NAME

nmrDraw − Graphics Interface for NMR Processing and Analysis

SYNOPSIS

nmrDraw [**−in** *inName*] [**−dir** *dirName*] [**−file** *fileExp*] [**−name** *defName*] [**−text** *textDir*] [**−read**] [**−cellX** *xPix*] [**−cellY** *yPix*] [**−type1** *small* | *medium* | *large*] [**−type2** *small* | *medium* | *large*] [**−square**] [**−focus**] [**−track**] [**−scroll**] [**−repaint**] [**−norepaint**] [**−frp** *repaintCount*] [**−dbg**] [**−verb**] [**−draw**] [**−clear**] [**−frzLevels** *Always* | *Sometimes* | *Never*] [**−frzZoom** *Always* | *Sometimes* | *Never*] [**−autoScale**] [**−grid**] [**−pix**] [**−image**] [**−peak**] [**−vert**] [**−zero**] [**−cursor**]] [**−relative**] [**−compress**] [**−iz** *zPlane*] [**−ia** *aPlane*] [**−func** *fnTab*] [**−proc** *scriptName*] [**−nosys**] [**−zfht**] [**−mult** *contFactor*] [**−plev** *numLevels*] [**−nlev** *numLevels*]] [**−hi** *firstHeight*] [**−plot** 1 | 2 | 3] [**−pcc** *numColors*] [**−pHue1** *hue*] [**−pHue2** *hue*] [**−pSat1** *saturation*] [**−pSat2** *saturation*] [**−pVal1** *value*] [**−pVal2** *value*] [**−ncc** *numColors*] [**−nHue1** *hue*] [**−nHue2** *hue*]] [**−nSat1** *saturation*] [**−nSat2** *saturation*] [**−nVal1** *value*] [**−nVal2** *value*] [**−XOR** *Always* | *Sometimes* | *Never*] [**−virt** *Always* | *Sometimes* | *Never*] [**−labMode** *Normal* | *XOR* | *Overlay*] [**−svri**] [**−colors** *clrList*] [**−color0** *zeroClr*] [**−color1** *1dClr*] [**−colorC** *cClr*] [**−colorG** *gridClr*] [**−colorX** *xClr*]] [**−colorY** *yClr*] [**−colorZ** *zClr*] [**−colorA** *aClr*] [**−colorL** *lClr*] [**−colorE** *eClr*]] [**xviewFlags**]

SPECIAL NOTE

This manual page is under development.

DESCRIPTION

NMRDraw is a User−oriented X11 graphical interface for inspecting and processing multidimensional NMR data. It works in conjunction with the nmrPipe program for spectral processing via UNIX pipes.

In its current implementation, **NMRDraw** is used to prepare data for use with computer−assisted analysis and assignment programs such as **PIPP** (Dan Garrett, NIH), **ANSIG** (Per Kraulis, Karolinska Institute), or **NMRView** (Bruce Johnson, Merck Pharmaceutical). NMRDraw facilities include:

Display of 2D Planes from either processed or unprocessed multidimensional data, including interactive and User−specified 2D Zoom, adjustable color schemes, and viewing of the next 2D plane in a series by a single mouse click.

Real−time display of one or more 1D slices superimposed over 2D spectral graphics, with interactive adjustment of zoom region, vertical scale, and vertical offset.

Interactive processing of 1D slices from any dimension of a spectrum, as well as automatic processing according to pre−defined schemes.

Real−time phase correction of one or more 1D slices simultaneously, with coarse and fine phase adjustment, interactive pivot point selection, and automatic reconstruction of imaginary data when needed.

An **nmrPipe** shell−script editor, for creating, saving, and executing multidimensional conversion and processing schemes.

Interactive adjustment of chemical shift calibration.

Color and monochrome PostScript hard copy plot generation.

Other extraction, display, and analysis facilities, including projections, graphics overlays from one or more spectra, and automated/interactive peak picking, are included or under development.

A TYPICAL SESSION WITH NMRDRAW

There are many possible scenarios for a session with **NMRDraw**; a typical session for processing and inspecting a 3D spectrum might include the following steps:

Use the **NMRDraw** Macro Edit facility to create, save, and execute a UNIX shell−script which converts an unprocessed spectrometer format data file to an **nmrPipe** format data file.

Read and display the converted, unprocessed data file; inspect the raw data to see whether it was acquired and converted successfully.

