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This file describes commands accessed via the Main menu. It is recommended to enable the "Help Balloons" option. Additional Info can also be found using the "Help Starting" command, which explains how to setup a configuration file, save settings and reload an already defined configuration.

When starting, the best is to create a working directory. The next step is creating contour files, using sgi2cindy program utility, or from Gifa using the fplot command, or from Cindy reading a 2rr Bruker file and writing contours to a file. When all the needed contour files are created (like COSY, TOCSY and NOESY contours) then manual peak picking can be done.

A Peak layer must be created for each experiment type, i.e. one for the TOCSY/COSY and one for the NOESY type. One way for doing this is to use the Peaks New Menu, setting the Layer name and the file name with strings like "noesy.pks" and "tocsy.pks" to avoid confusion. At that stage these files are empty, and the peak picking is done using the "Tools" window, just by drawing simple lines starting at the center of each cross peak. When all peaks have been marked (peak annotation), a spin system file can be used. A sample file is found in the EXAMPLES directory and contains all the KEY words. Using the "SpinSys New" Menu just creates a minimal spin system layer (without the KEY words needed for sequential assignments) and is more simple to handle than the complete one. The extra KEY words can be added later.

A first utility is the "Peaks Build SpinSys" from the Menu which starts from a selected peak annotation in the finger print region (HA-HN cross peak) and extends it in 2D dimensions to find aligned annotations. Of course the selected Peak Layer must be the "tocsy.pks" layer, and only one Peak annotation should be selected from this layer. The "Peaks Build SpinSys" Menu creates a group of new lines, which make a 2D grid where each crossing shows an expected cross peak correlation. Since in the previous steps all COSY/TOCSY peaks have been peak picked this utility also counts the number of cross peaks found versus the number of cross peaks expected. The score value is displayed in the "Group name" field using the "Peaks Info" Menu which shows information of the selected Peak annotation or group of annotations. When the score is good enough the chemical shift values must be copied in the textual clipboard using the "Peaks Copy" menu. Adding these ppm values to the spin system layer is a matter of text editing. The spin system editor is opened by "SpinSys Edit" menu, and has copy/paste functionality.

Sequential connectivities can also be search starting from a spin system Layer and a "noesy.pks" peak layer. This can be done only if NOE and FIND key Words are found in the spin

system Layer file (refer to section 3.4 for details). This functionality is accessed via the “SpinSys Connect” menu. Chemical shifts of the sequential HN is displayed in the NOE columns and must be visually controlled before adding the chemical shift value of the sequential HN in the NEXT column of the spin system file. Connecting spin systems together according to sequence information is done by using the “SpinSys Connect sequence” Menu.

Translation from assigned NOE Peak annotations to constraints requires a PDB file, which is only used to get atom names. This PDB file can be build from X-plor or Dyana without any constraints and must contains the residues named and numbered according to the spin systems. Five Upper bounds classes are recognized by default and they are encoded from the Line width of the NOE Peak annotations. Pseudo atom corrections are automatically calculated.

Theoretical NOEs can be displayed (1/r⁶ approximation) from a calculated structure and superimposed on the spectra (Section 4.1).

