Practicum 4, Fall 2010

The acquisition time: weighting and linear prediction

Strychnine, dissolved in CDCl3

This demonstration develops the inverse relationship between time and frequency as we go back and forth between the FID, which occurs in time (it is time-domain data) and the NMR spectrum, which is displayed over a frequency axis (it is frequency-domain data).

Weighting functions are developed as a way to decrease the contribution to the spectrum of noise, and to correct for data truncation. They can also be used to enhance resolution, provided the data are of good quality.

Improving signal/noise with weighting

Again, we begin by acquiring a nice 1-dimensional spectrum.

Now click on the FID display button [1] to look at the corresponding FID (**Figure 1**).

Note that the axis is now a time axis [2], and it runs from zero to the value you used as the acquisition time (at) [3].

For best spectral resolution, the FID should have decayed to zero by the time at ends. However making at much longer collects noise only, and decreases the quality of the spectrum, because every point in the FID is combined to generate each point in the spectrum, by the Fourier transformation. Look at the X-axis while displaying the FID. Decide at what time the signal is essentially gone, and choose that time for use as your improved acquisition time [4].

Thus, in this instance, a better choice of at is 1.6 seconds.

You can make this decision at the same time as you adjust the sweep width, based on a trial spectrum.

You can also cause the software to simply not use all of the digitized data as input to the FID, and you can do so in a tapered way.

Under Processing>Weighting (**Figure 2**, [0]) activate 'Interactive Weighting' [1]. In the graphical display window, the bottom panel shows the FID [2], the middle panel shows the function that will be multiplied point-for-point with the FID [3] and the top panel shows what the Fourier transform of this product will be [4]. Neither of the latter two panels display anything yet.

Click next to 'sinebell' to activate a sine function [5].

Now the middle panel shows a sine function (**Figure 3**, [1]). Click in the upper panel using the RightMouse (RM) [2]. The anticipated spectrum appears as a preview (not shown).

The spectrum that results has distorted peak shapes (**Figure 4** [1]). Go to Process>Display, click 'Transform' and 'Display Spectrum' to get a better view. Click on 'Transform' in order to perform a new weighted Fourier transform incorporating the weighting function you just chose (**Figure 5**).

The strong negative excursions on each side of each signal are because the first point of the weighted FID will be zero, because the first point of the weighting function is zero. The value of the first point in the time domain determines the total integral under the spectrum after Fourier transformation. Thus in the sine-weighted spectrum, all the peaks have as much negative area as positive area, for a total area of zero, in theory.

To prevent the first point from having a zero value while nonetheless exploiting the sine function's decay to zero at long times, we shift it. In Processing>Weighting activate 'Interactive Weighting' [1] again and activate 'shift' [2] (**Figure 6**). Activate the spectrum preview by clicking in the top panel with the RM [3]. For shift, enter -1 * the value you have next to 'sinebell'. Now you see that the peaks are broader but no longer have negative dips on both sides. Their integrals are positive. To shift the sine bell so that its peak is at time=0, set the shift equal to -1 * the sine width.

The lines are broadened now because data are being squeezed to zero by the weighting function at time equal to the value used for the 'sinebell' parameter (look at the time axis in the lower panel of the interactive weighting display [4]).

After processing with your new weighting function, the 'shifted sinebell', determine the width at half-height of the signals in the frequency-domain spectrum by going to Process>Cursors/LineLists, and clicking on 'Transform' (**Figure 7**). Use the tools on the RHS to zoom in on a representative peak [0], place the cursor on it and click 'Place on nearest line' [1] then 'Show linewidth' [2]. In the space above the command line, as well as the RH response box at the bottom, the linewidth at half height is provided (2.55 Hz) along with the digital resolution [3].

Note that this screen also gives you the possibility of making the chosen line the center of the next spectrum you collect, by clicking on 'Move transmitter' [4]. This will change the value of tof (carrier frequency = 'transmitter offset') without changing the sweep width sw.

Go back to Processing>Weighting and activate 'interactive Weighting' again. Now set the shift to only -1* *half* the value in sinebell. This is a 45 ° shifted sine bell, as opposed to the previous 90 ° shifted sinebell. The peaks will now be a little shorter, but their linewidths should be a little longer. This weighting function also has the beneficial effect of cancelling out 'feet' that often accompany peaks, complicating integrals and causing streaks in 2D spectra. Thus, it is often used.

You can also select other weighting functions. The Gaussian function and the line broadening (an exponential decrease) both have full amplitude at the first point and therefore do not require shifting, although shifting is often helpful (see above) and is possible with the Gaussian. Try the different options !

Correcting for short a at with weighting

Sometimes we intentionally do not digitize the FID for as long as it takes to decay to zero. Sometimes this is because the sample contains one species with a very long T2 and that species is not of interest to us so we have optimized the experiment parameter in favour of other species present. Sometimes it is to keep the data set size smaller and easier to manipulate (eg. for 2D spectra). The result of having stopped data collection before the FID is really over is shown in **Figure 8**. In this case, the at chosen was longer than the T_2 of the major constituent of the sample (strychnine), but it was shorter than the T_2 of the TMS. Thus we see 'sinc wiggles' (feet) at the base of the TMS line [1] which is sharp (long T_2). These are a 'truncation artifact'. (Note that the lines of strychnine which are broader (shorter T_2) do not have sinc wiggles [2].)

There are two ways to 'fix' truncation artifacts without re-collecting the data. One is to apply a weighting function that compresses the data to zero at the time when the data collection ceased. The other is to apply linear prediction to extent the acquired data with synthetic 'predicted' data.

Figure 9 shows the Processs>Weighting interactive display with the truncated FID. (Note how the oscillations continue at the end of the data.)

Activate a Gaussian weighting function (**Figure 10**, [1]), click in the middle panel using the LM to extend or compress the Gaussian interactively [2] (the horizontal position of the mouse matters but not the vertical position within the middle panel) and note the effect on the preview of the frequency domain spectrum in the top panel [3] of the interactive weighting display. The sinc wiggles are gone, but the sharp line is broadened. In each instance, you will have to decide which is more important: no sinc wiggles or sharper lines.

Click on 'Transform' to apply your new weighting function and Fourier transform the spectrum. (**Figure 11** [1]). Compare the result with the spectrum in figure 8 that was not weighted prior to transformation.

Linear Prediction

If the at is shorter than the decay of the data, you can have sinc wiggles. If you want to remove those without broadening your lines, you need more time-domain data (narrower freq-domain lines need longer time-domain data).

The software 'knows' that the data you collected should be the sum of many cosine functions each with the frequency of one peak and each damped according to that peak's T_2 ($1/\pi\Delta\nu$). Thus, if you tell it how many strong lines there are in your spectrum (approximately), the software will fit your acquired data in terms of a sum of damped Cos' to obtain sets of ν and T_2 s. (It will also generate phases and amplitudes for each.) Then the software uses this set of parameters to calculate what the 'ideal' FID should be for any time points you want. If we want to extend a short FID, we will ask for 'forward' linear prediction and we will ask the software to predict the perfect FID for time points after we stopped actually digitizing data.

In **Figure 12**, the actual data are in black and the predicted data are in blue.

To generate synthetic (predicted) points that double the data, go to Process>More 1D (**Figure 13**).

A number of decisions are required. We need to tell the software whether to linear predict forward in time or backward (parameter lpop = 'f' or 'b') (**Figure 13** [1]).

We need to specify how many peaks are to be assumed in fitting our data and which actual data points are to be the basis for the fit to determine peak ν and T_2 for each peak. Having seen your spectrum, estimate the number of *strong* peaks, for example 16 (don't be too greedy). Enter this next to 'coeff' [2] (parameter = lpfilt). For forward linear prediction we do this by specifying the number of points to be used [3] (parameter lpnupts can be as large as np, the number of points you have), and the *last* data point to be used (strtlp, 'start lp' in Figure 13 [4]). Thus if you want to use points 1-609, give 609 as the number of basis points [3] and 609 as the last point [4]. (This is called the 'starting point', but the software looks *backward* from that point when doing forward linear prediction. Just one of those things . . . .)

If you chose to simulate 'n' signals you will need a minimum of 2*n data points, but you should really use at least twice that many. I chose to generate points based on a model dominated by 16 signals. This requires that I use at least 32 points as a basis for my simulation. In our case, with nice strong data, we can afford to use many more points than that. To use the entire first half of the FID, use 609 points, from point 609 back to the start.

Enter the number of 'predicted points' you would like to add to your FID [5] (parameter lpext). To double the length of your FID enter the same number as you see below in the box 'Acquired points' [6]. This number is fixed at the time you collect data, it is reported here for your convenience (parameter name np). If these are to be added after the last actual data point, then the first predicted point is 1+ np. Enter this value next to 'starting at' [7] (parameter strtext).

