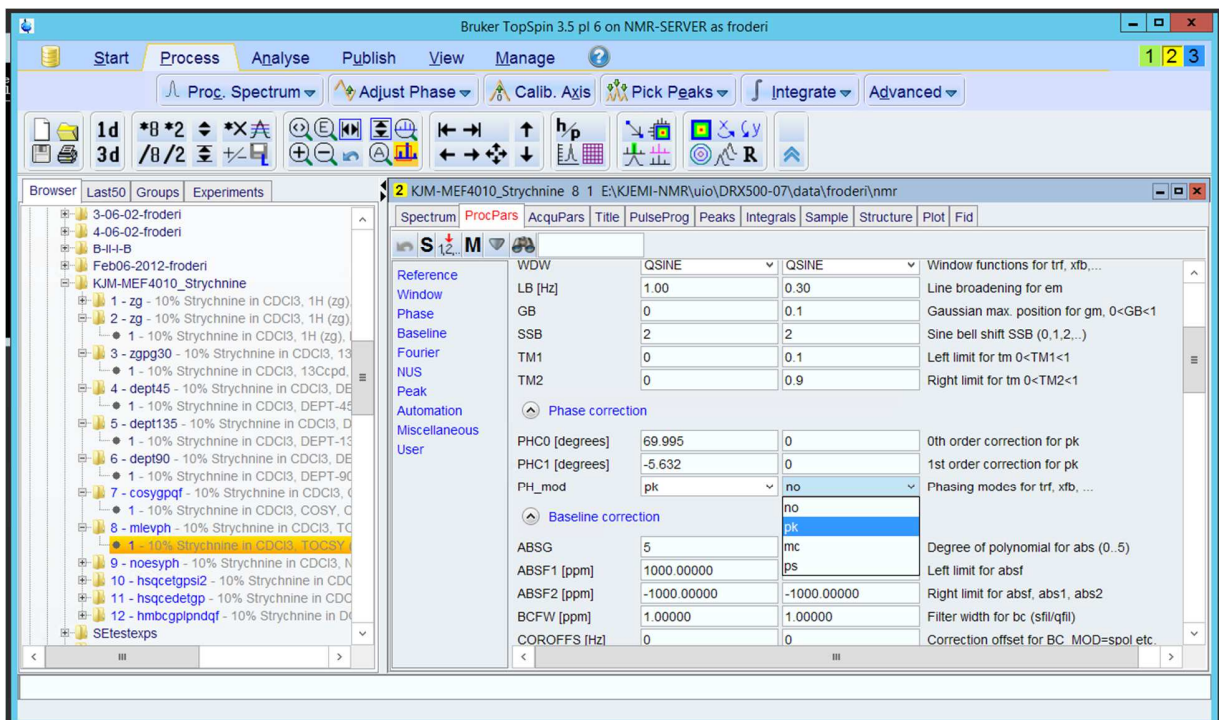
Change to phase correction for the F1 dimension if not done yet.
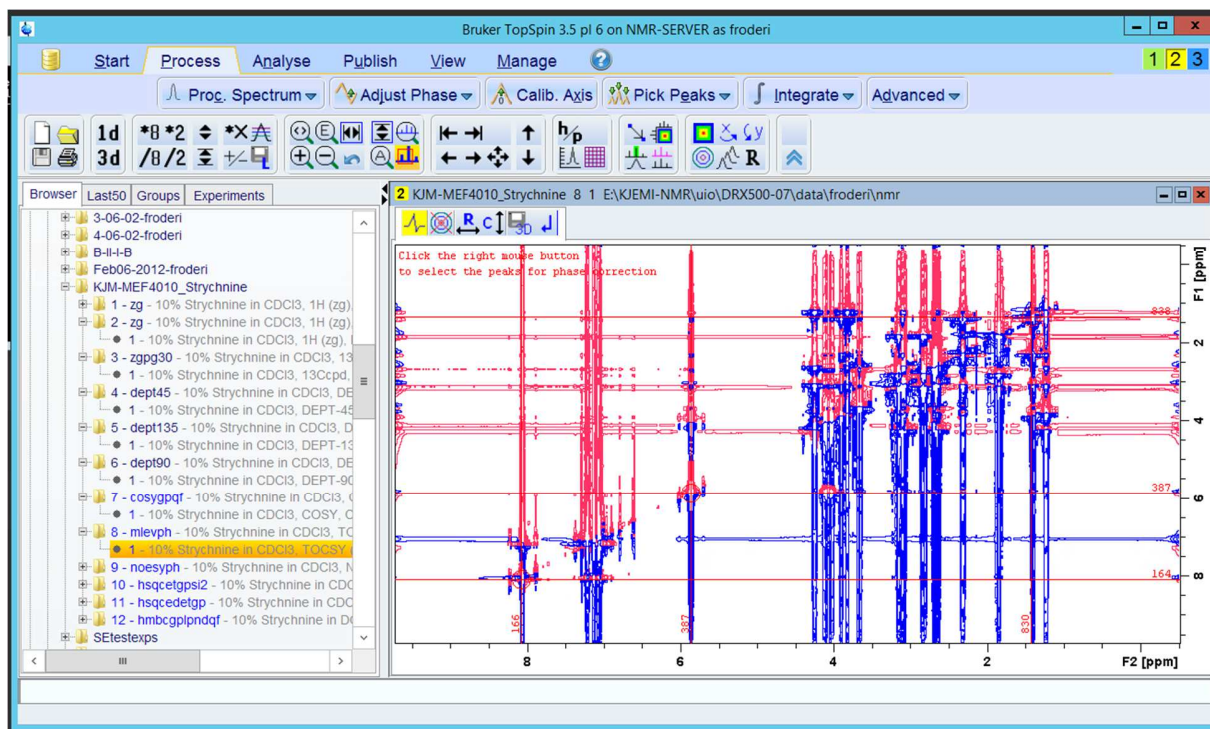
Add crosses to be used in the vertical phasing (F1). It is three of them here, but they are red.
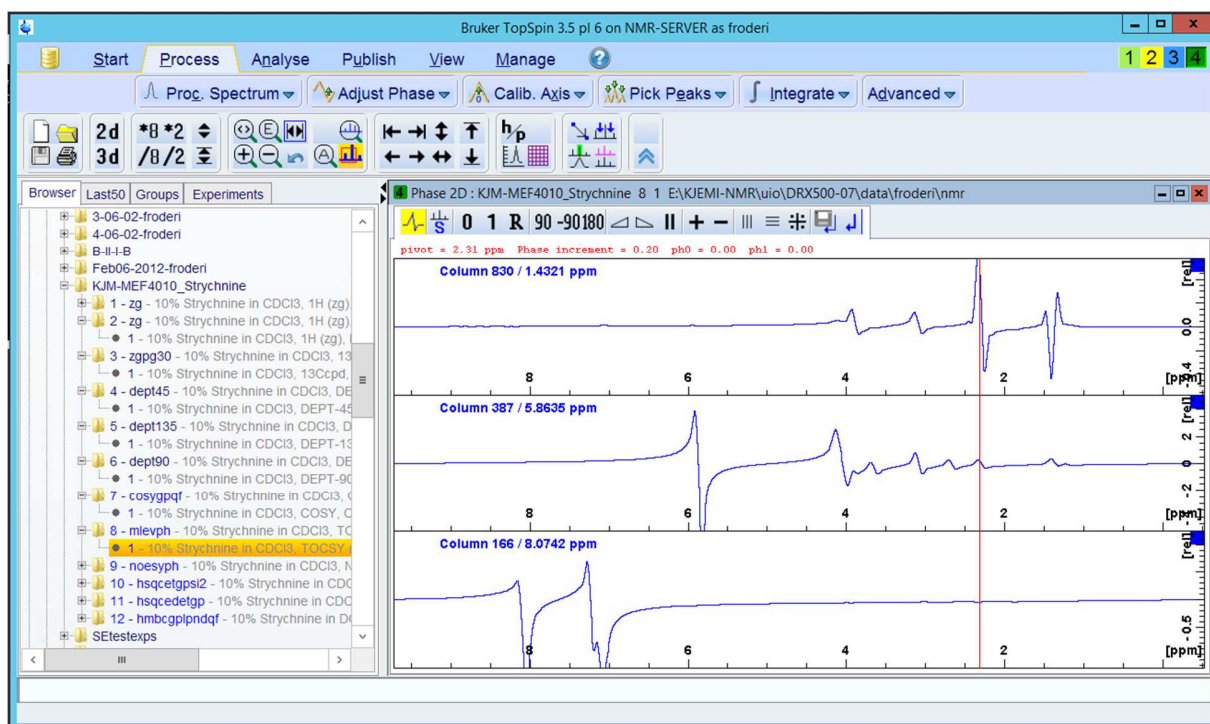
Use "0" and "1".
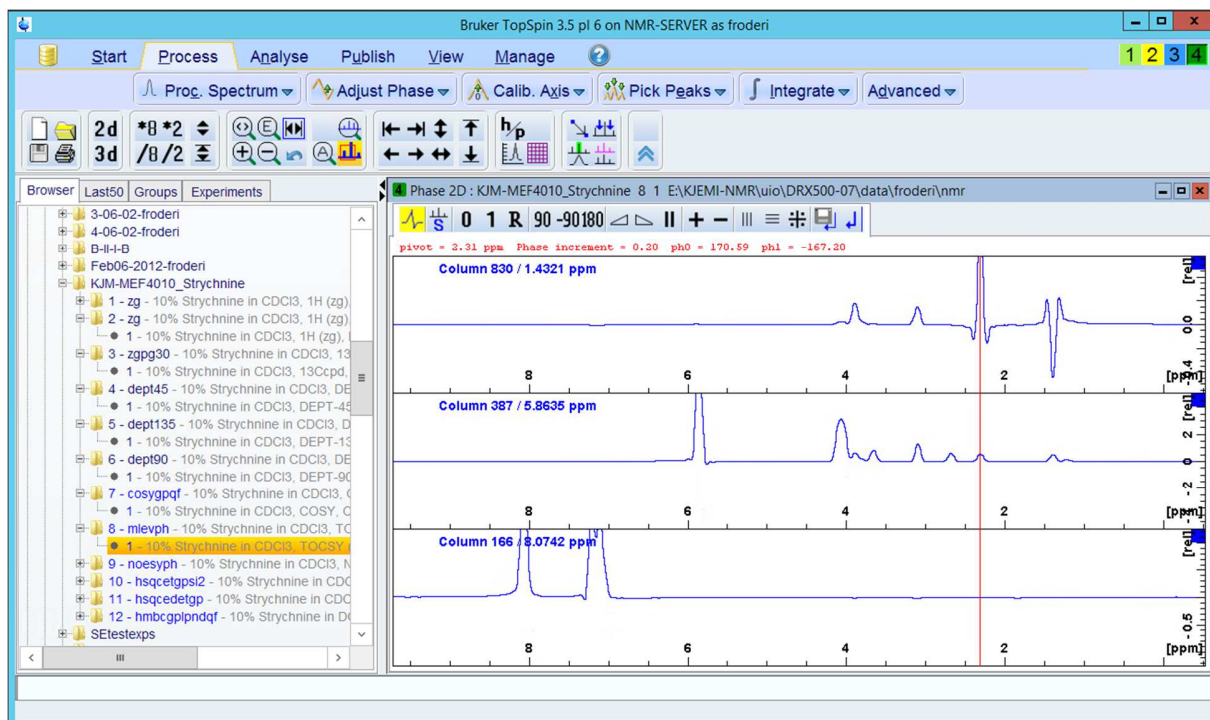
Save
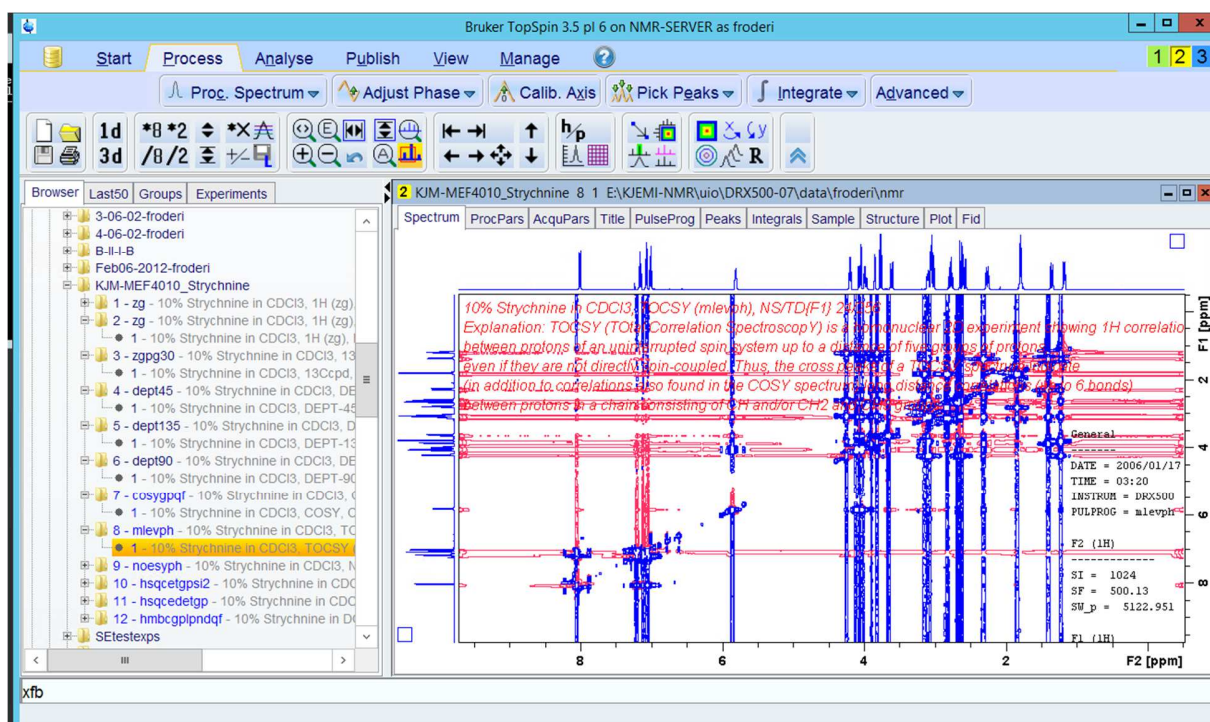
