6
Processing Data

Introduction

To turn data into a spectrum after acquisition, data must be Fourier Transformed. Use the **Process** tab to access other data-processing options: adjusting the weighting function, zero filling, linear prediction, phasing, and referencing.

Processing and plotting options can be accessed on the **Process/Basic** page.

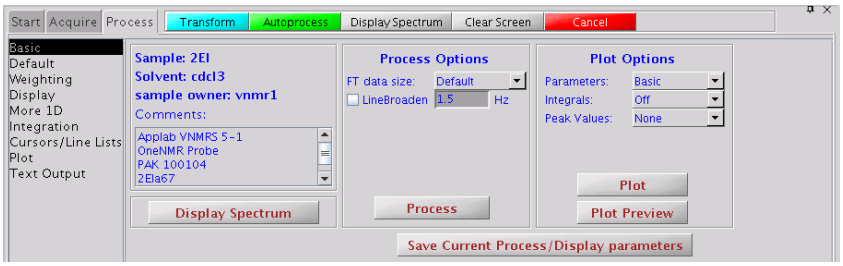


Figure 20 Process/Basic page

Other data processing options can be accessed on the **Process/Default** page.

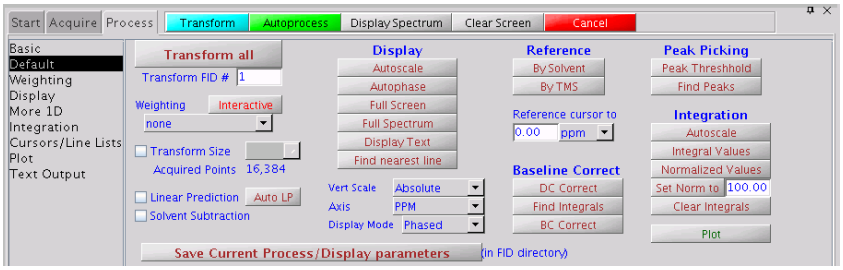


Figure 21 Process/Default page

Weighting Function

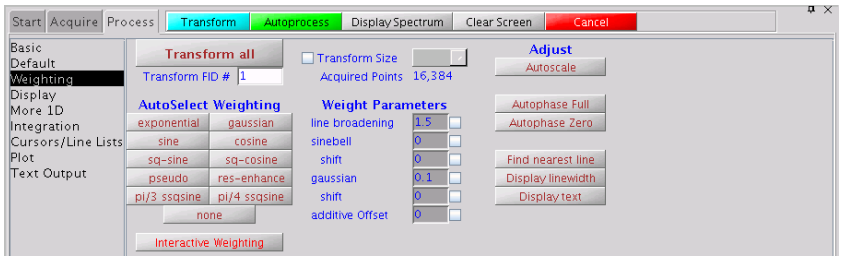


Figure 22 Process/Weighting page

The **Process/Weighting** page contains a full set of weighting-function action buttons. These automatically set the Weight parameters in the following way:

- **exponential** – A positive value gives the desired line broadening in Hz. This is also called a decaying exponential function. A negative value gives a resolution enhancement function. The parameter name is `lb`.
- **gaussian** – Time constant, in seconds, that defines a Gaussian function of the form `exp(-(t/gf)2)`.
- **shift** – shifts the center of the Gaussian function `exp(-((t-gfs)/gf)2)`.
- **sine** – A positive value, in seconds, applies a sinebell of the form `sin(t*p/(2*sb))`. A negative value applies a squared sinebell function of the form `sin2(t*p/(2*sb))`.
- **shift** – a sinebell shift constant, in seconds. It allows shifting the origin of the sinebell function according to the formula `sin((t-sbs)*p/(2*sb))`. Again, the square of this function is applied if `sb` is negative.
- **additive Offset** – An additive weighting constant that adds the constant `awc` to each value of the weighting function. It is applied after the sinebell and exponential function but before the Gaussian function.

As part of the Transform process, all weighting functions are set and applied simultaneously. Deselect the associated check box to remove a particular weighting function from use.

The effects of combining sinebell, exponential, and Gaussian weighting can be complicated and should only be used after experimenting with the individual parameters. The use of either Gaussian apodization (which leads to Gaussian line shapes) or line broadening (values greater than 0 lead to Lorentzian lineshapes) is especially critical for deconvolution.

Other line shapes cannot be handled by the deconvolution program, but may be appropriate for 1D resolution enhancement or for absolute-value 2D experiments. Weighting functions (other than exponential) can alter the relative areas of the resonances within a spectrum, and so they should be used with great care if quantitative results are required.

The **res-enhance** button sets defaults of a equal to 0.1 and `b` equal to 0.3 into the formulas `lb=-0.318/(a*sw)`, and `gf=b*sw`, thereby calculating "reasonable" values for the resolution enhancement parameters `lb` and `gf`. The arguments `a` and `b` can also be selected by the user.

Several macros exist that set weighting parameters to give certain window functions. These include gaussian, `pi3ssbsq`, `pi4ssbsq`, `sqcosin`, and `sqsinebell`.

The parameter `wtfile` is available for handling user-written weighting functions; see the manual *VnmrJ 3 User Programming* for details.

Interactive Weighting

Click the **Interactive Weighting** button on the Process panel to start interactive weighting.

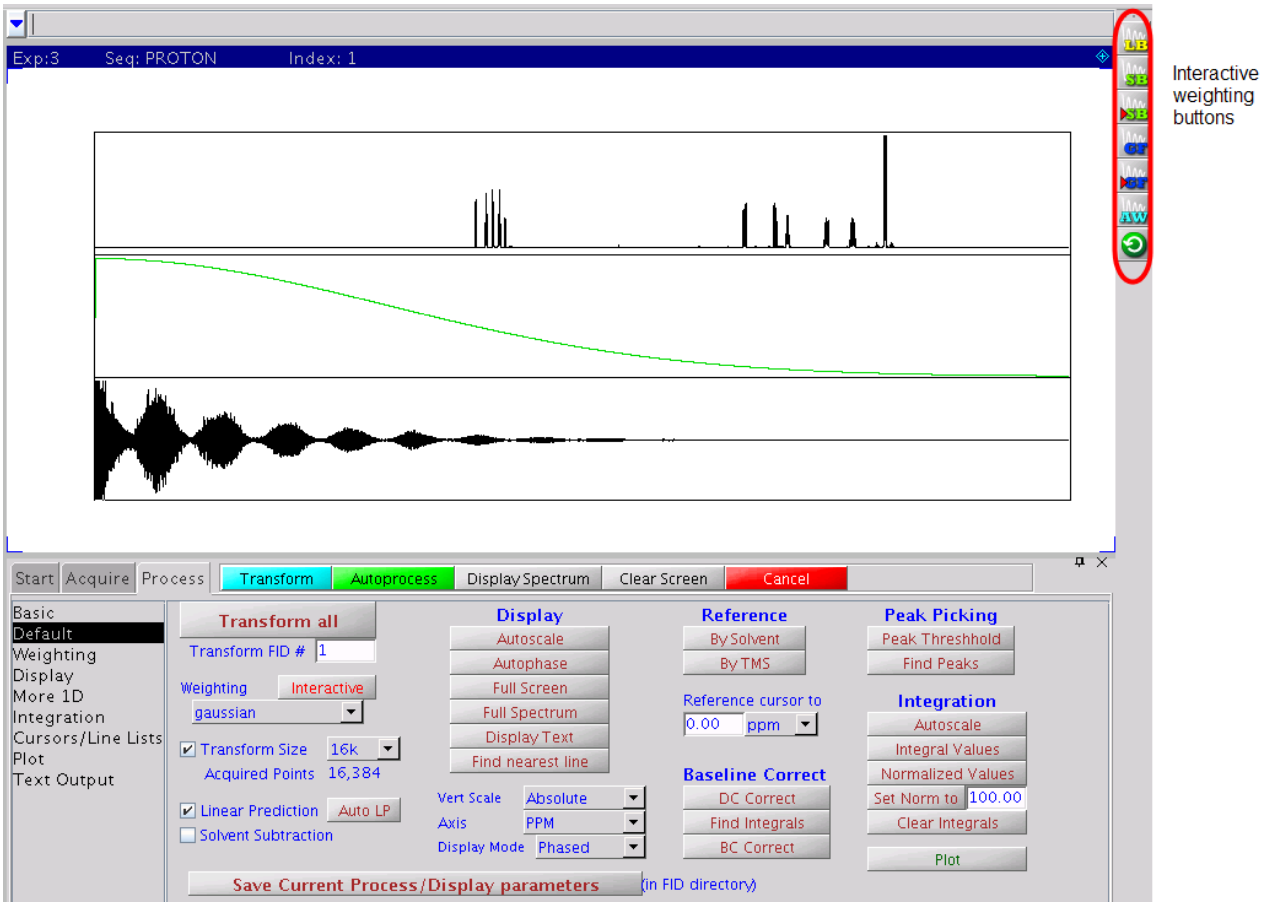


Figure 23 The graphics display for interactive weighting

Buttons next to the Interactive Weighting display provide access to the following functions:

Check box	Icon	Function
Line broadening		Selects line broadening or exponential weighting. A negative value gives resolution enhancement.
Sinebell		Selects the sinebell constant. A negative value gives squared sinebell. Change sign by clicking outside the box at the left.
Shifted Sinebell		Selects the sinebell shift constant (if sinebell is active).
Gaussian		Selects the Gaussian time constant.
Shifted Gaussian		Selects the Gaussian shift constant (if Gaussian is active).
Additive weighting		Selects the additive weighting constant.
Return		Returns to the previous menu.

Currently active weighting parameters can be changed by moving the cursor to the appropriate field in the weighting function box and pressing the left mouse button. New values for weighting parameters can also be typed in. Note that all other parameters, unless set to “not used”, are also used to calculate the weighting function.

Use the center mouse button within the FID box to adjust FID intensity (parameter `vf`). Use the center mouse button within the spectrum box to adjust spectrum intensity (`vs`). Use the right mouse button to turn the display of the transformed spectrum off and on. (It will be off by default whenever `fn > 25000`.)

Fourier Transformation

The **Transform all** button will Fourier transform one or more FIDs. It uses the Transform Size parameters, and weighting functions are simultaneously applied whenever any weighting options are selected. Other options listed on the **More 1D** page are also simultaneously applied (such as **Linear Prediction**, **Solvent Subtraction**, **FID Shift**, and **FID phase rotation**). The data processing options **Baseline Correct** and **Drift Correct** are only applied as separate discrete actions that are used after the Fourier Transform.

The Transform Size field is the number of points to be Fourier transformed (`fn`), and the number must be a power of two; typical numbers are 16384, 32768, or 65536 (listed as 16K, 32K, and 64K, where K is a multiplier of 1024). The most common entry for Transform Size is Default. This value specifies that however many data points (`np`) were acquired, the first power of two greater than or equal to `np` will be used as `fn`. If `fn` is greater than `np`, or if `fn` is 'n' and `np` is not a power of two, the remaining points in the transform are filled in with values of zero (zero-*filling*). (If `np` is <10% bigger than `fn`, the software will round down instead of up.) Thus, there is no explicit zero-filling command. This process is an implicit one governed by the relationship between `fn` and `np`. The number of complex data points is `fn`/2.

Phasing

Phasing spectra may be considered part of either data processing or data display. Performing a complex Fourier transformation produces two sets of data, referred to as the *cosine* and *sine* transforms, or the *real* and *imaginary* data sets, respectively. The absorption spectrum (peaks "in-phase") and the dispersion spectrum (peaks "out-of-phase") generally do not coincide with either the real or the imaginary channels, but must instead be produced from a linear combination of the two spectra.

Phasing can be adjusted using **Phase button**  for interactive phasing or using the **Autophase functions** on the **Process/Default** page.

Phase parameters

The process of phasing a spectrum requires the determination of an angle θ that can be used to "mix" these two data sets to produce one data set, according to the formula:

$$\textit{Absorption}\ \text{spectrum} = \textit{real}^{*}\ \cos\theta + \textit{imaginary}^{*}\ \sin\theta \qquad \text{[Eq. 1]}$$

The process is complicated by the fact that the phase angle θ is a function of frequency:

$$\theta = rp + (w - w0)\ /sw * lp \qquad \text{[Eq. 2]}$$

where `lp` (left or first-order phase) and `rp` (right or zero-order phase) are constants that must be determined.

The following is clear about the terms in Equation 2:

- `rp` is *frequency independent*. Changes in `rp` affect all peaks in the spectrum equally.
- `lp` is *frequency dependent*. Changes in `lp` affect peaks with a differing amount as a function of frequency.

There are several ways in which `lp` and `rp` can be adjusted:

- Like any parameter, they can be recalled with a particular parameter set. They can also be entered directly (for example, `lp=150`).

- Fully automatic phasing is also provided with the aph and aph0 commands. The aph command optimizes both the frequency-dependent (lp) and the frequency-independent (rp) parameters, and is independent of the starting point. The aph0 command adjusts only rp. The aphx macro optimizes parameters and arguments for the aph command. aphx first performs an aph then calculates a theoretical value for lp. If lp set by the aph is different from the calculated value by 10 percent, the calculated value is used and an aph0 is performed.

The command phase (phase_change) changes the phase of all peaks in the spectrum by adding phase_change to the current value of rp, and can remove any excess in rp more than 360°.

Autophase algorithm

The automatic phasing algorithms aph and aph0 have the following features:

- Weighting parameters do not affect the algorithms.
- Spectra with very low signal-to-noise can be phased.
- In vivo spectra can be phased, which is very difficult for most autophasing algorithms.
- Spectra with inverted lines can be phased. Such spectra include APT or DEPT data or selectively inverted lines obtained with shaped pulses. This type of phasing is difficult for traditional autophasing algorithms.

The autophasing algorithm uses many rules that are used in a manual phasing procedure. First, it finds the peak areas. Then, it estimates the correct phase for each peak. An initial guess of the first-order phasing parameter lp is made based upon the estimated phases of two “normal” peaks. The peaks are categorized into three classes: normal, inverted, and bad. The peaks in the normal and inverted group will be used to find the optimal values for the phasing parameters lp and rp. A final check is made to determine whether autophasing was successful or unsuccessful.

Algorithms are complicated but fairly “intelligent.” The key point of an algorithm is to use a set of fuzzy rules to estimate the correct phase for each peak. The use of these rules makes an algorithm less sensitive to the signal-to-noise ratio, the weighting parameters, and the baseline quality. Fuzzy logic also makes it possible to do the classifications on the peaks.

The command `aphb` autophases Bruker data. See the *Command and Parameter Reference* for more information about this command.

Spectrum display

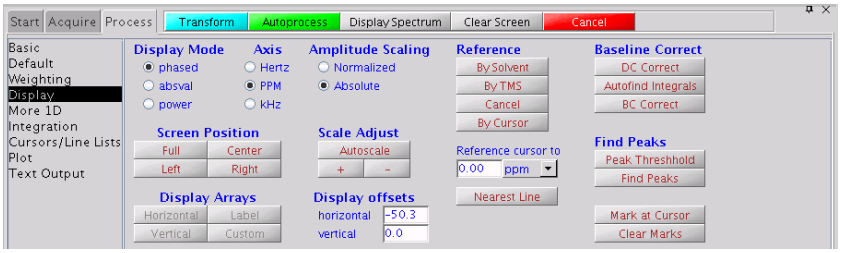


Figure 24 Process/Display page

The displayed spectrum is calculated in one of the following four *mutually exclusive* modes. The first three can be selected by radio buttons in the **Process/Display** page.

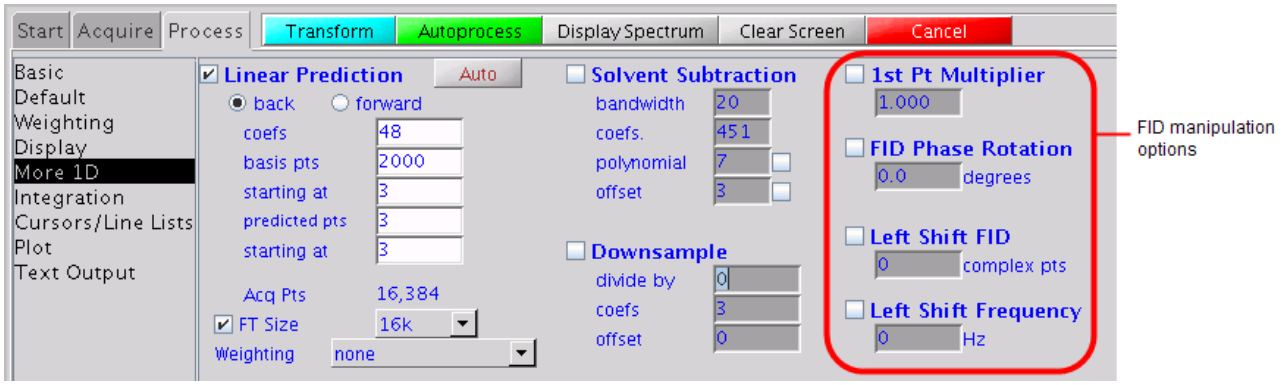
- The *phase-sensitive mode* is selected by the command `ph`. In this mode, the displayed spectrum is calculated using the phase parameters `lp` and `rp`. This is the most commonly used mode.
- The *absolute-value mode* is selected by the command `av`. In this mode, the displayed spectrum is calculated according to the equation
- $absorption\ spectrum(\omega) = (real^2\ (\omega) + imaginary^2(\omega)^{1/2}$
- The *power mode* is selected by the command `pwr`. In this mode, the displayed spectrum is the square of the displayed spectrum calculated in the absolute value mode.

- The *phase-angle mode* is selected by the command `pa`. In this mode, each point in the displayed spectrum is the arc-tangent of the phase angle of the real and imaginary point.

Once a spectrum is displayed using the interactive display command `ds`, the spectrum can be interactively phased by selecting the **Phase** button from the graphical tool bar. When the spectrum is in the Phase mode, the integral and cursors are not displayed.