There is another choice related to your Fourier transformation operation. Even though we have np=1218, we can choose any power of two for the output of our Fourier transform. To use all 1218 input points, we would choose to output to 2048 (next biggest power of 2). What is done is that the input is augmented to 2048 points too by addition of a string of zeros after the last data point (zero-filling). When we linear predict, we will be doing a better job, but putting simulated data there instead. However if our simulated points make the FID so much longer that it now excees 2048 points, we may increase the Fourier transform size to 4096, or 4k [8] (parameter fn, or Fourier number).

This will determine the digital resolution, the number of Hz per point. Since you would like digital resolution better or equal to your spectral resolution (that is to say a smaller number of Hz / point), make fn large enough that the digital resolution is a smaller number than 1/2 your sharpest line's width at half height. These values can be checked on a line by going to Process>Weighting, placing the cursor on the line and clicking on 'Display Linewidth' (**Figure 11** [4]). (Alternately, type **dres**). You don't need to collect new data if fn is too small, just increase it and Fourier transform again by clicking on 'Transform'.

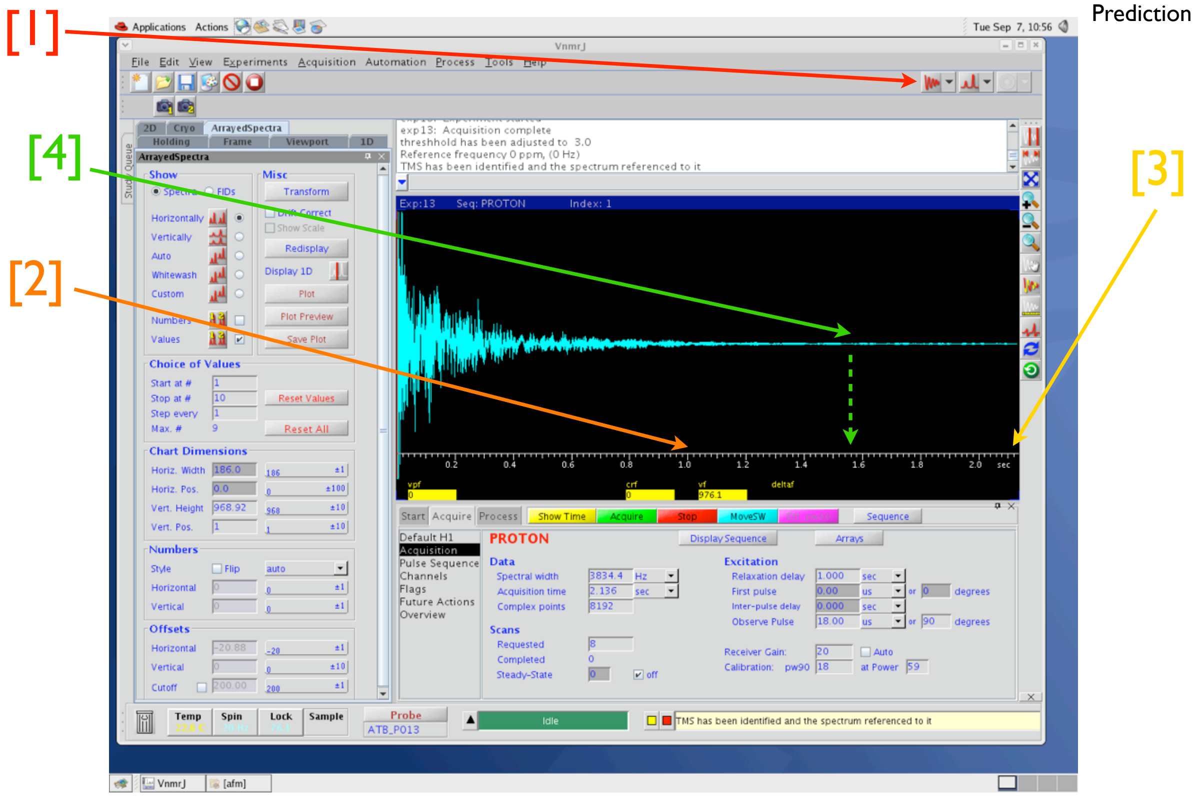
Figure 14 shows the spectrum that was acquired with a very short 0.3 s at, but augmented with linear prediction to double the FID length. In this case no weighting was applied in order to show the effect of linear prediction alone. The analogous spectrum that was not linear predicted is shown in **Figure 15**.

To get the best possible spectrum from the short-at data set, combine the use of linear prediction and weighting, by activating weighting in the linear prediction window (**Figure 15** [1]). (go to Processing>Weighting to double the Gaussian length in accordance with your new doubled FID length. If you used a shifted Gaussian, also double the shift.) You can double these in the command line by typing **gf=2*gf** (Gaussian function is now twice the previous Gaussian function) and **gfs=2*gfs** (Gaussian shift is now twice the previous Gaussian shift).

In figures 13, 14 and 15 compare both the line widths of the signals and the magnitude of truncation artifacts (sinc wiggles at the base of sharp signals).

For completeness' sake, **Figure 16** shows how the meanings of the linear prediction parameters change when one uses linear prediction to fix early points, by 'backward' linear prediction (black data are actual data to be used as the basis for a fit and blue are data that are predicted and will overwrite bad initial data points). In this case the choice of the number of signals to model ('coef' or lpfilt) and number of actual data are the same, but now the data points to be used as the basis for the fit extend from the first point to be used ('starting at' = strtlp) out to later times by a number of points called 'basis pts' or lpnpts. The first predicted point will be at 'starting at' (strtext) and will extend backwards for a number of points you enter as 'predicted points' (lpext)

Figure 1
Weighting & Linear
Prediction



exp13: Acquisition complete
threshhold has been adjusted to 3.0
Reference frequency 0 ppm, (0 Hz)
TMS has has been identified and the spectrum referenced to it

Exp:13 Seq: PROTON Index: 1

vf 976.1

Show: ● Spectra ○ FIDs

Choice of Values: Start at # 1; Stop at # 10; Step every 1; Max. # 9

Chart Dimensions: Horiz. Width 186.0; Horiz. Pos. 0.0; Vert. Height 968.92; Vert. Pos. 1

Offsets: Horizontal -20.88; Vertical 0; Cutoff 200.00

PROTON

Data: Spectral width 3834.4 Hz; Acquisition time 2.136 sec; Complex points 8192

Scans: Requested 8; Completed 0; Steady-State 0 ☑ off

Excitation: Relaxation delay 1.000 sec; First pulse 0.00 us or 0 degrees; Inter-pulse delay 0.000 sec; Observe Pulse 18.00 us or 90 degrees

Receiver Gain: 20 □ Auto

Calibration: pw90 18 at Power 59

TMS has been identified and the spectrum referenced to it

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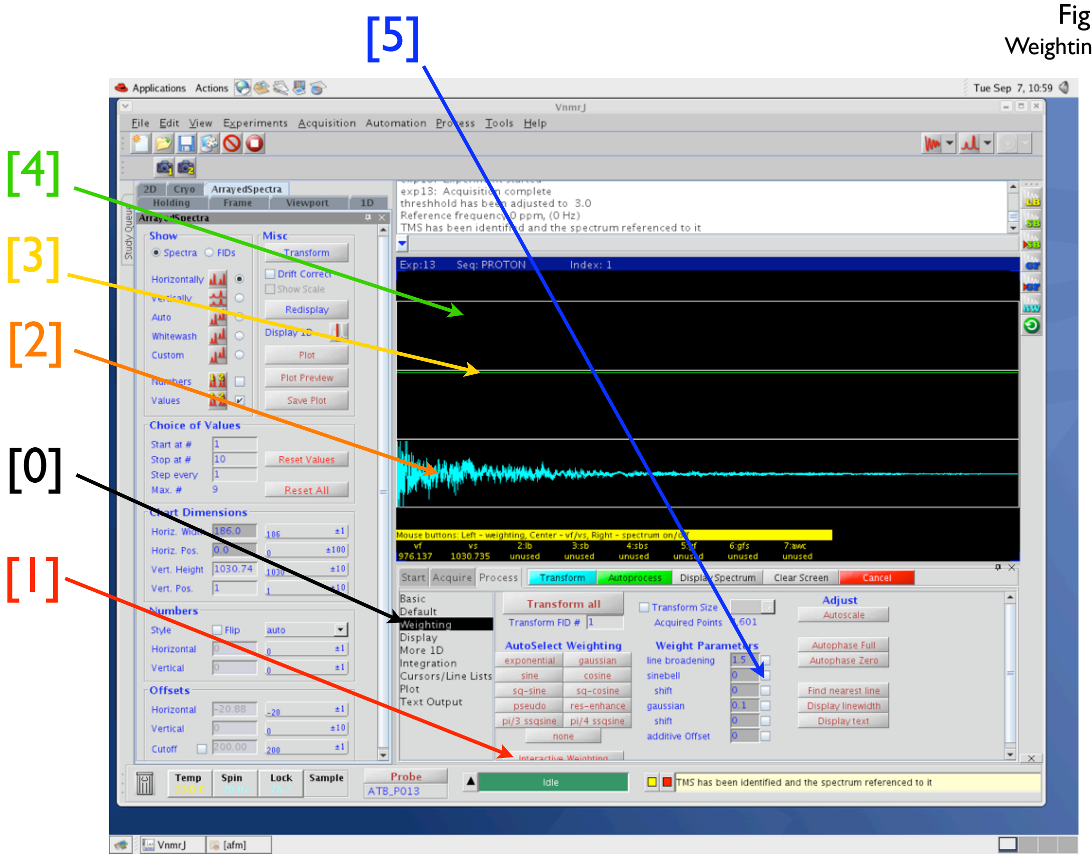
Figure 2
Weighting & Linear
Prediction



exp13: Acquisition complete
threshhold has been adjusted to 3.0
Reference frequency 0 ppm, (0 Hz)
TMS has been identified and the spectrum referenced to it