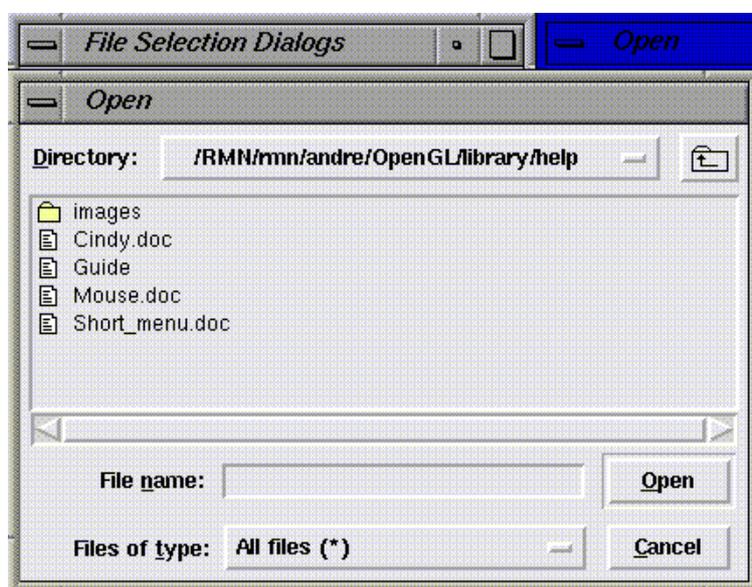
1. Spectrum

This menu is used to read, write and manage spectra. The “Reduction” item is specific to 2D spectra and allows fast overview of the spectral area.

1.1. Open

Shows the File Selection Dialogs which is the same used when opening any kind of file.

- a) Enter the name of the file to open or Browse ...
- b) Give a name for the Displayed Layer ...
- c) Select the Format. By Default All Types will be recognized ...
- d) Click to Open the File ...



There are two windows : the Open window is used to selected the files and test if they can be accessed by the user. The other is the File selection Dialogs window used for file reading.

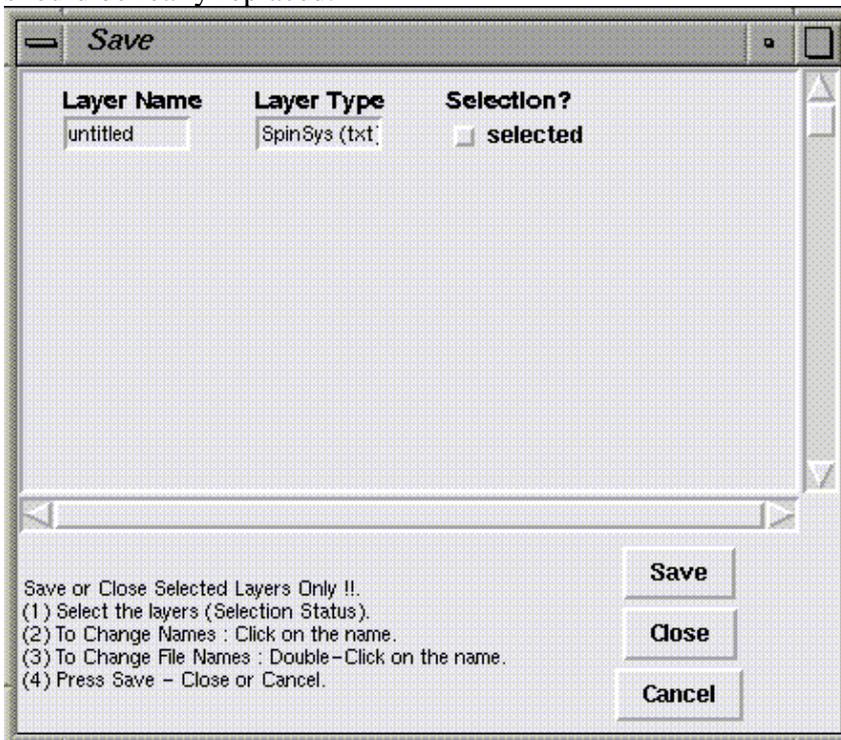
Files are opened in two steps, first file selection is done within the Open window (click Open to select one file – this just try to see if it can really be accessed). Then from the “File Selection Dialogs” window click Open. This will check for file types and will open the file adding it to the Layer stack.