Fourier transform in 2 dimensions. Followed by abs1 and abs2 and maybe syma. If bad result from syma do it all again without syma.
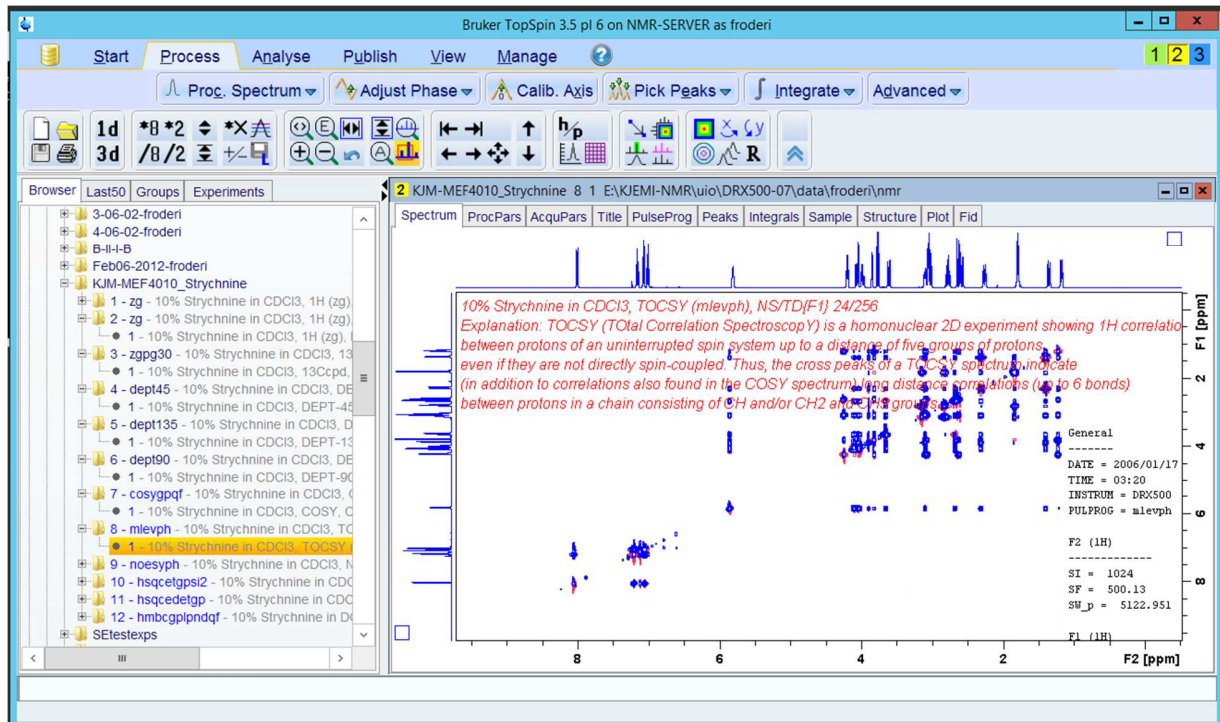
Result after adjusting the intensity.
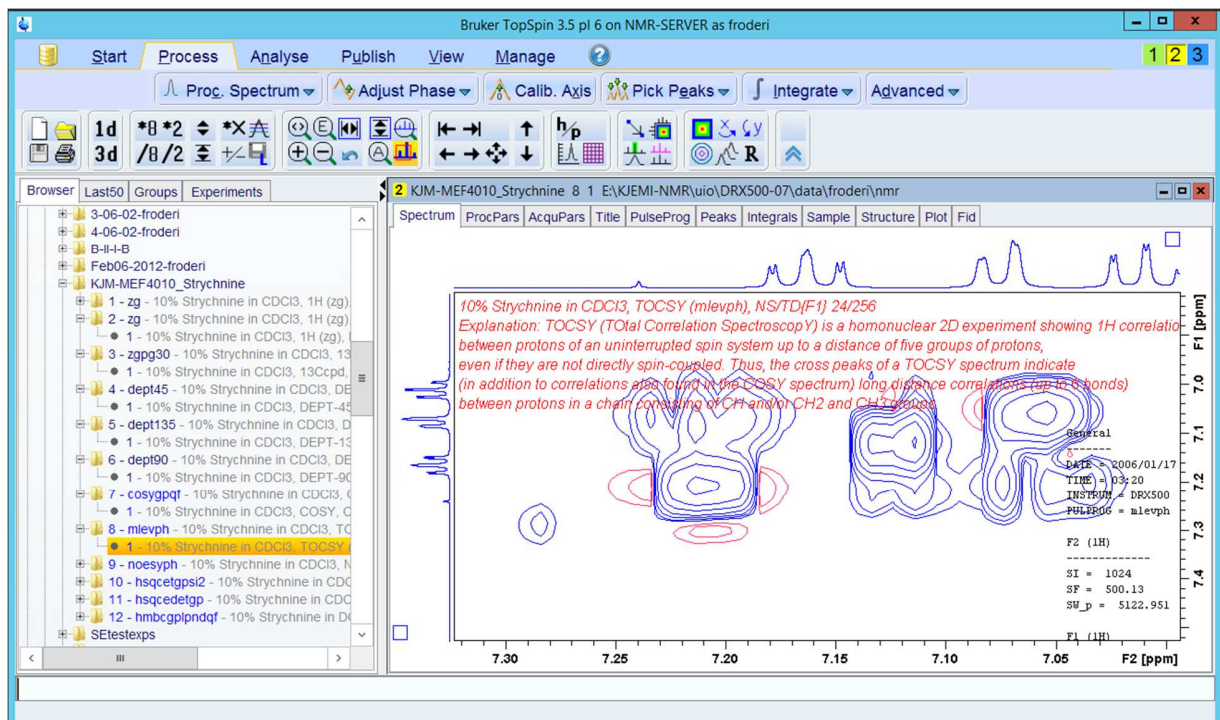
The 2D diagonal peak for the impurity CHCl$_3$ in the solvent CDCl$_3$ is not yet aligned with the 1Ds.
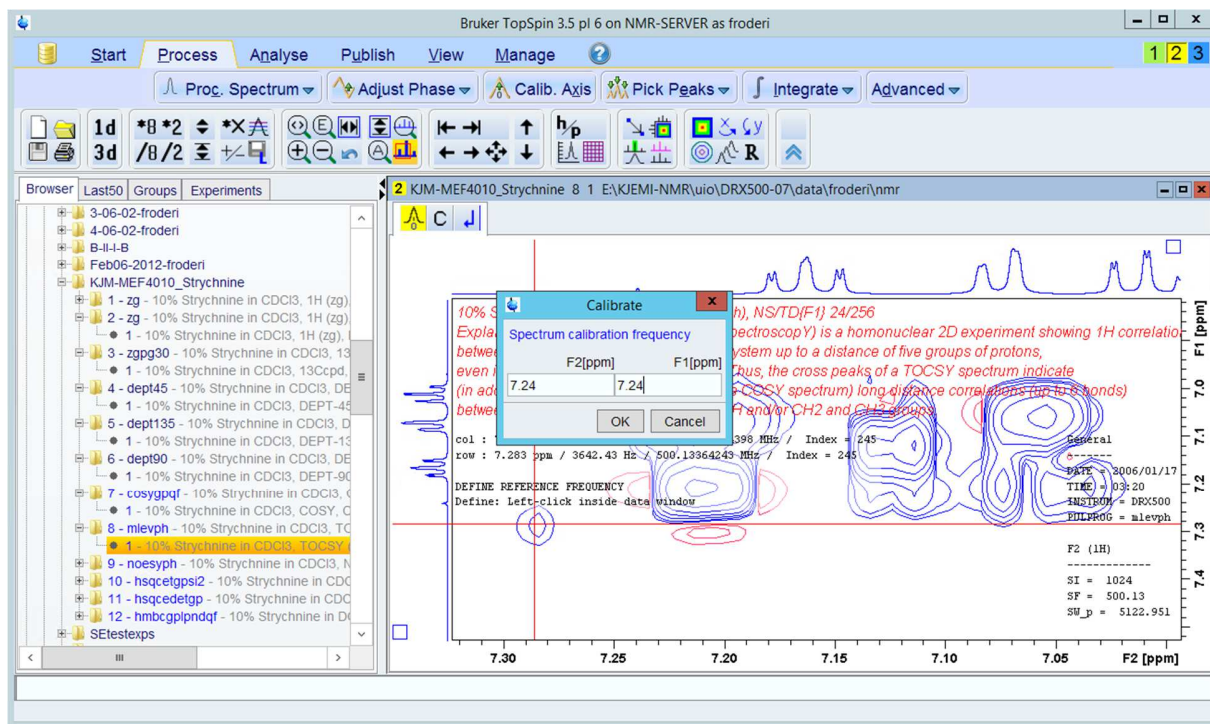
Do the alignments. Calib Axis and so forth.