Exp:13 Seq: PROTON Index: 1

Mouse buttons: Left - weighting, Center - vf/vs, Right - spectrum on/off

vf	vs	2:lb	3:sb	4:sbs	5:gf	6:gfs	7:awc
976.137	1030.735	unused	unused	unused	unused	unused	unused

Chart Dimensions: Horiz. Width 186.0; Horiz. Pos. 0.0; Vert. Height 1030.74; Vert. Pos. 1

Transform FID # 1

□ Transform Size

Acquired Points 8601

Weight Parameters: line broadening 1.5; sinebell 0; shift 0; gaussian 0.1; shift 0; additive Offset 0

TMS has been identified and the spectrum referenced to it

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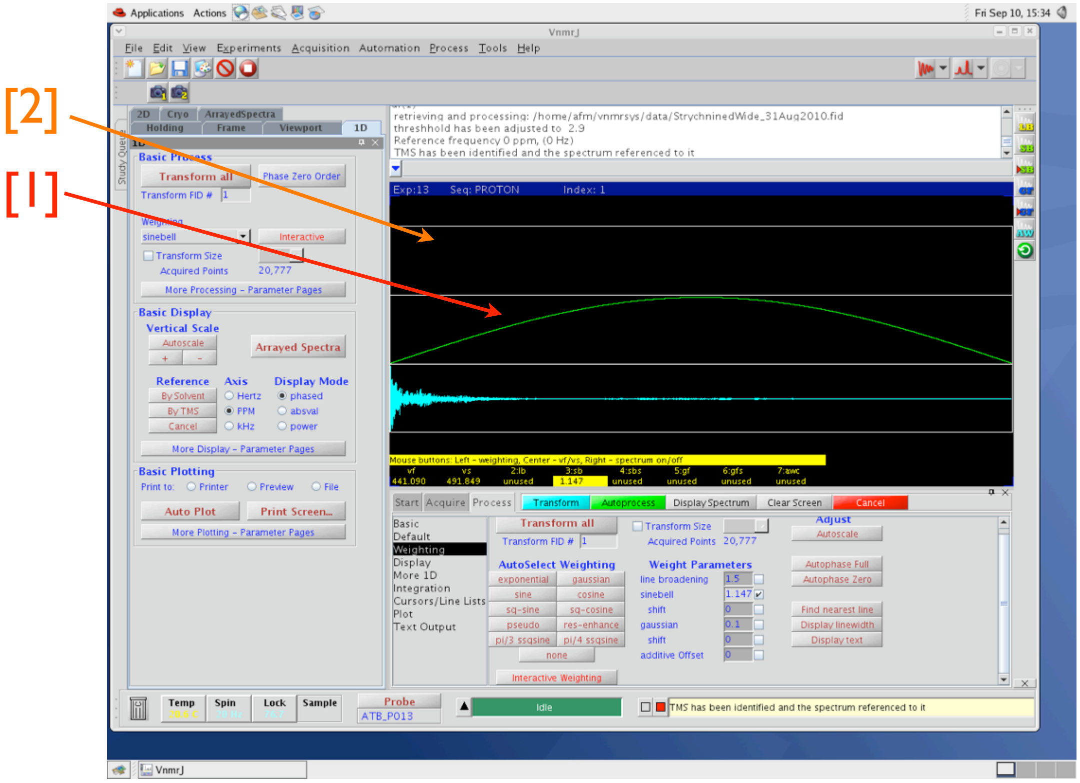
Figure 3
Weighting & Linear Prediction



```
retrieving and processing: /home/afm/vnmrsys/data/StrychninedWide_31Aug2010.fid
threshhold has been adjusted to  2.9
Reference frequency 0 ppm, (0 Hz)
TMS has been identified and the spectrum referenced to it
```

```
Mouse buttons: Left - weighting, Center - vf/vs, Right - spectrum on/off
   vf        vs       2:lb     3:sb     4:sbs    5:gf     6:gfs    7:awc
441.090   491.849   unused   1.147    unused   unused   unused   unused
```

Transform FID # 1
Weighting: sinebell
□ Transform Size
Acquired Points 20,777

Weight Parameters
line broadening 1.5 □
sinebell 1.147 ☑
shift 0 □
gaussian 0.1 □
shift 0 □
additive Offset 0 □

TMS has been identified and the spectrum referenced to it

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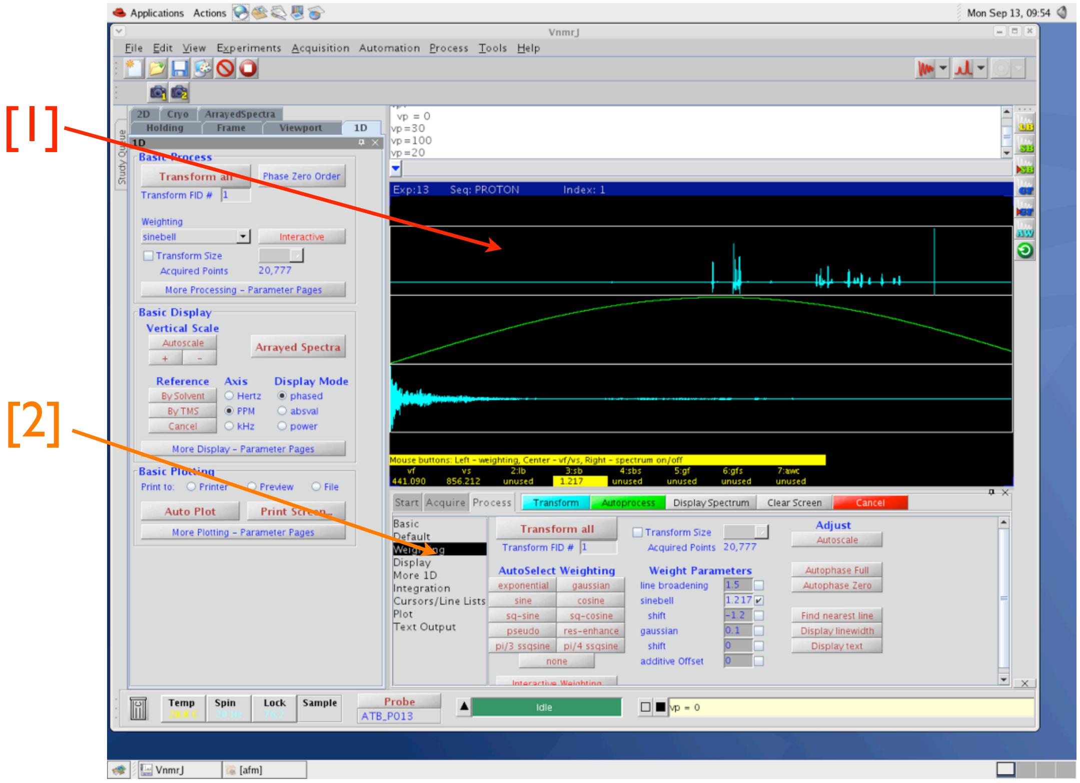
Figure 4
Weighting & Linear Prediction



```
vp = 0
vp=30
vp=100
vp=20
```

```
Mouse buttons: Left - weighting, Center - vf/vs, Right - spectrum on/off
   vf        vs       2:lb     3:sb     4:sbs    5:gf     6:gfs    7:awc
441.090   856.212   unused   1.217    unused   unused   unused   unused
```