1.2. Save & Close

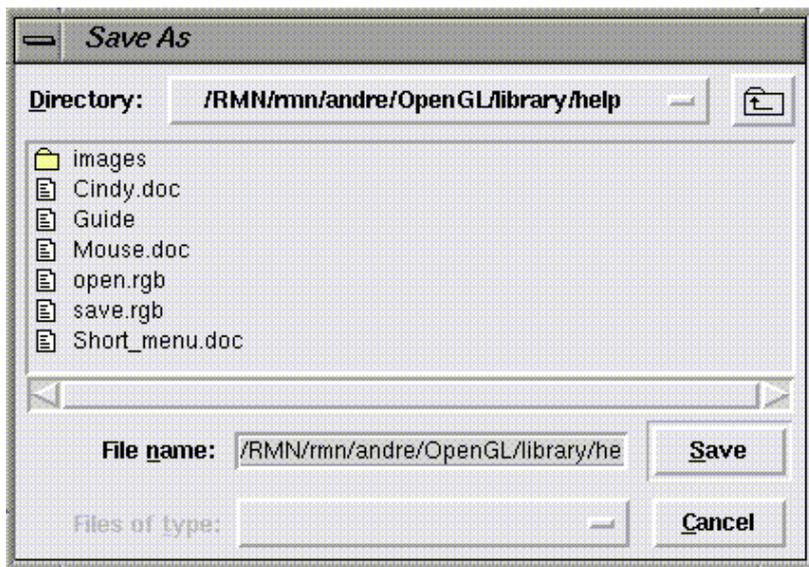
Shows a file selection dialog used to Save **or** Close loaded layers.

- a) First select the layer(s) to save or close
- b) Double-click on the name to change the file name & return
- c) Click on Save or Close button

Normally steps “a” and “c” are sufficient to save or close loaded layers. With step “b” a new window shows up which requires a file name. If the file already exists then the user is asked if it should be really replaced.



Step “b” is used to change the file name associated to a given layer.

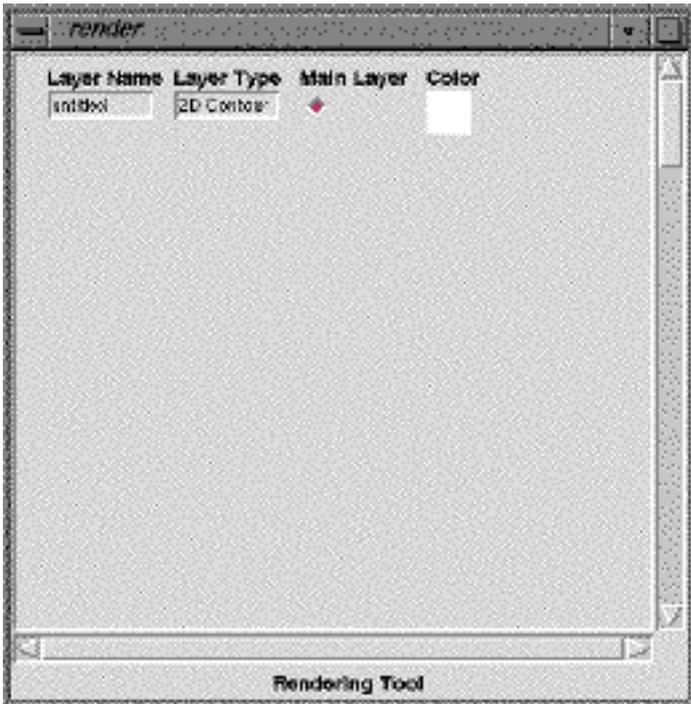


1.3. Render

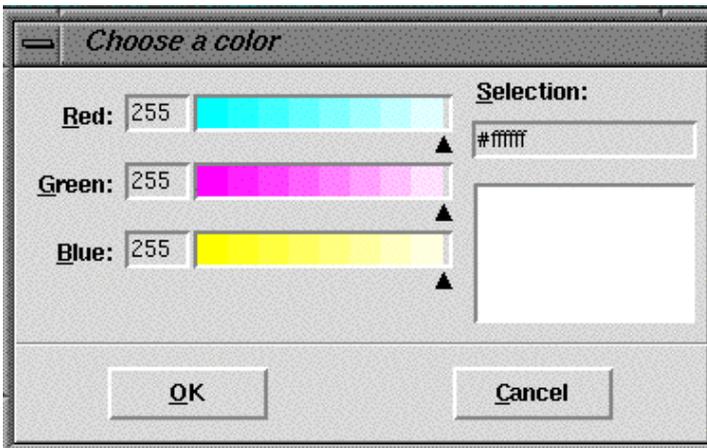
This menu is used to change color setting and to define the main layer.