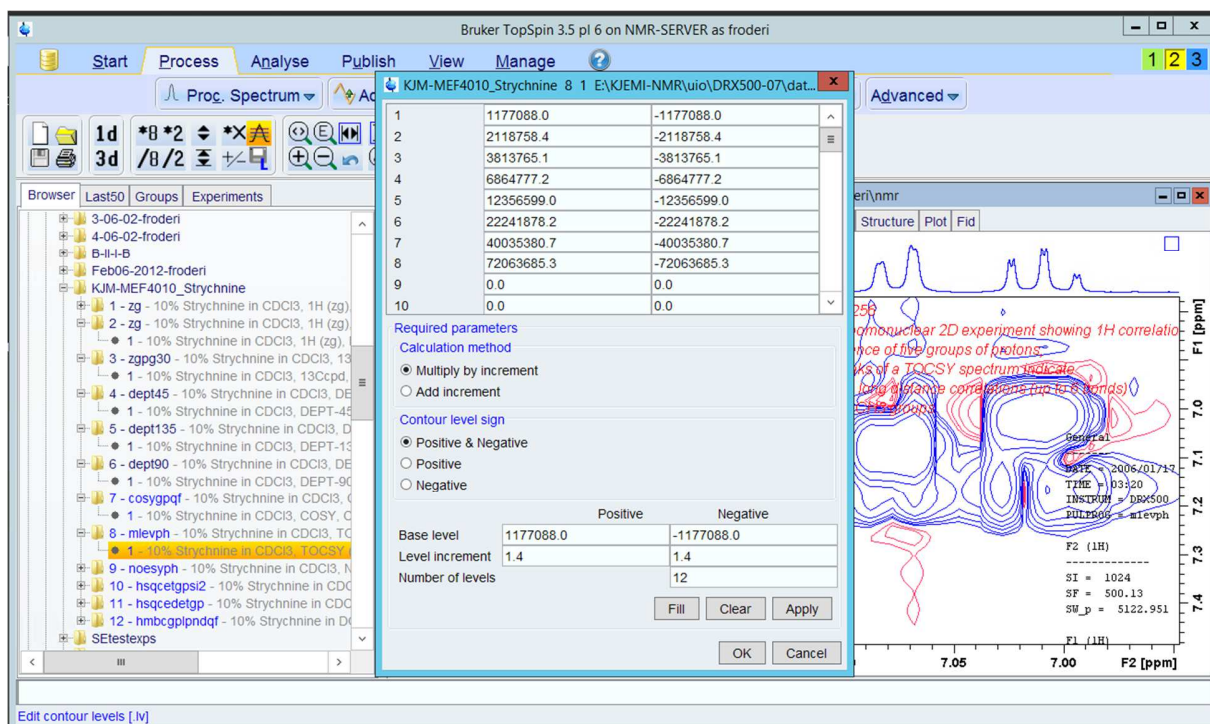
Want more contours? Change Number of levels and Level increment followed by Fill, Apply and OK.
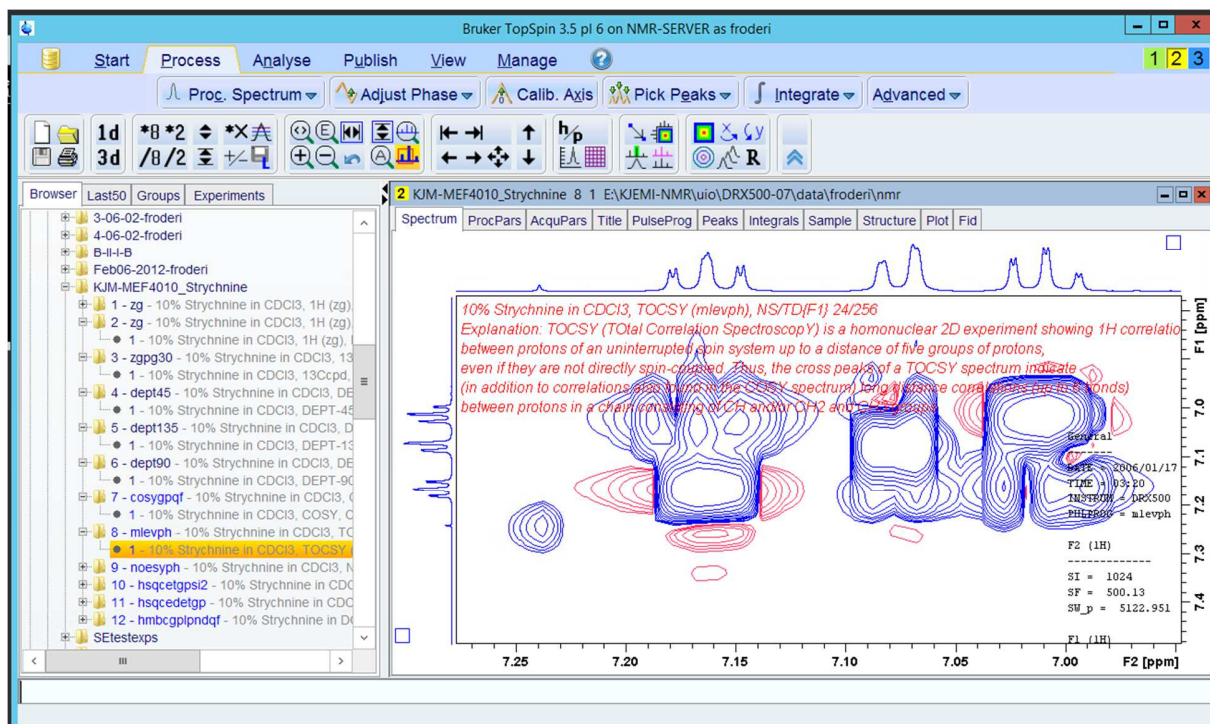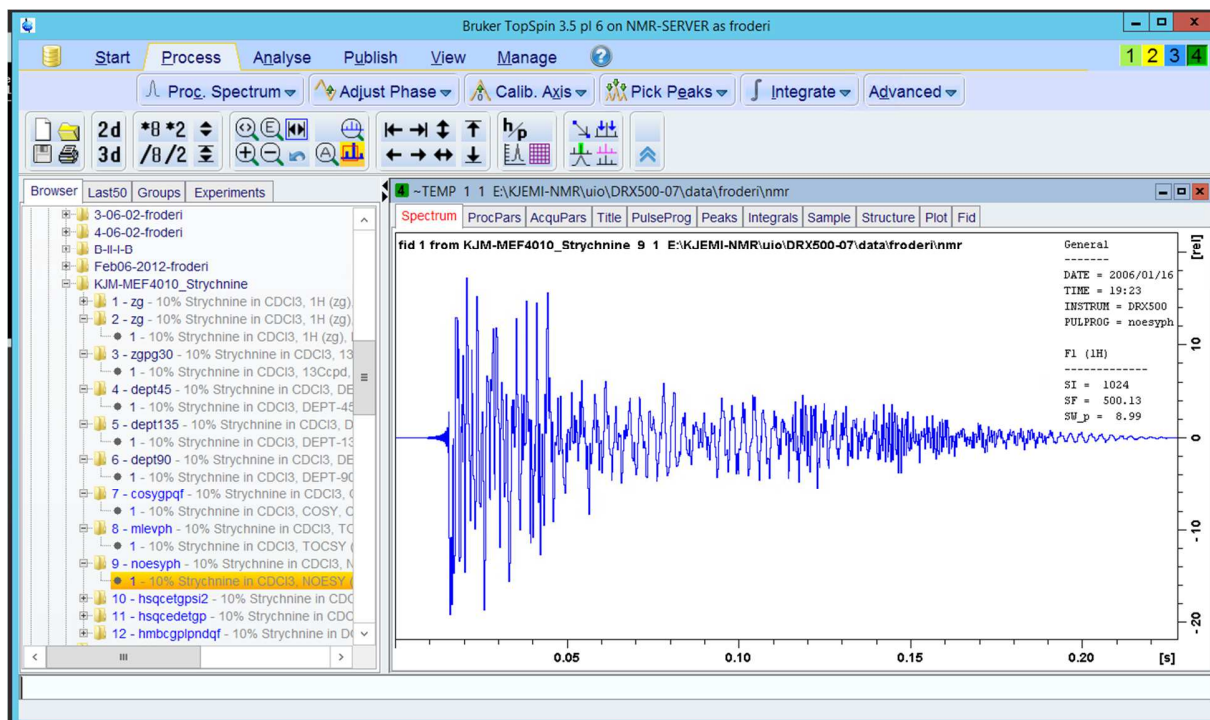
Play with the contour adjustment tool.
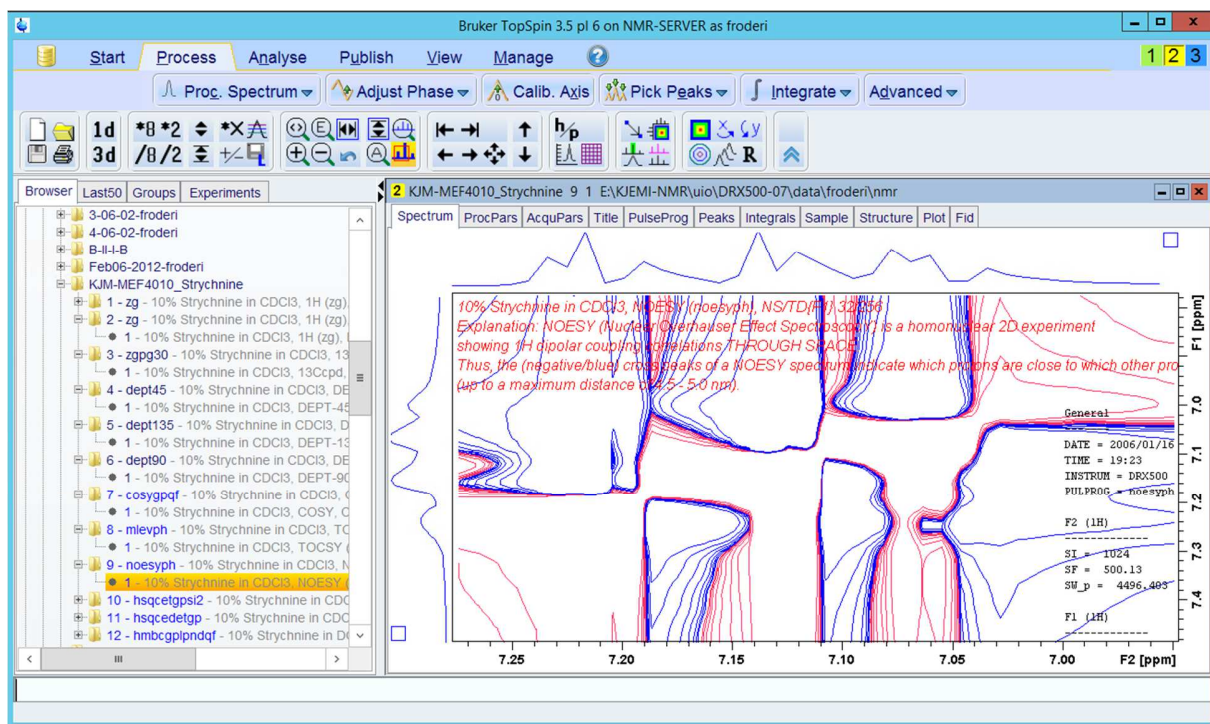
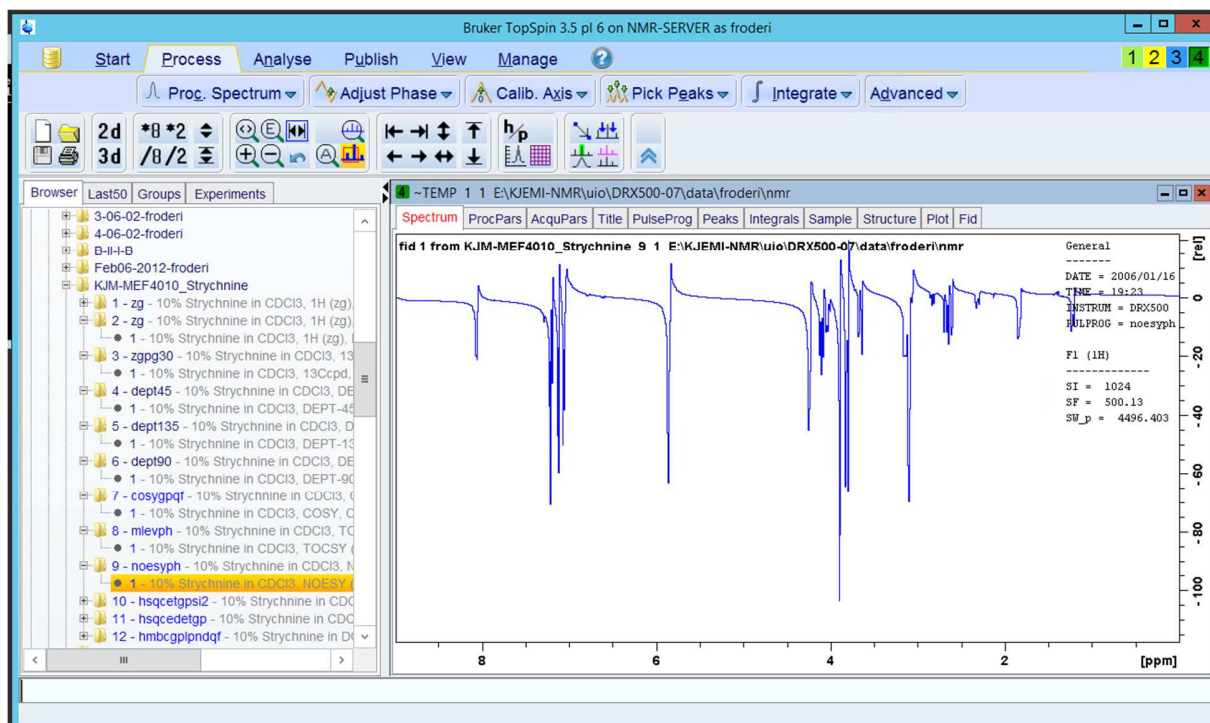Open the NOESY experiment and realize that