Transform FID # 1
Weighting: sinebell
□ Transform Size
Acquired Points 20,777

Weight Parameters
line broadening 1.5 □
sinebell 1.217 ☑
shift -1.2 □
gaussian 0.1 □
shift 0 □
additive Offset 0 □

vp = 0

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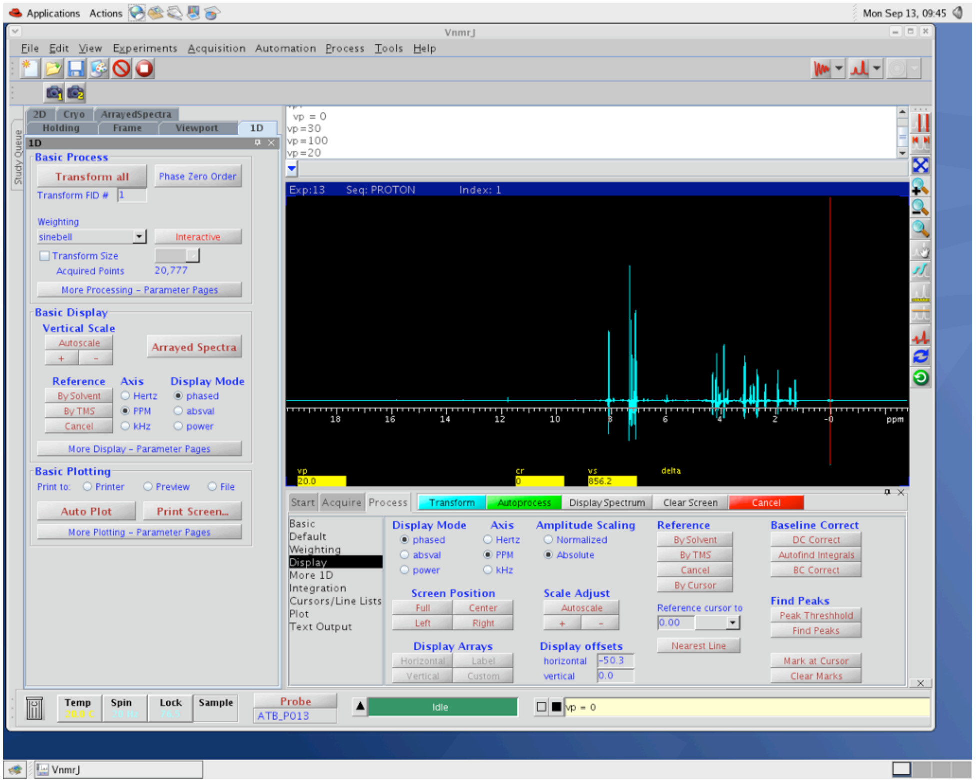
Figure 5
Weighting & Linear Prediction



Mon Sep 13, 09:45

```
 vp = 0
vp=30
vp=100
vp=20
```

Exp:13 Seq: PROTON Index: 1

Weighting: sinebell

Transform FID # 1

Acquired Points 20,777

vp 20.0 cr 0 vs 856.2

Reference cursor to 0.00

horizontal -50.3

vertical 0.0

Idle

vp = 0

Probe ATB_P013

Applications Actions
VnmrJ
File Edit View Experiments Acquisition Automation Process Tools Help
2D Cryo ArrayedSpectra
Holding Frame Viewport 1D
Study Queue
Basic Process
Transform all
Phase Zero Order
Interactive
Transform Size
More Processing - Parameter Pages
Basic Display
Vertical Scale
Autoscale
+ -
Arrayed Spectra
Reference Axis Display Mode
By Solvent By TMS Cancel
Hertz PPM kHz
phased absval power
More Display - Parameter Pages
Basic Plotting
Print to: Printer Preview File
Auto Plot Print Screen...
More Plotting - Parameter Pages
18 16 14 12 10 8 6 4 2 0 ppm
delta
Start Acquire Process
Transform Autoprocess Display Spectrum Clear Screen Cancel
Basic
Default
Weighting
Display
More 1D
Integration
Cursors/Line Lists
Plot
Text Output
Display Mode: phased absval power
Axis: Hertz PPM kHz
Amplitude Scaling: Normalized Absolute
Reference: By Solvent By TMS Cancel By Cursor
Baseline Correct: DC Correct Autofind Integrals BC Correct
Screen Position: Full Center Left Right
Scale Adjust: Autoscale + -
Find Peaks: Peak Threshhold Find Peaks
Nearest Line
Display Arrays: Horizontal Label Vertical Custom
Display offsets
Mark at Cursor
Clear Marks
Temp Spin Lock Sample
Probe

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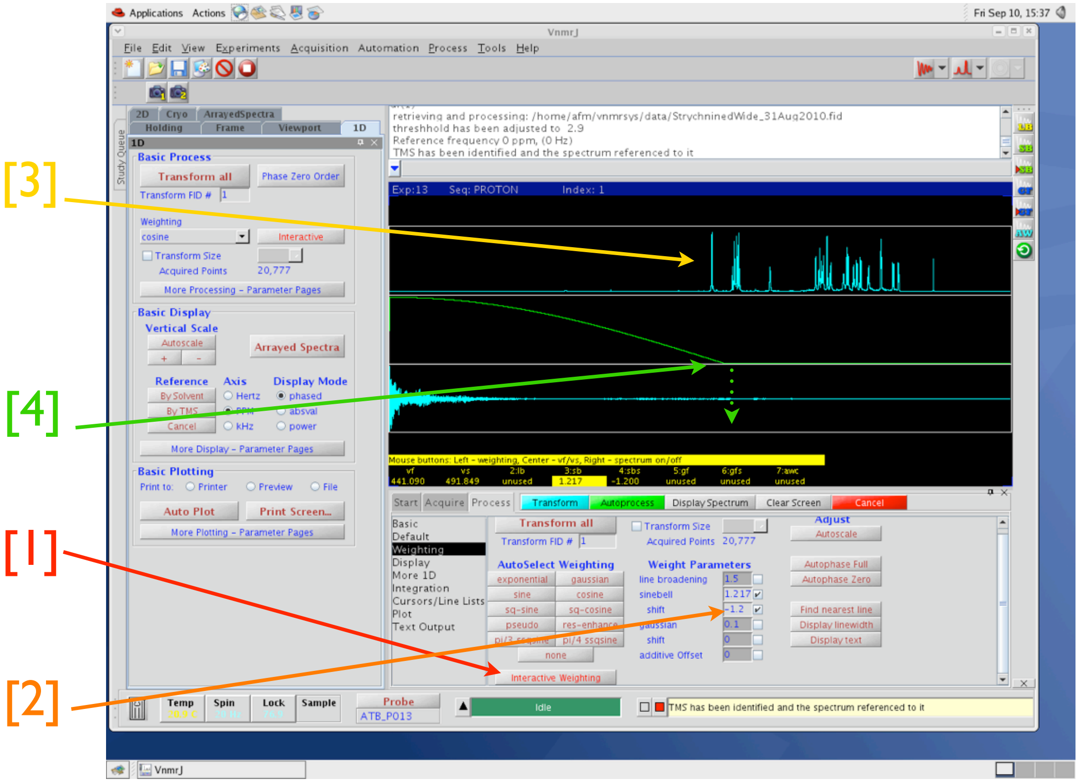
Figure 6
Weighting & Linear Prediction



Fri Sep 10, 15:37

```
retrieving and processing: /home/afm/vnmrsys/data/StrychninedWide_31Aug2010.fid
threshhold has been adjusted to  2.9
Reference frequency 0 ppm, (0 Hz)
TMS has been identified and the spectrum referenced to it
```

Exp:13 Seq: PROTON Index: 1

Weighting: cosine

Transform FID # 1

Acquired Points 20,777

Mouse buttons: Left - weighting, Center - vf/vs, Right - spectrum on/off

vf	vs	2:lb	3:sb	4:sbs	5:gf	6:gfs	7:awc
441.090	491.849	unused	1.217	-1.200	unused	unused	unused

Weight Parameters

line broadening	1.5	□
sinebell	1.217	☑
shift	-1.2	☑
gaussian	0.1	□
shift	0	□
additive Offset	0	□