Advanced Data Processing

This section covers the functions available on the **More 1D** page: advanced data processing, including linear prediction, FID shifting, FID phase rotation, and frequency shifting.



FID manipulation

Check Box	Function
1st Pt Multiplier	Allows correction of the first point of the FID if it is distorted. See the `fpmult` parameter in the *VnmrJ 3 Command and Parameter Reference*.
FID Phase Rotation	The parameter `phfid` is a zero-order FID phasing constant. If `phfid` is set to a value other than `'n'`, the FID is phase-rotated by `phfid` degrees before weighting or Fourier transformation is performed.
Left Shift FID	The parameter `lsfid` is a constant used in left-shifting the FID. If `lsfid` is set to a value other than `'n'`, the FID is left-shifted by `lsfid` complex points before weighting or Fourier transformation is performed. The value for `lsfid` must lie between 0 and `np`/2. The `tmove` macro provides a graphical method of setting the parameter `lsfid`—position the left cursor at the place that should be the start of the FID, then enter `tmove` to adjust the parameter `lsfid`.
Left Shift Frequency	Sets the frequency shift of spectral data, in Hz. See `lsfrq` in the *VnmrJ 3 Command and Parameter Reference*. Sets a frequency shift of spectral data, in Hz, with a negative value resulting in peaks being shifted upfield (to the right) and a positive value in peaks being shifted downfield (to the left). `lsfrq` operates in the time domain on complex FID data, and so the desired value must be entered prior to Fourier transformation.

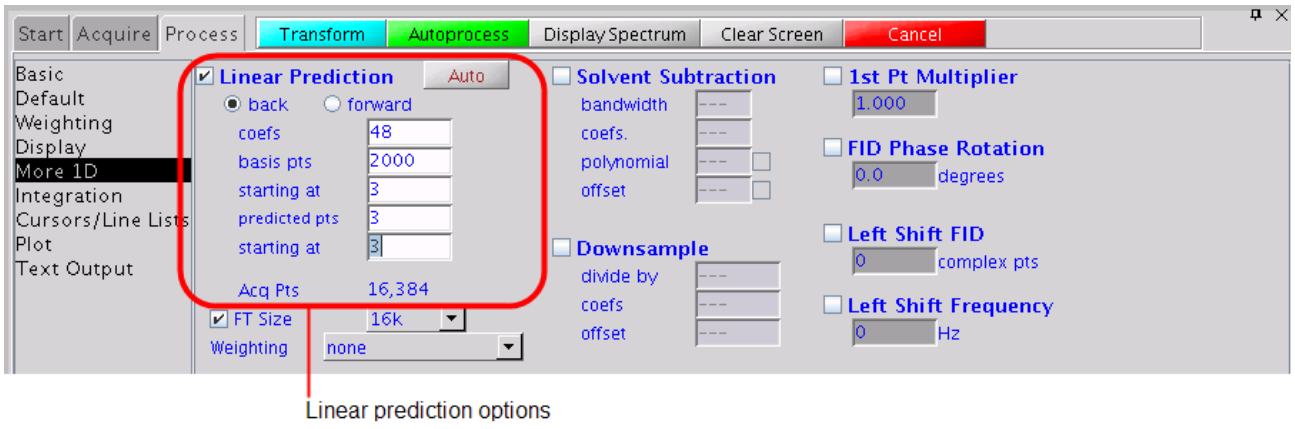
Data processing methods

All data processed in VnmrJ 3 are processed by using the Fourier transform, but there are three variations, which are governed by the `proc` parameter:

- Two orthogonal (real and imaginary, or x and y) data points are sampled at the same time and form a single complex data point in the FID. Such data are processed using a normal complex Fourier transformation, using `proc='ft'`.
- Some spectrometers (Bruker Instruments) acquire pseudo-quadrature data by sampling two orthogonal data points sequentially, rather than simultaneously. Such data must be processed using a real Fourier transformation, with `proc='rft'`.
- For complex data only, it is possible to include "linear prediction," as part of the data processing. `proc='lp'` is used to trigger this operation.

Linear prediction

Use the **Linear Prediction** page to control linear prediction and to adjust its parameters.



Linear Prediction in VnmrJ 3

Linear prediction is incorporated into the Fourier transform routine, so that you do not normally see the "improved" FID, but merely the resulting spectrum (which results from Fourier transforming the linear predicted FID). This is accomplished by selecting the **Linear Prediction** check box in the Linear Prediction panel and clicking on the **Transform**

button.

Enter `ft('noft')` to suppress display of the linear-predicted spectrum and perform all the steps of the Fourier transform routine except the actual Fourier transformation. Real points of the FID are displayed by setting `lp=0 rp=0`, or display the imaginary points by setting `lp=0 rp=90`.

Linear prediction involves solving a series of equations for appropriate coefficients based on the actual FID. It involves quite a number of parameters and can be somewhat tricky to optimize (if not optimized properly, or if the data are not amenable, the analysis may simply fail, just like any least-squares fit process may fail to converge).

Linear prediction can be run in an iterative fashion by arranging the LP parameters–first extending backward, then forward, and backward again for more complex problems.

Why Use Linear Prediction?

Raw time-domain data acquired during a pulsed NMR experiment can have two flaws:

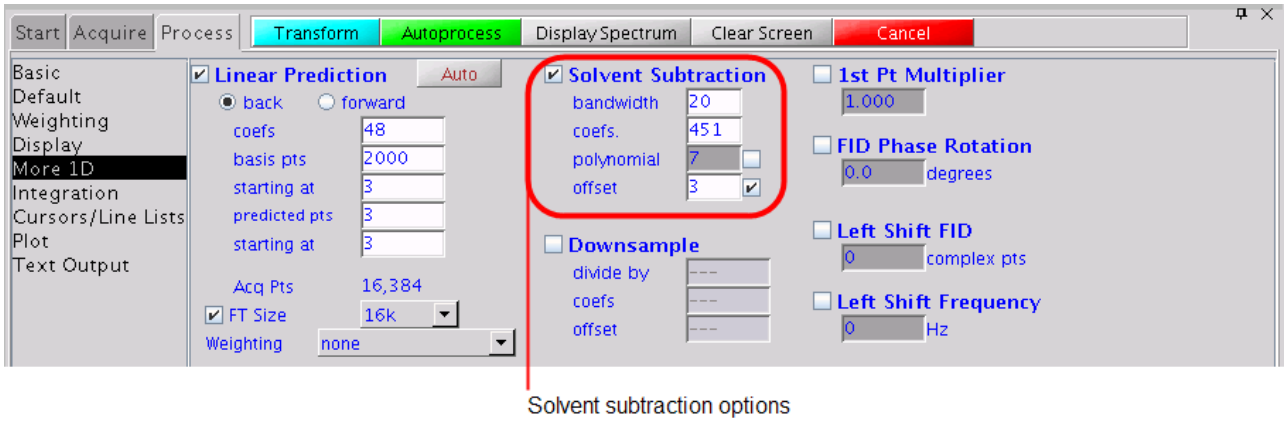
- Early points in the FID may be distorted due to a host of hardware characteristics, such as preamplifier saturation and probe ringing. Even on a perfect spectrometer, these distortions cannot always be avoided.
- The acquisition time of each FID may have been too short to allow for full decay of the signal, leading to distortion in the Fourier transformed spectrum.

Both types of distortions can be solved using *linear prediction*. This uses the “good” part of the FID to analyze for the frequencies that are present in the signal, and then uses that information to extend the FID either in a reverse direction (to “fix” the first few “bad” points) or in a forward direction (to eliminate truncation problems, or even single “bad” points). Following this process, the “new, improved” FID is then Fourier transformed in the usual way.

See H. Barkhuijsen, R. de Beer, W.M.M.J. Bovee, and D. van Ormondt, *J. Magn. Reson.*, 61, 465-481 (1985) for more information on the algorithm implemented in the software, and on linear prediction in general.

Solvent subtraction filtering

Numerous solvent suppression pulse sequences exist that reduce the signal from a large solvent peak to a level where the desired resonances can be observed. Often, however, experimental solvent suppression does not entirely eliminate an unwanted solvent peak. Digital filtering of the data can further suppress or eliminate a solvent peak.



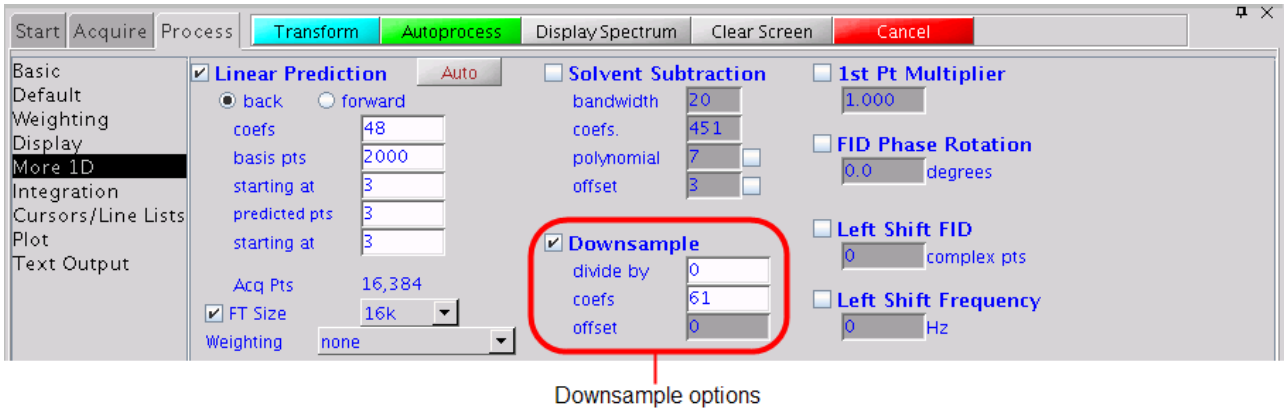
VnmrJ 3 incorporates two algorithms for solvent subtraction by digital filtering:

- bandwidth — Sets the value of `ssfilter` to specify the full bandwidth of the low-pass filter applied to the original FID to yield a filtered FID. Its default value is 100 Hz.
- coefs. — Sets the value of `ssntaps` to specify the number of taps (coefficients) used for the digital filter. The default value is 121, but the value can range from 1 to `np`/4. The more taps in a filter, the flatter the passband response and the steeper the transition from passband to stopband, giving a more rectangular filter. An increased number of taps also increases the computational time dramatically (so that it might become noticeable). The default is suitable for low-frequency suppression option.
  A value between 3 and 21 works better for the zero-frequency suppression option.

- polynomial — Sets the value of `ssorder` to determine the polynomial used to create a low-pass filter applied to the FID acquired with the solvent on resonance. The resulting FID is subtracted from the original FID to remove the on-resonance frequencies. Transforming the resulting FID produces a solvent-subtracted spectrum. Another name for this is zero-frequency suppression.
- offset — Sets the value of `sslsfrq`, which adjusts the location of the solvent-suppressed region of the spectrum. Setting `sslsfrq` to a non-zero value shifts the solvent-suppressed region by `sslsfrq` Hz. Setting `sslsfrq` to `'n'` (the default value) solvent suppresses a region centered about the transmitter frequency. The parameters may be arrayed to achieve multiple-frequency suppression.
  The quality of zero-frequency suppression diminishes rapidly as the solvent peak moves off the exact center of the digital filter. Adjust `sslsfrq` to move the center of the filter to within ± 0.2 Hz of the solvent peak for optimal solvent suppression.

Downsample

User-controlled downsampling is not routinely needed on data acquired on newer consoles, but it can be used on virtually all NMR data if desired.



- divide by — Sets the value of the downsampling factor that will be applied after digital filtering. The spectral width of the data set after digital filtering and downsampling is `sw` divided by `downsamp`, where `sw` is the acquired spectral width.

- coefs — Sets the value of `dscoef` to specify the number of coefficients used in the digital filter. This parameter is automatically adjusted by VnmrJ 3 to give filter cutoffs that are the same value of `downsamp` by using `dscoef*downsamp/2` coefficients in the digital filter. VnmrJ 3 always rounds `dscoef*downsamp/2` to an odd number. The default is 61.
- offset — Sets the value of a bandpass filter, in Hz, that is not centered about the transmitter frequency. A positive value selects a region upfield from the transmitter frequency; a negative value selects a downfield region.

Interleave FIDs

The `ilfid` command converts a multiple FID element into a single FID by interleaving the FIDs. When invoked in an experiment of `nf` FIDs, each of `np` points, `ilfid` sorts the data into a single FID of `np*nf` points that can then be transformed. The interleaving takes the first complex point of each of the `nf` FIDs and places them in sequential order in the new FID. It then takes the second complex point from each of the `nf` FIDs and appends them sequentially to the new FID. This operation is repeated for all complex points. Although `ilfid` adjusts `np` and `nf`, it does not alter other parameters such as `sw`. See the *VnmrJ 3 Command and Parameter Reference* for further information on `ilfid`, including an example.

CAUTION Because `ilfid` alters the data irrevocably, it is strongly recommended to save the FID before using `ilfid`.

7
Displaying FIDs and Spectra

Displaying a FID or 1D Spectrum

Click the **Display FID** graphics control button to display a FID. Click the **1D Spectrum** graphics control button to display a 1D spectrum.

FID display

An FID is available for displaying upon completion of the acquisition of acquisition block size. Clicking the **FID** icon displays a FID and enables interactive manipulation of the FID display.

The FID display graphics buttons change to show that multiple FIDs can be viewed. Figure 25 shows a typical display with a FID and two vertical cursors (box mode).

The FID is also phase-rotated (zero-order only) by the number of degrees specified in the FID Phase Rotation field on the **Linear Prediction** page.

1D spectrum display

After data is transformed, a spectrum becomes available for display and plotting.

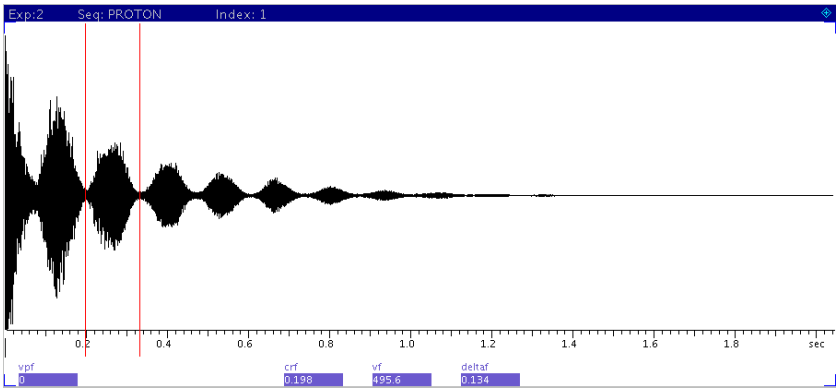


Figure 25 Interactive FID display

The normal spectrum display enables interactive manipulation of a single 1D spectrum. A spectrum is displayed by clicking on the **1D Spectrum graphics control** icon or by transforming a data set.

A spectrum displays in the graphics window similar to Figure 26.

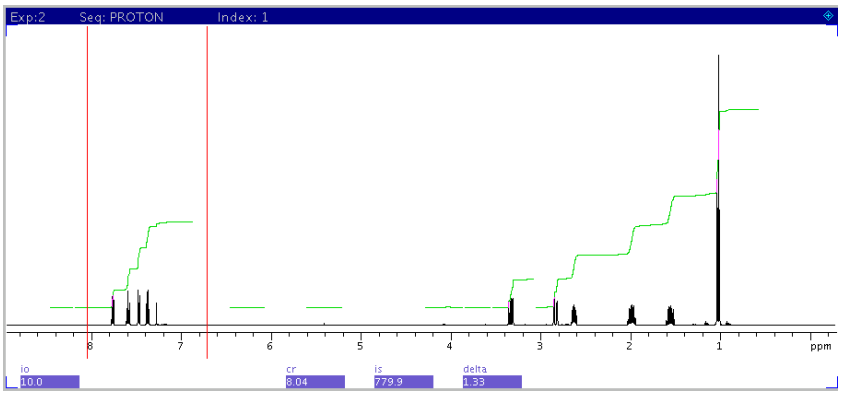


Figure 26 Interactive spectrum display

Display Tools

VnmrJ 3 provides interactive tools for creating individualized displays of NMR data.

Interactive display tools

These tools are described below:

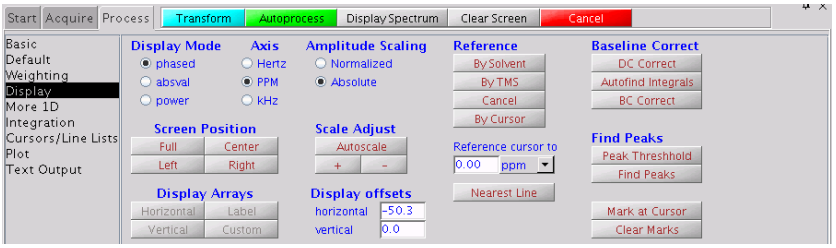
Mouse buttons	The mouse buttons correspond to the display parameters shown on the lower right part of the graphics window. The display parameter changes as different graphics control functions are selected. Typically, the left button controls the left cursor position, the middle button controls vertical scaling, and the right button controls the right cursor or delta between the two cursors.
Graphics control buttons	The graphics control bar next to the graphics canvas provides graphics control buttons for cursors, zooming, scales, grab and move, threshold, phasing, and refresh. Different functions appear for FID or spectrum display.
Display page	The **Display** page on the **Process** tab provides appropriate display parameters, including display mode, axis, and amplitude scaling.
Display menu	The **Display** menu provides tools for displaying multiple spectra, plotting, and creating insets.

A typical use of these tools might be to expand a region on a spectrum:

1. Display the spectrum – click the spectrum icon on the graphics control bar.
2. Select the region to expand – left click the spectrum to place the cursor on the left boundary of the region of interest, and right-click to designate the right boundary. Use the left mouse button to drag the left cursor and right button to drag the right cursor until the desired region is between the cursors.
3. Expand the region – click the magnifying glass icon on the graphics control bar.