the program has not become any better while maturing from version 1.3 to version 3.5. It still opens with the ppm scale from previous exp..
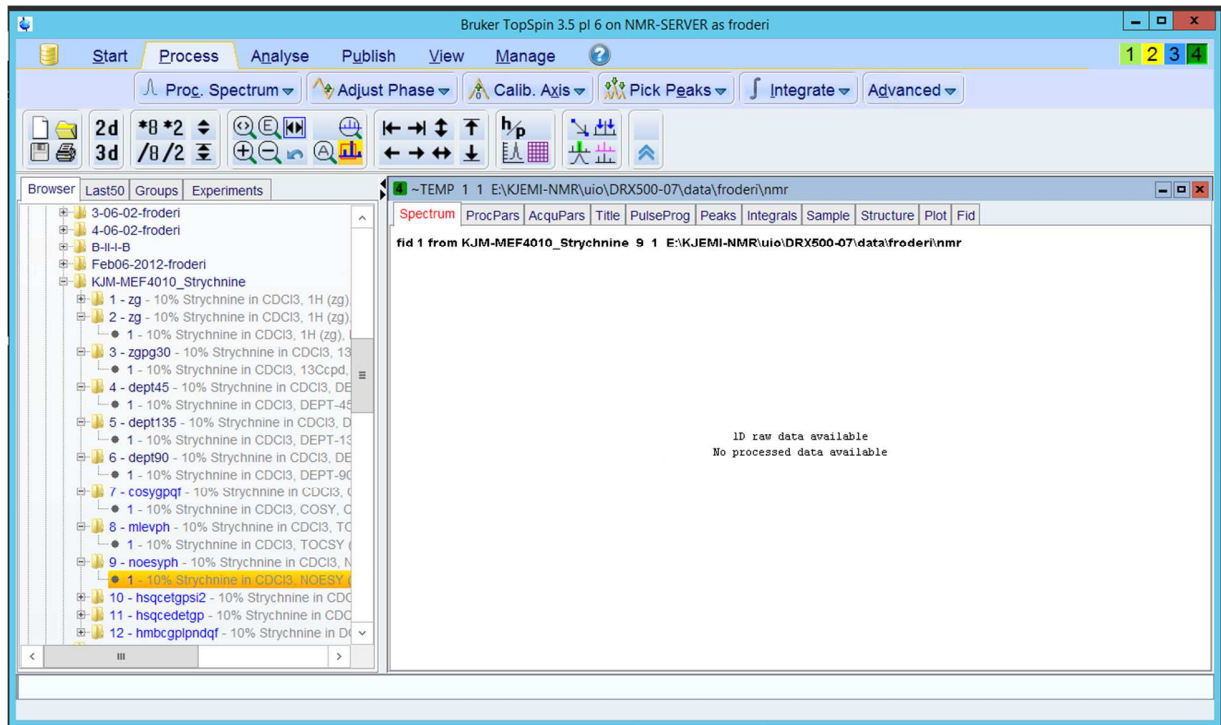
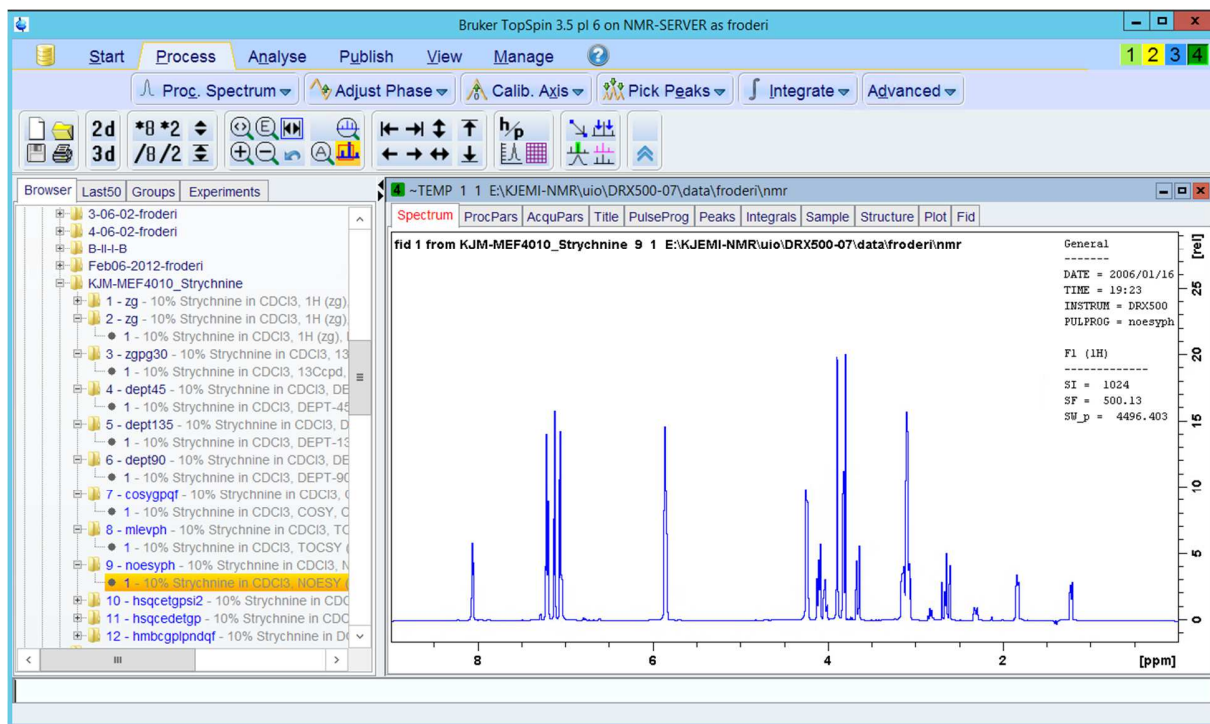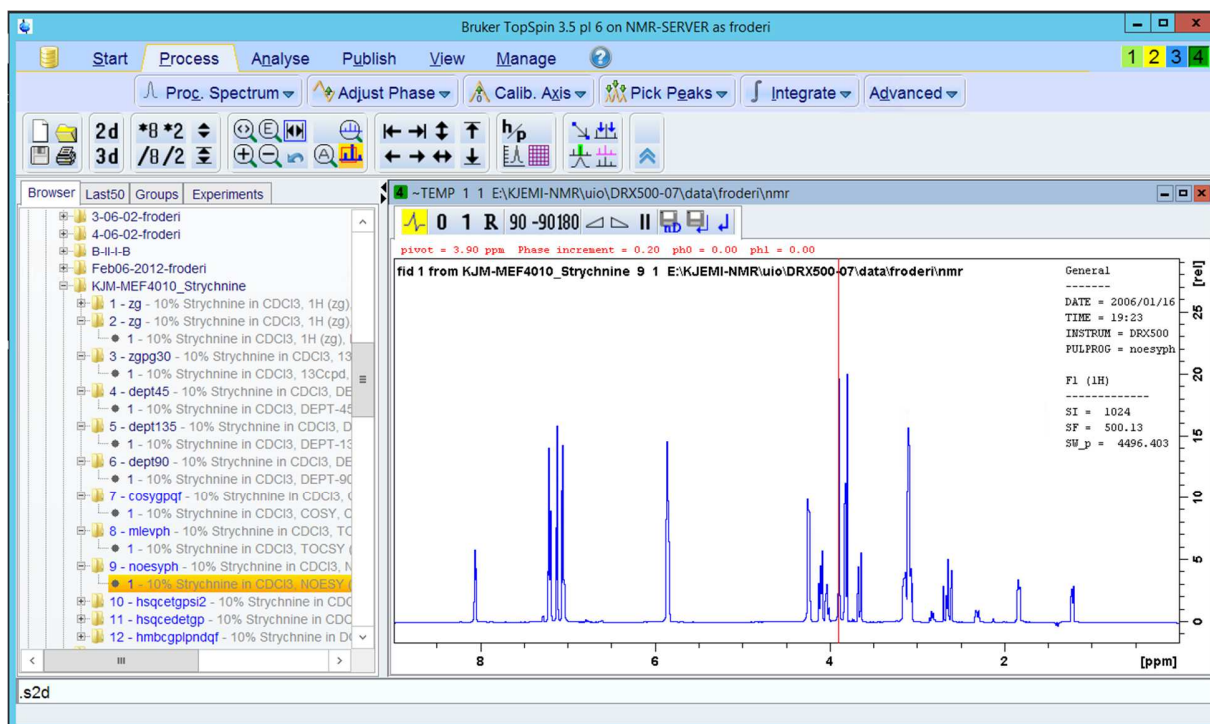rser 1 and rsr 1 give different result. Which one used above?
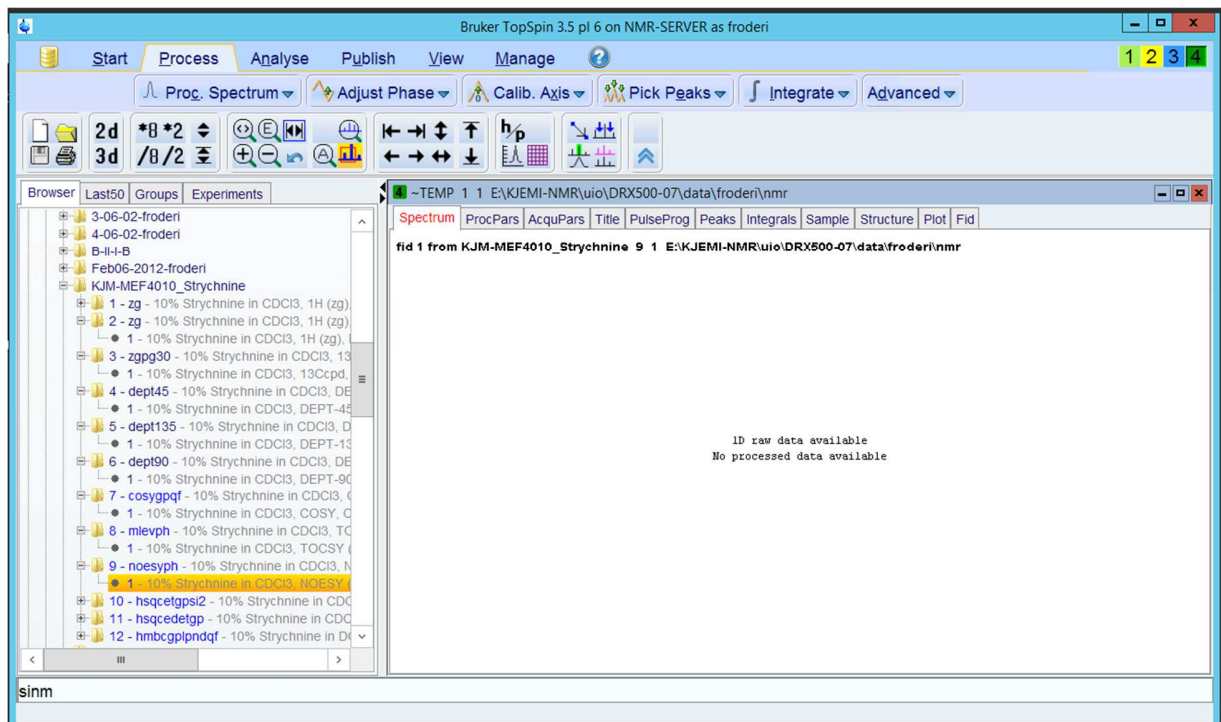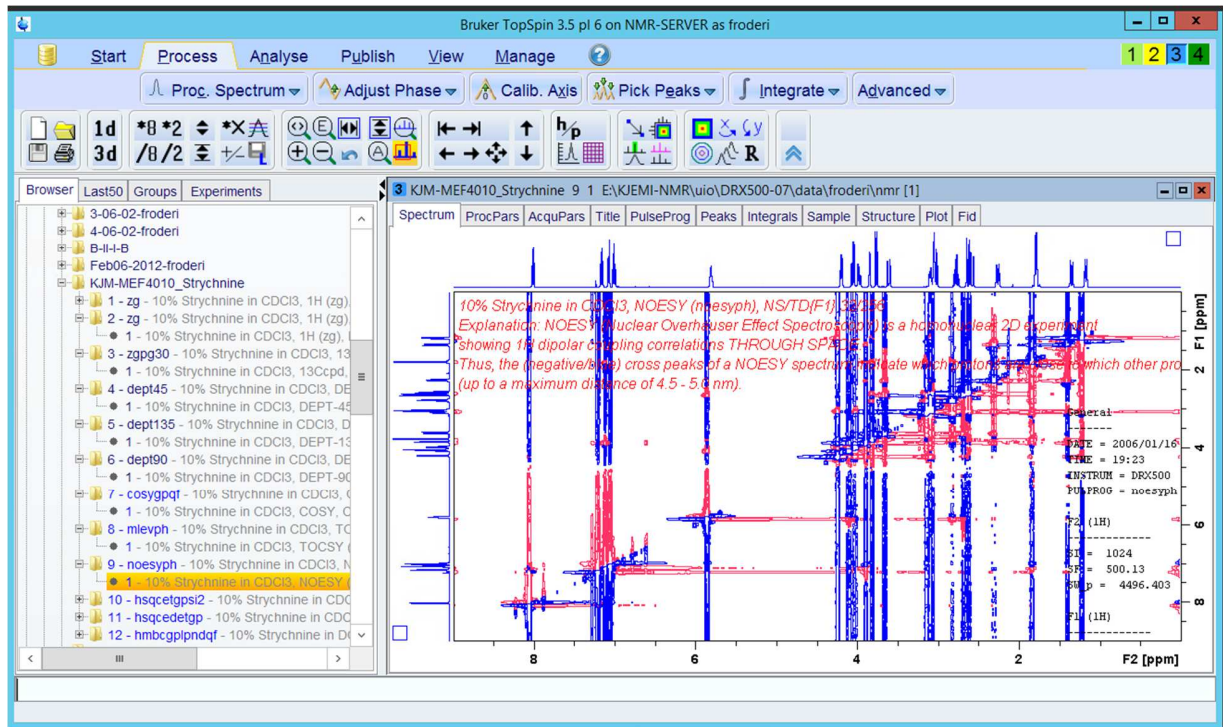