Interactively process a 1D slice from the data file; determine phase correction values and other processing parameters.

Create, save and execute a UNIX shell−script to process the first 2D plane from the data, using the interactively determined processing parameters.

Read and display the processed plane; evaluate the need for any additional processing, such as baseline correction.

Create, save, and execute a UNIX shell−script to process the entire 3D spectrum, incorporating the previous 2D scheme.

Read and display 2D planes, 1D slices, etc. from the processed 3D spectrum.

APPEARANCE OF NMRDRAW

NMRDraw has several components, which provide for informational text, command entry, and spectral display. The appearance and behavior of **NMRDraw** can be changed by command−line arguments and by other graphics parameters, especially the configuration parameters of the graphics environment (window manager) being used. The usual behavior of **NMRDraw** is described here:

By default, the **NMRDraw** *window* takes up the entire screen. The window *border* at the top edge of the screen describes the current functions of the mouse buttons, if any. It is also sometimes used to display information about the current data.

The *command panel*, which extends across the top of the nmrDraw window, contains pull−down menu buttons for command entry, numerical fields for specifying spectral locations and display parameters, and slider bars for adjusting phase correction values interactively. The command panel usually has a gray background.

The *canvas* takes up the remaining portion of the nmrDraw window; it has a purple background by default. The canvas contains a rectangular *spectral graphics area*, where displays such as contour plots will be drawn. By default, this graphics area has a black background. Many facilities of **NMRDraw** make use of the mouse; in these cases, the mouse buttons will perform one set of actions while the mouse pointer is inside the spectral graphics area, and a different set of actions when the mouse pointer is to the left or below the graphics area, in the purple borders. As mentioned above, the mouse button functions will be displayed the the topmost border of the NMRDraw window.

In addition to **NMRDraw's** primary window, one or more *pop−up windows* may appear during a session. These windows are used for special−purpose command entry, such as selection of the current data file. More than one pop−up may appear on the screen at a given time. As with **NMRDraw's** primary window, the top border of a pop−up will often display useful information. Most pop−ups have a **Done** Button, which should be used to close the pop−up and remove it from the screen. Note that if you remove a pop−up by other means, such as via window manager commands, you may not be able to use the pop−up again during the session.

NMRDRAW AND YOUR WINDOW MANAGER

As noted before, some functions of NMRDraw are under the control of the window manager, the program which coordinates the display of multiple windows on the screen. The window manager controls the behavior of the keyboard, mouse buttons, and window borders. It also controls default placement of windows on the screen, and the details of moving, re−sizing, iconifying and restoring windows. So, you may wish to investigate or adjust the details of your own window environment in order to make the best use of **NMRDraw**.

The current version of **NMRDraw** has been developed with the XView Toolkit V2.0, for use with X11R4. It has been used most extensively with the **twm** and **OpenLook** window managers. In these cases, the following aspects of the window environment seem to have the strongest influence on the behavior and appearance of **NMRDraw**:

Which mouse button is used to view pull−down menus, and which is used to select a command.

Whether pop–up windows are placed automatically or by hand.

Whether graphics drawn in overlapping or iconified windows is discarded or maintained.

The colors and fonts used for window borders, etc.

RUNNING AND EXITING NMRDRAW

In the usual installation, the **NMRDraw** program can be run by typing the command:

```
nmrDraw
```

This command executes the UNIX shell–script file called *nmrDraw*, which in turn runs the program itself, which is called *nmrdraw*. You can customize many aspects of **NMRDraw** by editing a version of the *nmrDraw* shell–script, to change the various arguments used to invoke the program.

You can also include arguments directly on the **NMRDraw** command–line. For instance, as a short–cut, you can specify the default data directory or data name:

```
nmrDraw –dir ft –name test%03d.ft3
```

In order to exit the **NMRDraw** program, you can select the **Quit NMRDraw** command from the **NMRDraw File** Menu. You can also exit the program by moving the mouse pointer into the spectral graphics area and typing the character **Q** (upper–case Q) at the keyboard.

ENTERING COMMANDS IN NMRDRAW

NMRDraw is operated by a combination of commands entered via the mouse and keyboard. Many commands and parameters are selected by using the mouse with *graphical items* on the screen; the general nature of some common graphical items is described in more detail below.