To change the color, you must click on the small colored square and select a new color. The changes are updated only for contour layers. By default the main layer is the first loaded contour. This setting may be changed by selecting a new main layer.

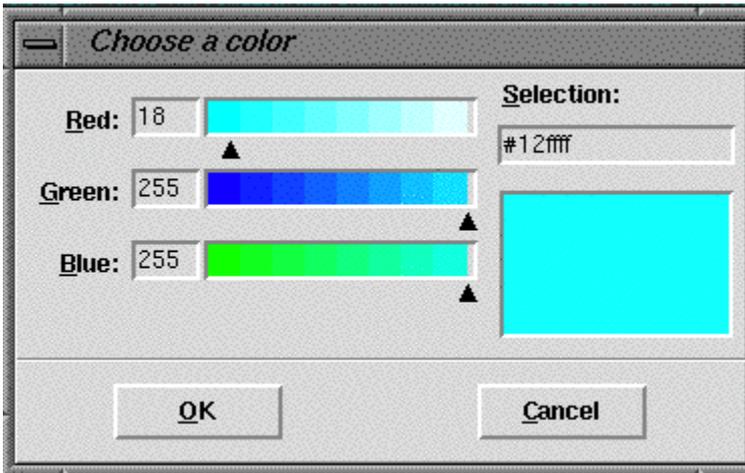
The window is divided in 4 columns (Layer Name, Layer Type, Main Layer, Color). The Layer Name and Layer type give the name (string) and the type (contour2D, annotation layer, spin system, PDB molecule). The Main layer field indicates the reference layer from which all other layers transformations are set (horizontal and vertical scales and translations) and ppm scales attached to.



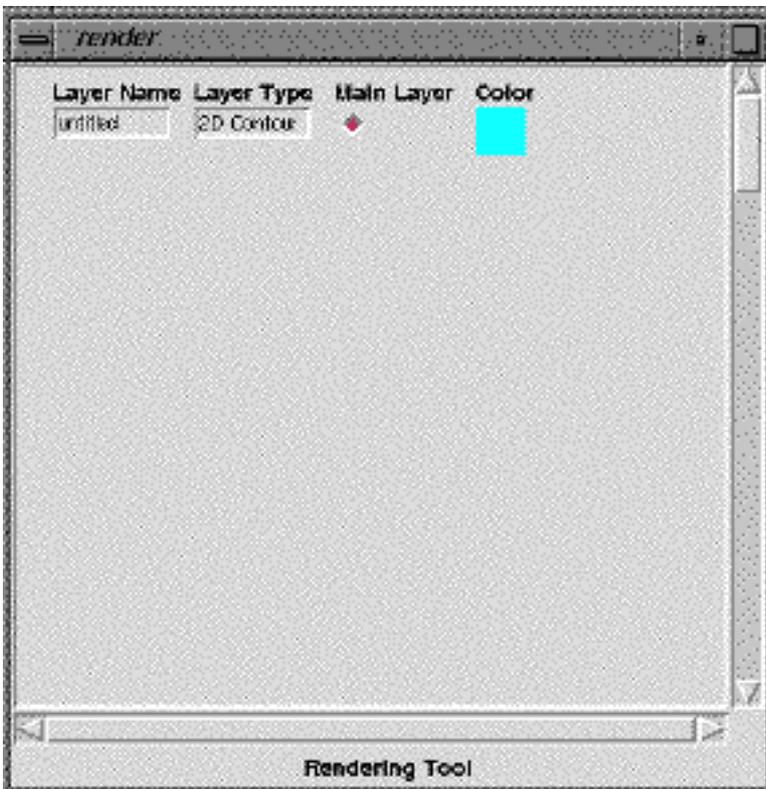
From the “render” window it is possible to Change the color settings. Just click on the square in the Color column. This opens a new window for choosing the color.



I selected light blue.



And pressed OK. The 2D contours are now displayed in the graphic window in blue color.