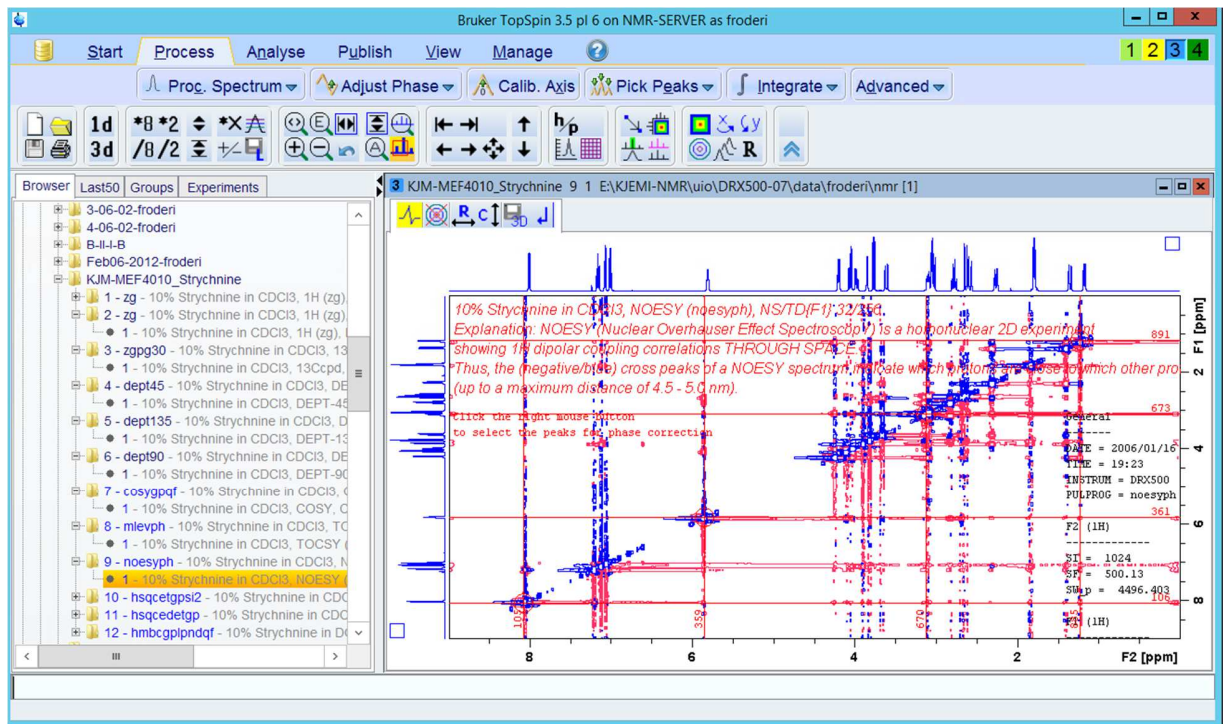sinm

The fid is visaible.

After ft

After apk and then realizing it is not possible to save the phasing to the whole 2D dataset.
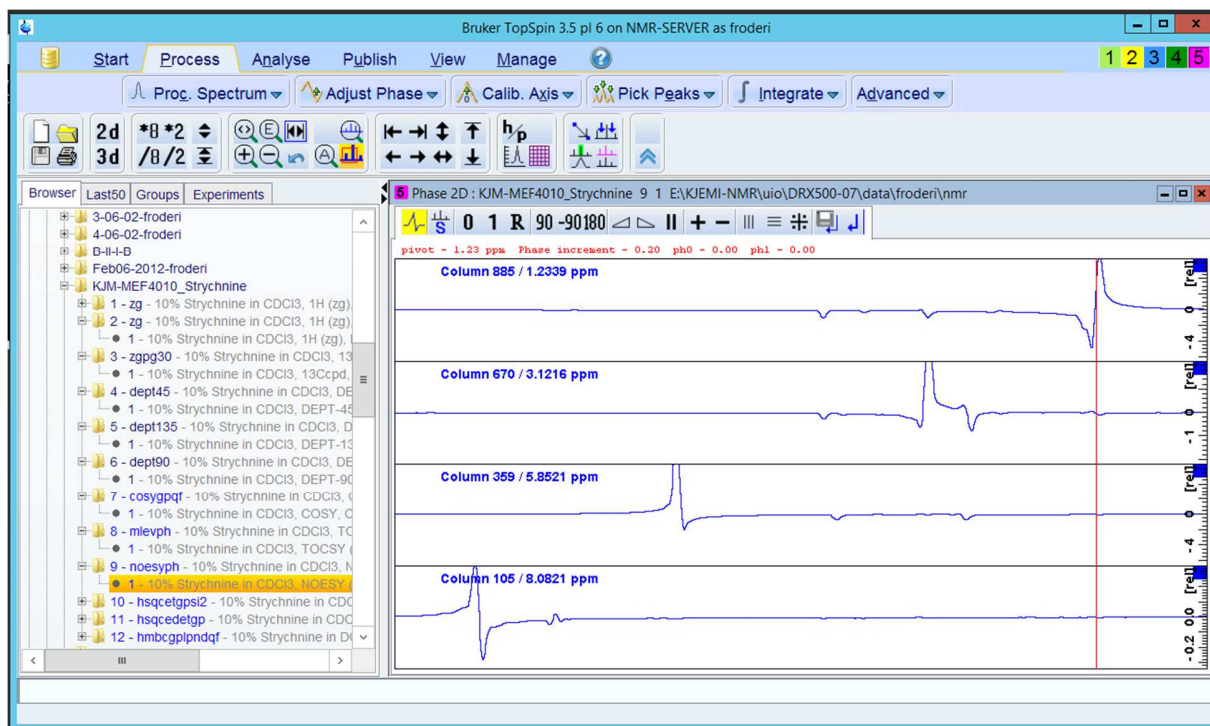

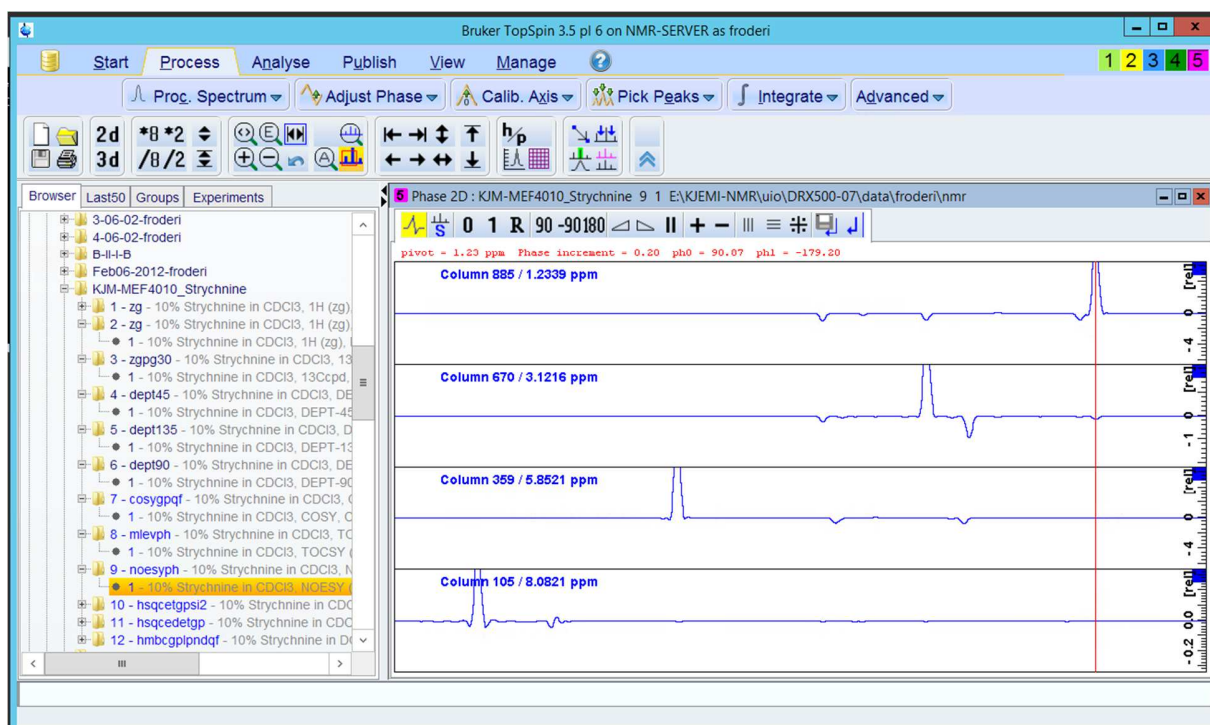Process and Adjust Phase to enable save. Use nD or simply saving?