The primary commands are selected via *Menu Buttons* in the command panel. For instance, the command to draw a contour plot on the screen is listed under the **Draw** pop–up menu as **"d) Contours"**, and can be selected via the mouse. As an alternative, the command can be selected from the keyboard without the need to use the mouse. In this case, the command can be selected by typing **d** (lower–case d), as indicated at the beginning of the Command Text.

You can only type commands from the keyboard if the *keyboard focus* is set to the spectral graphics area. This generally means that the mouse pointer will have to be positioned inside the graphics area before commands are entered. The outer edge of the graphics area will usually be hilighted to indicate that commands can be entered. You can restore keyboard focus at any time by moving the mouse pointer out of, then back in to, the graphics area.

SOME GRAPHICAL COMMAND ITEMS

Buttons

Buttons are graphical items intended to resemble actual push–buttons with rounded edges. They are used to display a single command or command choice. To select a Button's command, point to the Button with the mouse, and click the left mouse–button.

Example: most pop–up windows have a **Done** Button, which can be used to close the pop–up and remove it from the screen.

Menu Buttons

Menu Buttons are special Buttons which cause a pop–up menu of additional options to be displayed. Menu Buttons look like ordinary Buttons, but they also include a triangular caret symbol after the button text; this caret signifies that there is a menu associated with the button. To view the pop–up menu associated with a Menu Button, press and hold the right mouse–button; the menu will appear, and will stay on the screen as long as the mouse–button is held. Command options in the pop–up menu can be selected by dragging the mouse to highlight the desired option, then releasing the mouse.

The first command entry in any given menu is called the *default command*. The menus are often arranged so this default command is a commonly used one. As a short−cut, it is possible to select this default command without the need to pop−up the menu. To do this, use the left mouse−button (to select the default command) rather than the right mouse−button (used to make the pop−up menu appear). In this respect, Menu Buttons behave like ordinary Buttons, since the left mouse−button is used in both cases to select the Button's command.

Example: the **NMRDraw** Command Panel includes Menu Buttons marked **File**, **Draw**, and **Mouse**. The default commands for these menus are the often−used options to read a file, draw a contour plot, and view 1D slices.

Character Text Item

Character Text Items are one−line regions on the screen used for entering text information such as a file name from the keyboard. Text Items have a *label* on the left−hand side, followed by a horizontal line where text typed from the keyboard will be entered. In order to enter text into a Text Item, point to the item with the mouse and click the left mouse−button before typing from the keyboard. In some cases, entering a carriage return at the end of the input line will cause **NMRDraw** to perform some action related to the input text.

Example: the **Select File** pop−up window includes Text Items which are used to specify the current data file and directory; these text items are labeled "File:" and "Directory:". Typing a file name in the "File:" field followed by a carriage return will cause **NMRDraw** to read the specified file.

Floating−Point Text Item

Floating−Point Text Items look the same as character text items, but they are used specifically to enter floating−point numbers. They will have a floating−point number as a default value.

Example: the command panel includes floating−point text items labeled "P0:" and "P1:"; these are used to display or change the current phase correction values.

Integer Text Item

Integer Text Items look the same as character text items, but they also include a pair of square caret buttons to the right of the one−line text field. As the name implies, the integer text item is used for entering an integer value; the caret buttons can be used to increment or decrement the current integer value.

Example: the command panel includes integer text fields labeled "X:", "Y:", "Z:", and "A:", used for displaying or setting the point locations of 1D and 2D data being displayed.

Slider Bar

Slider bars are used for interactive specification of some continuous value, for instance zero or first order phase. Slider bars have the appearance of a rectangular button in a vertical or horizontal groove. The value associated with a Slider can be adjusted by pointing to the Slider's Button with the mouse, then dragging the mouse with the left mouse−button pressed. In addition, you can increment or decrement the slider value by clicking left mouse−button while pointing to either end of the Slider bar groove.

Example: the command panel includes a pair of slider bars marked "P0:" for coarse and fine zero−order phase, and a second pair of slider bars marked "P1:" for first order phase.

Edit Window

An Edit Window is a rectangular region used for displaying or editing lines of text. You can enter text at a particular position in the window by first pointing to that position with the mouse and clicking the left mouse−button, then typing text at the keyboard. In addition, pressing and holding the right mouse−button in an Edit Window will create a pop−up menu of text editing options, which allow you to read or save text files, cut and paste text selections, and so on.

Example: the command **Macro Edit** in the **File Menu** will create a pop−up which includes a light−blue Edit Window, used for creating UNIX shell−scripts that do spectral processing.