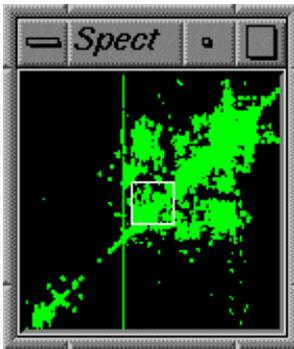


NOTE : The first “2D contour” is set by default to be the “Main Layer” (to which ppm scales are attached).

1.4. Reduction

Opens a spectrum reduction window corresponding to a snapshot of the main layer.

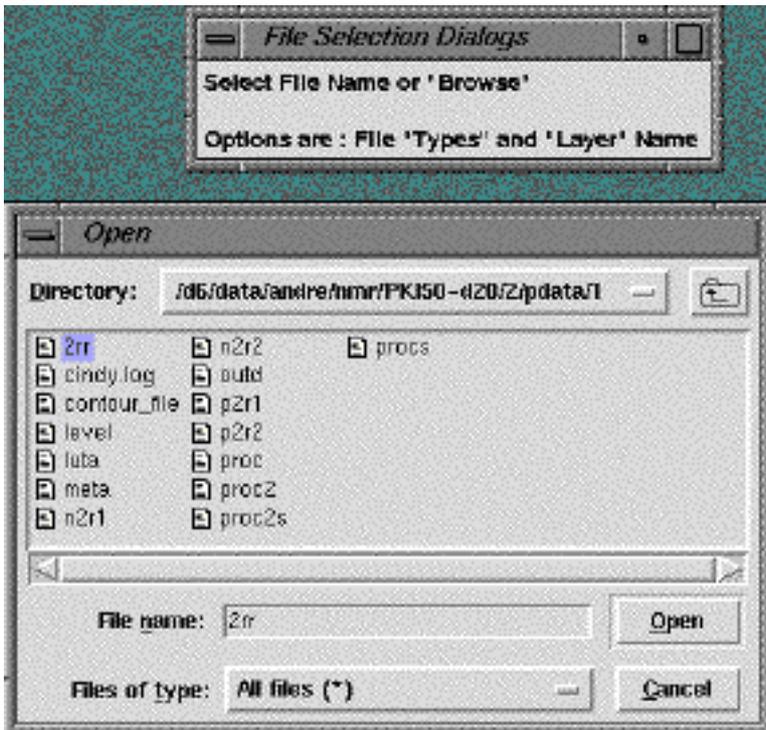
It is useful to zoom in/out and gives an overall view of the spectrum. Click the left button to center the zoom area. Click middle button and drag it to define a new zoom area.



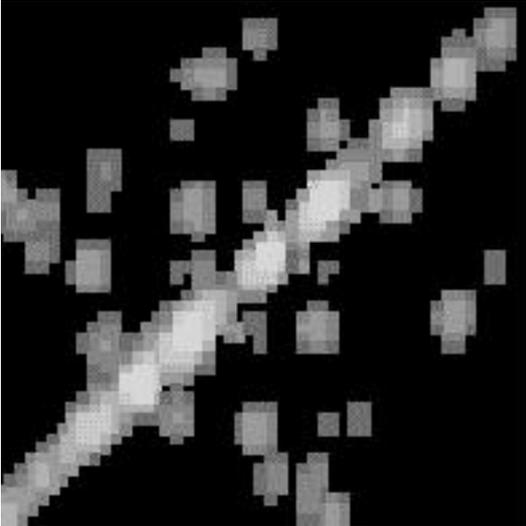
1.5. Levels

Opens a double column window to selected negative and positive levels. This is enabled when a 2D Bruker file is open. To view the new levels click on “Levels” . To compute contours click “Contours”.

The first step is to open a Bruker file (the 2rr file)



Click Open in the “Open” Window, then Open again in the “File Selection Dialogs” window. The spectrum will appear as intensity pixels in the main graphic window.