Idle

TMS has been identified and the spectrum referenced to it

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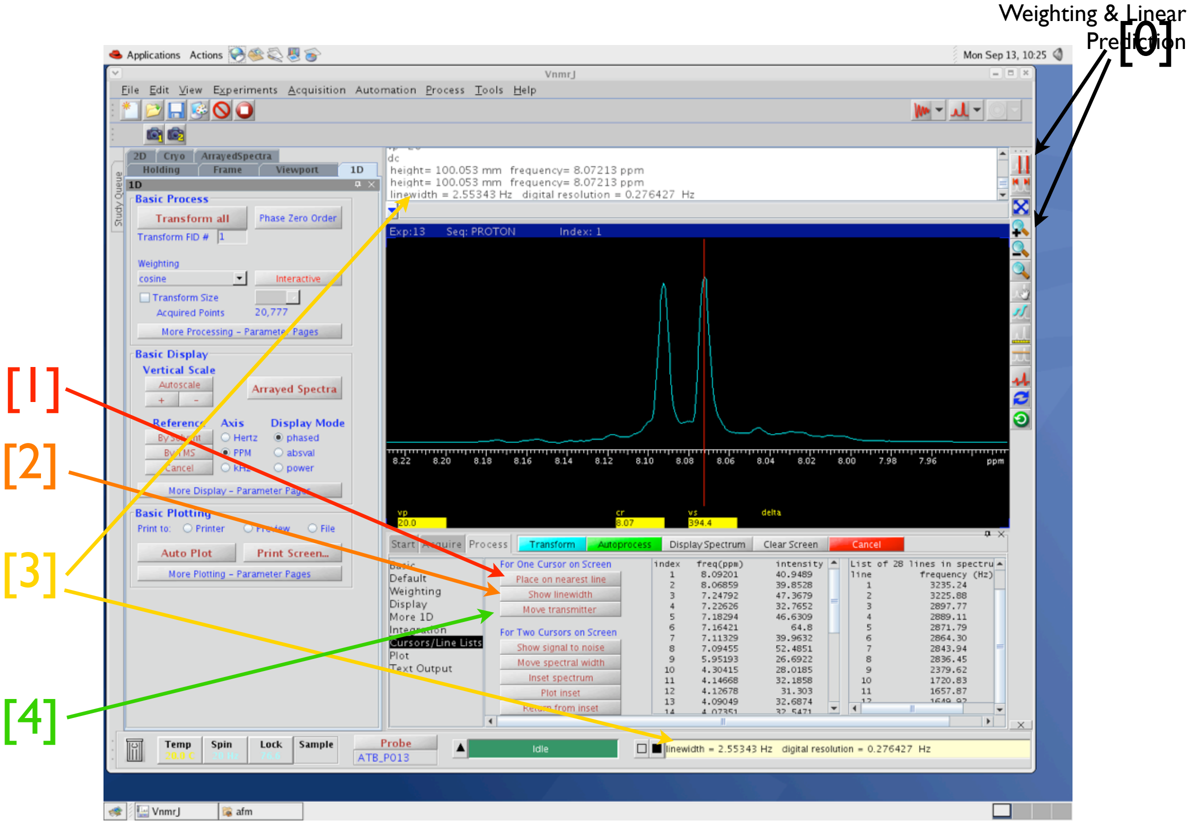
Figure 7
Weighting & Linear Prediction



Transform FID # 1

Weighting: cosine

☐ Transform Size

Acquired Points 20,777

Axis: ● PPM

Display Mode: ● phased

```
dc
 height= 100.053 mm   frequency= 8.07213 ppm
 height= 100.053 mm   frequency= 8.07213 ppm
 linewidth = 2.55343 Hz   digital resolution = 0.276427  Hz
```

Exp:13   Seq: PROTON   Index: 1

```
index    freq(ppm)     intensity
   1      8.09201       40.9489
   2      8.06859       39.8528
   3      7.24792       47.3679
   4      7.22626       32.7652
   5      7.18294       46.6309
   6      7.16421          64.8
   7      7.11329       39.9632
   8      7.09455       52.4851
   9      5.95193       26.6922
  10      4.30415       28.0185
  11      4.14668       32.1858
  12      4.12678        31.303
  13      4.09049       32.6874
  14      4.07351       32.5471
```

```
List of 28 lines in spectru
line            frequency (Hz)
   1               3235.24
   2               3225.88
   3               2897.77
   4               2889.11
   5               2871.79
   6               2864.30
   7               2843.94
   8               2836.45
   9               2379.62
  10               1720.83
  11               1657.87
  12               1649.92
```

linewidth = 2.55343 Hz   digital resolution = 0.276427 Hz

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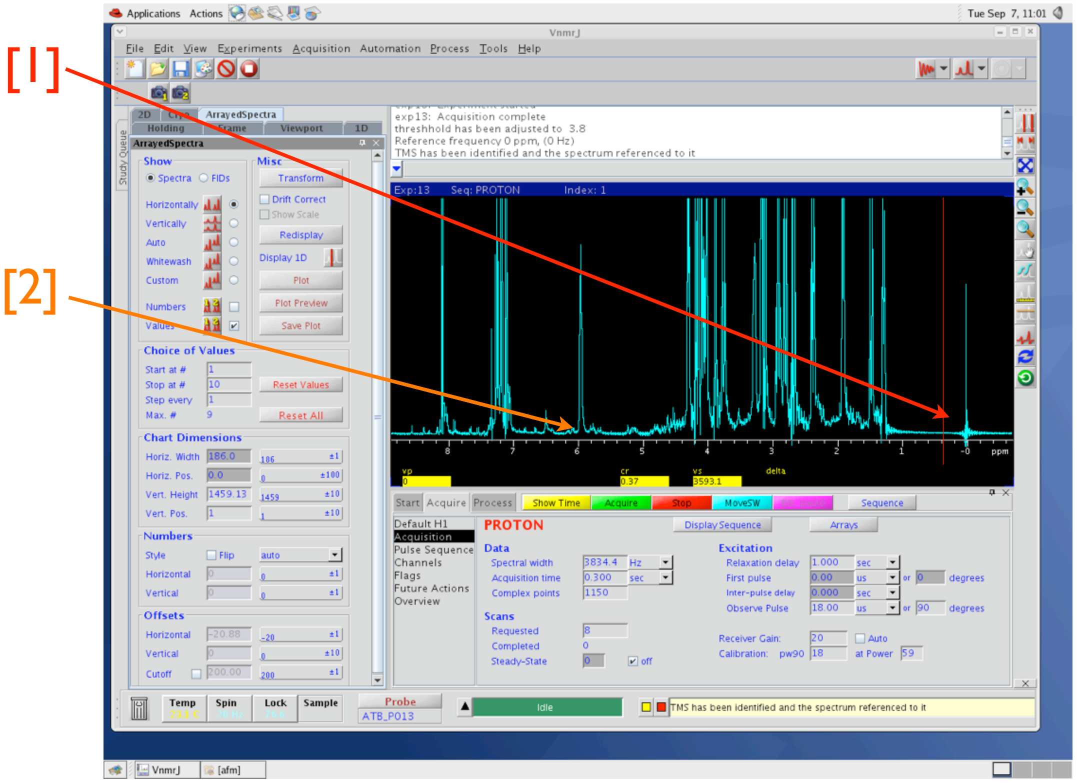
Figure 8
Weighting & Linear Prediction



```
exp13:  Acquisition complete
threshhold has been adjusted to  3.8
Reference frequency 0 ppm, (0 Hz)
TMS has been identified and the spectrum referenced to it
```

Exp:13   Seq: PROTON   Index: 1

Show: ● Spectra ○ FIDs

Horizontally ●

☐ Drift Correct

☐ Show Scale

Numbers ☐

Values ☑

Choice of Values

Start at # 1

Stop at # 10

Step every 1

Max. # 9

Chart Dimensions

Horiz. Width 186.0 186 ±1

Horiz. Pos. 0.0 0 ±100

Vert. Height 1459.13 1459 ±10

Vert. Pos. 1 1 ±10

Numbers

Style ☐ Flip auto

Horizontal 0 0 ±1

Vertical 0 0 ±1

Offsets

Horizontal -20.88 -20 ±1

Vertical 0 0 ±10

Cutoff ☐ 200.00 200 ±1

PROTON

Data

Spectral width 3834.4 Hz

Acquisition time 0.300 sec

Complex points 1150

Scans

Requested 8

Completed 0

Steady-State 0 ☑ off

Excitation

Relaxation delay 1.000 sec

First pulse 0.00 us or 0 degrees

Inter-pulse delay 0.000 sec

Observe Pulse 18.00 us or 90 degrees

Receiver Gain: 20 ☐ Auto

Calibration: pw90 18 at Power 59

TMS has been identified and the spectrum referenced to it

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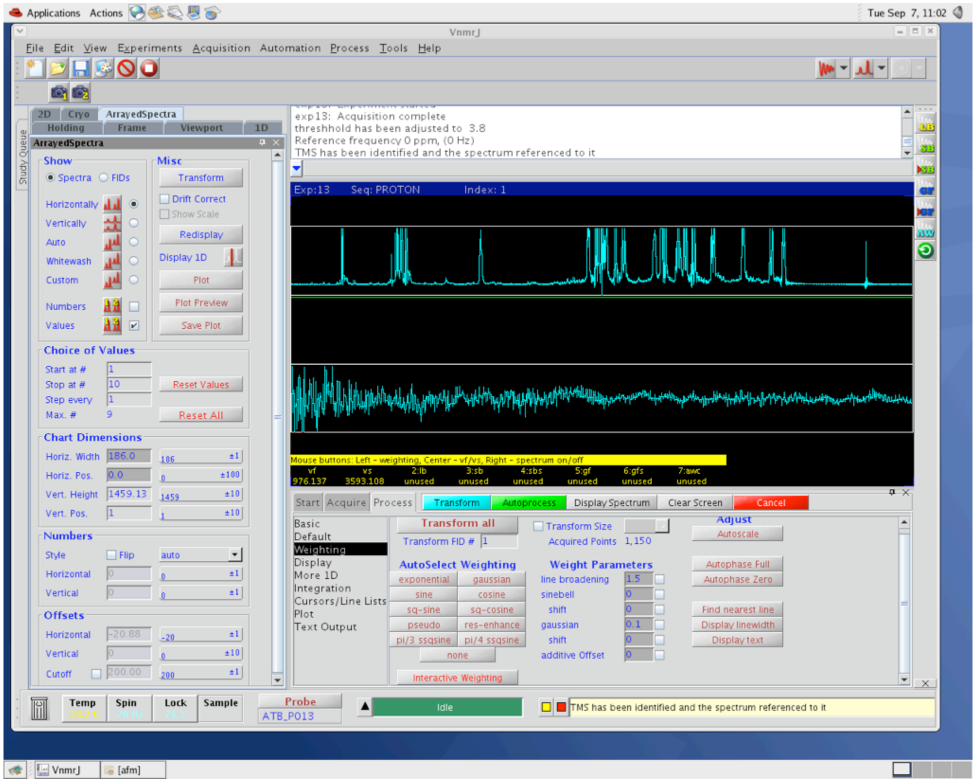
Figure 9
Weighting & Linear Prediction



exp13: Acquisition complete
threshhold has been adjusted to 3.8
Reference frequency 0 ppm, (0 Hz)
TMS has been identified and the spectrum referenced to it