Display parameters

FID and spectral display is governed by parameters on the **Display** page.



Display Mode

The Display Mode parameters set the display mode along the directly or indirectly detected dimension.

Phased	Each real point in the displayed spectrum is calculated from a linear combination of real and imaginary points comprising each respective complex data point.
Absval	(Absolute value mode) Each real point in the displayed spectrum is calculated as a square root of the sum of squares of the real and imaginary points comprising each respective complex data point.
Power	Each real point in the displayed spectrum is calculated as a sum of squares of real and imaginary points comprising each respective complex data point.

Axis

The Axis parameters set the labeling of plot scales, peak frequencies, etc. Typically, FID display is in seconds, and spectrum display is in PPM, Hz, or kHz.

Amplitude scaling

The amplitude scaling, or vertical scale, parameters set the scale intensities for the display:

Normalized	The largest peak in the spectrum is automatically found, then the display is normalized to make the peak vertical scale on the plot in millimeters.
Absolute	The appearance on the display screen is used as a guide to adjust the vertical scale to produce the desired height. This mode enables comparing intensity from one experiment to another, a necessity for *all* arrayed experiments.

For vertical scaling, full scale on the screen represents full scale on the plotter. This relationship is used to adjust the vertical scale in the Absolute display mode, because vertical scale is not the height of the largest peak. Use the Normalized amplitude scaling mode when the largest peak is to be off-scale.

An exception to the general rule of plotting is provided by the `wysiwyg` parameter. This parameter is set in the **Edit > System settings** window, on the **Display/Plot** tab: *Set display from plotter aspect ratio* (wysiwyg).

Checked	Scales the image to the current plotter setting (wysiwyg).
Unchecked	Scales the image to the full window, which is easier to view. This option scales the window but does not change the ratio of the image.

Screen position

The screen position parameters set the horizontal position of the display on the screen and the plotter. Clicking one of the buttons updates the display:

Full	Display or plot on the entire screen or page.
Center	Display or plot in the center of the screen or page.
Left	Display or plot in the left half of the screen or page.
Right	Display or plot in the right portion of the screen or page.

Controlling cursors and vertical scale

Click the mouse buttons in the graphics display window to position cursors and adjust the FID or spectral vertical scale and position.

Left cursor	Click the left mouse button to position the cursor and update the value displayed for the `crf` or `cr` parameter (`crf` for a FID or `cr` for a spectrum).
Right cursor (box)	Click the right mouse button to display and position a second cursor to the right of the original cursor. The value of the parameter `deltaf` for a FID or `delta` for a spectra changes with the position of the right cursor and is the difference in seconds or Hz between the two cursors.
Two cursors	If both cursors are displayed, the left mouse button moves both cursors simultaneously, leaving the distance between them (`deltaf` or `delta`) unchanged.
Vertical scale	Click the middle mouse button to adjust the vertical scale of the FID (`vf` parameter) or spectrum (`vs` parameter).
Vertical position	Adjust the vertical position of the FID by clicking and holding the middle mouse button near the left edge of the graphics display and sliding the FID or spectrum up or down. The value of `vpf` or `vp` (or `vpfi` if the imaginary channel) is will change.

Display limits

The screen position buttons (**Full**, **Enter**, **Left**, **Right**) on the **Display** page place the display and plot in the desired portion of the page.

The `wysiwyg` parameter is useful for scaling the image to a full window instead of the same size as the plot. This parameter is set in the **Edit > System** settings window, on the **Display/Plot** tab: Set *display from plotter aspect ratio* (wysiwyg).

Checked	Scales the image to the current plotter setting (wysiwyg).
Unchecked	Scales the image to the full window, which is easier to view. This option scales the window but does not change the ratio of the image.

Graphics Control Buttons

The graphics control bar for the active viewport is to the right of the graphics canvas. Use the buttons in the bar to control the interactive display in the graphics canvas.

Common graphics display toolbar controls

The following tools are common to 1D, nD, and fid display toolbars.

Icon	Description
	Zoom in
	Zoom out
	Select zoom region
	Redraw display
	Return to previous tool menu

1D display spectrum toolbar controls

Icon	Description
	One cursor in use, click to toggle to two cursors
	Two cursors in use, click to toggle to one cursor
	Click to expand to full spectral display
	Pan or move spectral region
	Display integral
	Display scale
	Toggle threshold on or off
	Phase spectrum

Display FID toolbar controls

Icon	Description
	One cursor in use, click to toggle to two cursor
	Two cursors in use, click to toggle to one cursor
	Click to expand to full FID display
	Pan and stretch
	Click to show real and imaginary
	Click to show real and zero imaginary
	Click to show real only
	Toggle scale on and off
	Phase FID

Main nD Display Bar Tools

Icon	Description
	Display color map and show common nD graphics tools
	Display contour map and show common nD graphics tools
	Display stacked spectra and show common nD graphics tools
	Display image map and show common nD graphics tools

nD graphic tools

Icon	Description
	One cursor in use, click to toggle to two cursors
	Two cursors in use, click to toggle to one cursor
	Click to expand to full display
	Pan and stretch
	Show trace
	Show projections
	Click  to show horizontal maximum projection across the top of the 2D display
	Click  to show horizontal sum projection across the top of the 2D display
	Click  to show vertical maximum projection down the left side of the 2D display
	Click  to show vertical sum projection down the left side of the 2D display
	Rotate axes
	Increase vertical scale 20%.
	Decrease vertical scale 20%
	Phase spectrum
	Click  to select the first spectrum
	Click  to select the second spectrum
	Enter peak pick menu

Phasing

The **Phase** button starts the interactive phasing mode. Any integral and cursors that are displayed along with the spectrum are removed. The width of the update region is set by the *Spectrum updating during phasing (0-100)* field in **Edit > System settings > Display/Plot** tab, which sets the percentage of the screen display to be updated.

FID phasing

The **Phase** button activates the interactive phasing mode:

1. Position the mouse arrow on a FID region of interest, about halfway vertically up the screen, and click the left mouse button.

   A horizontal cursor intersects at the mouse arrow, and two vertical cursors are placed on either side of the mouse arrow. A small region of the FID is displayed in a different color if a color display is present. Only this spectral region is interactively updated.

2. Move the mouse above or below the horizontal cursor, but within the two vertical cursors. Click the left or right button to adjust the FID phase parameter `phfid`.

   Click the mouse above the horizontal cursor to increase `phfid`. Click below the horizontal cursor to decrease `phfid`. Place the mouse arrow right on the horizontal cursor and click the left button to restore the initial phase.

3. To exit the interactive phasing mode, make another selection from the menu. Select the **Cursor** or **Box** button if no other choice is desirable.

Spectrum phasing

1 Position the mouse arrow on a spectral region of interest toward the right side of the spectrum, about halfway vertically up the screen, and click the left mouse button.

   A horizontal cursor will intersect at the mouse arrow. Two vertical cursors will be placed on either side of the mouse arrow. A region of the spectrum will be displayed in a different color if a color display is present, and only this spectral region will be interactively updated (for the case of less than 100% updating).

2 Move the mouse above or below the horizontal cursor, but within the two vertical cursors. Click the left or right button to adjust the zero-order or frequency-independent phase parameter `rp`.

   - Click above the horizontal cursor to increase `rp` (cause a clockwise rotation of the peaks).
   - Click below the horizontal cursor to decrease `rp` (and cause a counter-clockwise rotation).
   - Place the arrow on the horizontal cursor and click the left button to restore the initial phase.

   The left and right buttons of the mouse differ only in their sensitivity. Full scale (top to bottom of the screen) corresponds to approximately 180° for the left button, and 20° for the right button. The left button is a "coarser" adjustment, and the right button is a "finer" adjustment.

3 Move the mouse arrow to another region of the spectrum, near the left edge of the display, outside the vertical cursors, and click the left mouse button again.

   The frequency-independent phase-correction made so far is first applied to the entire spectrum. A new horizontal cursor is displayed at the mouse arrow, and two new vertical cursors are displayed on either side of the mouse arrows. The mouse now controls the first-order or frequency-dependent phase parameter `lp`.

4 Click the left or right button above or below the horizontal cursor to increase or decrease `lp` so that the phase at the center of the previous region bracketed by the vertical cursors is held constant.

This process eliminates or substantially reduces the necessity to iteratively adjust the two parameters `rp` and `lp`. As with the zero-order correction, the left button acts as a “coarse” adjust, and the right button as a “fine.”

Define a new update region by clicking the mouse outside the two vertical cursors.

Subsequent first-order phase changes cause the zero-order phase to be adjusted so that the phase angle at the center of the previous region bracketed by the vertical cursors remains constant. Click the **Phase** button again if to return to the zero-order phase correction.

Adjust the vertical scale and apply the latest phase correction by clicking the middle mouse button at the top of a peak that is on scale. This leaves the vertical scale unaffected but recalculates the phase of the entire spectrum. Clicking the center button above or below the peak raises or lowers the vertical scale.

5 Exit the interactive phasing mode by clicking another graphics control button.

Line Tools

Find nearest line and line resolution

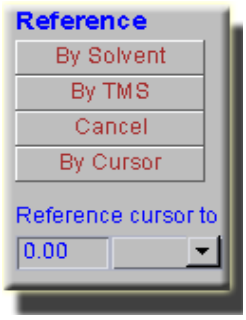
1. Place a cursor near the line of interest.
2. Select the **Process** page and click the **Find nearest line** button. The cursor moves to the nearest line and displays its height and frequency (in Hz and ppm) in the message window.
3. Click **Display** linewidth to display the resolution of a line, as well as the limiting digital resolution of the spectrum. The resolution is determined by a width at half-height algorithm and not by least-squares.

Display line list

1. Click the **Threshold** graphics control button and use the middle mouse button to vertically position the yellow threshold line.
2. Select the **Line List** page and click the **Display Line List** button. This process displays line frequencies and intensities that are above a threshold.

Spectral Referencing

Frequency referencing is set on the **Display** page.



Button	Description
By Solvent	Reference the spectrum for selected solvent.
By TMS	Reference the spectrum to a TMS line. In the case of other signals (for example, from silicon grease) immediately to the left of the TMS line (even if they are higher than the reference line), `tmsref` tries avoiding those signals by taking the line furthest to the right in that area, as long as it is at least 10% of the main Si-CH3 signal. Large signals within 0.6 ppm for 1H (or 6 ppm for 13C) to the right of TMS might lead to mis-referencing.
Cancel	Clears the reference line by removing any spectral referencing present, and turns off referencing.
By Cursor	References the spectrum based on the current cursor position. To reference the spectrum based on a line position in the spectrum, first use the **Find nearest line** button on the **Process** page, then click **By Cursor**.

Table 11 Parameters used in spectral referencing

Reference line (frl)	The distance, in Hz, of the reference line from the right edge of the spectral window. This line is the spectral position used to set the referencing. It can be the signal of a frequency standard (such as TMS), or any line (such as a solvent signal) with a known chemical shift (in ppm), or a position in the spectrum where such a line is expected to appear.

Table 11 Parameters used in spectral referencing (continued)

Reference position (rfp)	The difference between the reference line and the reference frequency (zero position of the scale) in Hz. Referencing a spectrum using the signal of a frequency standard, such as TMS, use reference position is 0. The distance of the reference frequency from the right edge of the spectrum is *reference line reference position*.
Spectrometer frequency	The absolute frequency, in MHz, of the center of the spectrum (the transmitter position). Use the `spcfrq` command in order to see the accurate value of the spectrometer frequency (`sfrq` parameter).
Reference frequency	The frequency, in MHz, of the frequency standard, that is, the zero position of the frequency scale, and the divider (unit) for the calculation of ppm scales (`reffreq`).

The **By Solvent** and **By TMS** buttons assume that the system is locked (and that the lock solvent is defined in `/vnmr/solvents`). Ensure that the field offset has been adjusted so that the lock frequency is on resonance with a sample of similar susceptibility if the experiment is to run unlocked and these buttons are used to set the field offset. Adjust the field offset is adjusted using the following procedure:

1 Insert a sample with deuterated solvent.

2 Adjust `z0` (or `lkof`) in acqi so that the lock frequency is on resonance.

3 Switch off the lock.

4 Insert the non-deuterated sample.

The accuracy of the solvent and **TMS** referencing buttons is mostly limited by the accuracy of the chemical shift of the lock resonance line, which may depend on the concentration and the chemical properties (acidity/basicity) of the components in the sample. But they should normally be accurate enough to find an actual reference line close to its predicted position.

Estimate the position of the reference frequency in spectra from unlocked samples, provided the spectrometer is first locked on a sample with similar susceptibility, then the lock is disengaged and the field offset adjusted such that the lock signal is on-resonance. Now, acquire a spectra without lock and calculate their (estimated) referencing using `setref`, provided the solvent parameter is set to the solvent that was

last locked on.

Display an Inset Spectrum Using Viewport Tab

Viewport tab

Click the **Viewport** tab to display the viewport controls. If the tab is not visible, click **View** on the main menu and select **Viewport**.

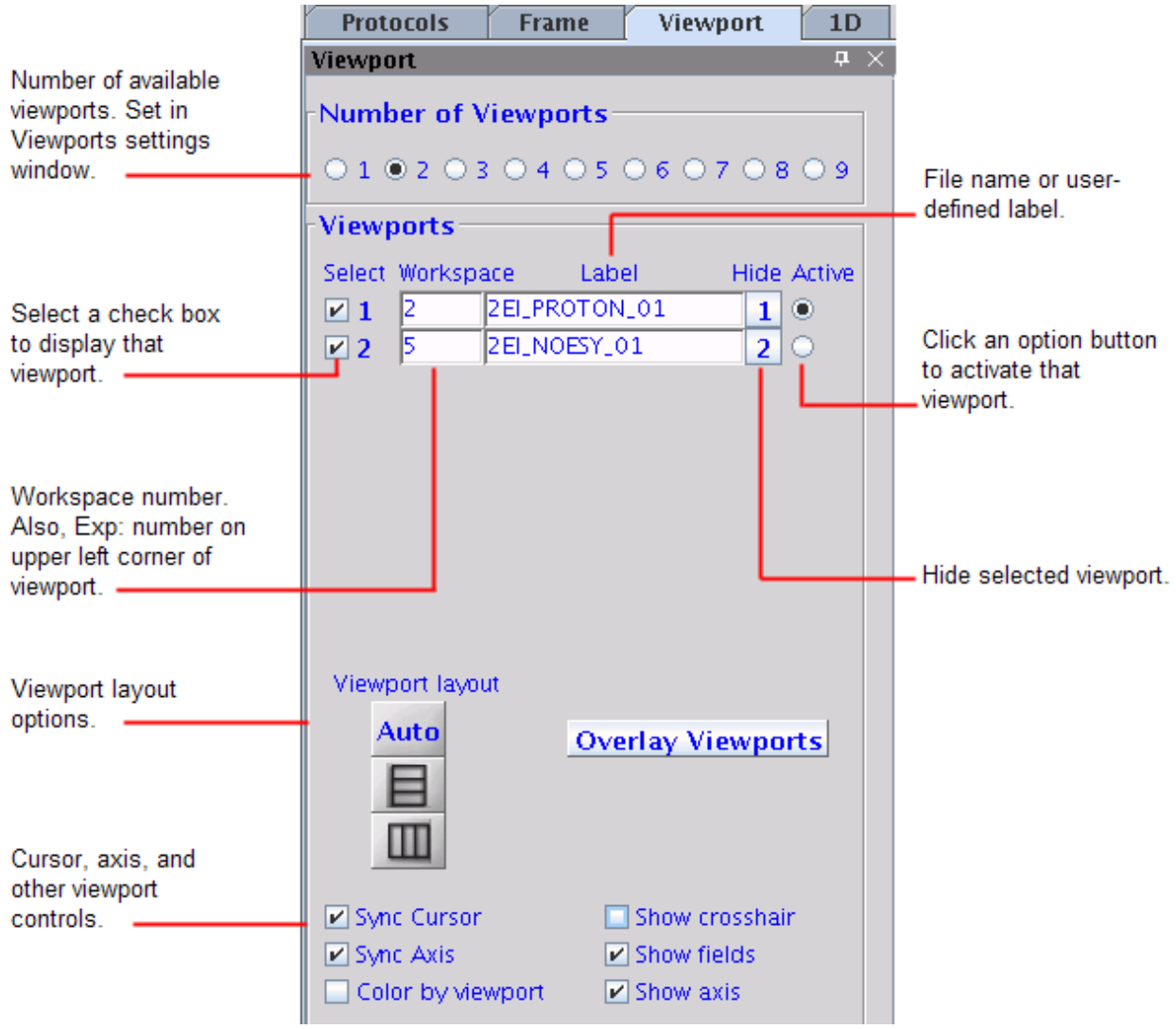


Figure 27 Viewport tab and controls

Frame Tab

The **Frame** tab, see Figure 28, of the viewport tab has the following tools, button, and check boxes:

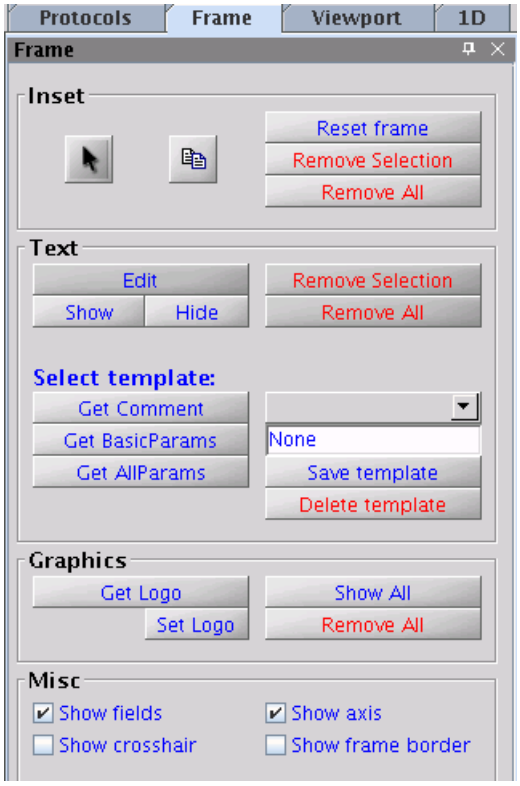


Figure 28 Frame tab and controls

Table 12 Viewport tools

Icon	Function
	Default mode — left mouse click moves the left cursor and right mouse click moves right mouse cursor.
	Inset mode — left mouse drag a box over a spectrum region creates an inset frame of the region. A viewport can have multiple inset frames. Exit inset mode — release mouse button.