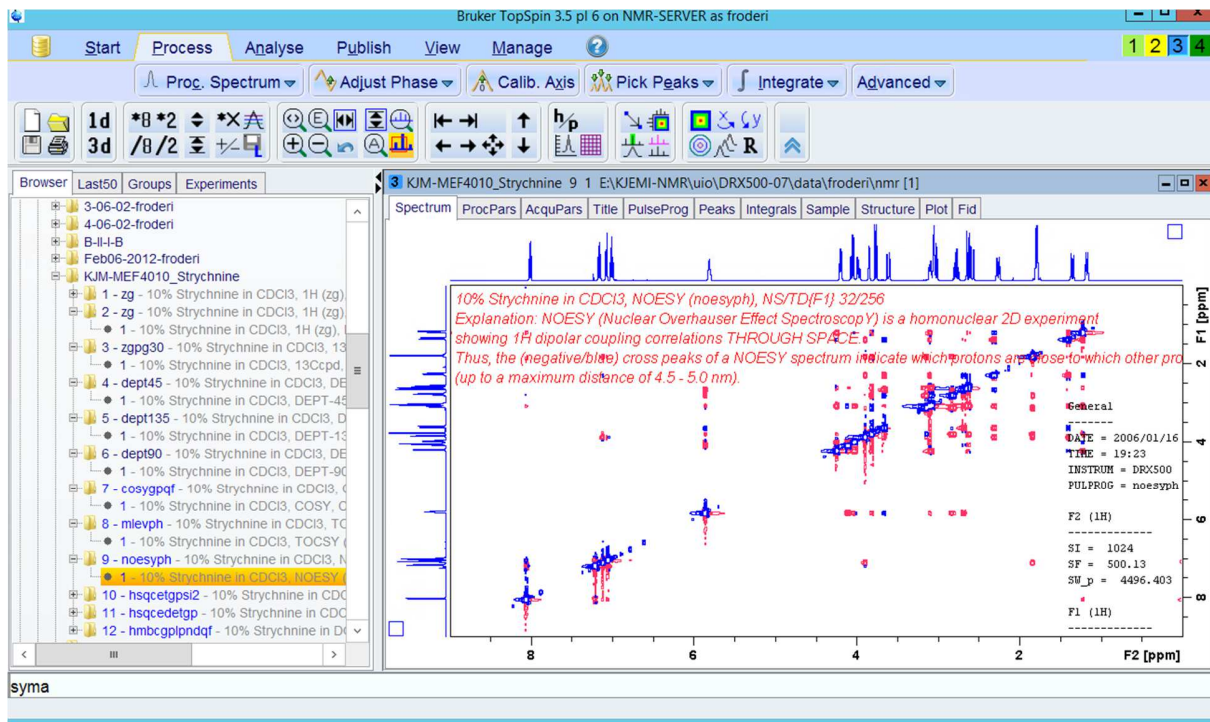Xfb after fixing the horizontal phasing – almost.

Process, Adjust Phase and adding the horizontal lines – at positions with signals, crosshairs in the diagonal. Selecting columns.
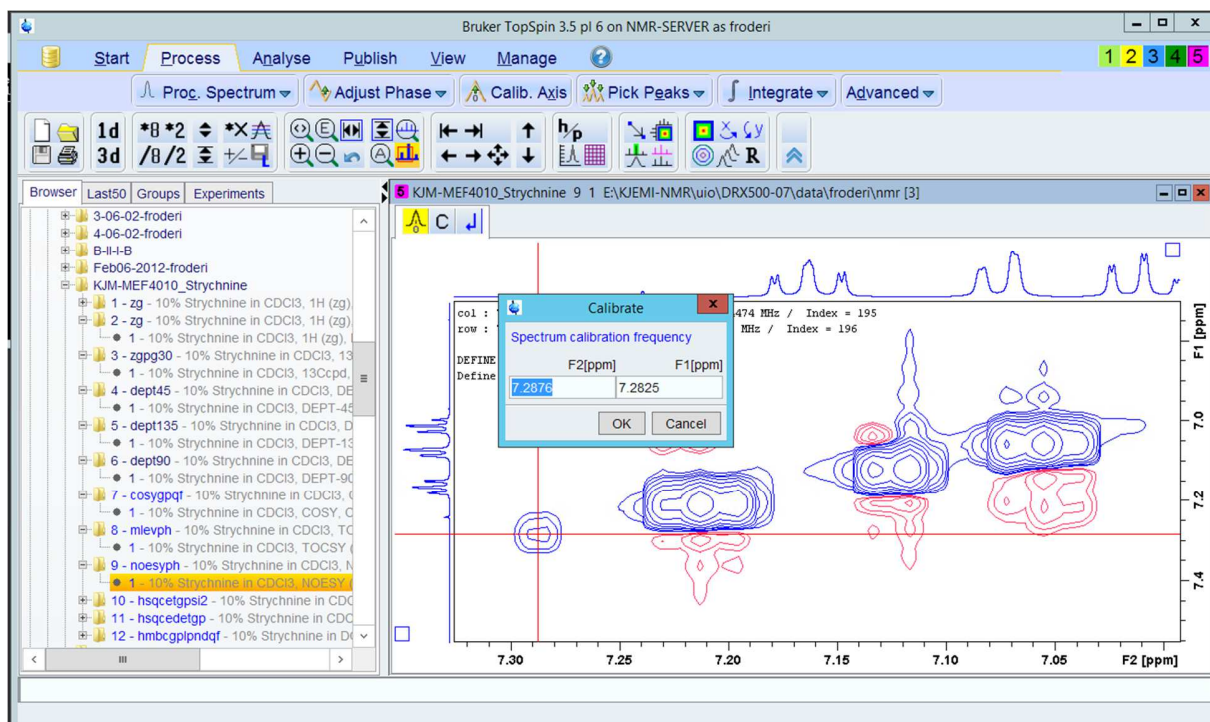
Fixing up the slices. Both positive and negative peaks are to be expected.
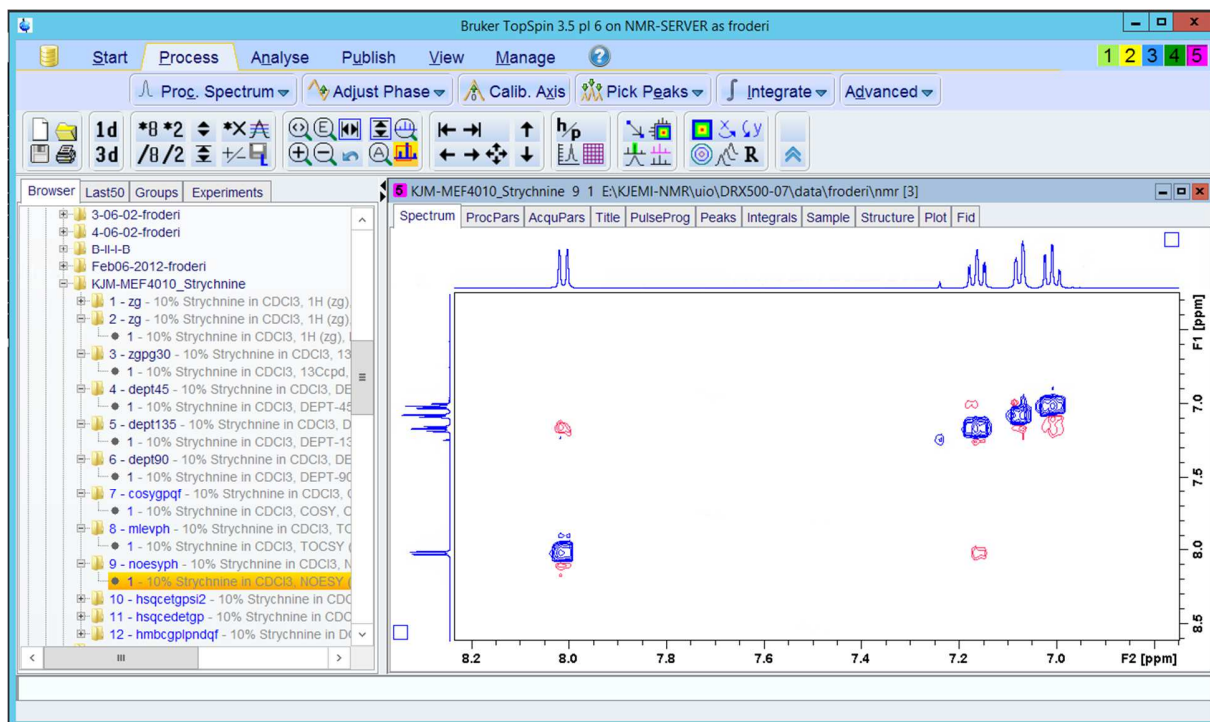

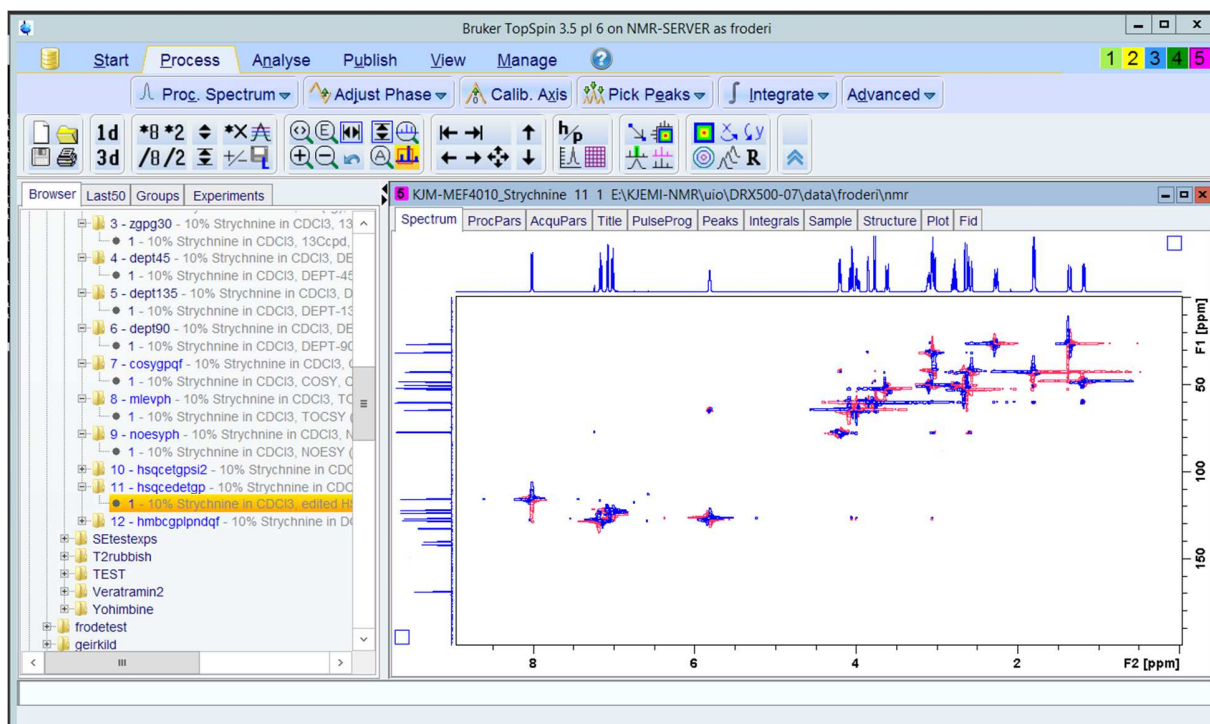
Quite good. Save it.