THE COMMAND PANEL

The command panel contains several graphical items for adjusting commonly−used parameters. An outline of the functions of these items follows:

X: Use this to increment, decrement, or select a particular 1D slice when viewing 1D slices from the X−Axis of the current data.

Y: Use this to increment, decrement, or select a particular 1D slice when viewing 1D slices from the Y−Axis of the current data.

Z: Use this to increment, decrement, or select a particular Z−Axis plane. Under default settings, the plane will be automatically read and drawn with the previous zoom region and contour settings. This option requires selection of data as a 3D or 4D template.

A: Use this to increment, decrement, or select a particular A−Axis coordinate. Under default settings, a new plane will be automatically read and drawn with the previous zoom region and contour settings. This option requires selection of data as 4D template.

Plus: Use this to change the number of positive contour levels to use the next time the data is drawn.

Minus: Use this to change the number of negative contour levels to use the next time the data is drawn.

First: Use this to select the height of the first contour used the next time the data is drawn. Negative contours will begin at the negative of this height.

Factor: Use this to select the spacing factor between adjacent contours used the next time the data is drawn.

(+) Use this button to increment the first contour height used the next time the data is drawn.

(-) Use this button to decrement the first contour height used the next time the data is drawn.

P0: (Sliders)

These sliders control the coarse and fine zero−order phase applied at the selected pivot point of the current 1D spectra. These sliders will only work if a 1D slice is selected, and the Phasing Toggle button is ON.

P1: (Sliders)

These sliders control the coarse and fine first−order phase correction. These sliders will only work if a 1D slice is selected, and the Phasing Toggle button is ON.

P0: (Text)

Displays or changes the current P0 phase value; this value can be used directly with **nmrPipe** regardless of the pivot setting.

P1: (Text)

Displays or changes the current P1 phase value; this value can be used directly with **nmrPipe** regardless of the pivot setting.

Pivot: Displays or changes the position of the phasing pivot. The pivot position can also be selected via the mouse when viewing 1D slices.

Phasing Toggle

This toggle button must be set to ON in order to apply phasing to the current 1D data. But, once the toggle is turned ON, the current 1D spectra will not be rephased until a slider or phase value is adjusted.

THE FILE MENU

The **File Menu** includes commands to select the spectral data of interest, as well as commands to read or re-read the selected data. It also includes commands for creating and modifying other kinds of files, such as UNIX shell−scripts. Importantly, the File Menu includes the command used to Exit from NMRDraw.

Read This command reads a 2D file plane into NMRDraw's data memory; depending on the **2D Settings**, a 2D plot of the plane may be drawn automatically once the data is read. The name of the data to read is specified by the **Select File** command in the **File Menu**; 1D and 2D data sets are selected according to their file names, while 3D and 4D data are selected according to their template names. In the case of 3D and 4D data, the Z-Axis and A-Axis locations for the plane to read are taken from the **Z:** and **A:** fields in the command panel.

Select File
This command is used to specify the file or template name of the spectral data to read. Select 1D and 2D data according to their file names. Select 3D and 4D data according to their template names.

Read Only
This command is similar to the **Read** command in the File Menu, however it will not cause any graphics to be drawn regardless of other settings. Use this command if you would like to adjust the display parameters before a plot is drawn.

Previous Data
This command will read the previous data file. It is commonly used to switch between orthogonal planes of a 3D dataset, as created by commands in the **1D Menu**.

Parameters
This command displays the file parameters of the current spectral data. The parameter listing is generated by the program **showhdr;**, it is displayed in the **Info Window**, which will pop up automatically.

Calibrate PPM
Provides a pop−up to re-calibrate the chemical shifts of any axis in the current data:

1. Change the axis selection, axis label, or any other parameter which needs to be adjusted.

3. Enter the PPM value for the selected point; the default point will be set according to the positions of the last 1D slices being viewed.

4. Use the "Apply" button to re-calculate the chemical shifts according to the new parameters.

5. Use the "Save" button to write the new calibration data.

Macro Edit
This command is used to create and execute UNIX shell−scripts for spectral processing. It provides a point−and−click text editor augmented with a series of predefined conversion and processing scripts. It also allows edited scripts to be saved on the disk and executed. Note that this command could use much more documentation here.

Hard Copy Plot
This command creates simple PostScript plots of the current data, and optionally sends the plots to a printer queue. The plots are generated according to the current display settings such as first contour height, number of contour levels, etc.