Inset frame buttons

The buttons delete one or all inset frames and restore the default frame to full size.

Button	Function
Delete Inset	Delete the selected inset.
Delete all	Delete all inset frames.
Full size	Restore the default frame to its full size.

Display check boxes

The check boxes control optional display features.

Check box	Function
Cross hair	Display cross hair and chemical shift(s) of the cursor position when the mouse is moved over the spectrum. A useful function when the fields are not shown, not in cursor mode (default mode), or when chemical shift of a peak without moving the left cursor is required while in the cursor mode.
Fields	Display `cr, delta, vp` etc... fields at the bottom of the viewport.
Axis	Show scale of the axis.
Show frame border	Check the box to display a box around the frame. Un-check the box to display the four corners of the selected frame as *hot spots* for resizing. No border or corner will be displayed if a frame is not selected. An empty frame is not visible until it is selected.

Working with viewports and inset frames

All VnmrJ 3 graphics are displayed in frame(s). The viewport has a default frame that occupies the entire viewport graphics area. An inset frame initially shares the same workspace and data as the original frame and is manipulated in the same way as the default frame.

Creating an inset frame

An inset frame has the full capability of the default frame. The only difference is that the default always exists, while an inset frame can be created and removed. Create an inset frame within the default viewport frame as follows:

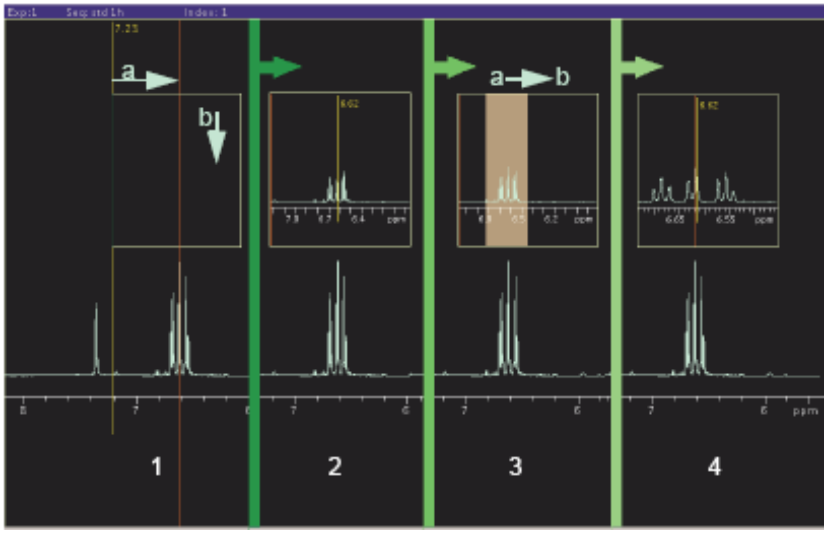


Figure 29 Creating an inset frame

1 Select the inset mode tool  .

2 Place the cursor at the low field (left) side of the region to be expanded as shown in Figure 29 frame 1a.

3 Hold the left mouse button down and drag the inset window to the high field (right) side of the region.

4 Drag the cursor down to set the height of the inset frame as shown in Figure 29 frame 1b.

5 Release the mouse button to create the inset frame, see Figure 29 frame 2.

Zooming in on a region within an inset frame

1. Select the default mode tool  .
2. Click inside the frame to make the frame active.
3. The frame has a yellow border when it is active and white border when it is inactive (these are the default colors of inactive and active frames).
4. Select the zoom mode tool  .
5. Place the cursor at the low field (left) side of the region to be expanded as shown in Figure 29 frame 3a.
6. Hold the left mouse button down and drag the inset window to the high field (right) side of the region, Figure 29 frame 3b.
7. The region selected is indicated by a transparent gray rectangle.
8. Release the mouse button and the selected region expands to fill the inset box, Figure 29, frame 4.

Resizing an inset frame

1. Select the default mode tool  .
2. Click inside the frame to make the frame active. An active frame has a yellow border.
3. Move the mouse cursor to a corner of the inset frame. The cursor changes from a single-headed arrow to a double-headed arrow.
4. Hold down the left mouse button and grab the corner of the frame.
5. Drag the corner to resize the frame.
6. Release the mouse button when the frame is at the desired size.

Moving an inset frame

1 Select the default mode tool  .

2 Click inside the frame to make the frame active. An active frame has a yellow border.

3 Move the mouse cursor to an edge of the inset frame. The cursor changes from a single-headed arrow to a four-headed arrow.

4 Hold down the left mouse button and grab the edge of the frame.

5 Drag the frame to the new position.

6 Release the mouse button when the frame is at the desired position.

Stacked 1D Display

Stacked display using the main menu display

1 Click **Display** on the main menu.

2 Select a display mode from the drop-down menu:

- Display Multiple Spectra Horizontally
- Display Multiple Spectra w/ Labels
- Display Multiple Spectra Vertically
- Increase vertical Separation by 20%
- Decrease vertical Separation by 20%
- Create an Inset of the current Display

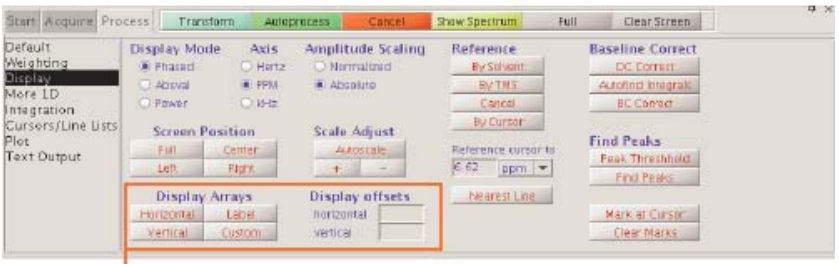
– Save Current Display Parameters

– Plot Current Display before Making Inset

– Make Inset

– Plot Inset and Return Original Display

Stacked display using the display page



1 Click the **Process** tab.

2 Select the **Display** page.

3 Click a **Display Arrays** button:

- **Horizontal** – Display arrayed spectra horizontally and divide available display width into equal portions.
- **Vertical** –Display arrayed spectra stacked vertically with each spectrum displayed using the full width of the screen.
- **Label** – Add a label to the spectra.
- **Custom** – Use a custom Label.

4 Enter values for the Display offsets

- **Horizontal** – Enter a value in mm for the separation between spectra.
- **Vertical** – Enter a value in mm for the separation between spectra.

Stacked spectra display using the graphics tools

Icon	Function
	Display the first arrayed spectrum and display 1D graphics toolbar with the following icons at the top (or left side if the bar is horizontal).
	Display the next spectrum.
	Display the previous spectrum.
	Display arrayed spectra stacked vertically with each spectrum displayed using the full width of the screen.
	Display arrayed spectra horizontally and divide available display width into equal portions.
	Hide or show axis under the spectra.
	Label the spectra.
	Return to previous graphics display tool.

Stacked FID Display Using the Graphics Tools

Icon	Function
	Display the first arrayed FID and display 1D FID graphics tool bar with the following icons at the top (or left side if the bar is horizontal).
	Display the next FID.
	Display the previous FID.
	Display arrayed FIDs stacked vertically with each spectrum displayed using the full width of the screen.
	Display arrayed FIDs horizontally and divide available display width into equal portions.
	Label the FIDs.
	Return to previous graphics display tool.

Aligning and Stacking Spectra

Requirements for aligning and stacking spectra

Spectra can be a mixture of 1D and 2D data sets, all 2D data sets, or all 1 D data sets provided these requirements are met:

- All selected viewports need to use a common scale.
- Data in the viewports may have different nuclei, different spectrum width, or different spectral regions. The common scale is determined based on data in all selected viewports and determines whether alignment or stacking is possible. Overlaid and stacked spectra are drawn based on the common scales.
- Alignment is enabled if more than one axis in more than one viewport has the same axis (H1, C13 etc.).
- Stacking is enabled when data in all viewports have the same axis/axes.

Setting up stacked aligned spectra

1. Select the **Viewport** tab from the vertical tabs panel.
2. Load each data set into a different viewport and process the data. Data must meet the requirements mentioned in “Requirements for aligning and stacking spectra” .
3. Select viewports containing spectra to overlay by placing a check in the check box under **select**.
4. Click the **Overlay Viewports** button to overlay all selected viewports.

The **Stack Spectrum** button, Figure 30, is displayed below the **Overlay Viewports** button if all spectra have the same dimension (all 1D or all 2D) and all axis/axes (nuclei) match. Stacked spectra are aligned and each spectrum is shifted along x and y. The shift between spectra is specified by x and y offset in the entry fields below the **Stack Spectrum** button. Spectral axes are also synchronized to enable zoom and pan of the spectrum without losing the alignment.

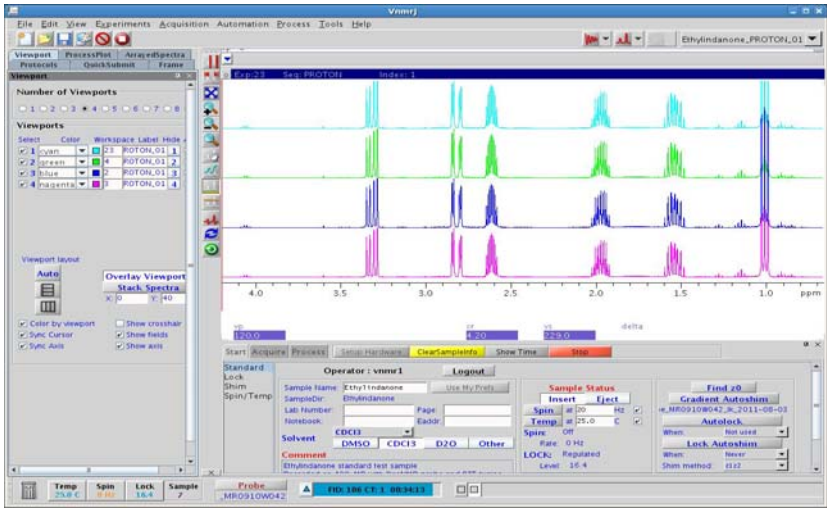


Figure 30 1D stacked spectra

The **Align Spectra** button, Figure 31, is available if it is a mix of 1D and 2D spectra when multiple spectra are overlaid. All 2D spectra must have matching axes. All 1D data must match one of the 2D axes. 1D spectra are aligned and displayed at the margins of the 2D spectrum. 1D spectrum will be rotated if necessary to align with the 2D spectrum. Zoom and pan are synchronized when the spectra are aligned.

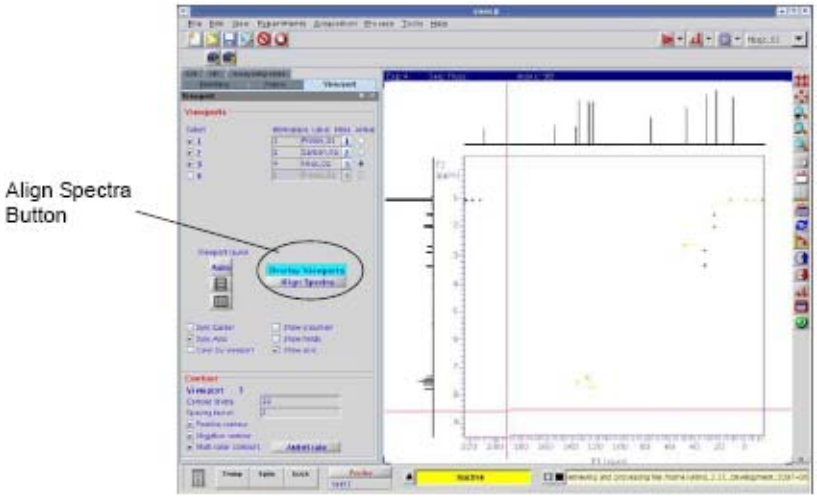


Figure 31 2D spectra with overlaid 1D's

The **Stacked Spectrum** button for 2Ds, Figure 32, is displayed below Overlay Viewport if all 2D spectra axes and nuclei match. Spectral axes are synchronized to enable zoom and pan of the spectra without losing alignment.

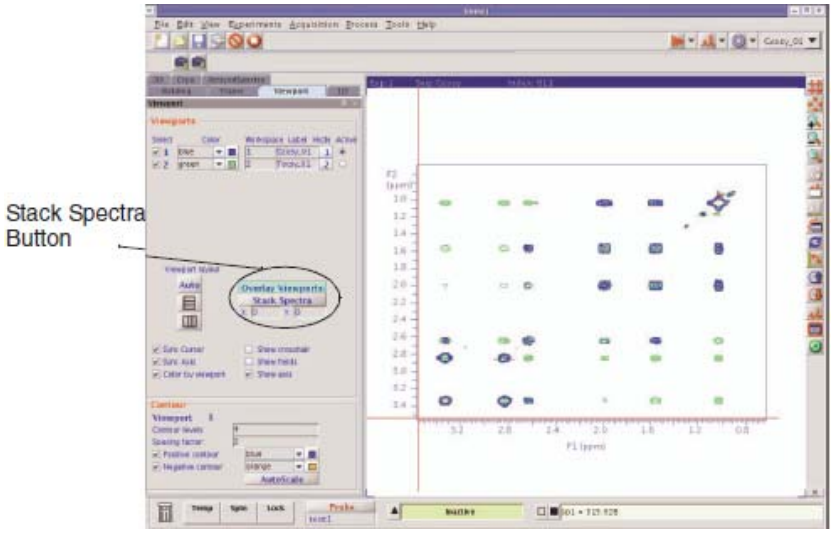
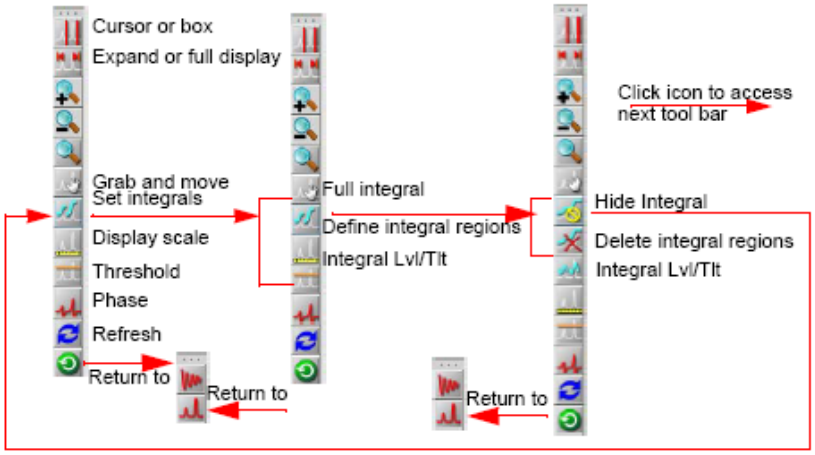
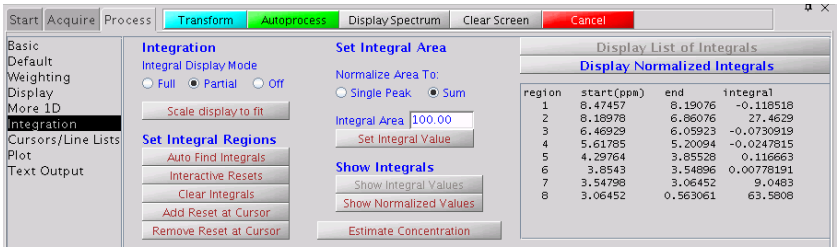


Figure 32 Stacked overlaid 2D spectra

Integration

This section describes methods and tools for displaying and plotting integrals.





Interactive zero- and first-order baseline correction mode

The **Integral Lvl/Tlt** button activates interactive zero and first order baseline correction mode. The zero order correction is represented by the `lvl` parameter; the first order correction is represented by the `tlt` parameter. If no integral is displayed when the **Integral Lvl/Tlt** button is activated, the integral is automatically displayed.

1 Left-click an integral region of interest, about halfway vertically up the screen.

   A horizontal cursor intersects at the mouse arrow. Two vertical cursors are placed on either side of the mouse arrow.

2 Right or left-click above or below the horizontal cursor, but within the two vertical cursors, to adjust the zero-order baseline correction parameter `lvl`.

- Clicking above the horizontal cursor increases `lvl`.
- Clicking below the horizontal cursor decreases `lvl`.
- Clicking on the horizontal cursor restores the initial baseline correction value.

3 Left-click another region of the spectrum, outside the vertical cursors.

A new horizontal cursor is displayed at the mouse arrow, two new vertical cursors are displayed on either side of the mouse arrow, and a single vertical cursor is displayed in the middle of the region where `lvl` was being updated. The mouse now controls the first-order baseline correction parameter `tlt`.

4 Right or left-click above or below the horizontal cursor to increase or decrease `tlt`, and change `lvl` so that the total drift correction at the single vertical cursor in the middle of the previous region is held constant.

This process eliminates or substantially reduces the necessity to iteratively adjust the two parameters `lvl` and `tlt`. As with the zero-order correction, placing the mouse arrow right on the horizontal cursor and clicking the mouse button will restore the initial baseline correction values.