After xfb.   Adjust with abs 1 and abs 2? If symmetrizing - are you using sym or syma?
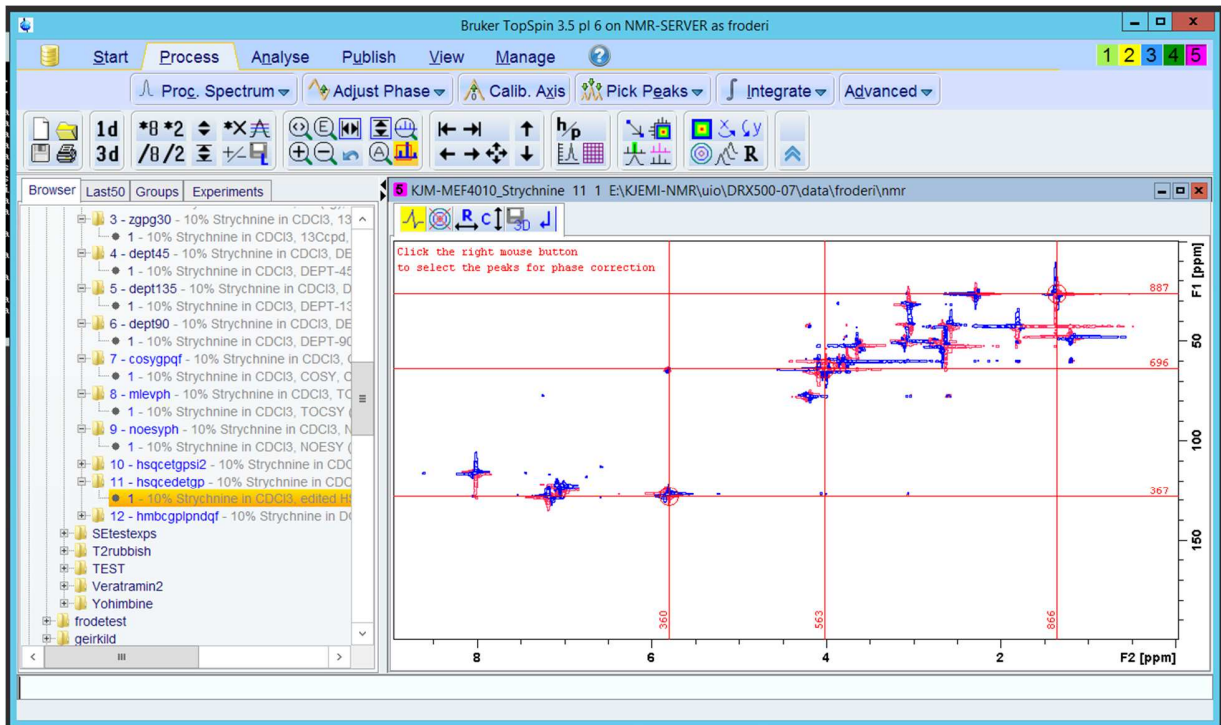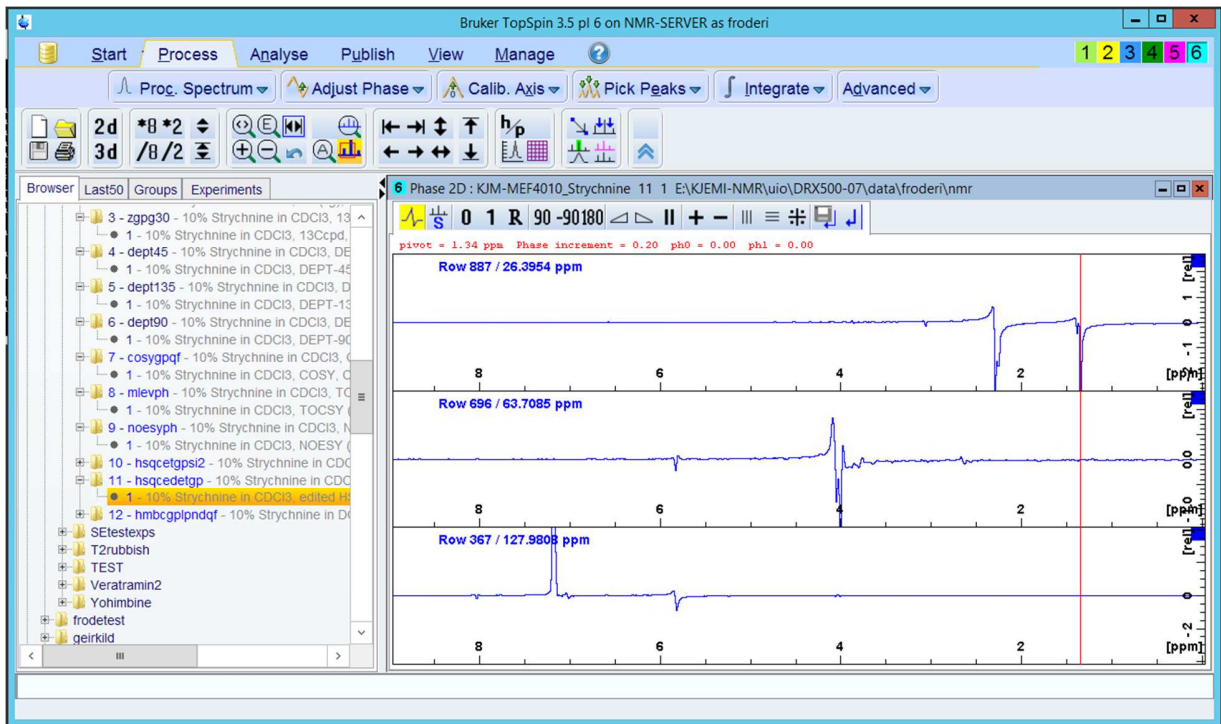

Fixing up the calibration.

Cute.