Exp:13 Seq: PROTON Index: 1

Mouse buttons: Left - weighting, Center - vf/vs, Right - spectrum on/off

vf	vs	2:lb	3:sb	4:sbs	5:gf	6:gfs	7:awc
976.137	3593.108	unused	unused	unused	unused	unused	unused

● Spectra ○ FIDs
Horizontally ●
□ Drift Correct
□ Show Scale
Display 1D
Numbers □
Values ☑

Choice of Values
Start at # 1
Stop at # 10
Step every 1
Max. # 9

Chart Dimensions
Horiz. Width 186.0
Horiz. Pos. 0.0
Vert. Height 1459.13
Vert. Pos. 1

Numbers
Style □ Flip auto

Offsets
Horizontal -20.88
Cutoff □ 200.00

□ Transform Size
Transform FID # 1
Acquired Points 1,150

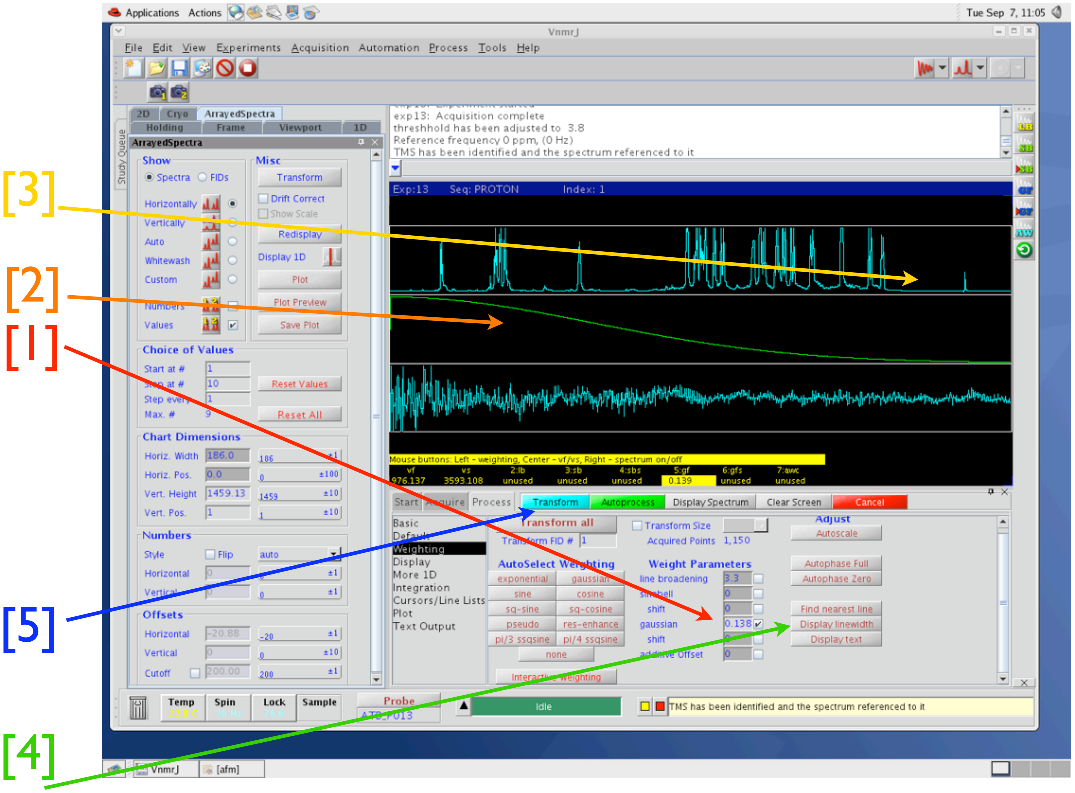
Weight Parameters

line broadening	1.5	□
sinebell	0	□
shift	0	□
gaussian	0.1	□
shift	0	□
additive Offset	0	□

Probe ATB_P013

TMS has been identified and the spectrum referenced to it

Figure 10
Weighting & Linear Prediction



exp13: Acquisition complete
threshhold has been adjusted to 3.8
Reference frequency 0 ppm, (0 Hz)
TMS has been identified and the spectrum referenced to it

Exp:13 Seq: PROTON Index: 1

Mouse buttons: Left - weighting, Center - vf/vs, Right - spectrum on/off

vf	vs	2:lb	3:sb	4:sbs	5:gf	6:gfs	7:awc
976.137	3593.108	unused	unused	unused	0.139	unused	unused

Choice of Values
Start at # 1
Stop at # 10
Step every 1
Max. # 9

Chart Dimensions
Horiz. Width 186.0
Horiz. Pos. 0.0
Vert. Height 1459.13
Vert. Pos. 1

□ Transform Size
Transform FID # 1
Acquired Points 1,150

Weight Parameters

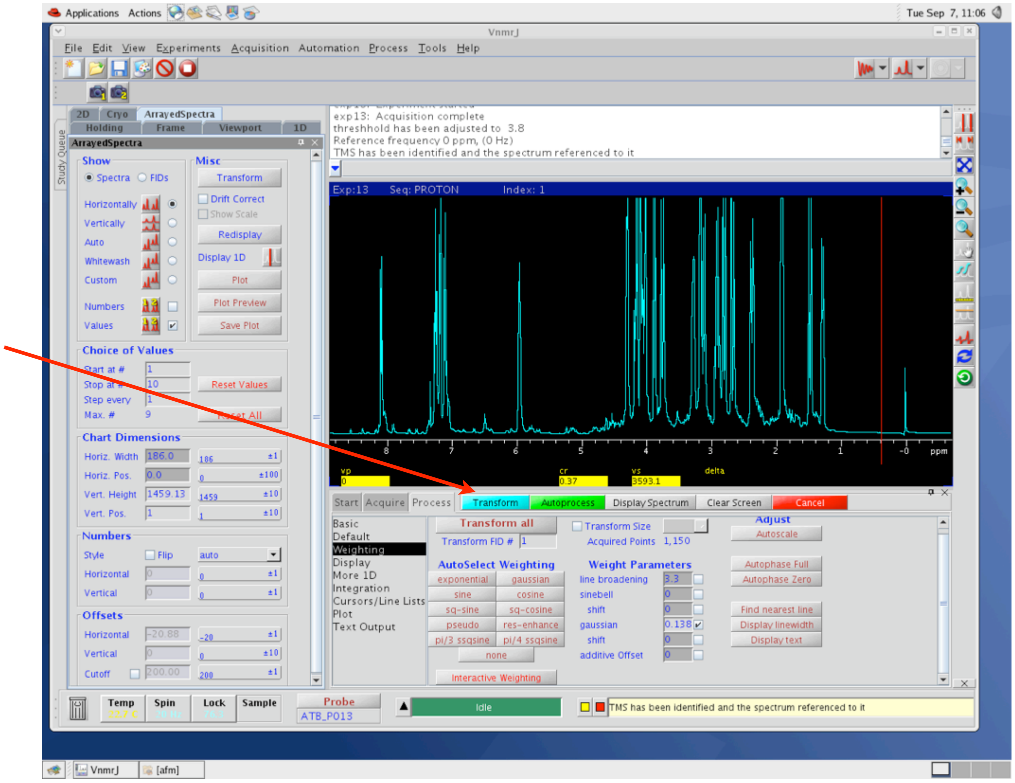
line broadening	3.3	□
sinebell	0	□
shift	0	□
gaussian	0.138	☑
shift	0	□
additive Offset	0	□

Probe ATB_P013

TMS has been identified and the spectrum referenced to it

Figure 11
Weighting & Linear Prediction

[1]



```
exp13:  Acquisition complete
threshhold has been adjusted to  3.8
Reference frequency 0 ppm, (0 Hz)
TMS has been identified and the spectrum referenced to it
```