Info Window
This command pops up the **Info Window**, a text editing window used for displaying information such as file parameters.

Quit NMRDraw
This command exits the NMRDraw program; no confirmation to exit is requested.

THE DRAW MENU

Contours
Draws a 2D contour plot of the current data on the screen, using the current contour settings.

PixMap
Draws a 2D pixmap of the current data on the screen, using the current contour settings. It is used as the default mode for drawing mixed time−frequency mode planes.

Dot Plot
Draws a 2D dotplot of the current data. The dotplot is a display which shows intensity as a varying density of dots. It is used as the default mode for drawing time−domain data planes.

Clear Graphics
Erases the spectrum in the graphics area.

Erase Screen
Erases the entire screen, both inside and outside the graphics area.

2D Full Restores the full view of the current data plane.

2D Toggle
Toggles the 2D display on or off by changing the colormap.

2D Colors
Provides a pop−up for adjusting the range of colors used to display positive and negative data.

Estimate Noise
Estimates the standard deviation of the spectral noise, and resets the first contour height accordingly. Note that the estimate may be crude.

2D Limits
Provides a pop−up for selecting a data region in spectral units such as PPM.

2D Settings
Provides a pop−up for selecting various 2D drawing properties, such as whether or not to use grid lines.

THE MOUSE MENU

The **Mouse Menu** provides a list of functions that are performed interactively with the mouse, such as extracting and drawing 1D slices from the current data. Whenever the mouse is active, the topmost border of **nmrDraw** will report the functions of the mouse buttons. The buttons perform different actions depending on whether the mouse pointer is inside the spectral graphics region, or outside in the purple borders.

When a given slice is extracted with one of the **Mouse Menu** commands, several other commands can be used on it:

It can be kept on the screen with other 1D slices using the **Append 1D** command in the **1D Menu**.

It can be phase corrected interactively using the tools in the command panel.

It can be processed or inverse−processed using **NMRPipe Command** or **Auto−Process 1D** in the **Proc Menu**

1D Horizontal
Real−time extraction of 1D slices from the horizontal axis of the current display. Mouse functions allow real−time vertical offset and scale adjustment, and graphical selection of phase pivot.

1D Vertical
Real−time extraction of 1D slices from the vertical axis of the current display. Mouse functions allow real−time vertical offset and scale adjustment, and graphical selection of phase pivot.

1D Both
Real−time extraction of 1D slices from both the horizontal and vertical axis of the current display at the same time. Mouse functions allow real−time vertical offset and scale

adjustment, and graphical selection of phase pivot.

1D Z-Axis
Extraction of individual 1D slices from along the Z−Axis of the current display. This requires that a 3D or 4D data template is selected.

1D A-Axis
Extraction of individual 1D slices from along the Z−Axis of the current display. This requires that a 4D data template is selected.

2D Location
Real−time display of cursor location and the corresponding data value. Information is displayed in the topmost border of **nmrDraw**.

1D Zoom
Provides a zoom−box for selecting and expanding a region of the current 1D slice being displayed.

2D Zoom
Provides a zoom−box for selecting and expanding a region of the current 2D plane being displayed.

Exit Mode
Turns off the current mouse function.

THE 1D MENU

The **1D Menu** contains some commands which effect or relate to the 1D data being viewed.

Append 1D
Appends the current 1D slice to the list of slices which will be kept on the screen. This allows two or more slices to be viewed at the same time.

Delete 1D
Deletes all the 1D slices being viewed from the screen.

1D Full Restores the full view of the current 1D slice.

1D Toggle
Toggles the 1D display on and off.

Extract 2D H
(3D Data Only) Extracts the orthogonal 2D plane which corresponds to the horizontal 1D slice currently selected. The 2D plane will be extracted as a file called "ext.dat". The **File Menu** command **Previous Data** can be used to return to the original 3D data.

Extract 2D V
(3D Data Only) Extracts the orthogonal 2D plane which corresponds to the vertical 1D slice currently selected. The 2D plane will be extracted as a file called "ext.dat". The **File Menu** command **Previous Data** can be used to return to the original 3D data.

Axis Toggle
Toggles the 1D axis display on and off.

1D Settings
Provides a pop−up which adjusts the properties of 1D displays, including whether the zero−level is displayed.