Each time the mouse is clicked outside the two vertical cursors, new vertical and horizontal cursors are displayed.

The left and right mouse buttons both adjust the baseline correction parameters and differ only in their sensitivity. The left button causes changes a factor of eight times larger than the right button, making the left button a “coarse” adjust and the right button a “fine” adjust. The overall sensitivity of these adjustments can also be controlled by the parameter lvltlt. This parameter is a multiplier, with a default value of 1.0, for the size of the changes. To make larger changes, make `lvltlt` larger than 1.0. To have finer control, set `lvltlt` to be between 0.0 and 1.0.

The middle mouse button adjusts the integral scale (parameter `is`) or the integral offset (parameter `io`), exactly as whenever an integral is displayed.

5 Exit the interactive baseline correction mode by clicking on another graphics control button.

Displaying integrals step-by-step

The following methods provide an opportunity to compare procedures. Before starting each procedure, be sure to obtain a typical spectrum.

1. Load a data file into the active viewport using the file browser or the Locator.
2. Transform the data if necessary.
3. Click the **Process** tab.
4. Select the **Integration** page.
5. Click an **Integration Display Mode** radio button: **Full**, **Partial**, or **Off**.
   - **Full** shows integrals over the entire spectrum, including the noise.
   - **Partial** shows even integrals regions and hides all the odd integral regions.
   - **Off** turns off the integral display.
6. Click **Auto Find Integrals** to automatically set the integral resets and display the data as set by the **Integration Display Mode** radio button.
7. Click the **Scale display to fit** button to automatically scale the display.
8. Set the integral area.
9. Enter a value in the Integral Area field.

10 Click one of the following radio buttons under the **Normalize Area to: page** region.

- **Single Peak** — selects the region or peak under the cursor as the reference and sets the single peak integral to the value in the Integral Area field when the **Set Integral Value** button is clicked.
- **Sum** — sets the entire integral to the value in the Integral Area field. Do not click the **Set Integral Value** button. This button sets the single peak reference.

11 Display the integral results as follows:

- **Single Peak** — both the **Show Integral Values** and **Show Normalized Value** buttons are active.
- **Integral Values**
  Click **Show Integral Values** to display the values of the integral regions on the screen below the spectrum.
  Click **Display Lists of Integrals** to list the display regions and the value of the integral over each region.
- **Normalized Integral Values**
  Click **Show Normalized Values** to display the values of the integral regions normalized to the reference region on the screen below the spectrum.
  Click **Display Normalized Integrals** to list the display regions and the value of the integral over each region normalized to the reference region.

Manual method

1 Load a data file into the active viewport using the file browser or the Locator.

2 Transform the data if necessary.

3 Click the **Process** tab.

4 Select the **Integration** page.

5 Click **Clear Integrals**.

Any currently defined integral reset points are cleared.

6 Set up the integral resets from left to right (down field to up field).

a Click the **Interactive Resets** button.

b Place the cursor to the left of the first integral region.

c Click the left mouse button.

d Move the cursor to the right of the first integral region.

e Click the left mouse button.

f Repeat Step b through Step e until all the required integral regions are defined.

7 Click **Scale display to fit** button to automatically scale the display.

8 Set the integral area:

a Enter a value in the Integral Area field.

b Click one of the following radio buttons under the N**ormalize Area to:** page region.

- **Single Peak** — selects the region or peak under the cursor as the reference and sets the single peak integral to the value in the Integral Area field when the **Set Integral Value** button is clicked.
- **Sum** — sets the entire integral to the value in the Integral Area field.
  Do not click the **Set Integral Value** button. This button sets the single peak reference.

9 Display the integral results as follows:

- **Single Peak** — both the **Show Integral Values** and **Show Normalized Value** buttons are active.
- **Integral Values**

  Click **Show Integral Values** to display the values of the integral regions on the screen below the spectrum.

  Click **Display Lists of Integrals** to list the display regions and the value of the integral over each region.

- **Normalized Integral Values**

  Click **Show Normalized Values** to display the values of the integral regions normalized to the reference region on the screen below the spectrum.

Click **Display Normalized Integrals** to list the display regions and the value of the integral over each region normalized to the reference region.

Command line equivalents for vnmrj 3 interface driven integration

Use the parameter page editor to view the commands on the current parameter page.

1. Click **Edit** on the main menu.
2. Select **Parameter Pages**.
3. Place the mouse cursor on a button or entry field.
4. Double-click (left mouse button).
5. Read the associated command next to the field Vnmr Command.

Baseline correction

Most operations performed on spectra assume a quality baseline. Line lists, integrations, resolution measurements, 2D volume integrations, etc., all measure intensities from "zero" and do not perform any baseline adjustments. If the baseline in your spectrum is not flat perform a baseline correction operation before performing further data reduction. Two types of baseline correction are provided, linear and non-linear, and are available using the buttons on the **Display** page.

Baseline correction commands

Using the beginning and end of the displayed spectrum to define a straight line to be used for baseline correction, the `dc` command turns on a linear baseline correction. `dc` calculates a zero-order baseline correction parameter `lvl` and a first-order baseline correction parameter `tlt`. The `cdc` command turns off this correction. The results of the `dc` or `cdc` command are stored in the `dcg` parameter, which can be queried (`dcg?`) to determine whether drift correction is active. If active, `dcg=''`; if inactive, `dcg='cdc'`.

The `bc` command performs a 1D or 2D baseline correction. The 1D baseline correction uses spline or second to twentieth order polynomial fitting of predefined baseline regions. `bc` defines every other integral, that is, those integrals that disappear in partial integral mode (`intmod='partial'`) as baseline and attempts to correct these points to zero. A variety of parameters can be used to control the effect of the `bc` command.

For more information about the `bc` command, see the entry for `bc` in the *Command and Parameter Reference*.

Integral reset points commands

The `z` command (or the equivalent button or icon) resets the integral to zero at the point marked by the displayed cursor. `z(reset1,reset2,...)` allows the input of the reset points as part of a command, instead of using the position of the cursor. Reset points do not have to be entered in order. The resets are stored as frequencies and will not change if the parameter `fn` is changed. The command `cz` (or the equivalent button) removes all such integral resets. `cz(reset1,reset2,...)` clears specific integral resets.

The `liamp` parameter stores the integral amplitudes at the integral resets points, and the `lifrq` parameter stores the frequencies of integral reset points, for a list of integrals. To display the values of `liamp`, enter `display('liamp')` with a **Text Output** page selected. Frequencies are stored in Hz and are not adjusted by the reference parameters `rfl` and `rfp`.

Integral regions commands

The region command divides a spectrum into regions containing peaks. A variety of parameters can be used to control the effect of the region command. For more information, see the *Command and Parameter Reference*.

Integral display and plotting commands

Display and plotting of the integral trace is independent of the values of the integrals. The height of the trace is controlled by the parameter `is` and can be interactively adjusted with the `ds` command. The macro `isadj(height)` (or the equivalent button) adjusts the integral height so that largest integral fits the paper or is height mm tall if an argument is provided, for example, `isadj(100)`.

The command dli (or the equivalent button) displays a list of integral values at the integral reset points. The frequency units of the reset points are defined by the parameter axis. The reset points are stored as Hz and are not referenced to rfl and rfp. The amplitudes are stored as actual values, they are not scaled. The integral values are scaled by the parameters ins and insref and the Fourier number. Typically, ins is set to the number of nuclei in a given region. For example, if a region represented a single methyl group, the following procedure would scale the integral values of that region:

1. Set ins=3.
2. Set insref to the Fourier-number-scaled-values of that integral.
3. Enter dli. The integral value of that region is displayed as 3 and all other integral values are accordingly scaled.

Integral value scaling can be interactively set with the ds command. The setint macro can also be used to adjust integral value scaling. The setint macro sets the value of an integral and scales integral values in conjunction with the command dli. Normalized integral values can also be selected. In this case, ins represents the total number of nuclei. The individual integral values will be scaled so that their sum is equal to ins. The normalized mode may be selected by setting insref to "not used." The integral is scaled by ins and insref.

Two commands are closely related to dli:

- nli is equivalent to dli except that no screen display is produced.
- dlni normalizes the values from dli using the integral normalization scale parameter ins and then displays the list.

The dpir command displays numerical integral values below the appropriate spectral regions, using the integral blanking mode in which only every other integral is plotted. The command dpirn shows the normalized integral values in an analogous fashion.

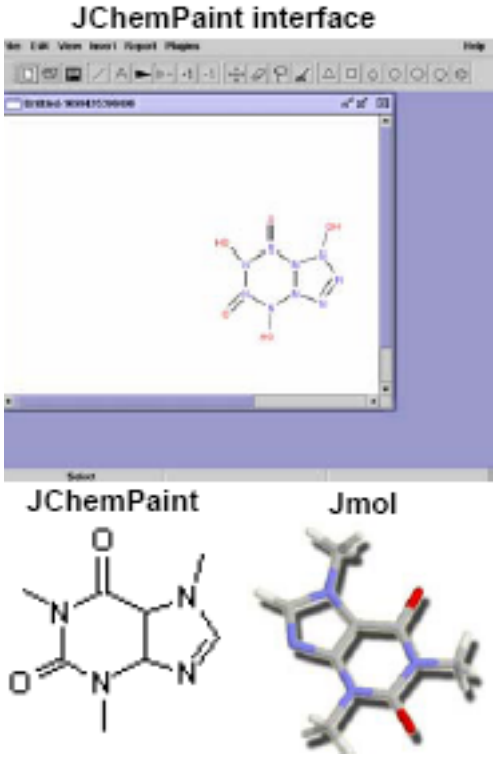
The pir command plots digital integral values below the spectrum, using the integral blanking mode in which only every other integral is plotted. The command pirn plots the normalized integral values in an analogous fashion.

Molecular Display and Editing (JChemPaint and Jmol)

Tools for editing, viewing, and printing molecular structures are installed as options with VnmrJ 3. These tools are derived from *JChemPaint* and *Jmol*.

JChemPaint and Jmol are open source software packages available from http://sourceforge.net/.

JChemPaint is a graphical editor for 2D molecular structures. Jmol is a visualization and analysis tool for 3D structures.



Running JChemPaint

1. Click **Tools**.
2. Select **Molecular Structures**.
3. Select **JChemPaint** menu.

See http://jchempaint.sourceforge.net for documentation.

File Formats

JChemPaint can edit, save, and export the file formats listed here.

Format	Action
MDL MOL	edit, save
SMILES	edit, save
IUPAC Chemical Identifier	edit
MDL SDF Molfile	edit
Chemical Markup Language	edit
Scalable Vector Graphics	save
CDK source code fragment	save
BMP	save
JPEG	save
PNG	save
TIFF	save
Gaussian Input	export

1. Save files as MDL MOL (*.mol) in one of the mollib directories: `/vnmr/mollib` or `~username/vnmrsys/mollib`.
2. Import an existing `mol` file into VnmrJ 3 by copying it into the `mollib` directory.
3. Click **Tools** on the main menu.
4. Select **Open**, browse to the file, and drag it to the VnmrJ 3 graphics screen.

Molecular structures

Molecular structures are displayed and manipulated in the VnmrJ 3 graphics window. View as many graphics as wanted. The graphics are displayed in the current experiment, and they are saved per experiment.

Use the following steps to display a molecular structure in the VnmrJ 3 graphics window:

1 Click **Tools** on the main menu.

2 Select **Browser**, browse to the `mollib` directory:

```
/vnmr/mollib or ~username/vnmrsys/mollib
```

3 Select the appropriate files and drag them to the VnmrJ 3 graphics window:

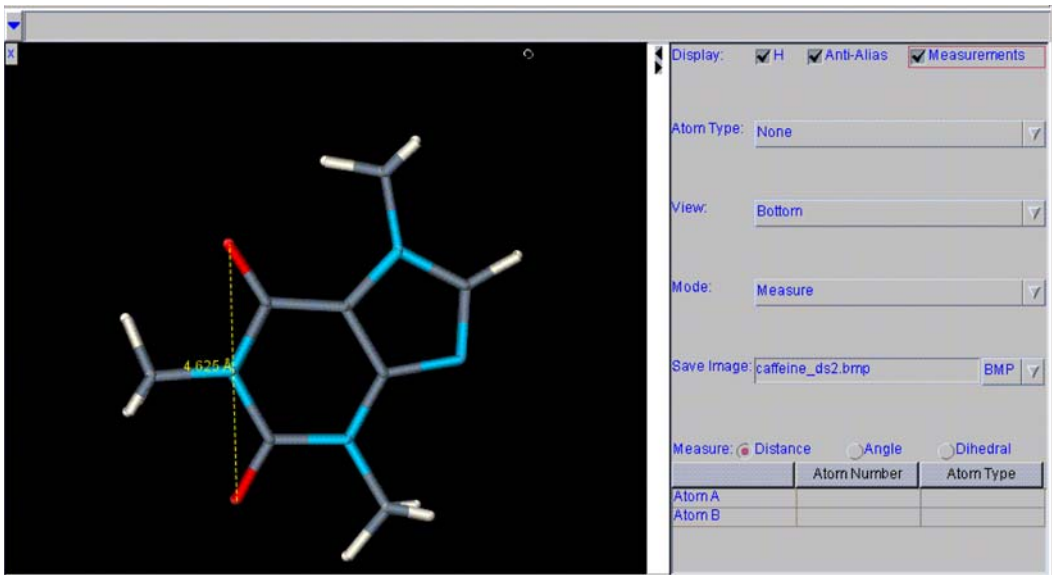
- Molecule file -- select a file from the `mollib` directory that ends in the `mol` extension.
- Graphic file -- open the icons directory and select a **TIFF**, **GIF**, **JPEG**, or **PNG** file.

After a molecular structure is displayed, use the mouse to move, resize, delete, or view the corresponding 3D version with Jmol.

To:	Do:
Select	Double-click the molecule.
Move	Select the molecule and drag with the left mouse button.
Resize	Select the molecule and drag with the middle mouse button.
Delete	Select the molecule and drag to the trash can.
View a molecule with Jmol	Select the molecule and click the right mouse button. This only works with MOL files. See Jmol Interface in *VnmrJ 3 Jmol Interface in VnmrJ 3*.

Jmol interface in VnmrJ 3

VnmrJ 3 provides some Jmol tools to view a molecule.



Menu	Description
Display	H– Displays hydrogen atoms. Anti-Alias – Turns on anti-aliasing and smooths the graphics display. Measurements – Displays measurements.
Atom Type	Displays the atoms with atomic symbols, atom types, atom numbers, or nothing.
View	Views the molecule from front, tom, bottom, right, or left.
Mode	Rotate – rotates the image. Zoom – zooms in/out. Translate – moves the image. Select – selects the atoms. Measure– measures distance, angle, or dihedral. See "Measuring a molecule" on page 196.
Save Image	Saves the molecule image as BMP, JPEG, PPM, PNG, or PDF. The image is saved in the directory `~username/vnmrsys/mollib/icons` with the name entered in the field. See "Saving a molecule image" on page 196.

Measuring a molecule

1 Select the measure mode: distance, angle, dihedral.

2 Click the appropriate atoms to create the measurement:

- distance – click two atoms.
- angle – click three atoms
- dihedral – click four atoms

3 Display the measurement by selecting the **Measurement** display option.

Saving a molecule image

1 Select the file format for the image: **BMP**, **JPG**, **PPM**, **PNG**, or **PDF**.

2 Enter a name for the image and add a file extension that corresponds to the file format chosen in step 1.

3 Press **Enter**.

The file is saved in the directory `~username/vnmrsys/mollib/icons/`.

Jmol display options

- Change the foreground color of the molecule window: enter the following command on the VnmrJ 3 command line:

  ```
  vnmrjcmd('mol','foreground','color')
  ```

  where `color` is a color name or a hex value. The foreground color by default is set to the most visible color according to the background color.
- Change the font of the labels on 3D molecule graphics: use the **Edit > Display Options** window and change the font of Plain Text.
- Click  to exit Jmol.

Full-Featured Jmol

Select **Tools > Jmol** to view a molecule with the full-featured Jmol software package,

See http://jmol.sourceforge.net/ for Jmol documentation.

Licenses for JChemPaint and Jmol

The licenses for JChemPaint and Jmol are included on the

VnmrJ 3 CD in the licenses directory.

8 Printing, Plotting, and Data Output

This chapter describes how users can print and plot data.

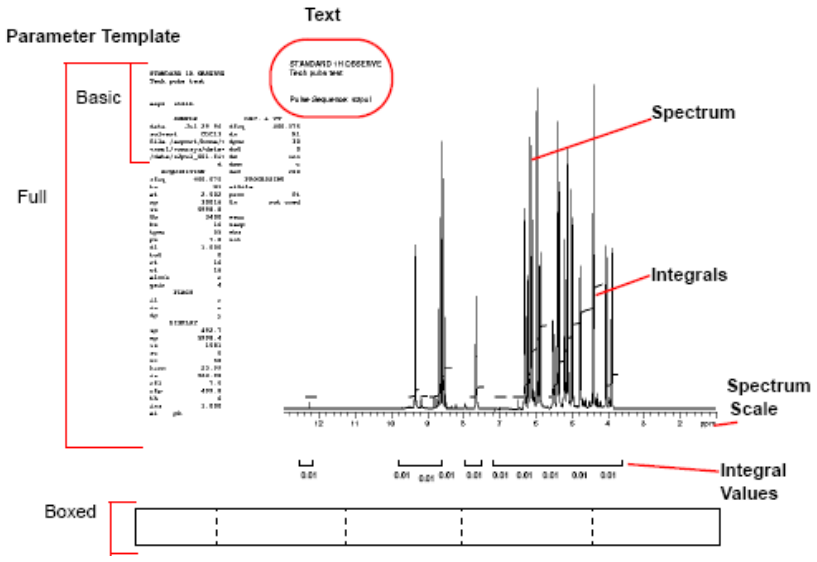


Figure 33 A general printout with several objects identified

Printing of the Graphics

After processing, the 1D or 2D spectrum is displayed in the graphics canvas so that the scale, expansion, and threshold can be adjusted.