● Spectra ○ FIDs

Start at # 1
Stop at # 10
Step every 1
Max. # 9

Horiz. Width 186.0   186
Horiz. Pos. 0.0   0
Vert. Height 1459.13   1459
Vert. Pos. 1   1

Style □ Flip auto
Horizontal 0
Vertical 0

Offsets Horizontal -20.88   -20
Vertical 0   0
Cutoff □ 200.00   200

vp 0   cr 0.37   vs 3593.1

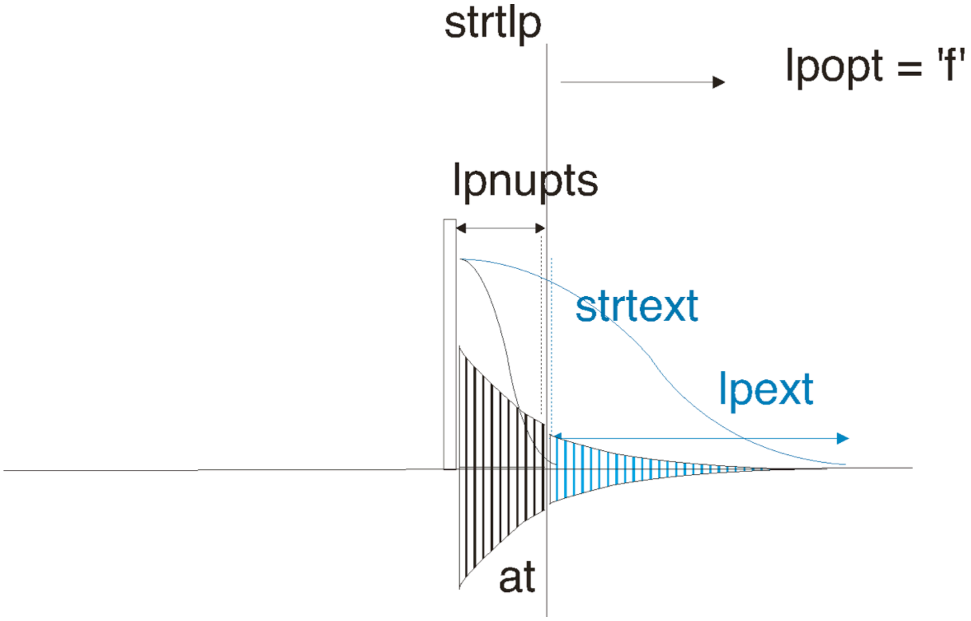
Transform FID # 1
□ Transform Size
Acquired Points 1,150

line broadening 3.3 □
sinebell 0 □
shift 0 □
gaussian 0.138 ☑
shift 0 □
additive Offset 0 □

Probe ATB_P013

TMS has been identified and the spectrum referenced to it

Figure 12
Weighting & Linear Prediction



strtlp

lpopt = 'f'

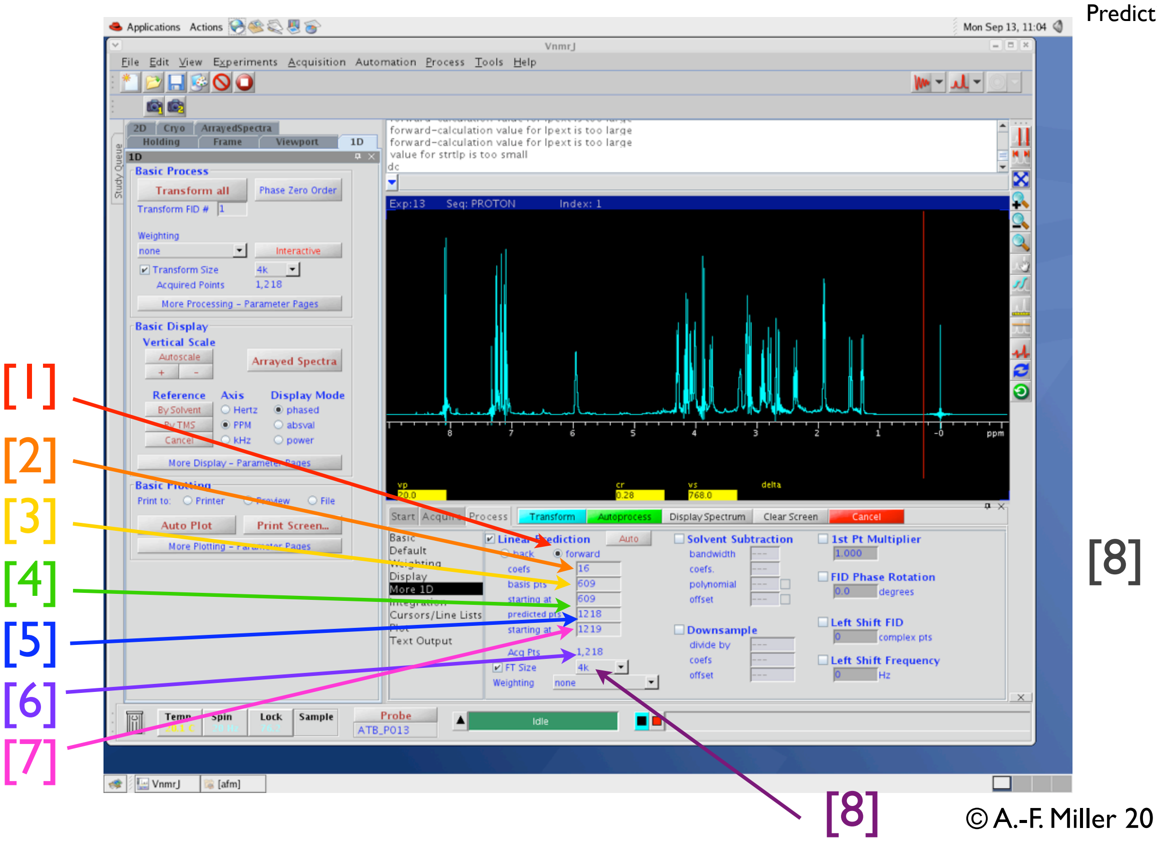
lpnupts

strtext

lpext

at

Figure 13
Weighting & Linear Prediction



```
forward-calculation value for lpext is too large
forward-calculation value for lpext is too large
value for strtlp is too small
dc
```

Exp:13 Seq: PROTON Index: 1

vp 20.0 cr 0.28 vs 768.0 delta

Basic Process: Transform all; Phase Zero Order; Transform FID # 1; Weighting none; Interactive; ☑ Transform Size 4k; Acquired Points 1,218; More Processing - Parameter Pages

Basic Display: Vertical Scale: Autoscale + -; Arrayed Spectra; Reference: By Solvent, By TMS, Cancel; Axis: ○ Hertz ● PPM ○ kHz; Display Mode: ● phased ○ absval ○ power; More Display - Parameter Pages

Basic Plotting: Print to: ○ Printer ○ Preview ○ File; Auto Plot; Print Screen...; More Plotting - Parameter Pages

☑ Linear Prediction (Auto)
○ back ● forward
coefs 16
basis pts 609
starting at 609
predicted pts 1218
starting at 1219
Acq Pts 1,218
☑ FT Size 4k
Weighting none

□ Solvent Subtraction: bandwidth ---; coefs. ---; polynomial ---; offset ---

□ Downsample: divide by ---; coefs ---; offset ---

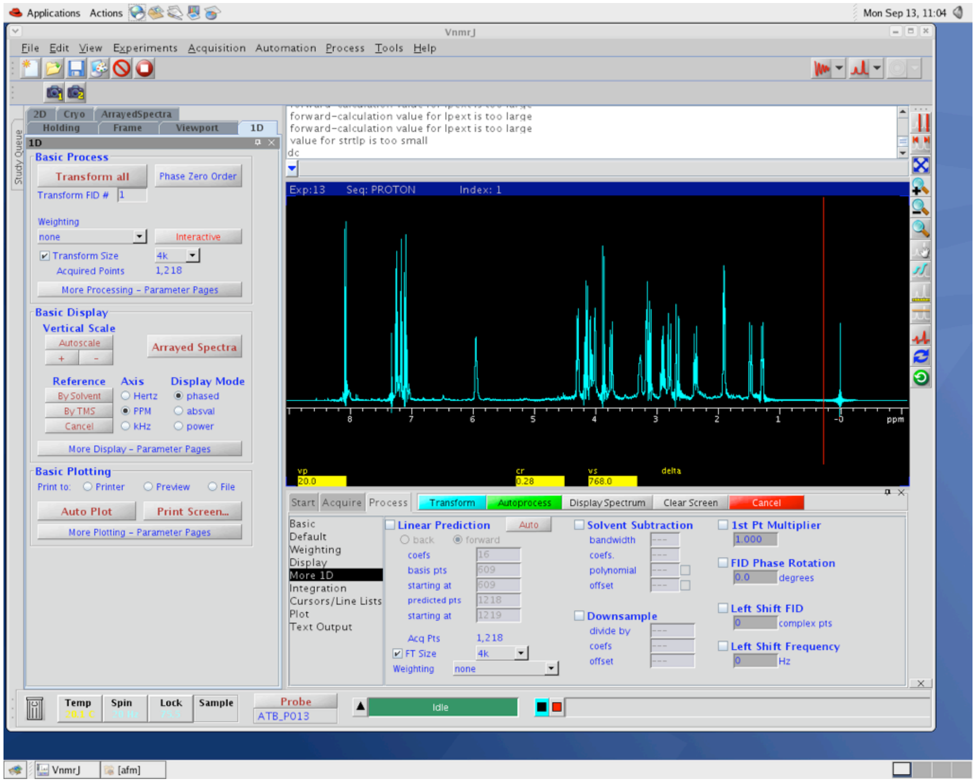
□ 1st Pt Multiplier 1.000

□ FID Phase Rotation 0.0 degrees

□ Left Shift FID 0 complex pts

□ Left Shift Frequency 0 Hz

Figure 14
Weighting & Linear Prediction



```
forward-calculation value for lpext is too large
forward-calculation value for lpext is too large
value for strtlp is too small
dc
```