THE PEAK MENU

The **Peak Menu** provides commands for automated and interactive peak detection in 1D-4D data. The peak detection is actually performed in the background by the **nmrWish** program. The commands in the peak menu are as follows:

Peak Detection
Activated the Peak Detection pop−up window. Use this window to view and adjust peak

detection settings, and to execute automated peak detect commands.

Draw Labels
Re−draws the peak labels; you can also use the

Erase Labels
Erases the peak labels; you can also use the

Peak Edit
Enters peak editing mode, described below.

THE PEAK DETECTION POP−UP

Peak Table:
Specifies the file name of the peak table to read or write.

Labels: Specifies what information is displayed by the peak labels. There is a pull-down menu to the right which lists the options. Note that peaks which have been identified as noise are always labeled with asterisks.

Read Reads the specified peak table; the peak table must already exist, and should have point coordinates which correspond to the current spectrum.

Write Writes the current peak table from memory to a file.

Clear Delete the current peak table in memory.

Edit This enables simple editing of the peak table in memory. In this version, there must already be a current peak table, either from "Read" or "Detect". When the "Edit" option is selected, the mouse can be used to insert, delete, or modify peak parameters. As with other mouse modes, the mouse button functions are given in the top border of nmrDraw. Once a peak table is edited, it should be saved using the "Write" option.

In the peak editing mode, the [Left] mouse button inserts a peak, the [Middle] mouse button can be used to adjust a peak value, and the [Right] mouse button will delete the nearest peak.

When using the middle mouse button to adjust a peak value, the value to be adjusted is the one selected for the label. This can be changed by the "Labels" option above. For example, if the assignment value "ASS" is selected for the label, you can modify the recorded assignment.

After clicking the middle mouse button over the peak to change, type in the new value followed by the <enter> key. Because of keyboard focus issues, you may have to move the mouse in and out of the graphics area before typing; using the −focus option of nmrDraw may help this.

Dimensions:
Sets the number of dimensions for the peak detection.

Settings ...
Activates the "Peak Detection Settings" pop−up, for specification of detection parameters described below.

Detect Select this button to detect peaks according to the current settings. This will be performed by creating and executing a new peak detection script "pk.tcl" in the current directory. Therefore, peak detection will only work if you have access permissions to create files in the current directory.

Done Use this button to dismiss the "Peak Detection" pop-up window.

PEAK DETECTION SETTINGS POP−UP

Filter Command:
The name of a command to execute after peak detection; when executed, the command will be given the name of the current peak table as its last argument. The intent of this option is to allow

special filtering of the peak table. For example, using the command "pkFilter.tcl" will generate a "simple" version of the peak table from the original one.

Chi2 Threshold:

This is a probability threshold for noise peak rejection by chi-square test. The chi-square test estimates the probability that the sum−of−squares intensity in the peak's neighborhood could be caused by random noise alone. To use this test, you must enter a reasonable "Noise:" value above. Increasing the chi2 threshold increase the rejection of peaks near the noise level. If the value is set to one or zero, no peaks will be rejected.

Noise: Enter an estimate of the standard deviation of the spectral noise here. The default value comes from an automated estimate. This parameter is used in the Chi-squared test to classify random noise peaks. It is also used to estimate errors in peak position due to random noise (parameters DX DY DZ and DA in the peak table).

Contour:

Specifies the minimum number of contour levels which define the "High:" and "Low:" peak detection thresholds.

High: The detection threshold for positive peaks. By default, it is set to the height of the first positive contour level in use when the "Peak Detection" pop-up window appears.

Low: The detection threshold for negative peaks. By default, it is set to the height of the first negative contour level in use when the "Peak Detection" pop-up window appears. If want want to detect positive peaks only, set this parameter to a large negative number.

DDX: ...

Size of the detection region in +/- points. A given point must be larger than all of the other points in this detection region in order to be detected as a peak.

IDX: ... Size of the parabolic interpolation region in +/- points. **IncX: ...** Defines how much of the spectral data is read into memory for peak detection. Values of zero will cause the entire spectral region to be read at once. Since some spectral data may be too large for this, it is possible to perform peak detection on automatically on overlapping regions. For example, if 3D peak detection is performed with a setting of IncX=0, IncY=0, IncZ=16, the data will be read and analyzed in 16−plane slabs. This will not effect determination of peak positions, widths, and heights, however it can effect the volume (VOL) and bounding region values (X1/X3 etc).