To print the spectrum:

1 Click **File** from the menu.

2 Select **Print Screen**.

The pop-up in Figure 34 appears.

3 Select the **name** of the printer to print to it.

4 Select the print area, either **Viewports** or **VnmrJ 3 Window**. Viewport will capture the contents of the Viewport, while VnmrJ 3 Window will capture the entire VnmrJ 3 window.

5 Choose the **number of copies** to print.

6 Click the **Print** or the **Preview** button.

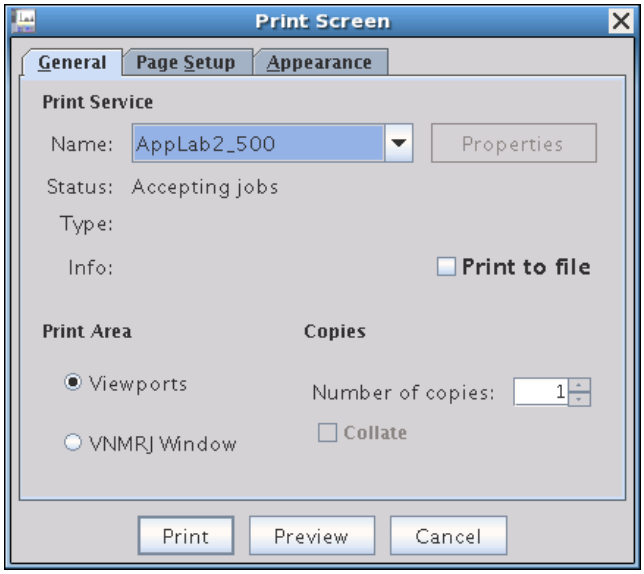


Figure 34 General tab of the Print Graphics pop-up

Printing a file

Select the **Print to file** check box. Figure 35 shows the pop-up that appears when the **Print to file** check box is selected and the **Print** button is clicked.

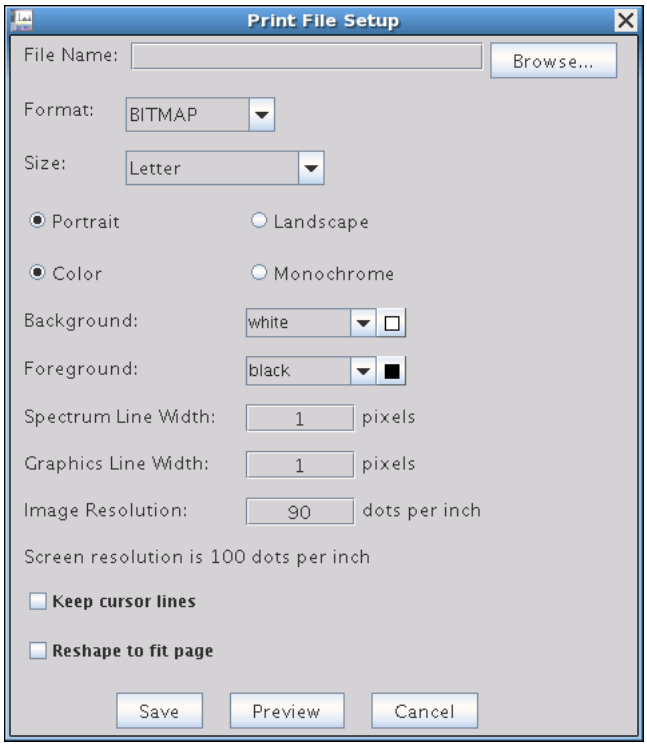


Figure 35 The **Print to File** pop-up

- **File Name**: name of the file to be saved.
- **Browse...**: allows one to browse to a folder to set the location where the file will be saved.
- **Format**: drop-down menu that offers a choice of various outputs.
- **Size**: drop-down menu that offers choice for paper size.
- **Orientation selection**: radio-button to set Portrait or Landscape.
- **Graphics color**: radio-button to select Color or Monochrome output.
- **Background** and **Foreground** color selection: Pull-down menus for various color choices.
- **Spectrum Line Width**: spectrum line width in pixels.
- **Graphics Line Width**: graphics line width in pixels.
- **Image Resolution**: image resolution in dots per inch.

- **Screen resolution**: the current screen resolution in dots per inch.
- **Keep cursor lines**: check box to include cursor lines as they appear in the graphics area.
- **Reshape graphics to fit paper**: check box to resize graphics to fit paper size.
- **Save**: saves output to File Name.
- **Preview**: starts Adobe Acrobat Reader and displays (without saving) the output.
- **Cancel**: closes Print to File pop-up (without saving).

The **Page Setup** and **Appearance** tabs (Figure 36 and Figure 37) allow for settings similar to the **Print File Setup** to be applied to the printed output. Additionally, entries are available for paper source, margins, and print quality (Draft, Normal, and High) while finer control of image resolution and preview is unavailable.

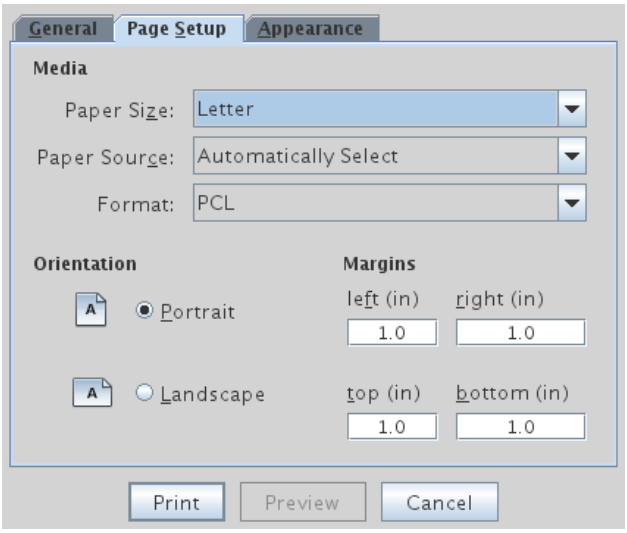


Figure 36 The Page Setup tab of the Print Graphics pop-up

- **Paper Source**: drop-down menu choices for tray a printer will use.
- **Margins**: margins on the sides of the page in inches (in).

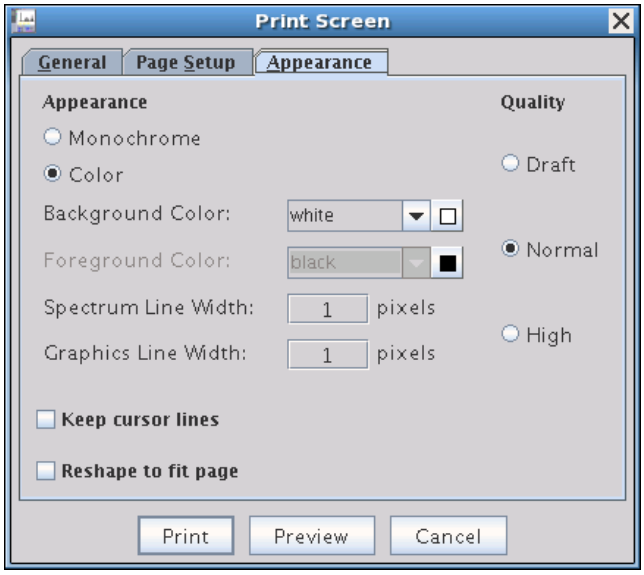


Figure 37 The Appearance Setup tab of the Print Graphics pop-up

- **Quality**: a choice of Draft, Normal, and High.

Plotting

Plotting is based around the concept of a plot file. Setting up and submitting a plot can be done from the vertical and horizontal panels and from the command line. The **Plot** parameter page is accessed from the **Process** tab after the spectrum or FID is displayed. Items selected on the **Plot** parameter page (Figure 38 and Figure 39) are added to a temporary plot file, and the **Plot Page** button submits the plot file to the plotter.

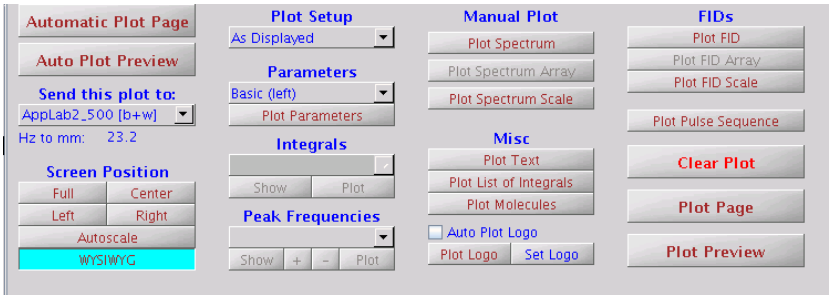


Figure 38 The Plot parameter page for a 1D data set

To plot:	Select:	Click:
Pulse sequence		**Plot Pulse Sequence**
FID		**Plot FID, Plot Page**
FID and scale		**Plot FID, Plot FID Scale, Plot Page**
Spectrum		**Plot Spectrum, Plot Page**
Spectrum and scale		**Plot Spectrum, Plot Spectrum Scale, Plot Page**
Spectrum, scale, and text		**Plot Text, Plot Spectrum, Plot Spectrum Scale, Plot Page**
Spectrum, scale, and parameters	**Parameter Template option**	**Plot Spectrum, Plot Spectrum Scale, Plot Page**
Spectrum, scale, and peak frequencies	**Peak Frequencies option**	**Plot Spectrum, Plot Spectrum Scale, Plot Page**
Spectrum, scale, and integrals		**Plot Spectrum, Plot Spectrum Scale, Integrals Plot, Plot Page**

To plot:	Select:	Click:
Spectrum, scale, and integrals, integral values	**Integrals option**	**Plot Spectrum, Plot Spectrum Scale, Integrals Plot, Plot Page**
Parameters only	**Parameter Template option**	**Plot Page**
Text only		**Plot Text, Plot Page**
Peak frequencies only	**Peak Frequencies option**	**Plot Page**
Integrals only	**Integrals option**	**Integrals Plot, Plot Page**
Scaled integral values only	**Integrals option**	**Integrals Plot, Plot Page**
Normalized integral values only	**Integrals option**	**Integrals Plot, Plot Page**
Molecules only		**Plot Molecules, Plot Page**
Logo only		**Plot Logo, Plot Page**
Using default settings to the printer		**Automatic Plot Page**
Using default settings to Adobe Reader for preview		**Auto Plot Preview**

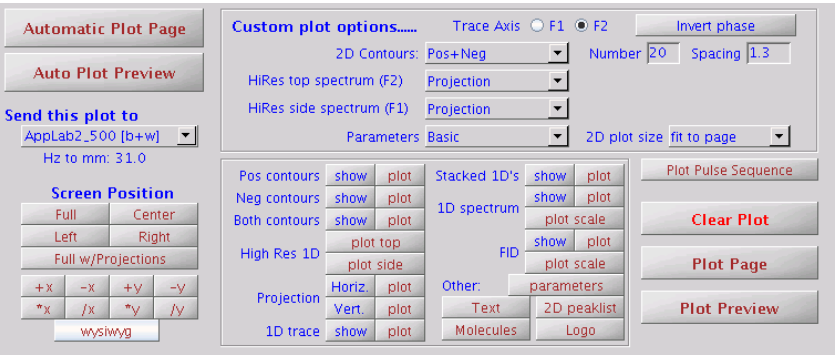


Figure 39 The Plot parameter page for a 2D data set

The **Clear Plot** button removes the plot file. The **Plot Preview** button starts Adobe Reader (Figure 40) and displays the output of the plot file. Some of the menu options in Adobe Reader are available for use. The **Automatic Plot Page** button executes the `plot` macro; then the `resetplotter` macro and the **Auto Plot Preview** button executes the macro `pageview('auto')` to generate the

output. The PlotView pop-up (Figure 41) appears during a preview, which allows the saving of the view to a pdf format file, sending the output to the default plotter, a file, and to one or more e-mail addresses.

The **Plot** parameter page for a 2D data set contains both- the **show** and **plot** buttons. **Plot** adds to a temporary plot file, **show** displays in the graphics area.

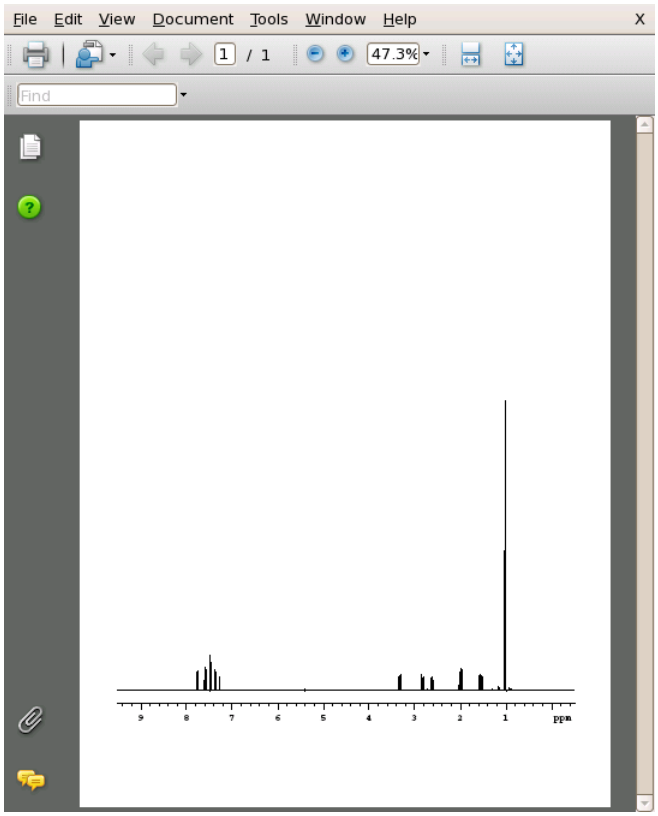


Figure 40 Preview of the plot file initiated from pressing the Plot Preview button

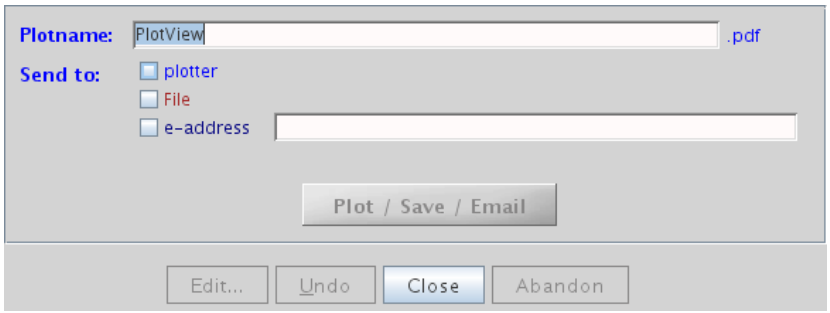


Figure 41 The PlotView pop-up

The **Basic** parameter page (Figure 42) contains **Plot** and a **Plot Preview** buttons; both have the same function as the **Automatic Plot Page** and **Auto Plot Preview** buttons found on the **Plot** parameter page.

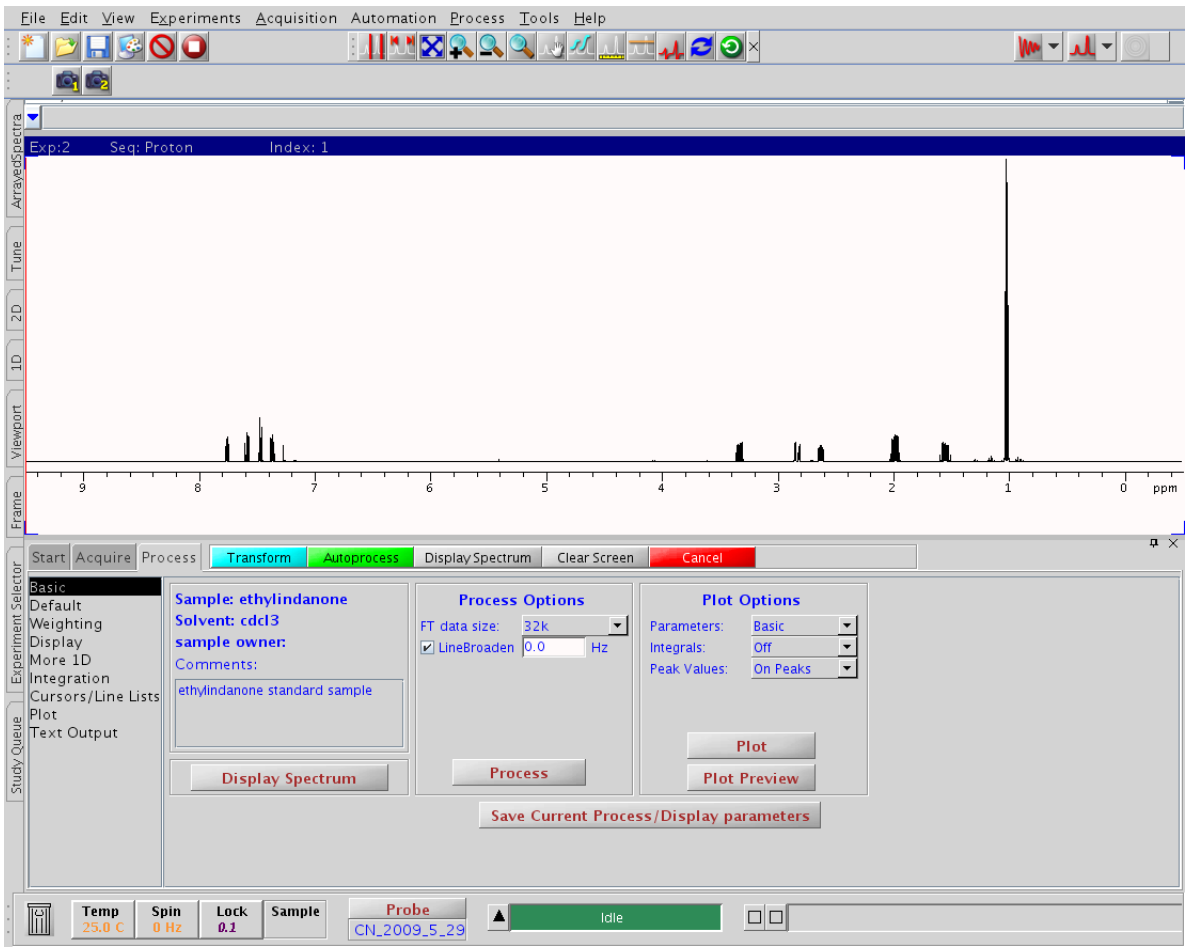


Figure 42 The Basic parameter page for a 1D data se

The **1D Vertical** parameter page contains four buttons in the **Basic Plotting** group.