Exp:13 Seq: PROTON Index: 1

vp 20.0 cr 0.28 vs 768.0 delta

Basic Process: Transform all; Phase Zero Order; Transform FID # 1; Weighting none; Interactive; ☑ Transform Size 4k; Acquired Points 1,218; More Processing - Parameter Pages

Basic Display: Vertical Scale: Autoscale + -; Arrayed Spectra; Reference: By Solvent, By TMS, Cancel; Axis: ○ Hertz ● PPM ○ kHz; Display Mode: ● phased ○ absval ○ power; More Display - Parameter Pages

Basic Plotting: Print to: ○ Printer ○ Preview ○ File; Auto Plot; Print Screen...; More Plotting - Parameter Pages

□ Linear Prediction (Auto)
○ back ● forward
coefs 16
basis pts 609
starting at 609
predicted pts 1218
starting at 1219
Acq Pts 1,218
☑ FT Size 4k
Weighting none

□ Solvent Subtraction: bandwidth ---; coefs. ---; polynomial ---; offset ---

□ Downsample: divide by ---; coefs ---; offset ---

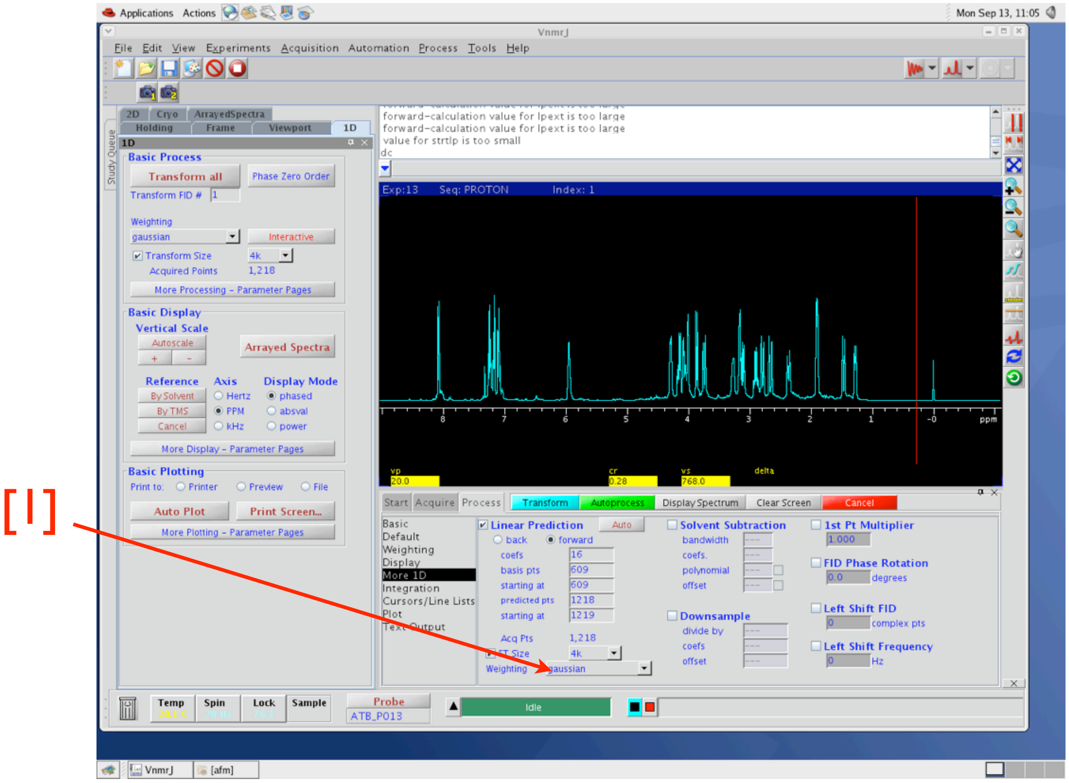
□ 1st Pt Multiplier 1.000

□ FID Phase Rotation 0.0 degrees

□ Left Shift FID 0 complex pts

□ Left Shift Frequency 0 Hz

Figure 15
Weighting & Linear
Prediction


[1]
VnmrJ
File Edit View Experiments Acquisition Automation Process Tools Help
Exp:13 Seq: PROTON Index: 1
vp 20.0
cr 0.28
vs 768.0
delta
Start Acquire Process
Transform Autoprocess Display Spectrum Clear Screen Cancel
Basic Default Weighting Display More 1D Integration Cursors/Line Lists Plot Text Output
Temp Spin Lock Sample Probe ATB_P013 Idle

```
forward-calculation value for lpext is too large
forward-calculation value for lpext is too large
value for strtlp is too small
dc
```

Basic Process: Transform all; Phase Zero Order; Transform FID # 1

Weighting: gaussian; Interactive

☑ Transform Size: 4k

Acquired Points: 1,218

Display Mode: ● phased ○ absval ○ power

Axis: ○ Hertz ● PPM ○ kHz

☑ Linear Prediction (Auto)

○ back ● forward

coefs	16
basis pts	609
starting at	609
predicted pts	1218
starting at	1219
Acq Pts	1,218
FT Size	4k
Weighting	gaussian

□ Solvent Subtraction: bandwidth ---; coefs. ---; polynomial ---; offset ---

□ Downsample: divide by ---; coefs ---; offset ---

□ 1st Pt Multiplier: 1.000

□ FID Phase Rotation: 0.0 degrees

□ Left Shift FID: 0 complex pts

□ Left Shift Frequency: 0 Hz

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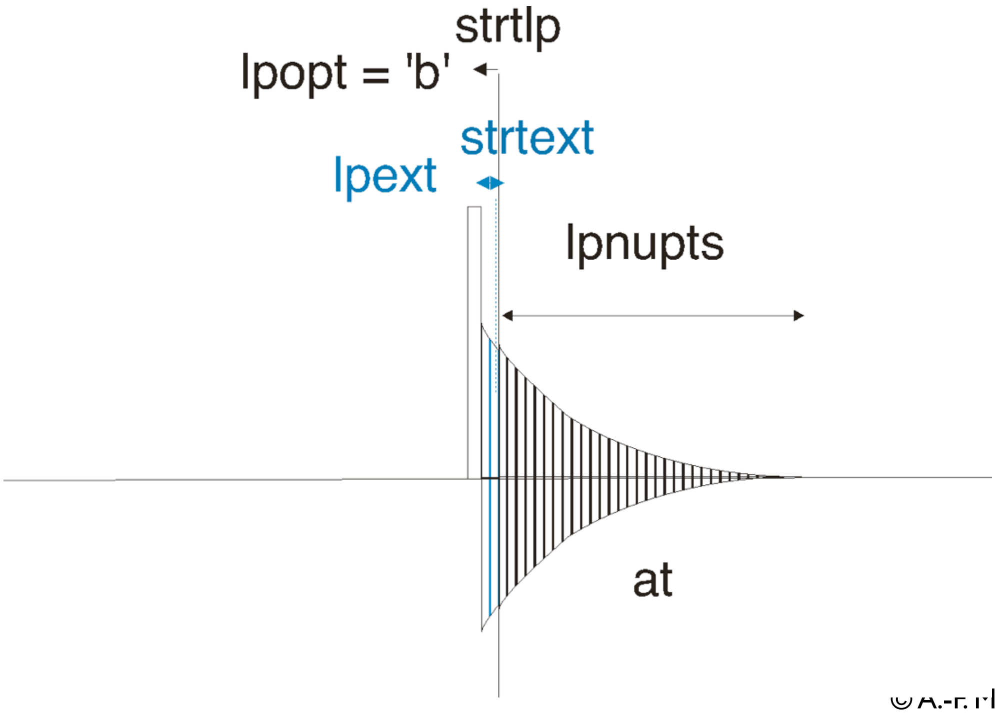
Figure 16
Weighting & Linear
Prediction



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