Local Noise:

By default, the Chi-square noise classification scheme uses a uniform noise estimate for all parts of the spectrum. Selecting one of the X Y Z or A checkboxes will allow for an adaptive noise estimate with respect to the selected dimension. This can help compensate for noise ridges. **Special Options** Currently, these options select how noise peaks are identified and handled:

Sinc Detect If this option is selected, the peak detection module will attempt to identify peaks which are due to truncation noise (sinc artifacts).

Reject Noise Peaks If this option is selected, any peak classified as noise (either random noise or truncation noise) will be automatically eliminated from the peak table.

Sinc Detect Parameters

The peak detection module attempts to identify truncation artifacts based on the details of window function and zero filling which were applied to each dimension of the data. By taking this information into account, it is possible to estimate for a given peak how far truncation wiggles would extend in each dimension before falling below the detection threshold. **XAdj: ...** In the artifact detection procedure, the height and extent of the truncation peaks are modeled as a profile which decreases as 1/X, where X is the distance from the peak center, and in order for a small peak to be classified as the truncation artifact of a larger peak, the smaller peak must fall below the profile. This value is used as a multiplying factor to increase or decrease the overall profile height. **XTol: ...** In order for a small peak to be classified as the truncation artifact of a larger peak, the two

peaks must align along a given dimension. This value specifies the tolerance in points for deciding whether two peaks are aligned. **XLW: ...** A rough estimate of the original linewidth in Hz in a given dimension before any window function was used.

Save Script
Selecting this command will save a new version of the peak detection script "pk.tcl" without executing it.

Done Use this button to dismiss the "Peak Detection Settings" pop-up window.

PEAK TABLE PARAMETERS

INDEX the unique peak ID number.

X_AXIS ...
the position of the peak in points, by parabolic interpolation.

DX ... estimate of the error in peak position due to random noise, in points.

X_PPM ...
the position of the peak in PPM, by parabolic interpolation.

X_HZ ...
the position of the peak in Hz, by parabolic interpolation.

XW ... the full width at half height in points, estimated by parabolic interpolation.

XW_HZ ...
the full width at half height in Hz, estimated by parabolic interpolation.

X1/X3 ...
coords of the bounding region surrounding the peak or its cluster in points.

HEIGHT
the peak height, estimated by parabolic interpolation.

DHEIGHT
the error peak height due to random noise, estimated by parabolic interpolation.

VOL the peak volume, estimated as the sum of intensities in the neighborhood of the peak maximum.

ASS location to hold assignment data.

PCHI2 the chi-square probability for the peak (i.e. probability that the peak could be due to random noise alone).

CLUSTID
identifies the cluster of peaks that a given peak overlaps. Peaks with the same CLUSTID value are considered to be in one overlapped group.

MEMCNT
the total number of peaks which are in a given peak's cluster (i.e. peaks which have the same CLUSTID value).

TYPE An integer describing the peak classification; currently 1 = Peak, 2 = Random Noise, 3 = Truncation artifact.

THE PROC MENU

The **Proc Menu** provides two ways to process the current 1D slice, as explained here:

NMRPipe Command
Provides a pop–up window for executing individual **nmrPipe** processing functions on the current 1D slice. To perform processing, enter the name of an nmrPipe function on the given command line, along with any additional arguments; For instance, "ft -inv" would be the command for inverse Fourier transform. As an alternative to typing the function and arguments, a small menu of common functions is provided. Once the function is entered, execute the processing by typing a carriage return, or by clicking the **Execute** button.

Auto-Process 1D

This command will execute a pre−defined macro which is responsible for processing the current 1D slice. The macro used is specified by the command−line argument **−proc** in the **nmrDraw** script. The default version of the macro will apply a window, zero fill, and FT to time−domain data; if the axis name is "HN", a solvent filter and extraction of an amide chemical shift range will also be applied.

In the case of frequency−domain data, inverse processing will be applied, automatically restoring the current 1D slice it to its original time−domain form as best as possible.

FILE OPTIONS

−in *inName*
Default Input Name, reads data on start−up.

−dir dirName
Default input directory.

−file fileExp
Expressions for directory list filter.

−name defName
Default Input Name, does not read data on start−up.

−text textDir
Help Text Directory.

−read Auto−Read on Startup.

GENERAL OPTIONS

−cellX *xPix*
Character Cell Width.

−cellY *yPix*
Character Cell Height. **−type1** *size* General specification for the NMRDraw ordinary font; use keywords "small", "medium", "large", or "extraLarge".