- **Auto Plot Page** does the same function as the **Automatic Plot Page** button in the **Plot** parameter page.
- **Auto Plot Preview** button does the same function as the **Plot** parameter page.
- **Print Screen...** button does the same function as **File / Print Screen**.
- **More Plotting – Parameter Pages** button opens the horizontal panel and displays the **Plot** parameter page.

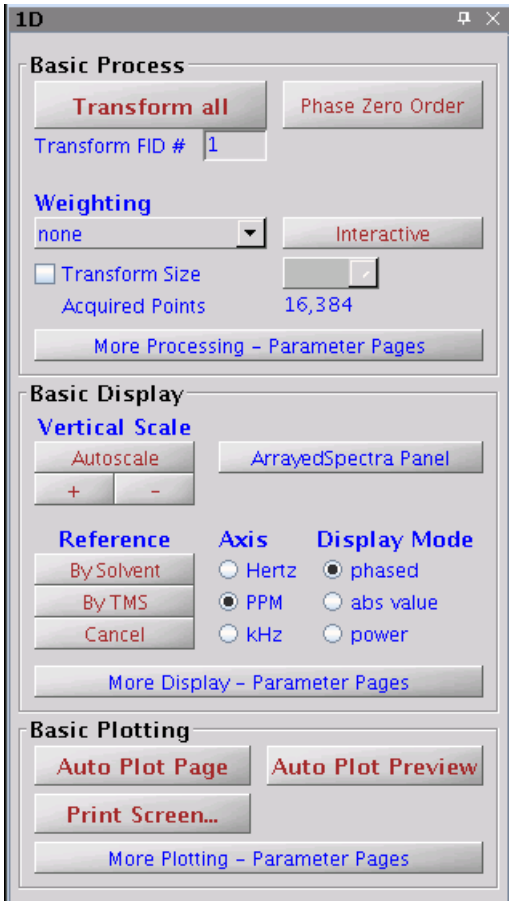


Figure 43 The 1D Vertical parameter page

Plot Designer

Plot designer provides the following tools:

- Interactive plot composition fine-tuning of the layout on the screen prior to plotting.
- Label spectra with text in various fonts and draw lines, boxes, and arrows.
- Save customer plot layouts and templates for reuse.
- Export plots for further annotation and incorporation into reports and publications.

System requirements

Plot Designer is a Java-based application. The Java Runtime Environment (JRE) provides an environment in which Java applications run. Any required updates are available from the update area of the Sun Microsystems Web site at http://www.sun.com.

Using plot designer

Select a viewport and process the data set for plotting.

Start the Plot Designer program as follows:

1 Click **File**.

2 Select **Create a Plot Design**.

The **Plot Designer** window opens. See Figure 44.

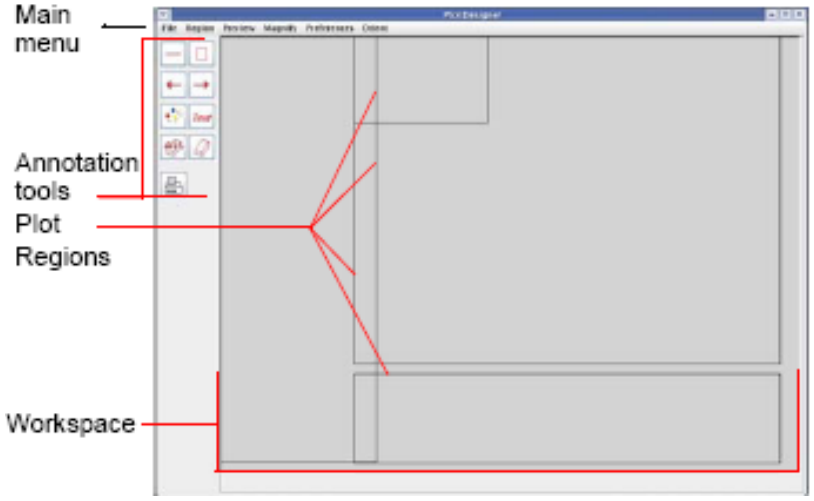


Figure 44 Plot Designer with current default template

3 Load a template:

a Click **File**.

b Click **Templates**.

c Click **Plot Template**.

d Select from the following standard templates or any custom user-created template:

deptB	dicom.default	chemParray	chemP1d
basic2D	oneD	Whitewash	ChemP2d

e Select **Use this template as default** to keep this as the template that loads each time Plot Designer is started. The name of the default template is shown on the message line above the **Plot Templates** window control buttons.

f Click **Open**.

4 Select **Preview** from the **Plot Designer** menu.

5 Select **All**.

The data from the active viewport is imported into the various regions of the template based upon the commands associated with each region.

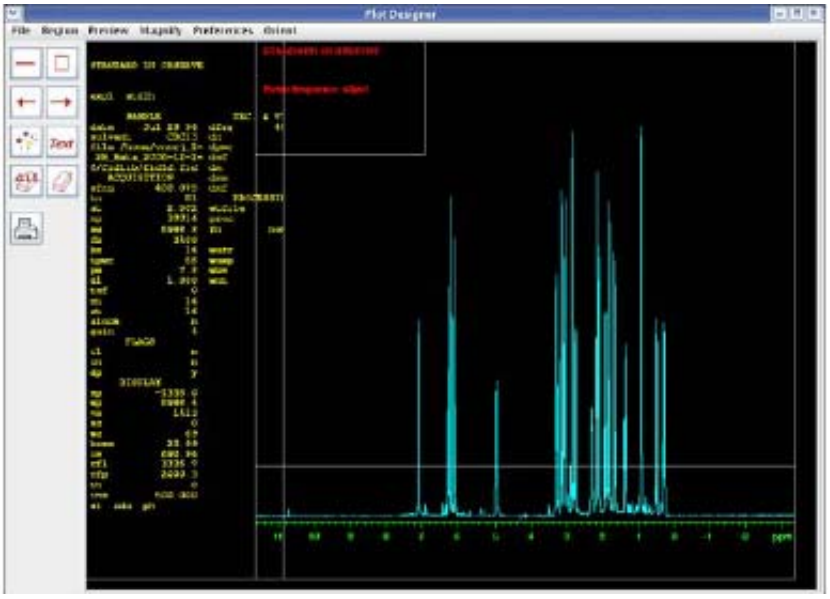


Figure 45 Default oneD template with imported data

Creating a customized template

Create a template from scratch or base a customized template on one of the supplied templates.

To prepare to customize a template:

1. Start Plot Designer.
2. Click **File**.
3. Select **Create a Plot Design**.
4. Load a template or use the default template.
5. Do any or all of the following:
   - Click a region to delete. See "Deleting a region" on page 211.
   - Delete all the regions. See "Clearing all regions from the workspace permanently" on page 211.
   - Add a new region. See "Adding a region" on page 212.
   - Edit an existing region: double on a region, click **Region** on main menu, select **Edit**, and enter the plotting command for the content of the selected region. See "Editing plotting commands in a new or existing plot region" on page 212
   - Add text and graphics elements: see "Adding and editing text and graphics elements" on page 213.

Deleting a region

1. Double-click a region.
2. Click **Region-Delete**.

Restoring a single deleted region

Click **Region-Undelete**.

Clearing all regions from the workspace permanently

Click **Delete All**: no undelete. Regions removed with Delete All cannot be restored with Undelete.

Adding a region

1 Click **Region** on main menu.

2 Select **New** (mouse cursor changes to a cross hair).

3 Draw the new region on the screen.

Editing plotting commands in a new or existing plot region

1 Double-click a region to make it active. Active regions have red borders with control handles.

2 Enter new plotting commands or edit existing plotting commands in the region editor window. Any plotting currently support plotting command is allowed.

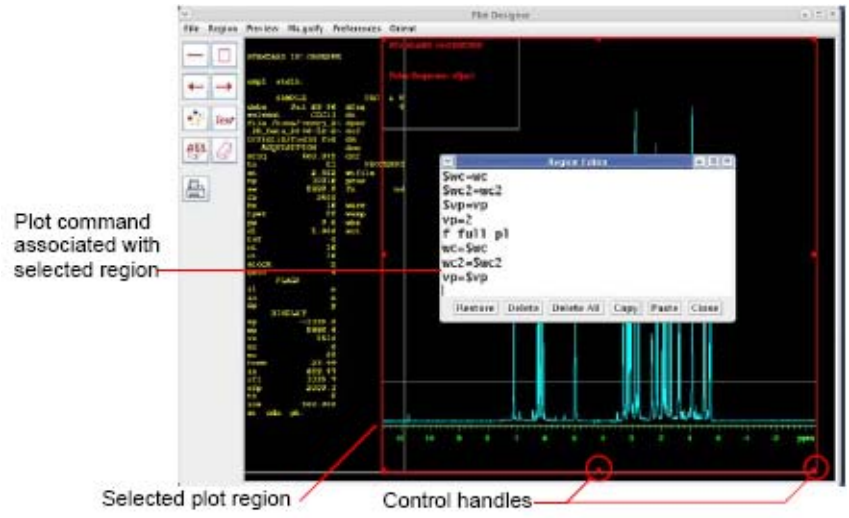


Figure 46 Editing a plot region commands

The **Region Editor** window control buttons as listed in Table 13 are found.

Table 13 Region editor buttons

Button	Function
Restore	Applies the original template to a region. Restores template to its original design if it was opened and changes were made to it, using this button.
Delete	Removes text. This option is not similar to Copy. Deleted text is not stored in a buffer. Do not use Delete to cut and paste text.
Delete all	Clears all text from the input area.
Copy	Duplicates text.

Table 13 Region editor buttons (continued)

Button	Function
Paste	Inserts copied text in the input area.
Close	Exits the Region Editor.

Resizing and moving plot regions and objects

Move an object or region by double-clicking on it and dragging the mouse across the workspace. The arrow keys can be used to move objects.

Resize a region by double-clicking on it, grabbing a control handle (see Figure 46) on the border, and dragging it to the new size.

Adding and editing text and graphics elements

Change the size and color of objects in a region with the **Item Preferences** window, shown in Figure 47.

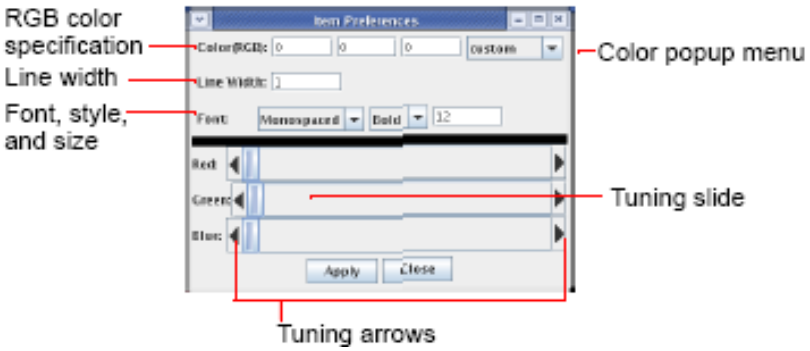


Figure 47 Item preferences window

Click **Region-Preferences** to open this window or click the **Item Preferences** icon , described in "Plot designer tools" on page 216.

Changing line width

Change the width of a line by doing the following procedure:

1. Highlight the line or region by double-clicking on it.
2. Enter a new width in the Line Width field.
3. Click **Apply** to change the line.
4. Click anywhere in the workspace to deselect the line.

Changing fonts

Plot Designer has three font families: Sans Serif, Monospace, and Serif. Fonts can be Plain, Bold, or Italic. Change the family, style, and size of a font as follows:

1. Highlight the text or region.
2. Click the **Item Preferences** tool  to open the **Item Preferences** window.
3. Choose a family, style, and enter a size in the Font field.
4. Click **Apply** to change the text.

Changing colors

Change the color of a line by doing the following:

1. Highlight the line or region.
2. Click the **color** button  to open a pop-up menu showing a range of colors.

   Move the tuning slider either left or right to change a color, or change a color by clicking on the left or right arrows in the Red, Green, and Blue fields. The values in the Color (RGB) field automatically change as the slider moves.
3. Click **Apply** when the required colors are selected.
4. Place the cursor anywhere in the workspace and click once to apply the color change.

Adding Text

Do the following to add text into your design:

1. Click the text input tool 

to open the text input window.
2. Type text in the field at the top of the window.
3. Customize the text by clicking on the desired options and entering a font size in the indicated field.
4. Click **Put** and drag the cursor into the workspace, then click once to paste in the text.

Use the following procedure to copy and paste text that is already on the workspace and change the font styles:

1. Highlight the text.
2. Click the text input tool 

to open the **Text Input** window shown in Figure 47.
3. Select a Font family and Font style, and enter a Font size.
4. Click **Put** to paste the text in the workspace.

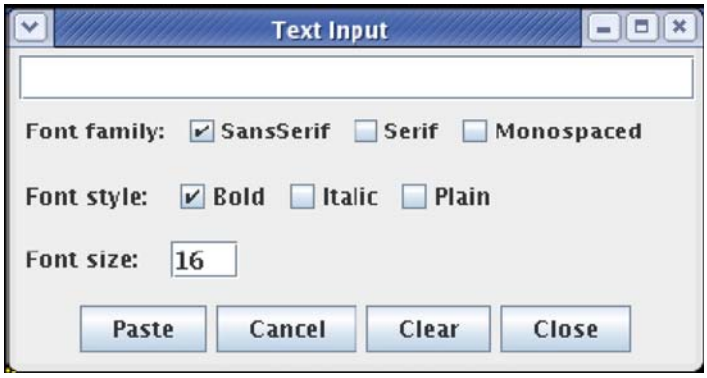


Figure 48 Text input window

Changing font color

Repeat the procedure given in"Changing colors" on page 214 to change font colors.

Saving a custom template

Save the custom a template as follows:

1. Click **File**.
2. Select **Templates** to open the **Plot Templates** window.
3. Enter a name in the **Template** field.

   Optional: Select the box next to **Use this template as default** to make the file the default template. The default template is automatically loaded when Plot Designer is started.
4. Click **Save** to store the template in `$vnmruser/templates/plot directory`.

   A warning is displayed if the saved template overwrites a current template.
5. Click **Cancel** to not replace the file.
6. Quit the **Plot Templates** window by clicking on **Close**.

Plot designer tools

The Plot designer tools are listed in Table 14. Press and hold down the left mouse button and drag the cursor in the workspace to use a drawing tool.

Table 14 Plot designer tools

Icon	Function	Description
	Line Drawing	Draws a line
	Box	Draws a box
	Arrows	Draws an arrowhead and places it at the origin of the line. Draws an arrowhead and places it at the point of the line
	Item Preferences	Sets the color and size of lines and fonts. Select an object to edit by double-clicking on it. See "Adding and editing text and graphics elements" on page 213 for a description of its properties.
	Text Input	Adds text into the design and controls the size and appearance of the text. See "Adding Text" on page 215 .

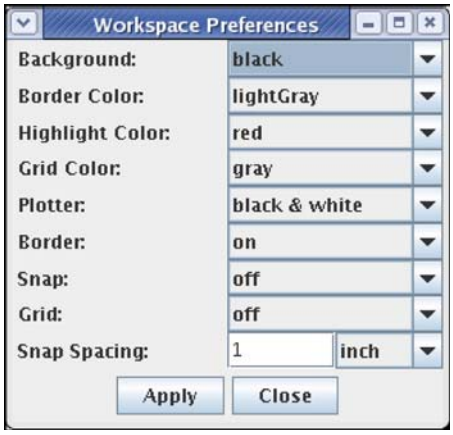
Table 14 Plot designer tools (continued)

Icon	Function	Description
	Erasers	The ALL eraser removes all objects The eraser tool removes selected objects. See also "Adding and editing text and graphics elements" on page 213, "Adding a region" on page 212, and "Deleting a region" on page 211.
	Print	Prints a file

Changing an aspect or property of plot designer

1 Click **Preferences** from the main menu.

2 Select **Set Up** to open the Workspace Preferences panel.



3 Click the corresponding button to open a pull-down menu.

4 Select a color preference.

5 Click **Apply** to execute the changes.

6 Click **Close** to exit the window.

Table 15 Workspace preference controls

Control	Function
Background	Changes the background color of the window
Border Color	Changes the color of the border surrounding the workspace
Highlight Color	Color of an object after double-clicking on an object to indicates that it is selected
Grid Color	Changes the color of the grid
Plotter	Selects a black and white or color plotter
Border	Shows (**on**) and hides (**off**) region borders
Grid	Shows (**on**) and hides (**off**) grid in the workspace
Snap	The center of the border of an object snaps to the grid when an object is created or moved if snap is turned **ON**. Turn Snap **OFF** to disable this feature.
Snap Spacing	Controls the amount of space on the grid to which an object snaps. Spacing is in inches, centimeters, or points.

Changing the shape of the plot designer window

Plot Designer can be viewed in two orientations- Landscape or Portrait (which is the default orientation). Change the shape of the **Plot Designer** window in the **Orientation** menu.

Changing the size of the plot designer window

Increase or decrease the size of the **Plot Designer** window by clicking on the sizes listed in the **Magnify** menu.