Moving over to HSQCEDETGP. Xfb if not processed already. Add the 1Ds on the sides.
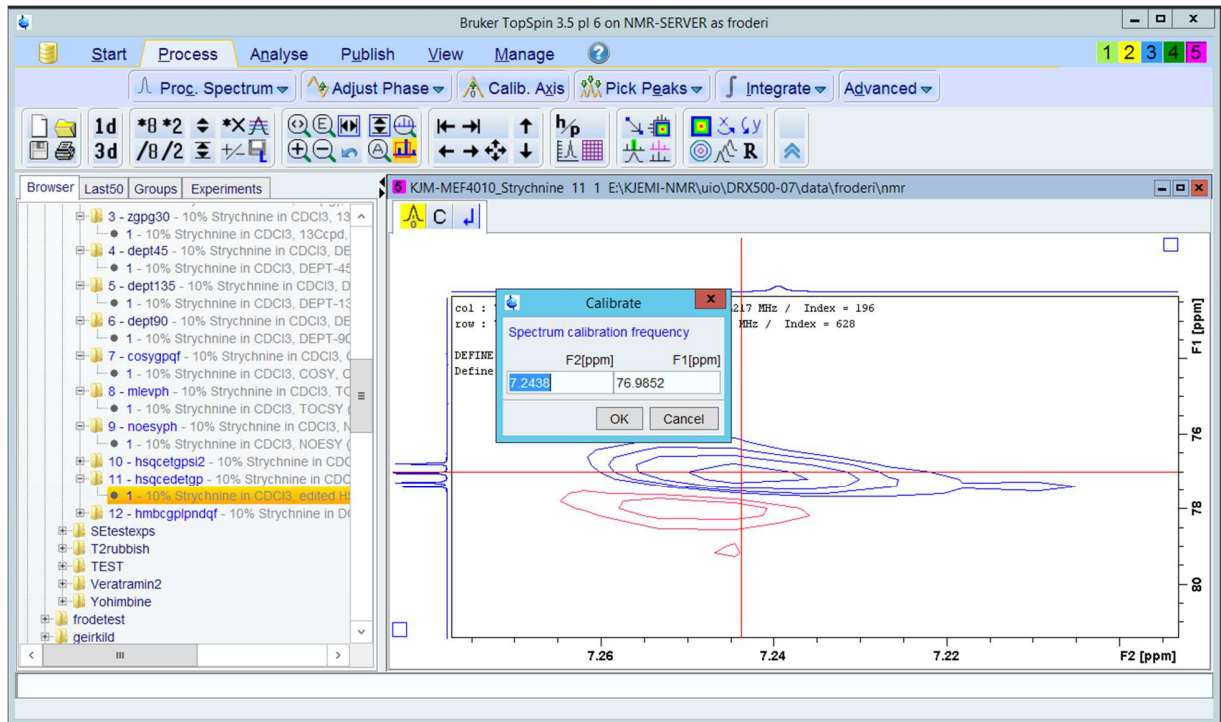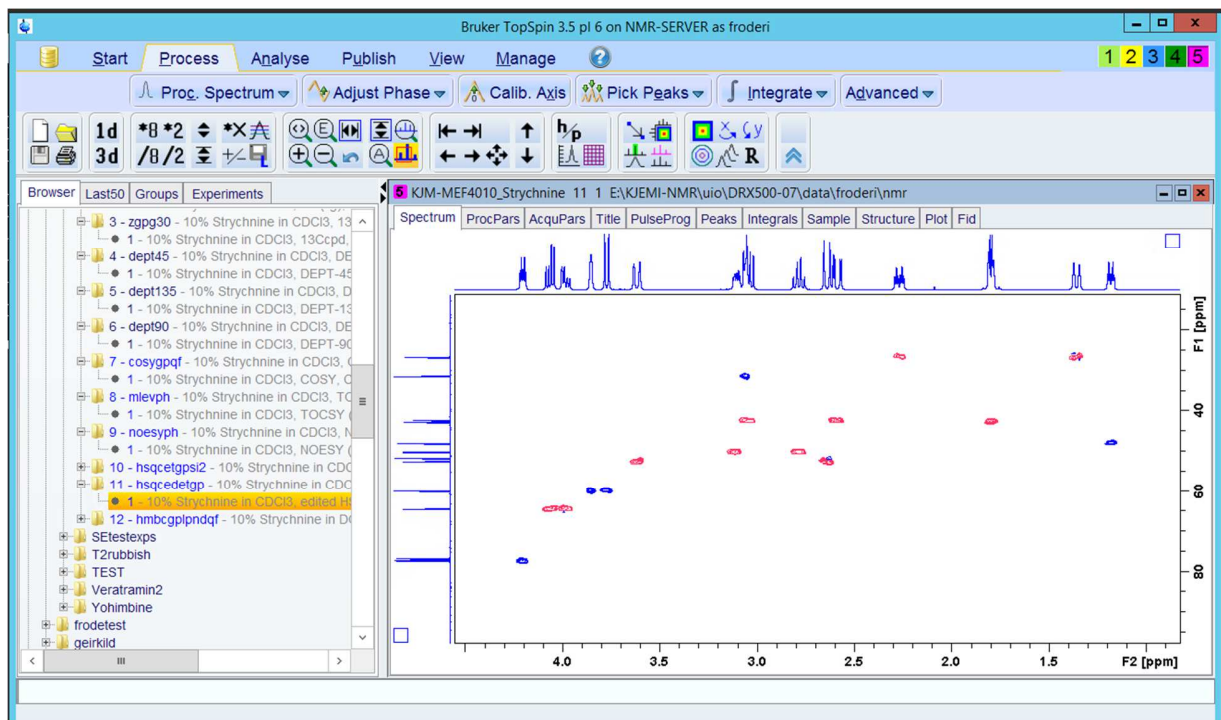
Do not use rser or rsr here.   Just add cross hairs. Phase vertically and horizontally – manually. There is no diagonal in this type of spectrum.
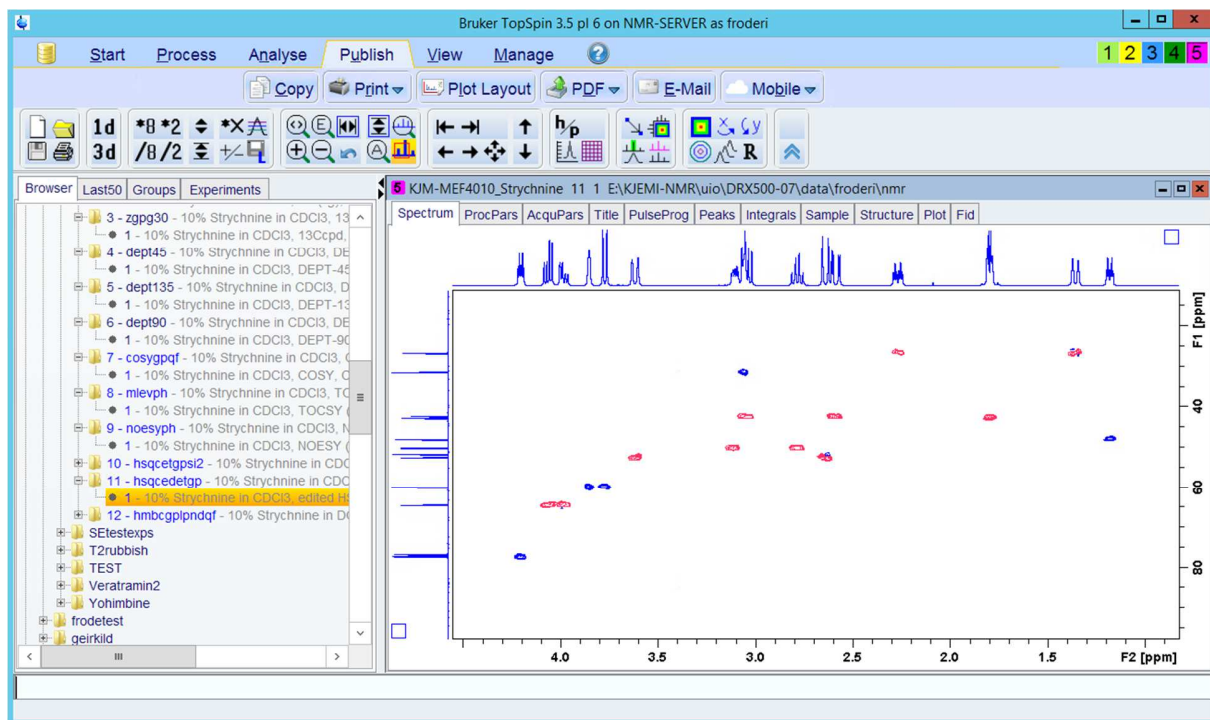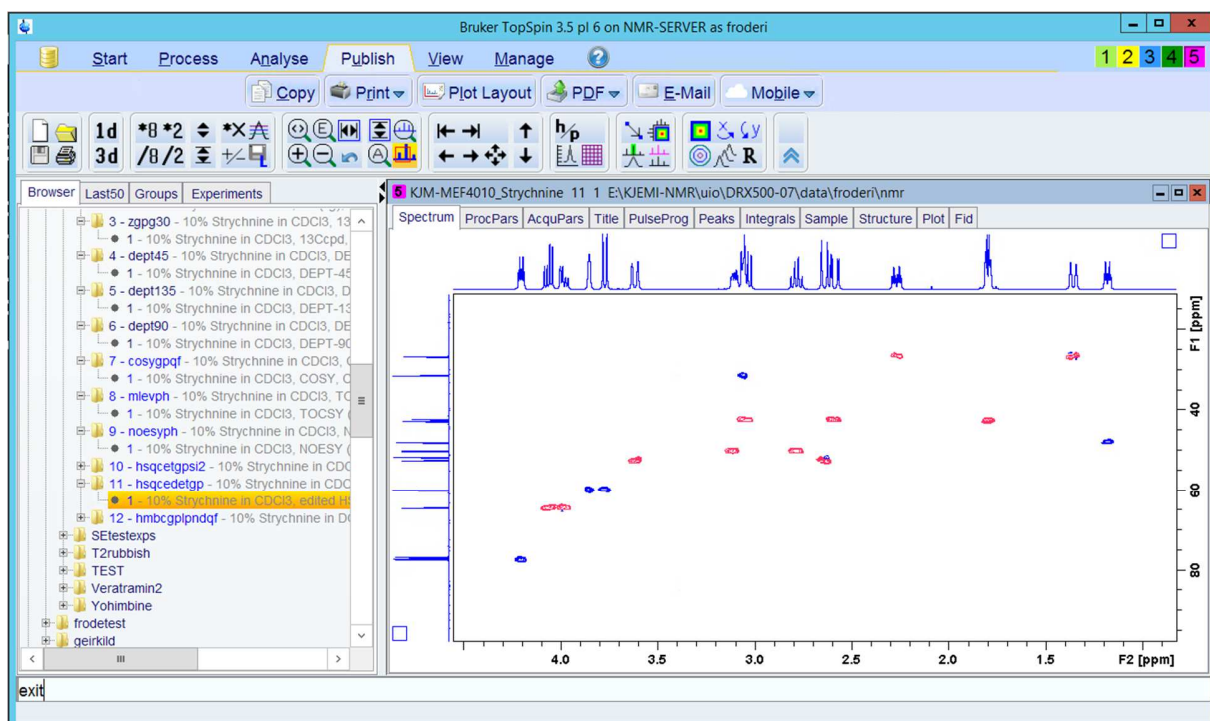

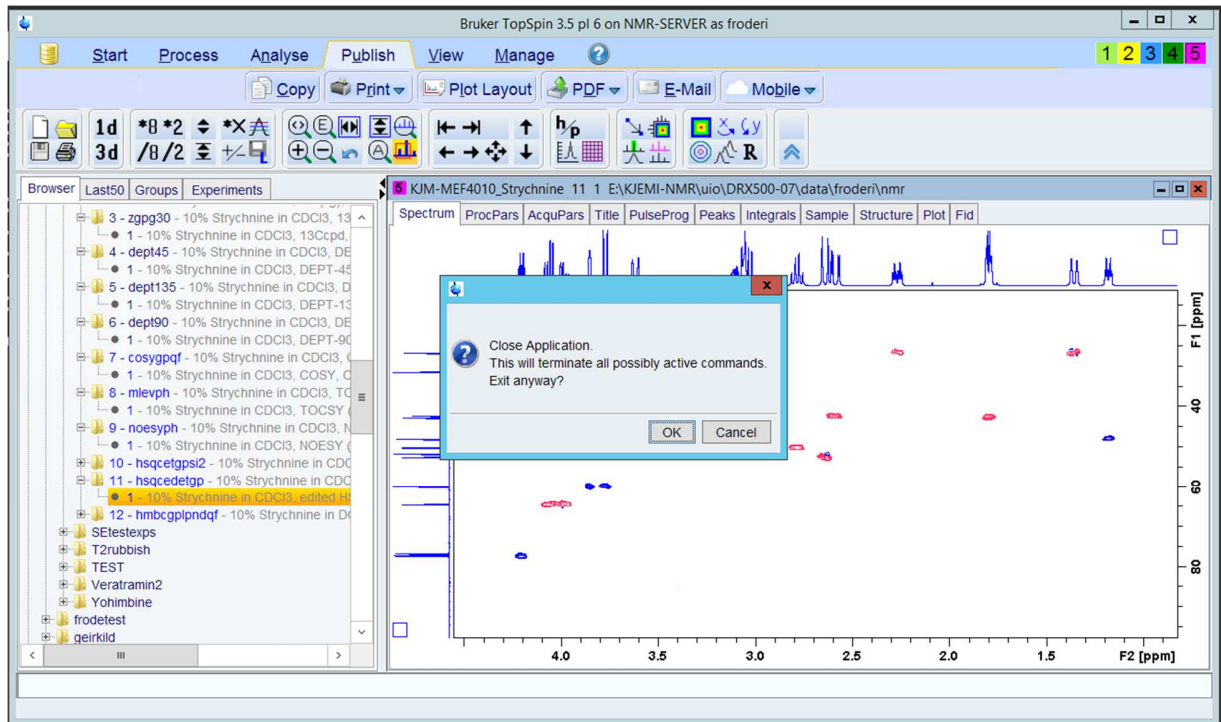Remove the two lower blue squares before phasing.

Calibrate.

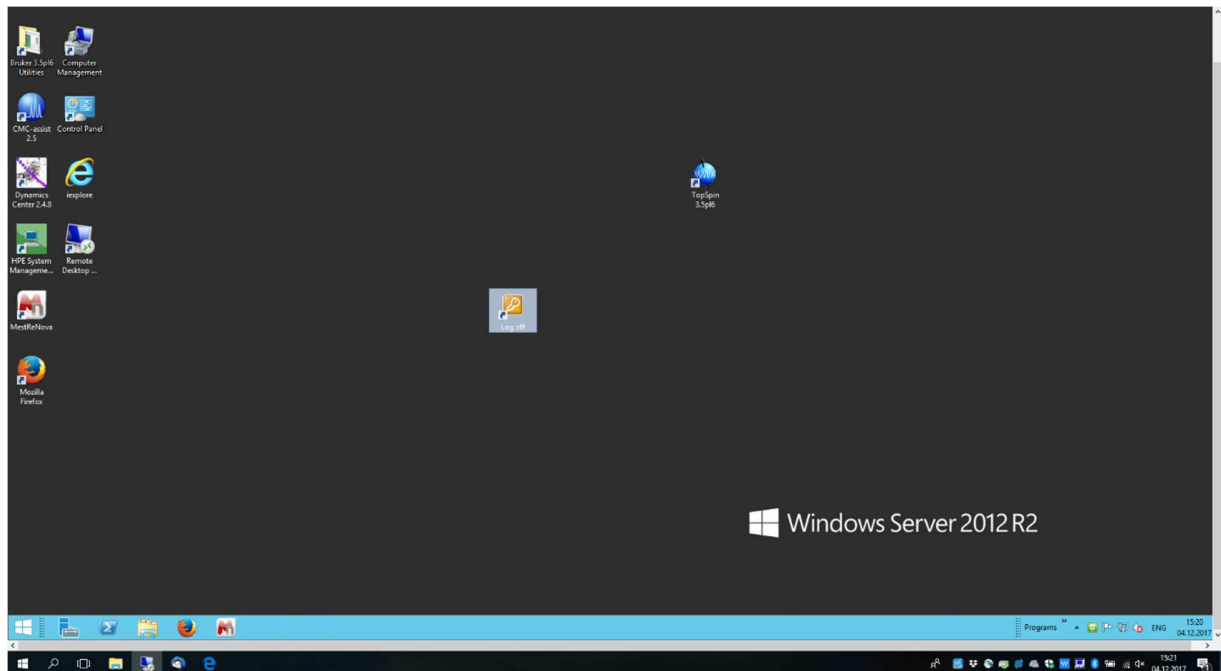See all the CH^2 groups in red? CH and CH$_3$ groups are in blue (here).

Copy it into your Word document. When working with your "real" sample all spectra shall be documented in your 10 pages report and also in your Power Point presentation.

Get out of the TopSpin program.

OK

Locate the Log off from the server.