−type2 *size*
General specification for the NMRDraw large font; use keywords "small", "medium", "large", or "extraLarge".

−square
Make the spectral graphics area square.

−track When a mouse mode is turned on, the default 1D location tracks the mouse.

−focus If this option is used, NMRDraw will attempt to get the keyboard focus automatically, making tasks such as peak editing easier.

−scroll Use Scrollable Panel.

−repaint
Force Manual Repaint Mode.

−norepaint
Avoid Manual Repaint Mode.

−frp First Repaint Count.

−dbg Debug Message Level.

−verb Toggle Verbose Mode On.

2D DISPLAY OPTIONS

−draw Auto−Draw with Read.

−clear Auto−Clear when Drawing.

−frzLevels
Freeze Contour Levels: Always Sometimes Never

−frzZoom
Freeze 2D Zoom Region: Always Sometimes Never

−autoScale
Auto−Calc Contour Level.

−grid Draw Grid Lines.

−pix PixMap Display is Default.

−image Image Display Setup.

1D DISPLAY OPTIONS

−vert Enable Vertical Plots.

−zero Draw 1D Zero Level Line.

−cursor
Draw 1D Position Cursor.

−relative
Relative 1D Scaling.

−compress
1D Display Compression.

COORDINATE OPTIONS

−iz Z−Plane Number.

−ia A−Plane Number.

PROCESSING OPTIONS

−func fnTab
Function Table Name.

−proc script
Processing script used for automatic 1D processing.

−nosys Suppress system calls.

−zfht Enable temporary zero fill with Hilbert transform.

CONTOUR LEVEL OPTIONS

−mult contFactor
Contour Level Factor.

−plev numLevels
Number of Positive Levels.

−nlev numLevels
Number of Negative Levels.

−hi firstHeight
First Contour Height.

2D DRAWING COLOR OPTIONS

−plot plotMode
Color mode for hard−copy plots; these will be selected from inside the program in future versions:
1 = Black and White
2 = Gray Scale (Not supported yet)
3 = Color

2D DRAWING COLOR OPTIONS

−pcc numColors
Positive Color Count.

−pHue1 hue
Positive colors, First Hue [0−1].

−pHue2 hue
Positive colors, Last Hue [0−1].

−pSat1 saturation
Positive colors, First Saturation [0−1].

−pSat2 saturation
Positive colors, Last Saturation [0−1].

−pVal1 value
Positive colors, First Value [0−1].

−pVal2 value
Positive colors, Last Value [0−1].

−ncc numColors
Negative Color Count.

−nHue1 hue
Negative colors, First Hue [0−1].

−nHue2 hue
Negative colors, Last Hue [0−1].

−nSat1 saturation
Negative colors, First Saturation [0−1].

−nSat2 saturation
Negative colors, Last Saturation [0−1].

−nVal1 value
Negative colors, First Value [0−1].

−nVal2 value
Negative colors, Last Value [0−1].

1D/2D OVERLAY DRAWING OPTIONS

−XOR XOR Drawing Keyword: Always Sometimes Never

−svri Server Image Color Palette.

−colors clrList
Color Name List.

−color0 zeroClr
Zero Line Color.

−color1 1dClr
Active 1D Plot Color.

−colorC cClr
Cursor Bar Color.

−colorG gridClr
Grid Line Color.

−colorX xClr
X−Axis 1D Plot Color.

−colorY yClr

Y−Axis 1D Plot Color.

−colorZ zClr
Z−Axis 1D Plot Color.

−colorA aClr
A−Axis 1D Plot Color.

−colorL lClr
Label Color.

−colorE eClr
Background Color.

Color Name Options:

`black`	`red`	`orange`	`yellow`
`green`	`blue`	`violet`	`cyan`
`magenta`	`lightGray`	`dimGray`	`white`

LEGAL NOTICE

This program and its related software is provided "as is". The NIH, the Laboratory of Chemical Physics, NIDDK, and the authors make no warranties, either express or implied, as to any matter whatsoever with respect to the software. In particular, any and all warranties of merchantability and fitness for any particular purpose are expressly excluded. In no event will the NIH, the Laboratory of Chemical Physics, NIDDK, or the authors be liable for any loss of profits, any incidental, special, exemplary, or consequential damages of any nature whatsoever (including without limitation, loss of use or other commercial or research loss) arising out of or relating to the use or performance of the software.