Saving a Plot File

Do the following procedure to save a plot:

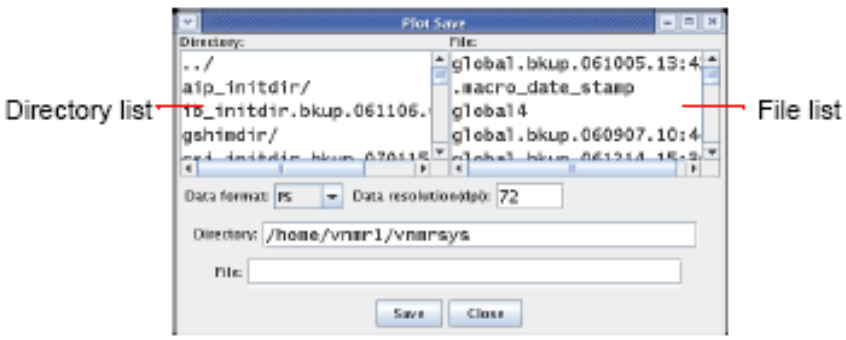


Figure 49 Plot save window

1 Click **File** in the **Main Menu**, then **Save Data** to open the **Plot Save** window shown in Figure 49.

2 Scroll down the list of directories and choose a directory or enter a path for the file in the Directory field.

3 Select a **Data format** for your file and enter a **Data resolution**. Table 16 lists the formats that are available.

Table 16 Output formats supported by plot designer

Format	Description
AVS	AVS X image file
BMP	Microsoft Windows bitmap image file
EPS	Adobe Encapsulated PostScript file
FAX	Group 3 FAX
FITS	Flexible Image Transport System
GIF	Compuserve Graphics Interchange Format (version 89a)
GIF87	Compuserve Graphics Interchange Format (version 87a)
JPEG	Compressed format from Joint Photographic Experts Group
MIFF	Magick image file format
PCD	Photo CD
PCX	ZSoft IBM PC Paintbrush file
PDF	Portable Document Format
PICT	Apple Macintosh QuickDraw/PICT file
PGM	Portable gray map
PNG	Portable Network Graphics
PS	Adobe PostScript file
PS2	Adobe Level II PostScript file
SGI	Irix RGB image file
SUN	Sun Rasterfile
TGA	Truevision Targa image file
TIFF	Tagged Image File Format
VIFF	Khoros Visualization image file
XBM	X11 bitmap file
XPM	X11 pixmap file
XWD	X Window System window dump image file

4 Label your file by entering a name in the File field.

5 Click **Close** to exit the window.

Printing a plot

Click the print tool. 

Exiting plot designer

Click **File-Quit**.

Any design in the window when Plot Designer is closed is automatically opened in the workspace the next time the program is started.

Color Printing and Plotting

Printer and Plotter color output is defined using the **Styles and Themes** window, which provides access to the display colors and the VnmrJ 3 interface colors.

Setting colors

View the current settings or define new color settings as follows:

1 Click **Edit**.

2 Select **Display options**.

The **Style and Themes** window opens. See Figure 50.

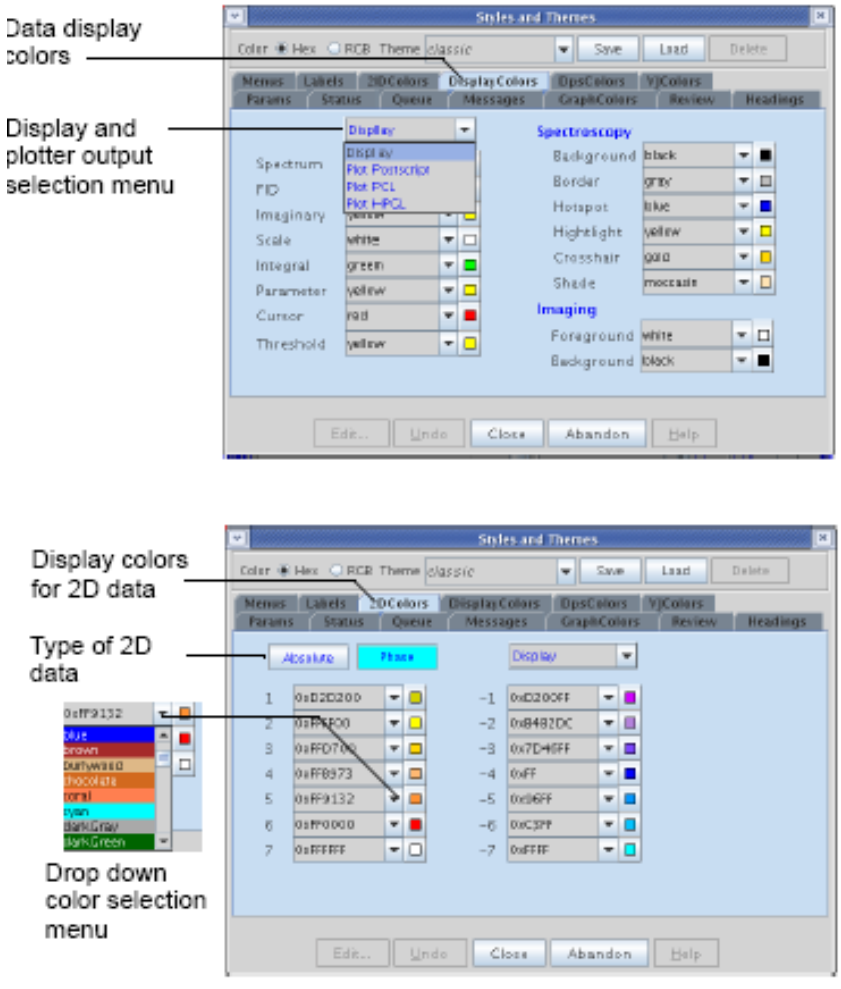


Figure 50 Styles and themes for display and 2D colors

3 Select the **Display** tab to set the colors for the spectra, axis, parameters, etc.

4 Click the **Display and Output** selection drop-down menu.

5 Select the output device: **Display, Plot Postscript, Plot PCL,** or **Plot HPGL**.

6 Select a color or keep the current color for each display or function shown.

7 Enter a **name** in the field next to the **Save** button to save the selection to a user defined file or continue with the next step to overwrite the current file.

8 Click **Save** to save the color selections to the specified file.

9 Click **2D colors**.

10 Click **Phase** to set the colors for this 2D display mode.

11 Select the output device: **Display, Plot Postscript, Plot PCL,** or **Plot HPGL**.

12 Select a **color** or keep the current color for each contour level.

13 Click **Absolute** to set the color for this 2D display mode.

14 Select a **color** or keep the current color for each contour level.

15 Enter a **name** in the field next to the **Save** button to save the selection to a user-defined file or continue with the next step to overwrite the current file.

16 Click **Save** to save the color selections to the specified file.

Loading a color file

To retrieve a color file:

1 Select a theme file from the **Theme** drop-down menu.

2 Click **Load**.

Changing or renaming a color file

To change the colors in a file:

1 Select a **theme file** from the **Theme** drop-down menu.

2 Click **Load**.

3 Follow the procedure in "Setting colors" on page 221.

4 Click **Save** to save the file.

To change the name of a color file:

1. Select a **theme file** from the **Theme** drop-down menu.
2. Click **Load**.
3. Enter a **new name** in the field next to the **Save** button.
4. Click **Save** to save the file.
5. Optional: To delete the file with the old name, see "Removing a color File" on page 223.

Removing a color File

To remove a color file from the list:

1. Select a theme file from the **Theme** drop-down menu.
2. Click **Load**.
3. Click **Delete**.

   The deleted file is removed from the bottom list box.
4. Click **OK**, when prompted, to delete the file, or **Cancel** to keep the file.

Closing the color selection window

Click **Close** to exit the window.

Sending a Plot via email

After selecting the options to and clicking the **Plot Preview** button in the **Plot** parameter page.

1. Enter a **Plot name** in the PlotView pop-up.
2. Select **File**.
3. Select **e-address**.
4. Enter valid email addresses in the entry field of e-address.
5. Press the **Plot / Save / Email** button.
6. Press the **Close** button when done.

There are advanced macros that can be issued from the command line (`eplot, epage, espec, fplot, fpage, efid, esampledir`), which can be used to send the output to an email address. See the *Command and Parameter Reference* for details on the usage of the macros.

Pasting text into a Text Editor or Other Application

Text output that appears in the **Integration**, **Cursors/Line Lists/Text Output** parameter pages can be pasted into a text editor or other application as shown in Figure 51, to be saved or used elsewhere.

1. Highlight the text to be pasted by clicking the left mouse button and dragging the mouse to the end of the desired text.
2. Release the mouse button at the end of the desired text. The selected text is highlighted indicating what has been selected.
3. Start the text editor or application and place the mouse cursor on the active document.
4. Click the middle mouse button to paste the highlighted text into the text editor.

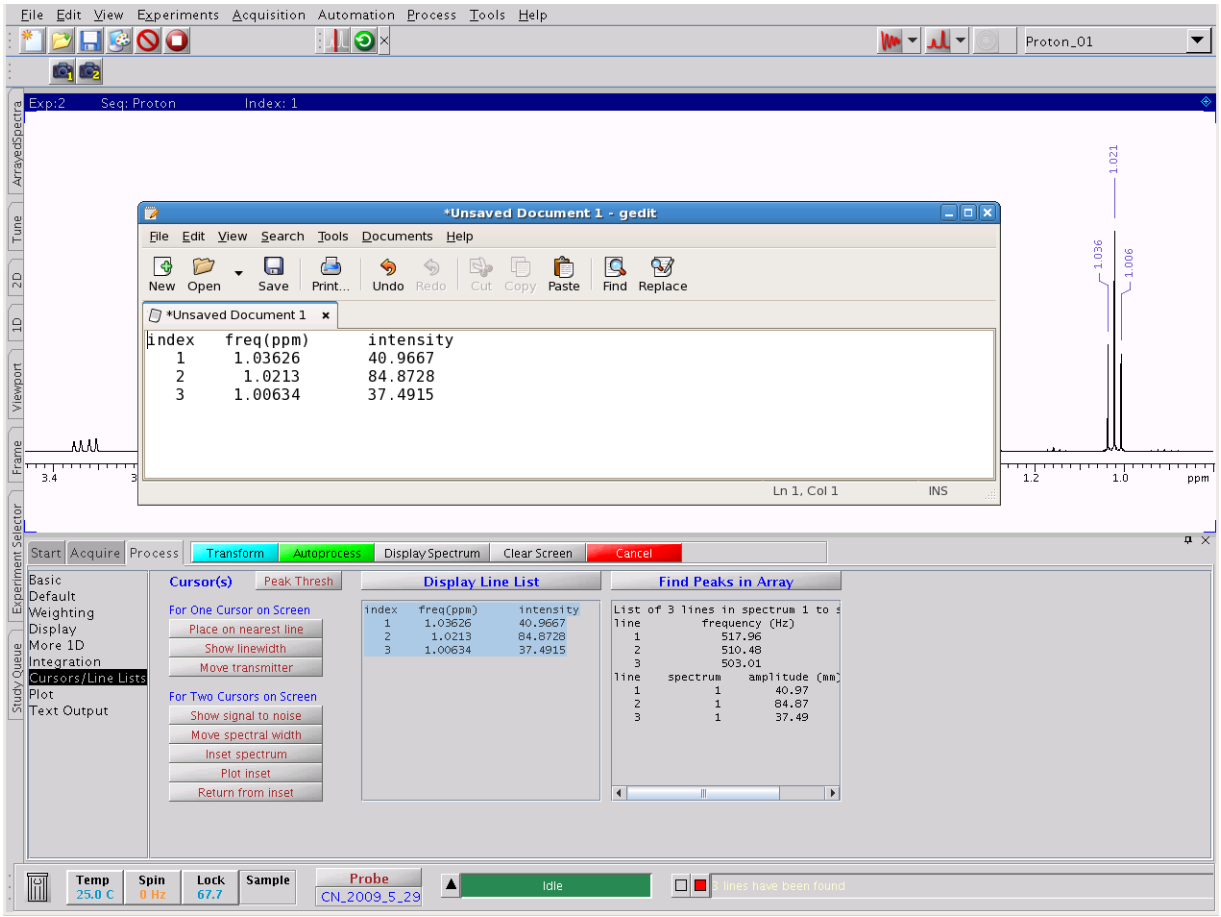


Figure 51 Contents of the Display Line List text box copied into the Linux gedit text editor

Advanced Printing Commands

Printing from within VnmrJ 3 is initiated with the `printon` command. Once the `printon` command is issued, all further output that normally appears in the text output window is redirected to a temporary file and no further output will appear in the text output window. When the `printoff` command is issued, the temporary file is sent to a printer, the file is purged from the system, and future text output is resumed to the text output window. This output includes the following:

- Parameter listings from `dg, dgl, da,` etc.
- Line listings from `dll`.
- Integral listings from `dli`.
- System configuration parameters generated by `config ('display')`.
- Text files using the text command.
- Results of calculations from `h2cal, adept, t1, t2,` etc.
- Any other information that some program or macro may write to the text window.

This output is saved in a temporary file in the VnmrJ 3 subdirectory `tmp`. The VnmrJ 3 parameter printer determines the printer to which the output is directed. When the `printoff` command is issued, VnmrJ 3 executes a UNIX script called `vnmrprint` that sends the temporary file to the printer using standard UNIX printing utilities. This script is supplied with the name of the temporary file to be printed, the name of the printer (corresponding to a `printcap` entry), and the type of printer (corresponding to a `devicetable` entry).

NOTE The `devicetable` information is used to distinguish PostScript printers. The `vnmrprint` script allows users to customize.

The macro `ptext(file)` prints out the text file given as an argument. For example, the command `ptext('/vnmr/psglib/DEPT.c')` prints the text file `DEPT.c`.

Print jobs for the currently active printer in VnmrJ 3 are held in a print queue. The `showprintq` macro displays the current print jobs in the print queue. The `killprint` macro will stop a print job and remove it from the print queue. Unless the user executing this macro is `root` (superuser),

only that the user's print job is deleted from the print queue.

Table 17 Printer-Associated commands and parameters

Commands	
`killprint`	Stop print job and remove from print queue
`printoff<('clear'|file)>`	Stop sending text to printer and start print operation
`printon`	Direct text output to printer
`ptext (file)`	Print out a text file
`showplotter`	Display currently defined plotters and printers
`showprintq`	Display print jobs in print queue
`vnmrprint*`	Print text files (UNIX)
`* vnmrprint printfile <printcap> <printer_type <clear|file>>`	
Parameter	
`printer {string}`	Printer device

Advanced Plotting Commands

Spectral plotting

The pl command plots the currently displayed region of the currently active spectrum, or spectrum plus integral (or the region which would be displayed if there were a spectral display on the screen). pl('int') plots the integral only. pl('pen2') plots the spectrum using pen number 2 of a multi-pen plotter.

The pscale command plots a scale under a spectrum. The syntax is:

pscale<(<axis><,vertical_start><,plot_start><,pen>)>

If the letter p, h, k, etc. is supplied as an optional argument for axis that is used instead of the current value of the parameter axis, the optional argument vertical_start defines the vertical position where the scale is drawn (the default is 5 mm below the current value of the parameter vp). The second optional argument plot_start is interpreted as a modified start of plot. The pen option defines the pen number to be used.

The ppf command plots peak frequencies in units specified by the axis parameter above the peaks, selecting only those peaks greater than th high. ppf('noll') plots peak frequencies using the last previous line listing while ppf('pos') plots only positive peaks. Other arguments for noise suppression (noise_mult) and label positioning work the same as the dpr command.

The pll command produces a columnar line list on a plotter, similar to what would appear on a printer. The output is automatically formatted into multiple columns, depending on the number of lines. The syntax is pll<(x,y,minimum_y)>. The arguments x and y are the x and y position of the upper left of the line list, and minimum_y is the minimum y at which to reset back to the top.

The plh command plots a proton spectrum based on parameters pltmod and intmod:

pltmod='off' sets no plotting.

pltmod='fixed' takes sp and wp as is.

pltmod='full' adjusts sp and wp to plot the full spectrum.

pltmod='yariable' adjusts sp and wp to plot only the

region of interest.

`intmod='off'` gives no integral.

`intmod='partial'` gives a series of integrals over each region.

`intmod='full'` gives a single integral over the entire spectrum.

Given a spectrum divided into regions by the `region` command or by the cursors in the `ds` program, the macro `aexppl<(expansion_factor)>` automatically plots each region at the horizontal scale requested (in Hz/ mm). The default scale is 2 Hz/ mm.

Several generic plotting macros, such as `plot` and `plot1d`, are available that call specialized plotting macros, depending on the user definition or other wise on the type of data in the experiment. For details, see *VNMR Command and Parameter Reference*.

Display limits

Because of the use of different plotters with different dimensions, the parameters `sc`, `wc`, `sc2`, and `wc2` need to be set differently to position plots and displays in the same relative position on the page. The full, center, left, and right commands do nothing more than modify `sc`, `wc`, `sc2`, and `wc2` to place the display and plot in the desired portion of the screen and page. The `f` command is used to set the `sp` and `wp` parameters to display a full spectrum. The `zoom(width)` macro adjusts the display limits to the width specified, in Hz, setting the limits to +/-width/2. Also available is the `split` macro, which repositions the left-hand cursor halfway between its original position and the position of the left cursor.

A scaling factor helpful for 1D plotting is the `hzmm` parameter, which contains the quotient of `wp` divided by `wc`.

The `wysiwyg` parameter is useful for scaling the image to a full window instead of the same size as the plot. Setting `wysiwyg='n'` sets a full display and `wysiwyg='y'` sets a plot display (the default).

Table 18 Plotting-Associated commands

Commands	Descriptions
`aexppl<(expansion_factor)>`	Automatic plot of spectral expansion