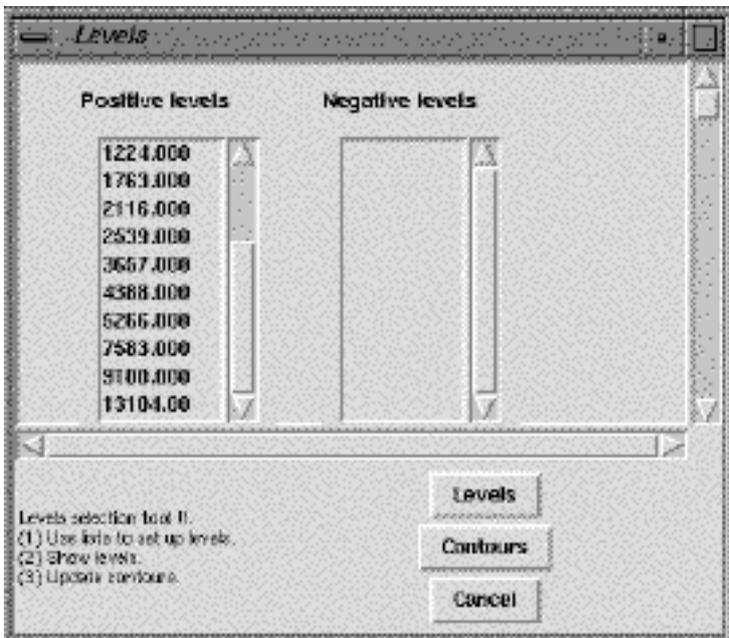


This is a black and white snapshot of a spectrum (intensity mode).

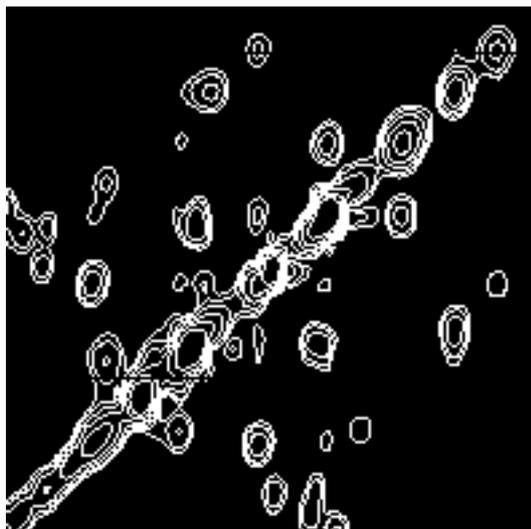
Levels from the Bruker level file are shown by default.

NOTE : levels are updated using the DEF PLOT command in Bruker software.

Double-click the left button to edit a new level. Double-click with the right button deletes the selected level. To show the new levels in the graphic window use the “Levels” button.



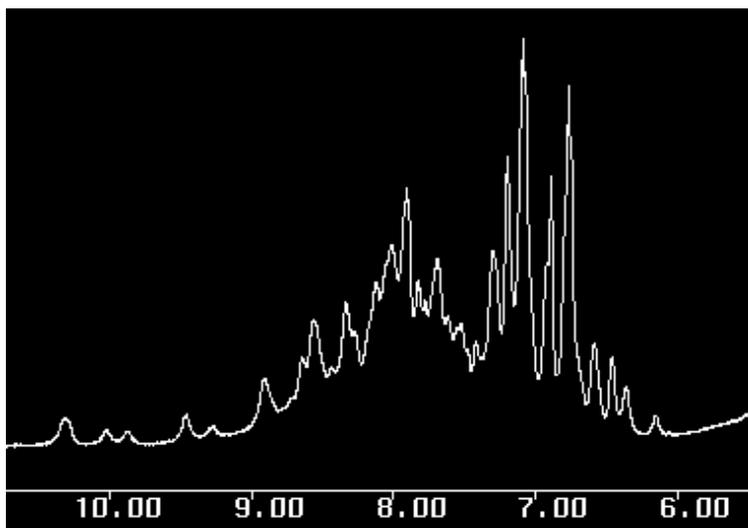
When the levels are those wanted by the user, clicking “Contours” makes a contouring with the selected levels, and contours should look like this :



Same spectrum in contour mode. This 2D contour Layer can now be saved on disk.

NOTE : Don't forget to change the file name before saving this contour file.

How looks a 1rr Bruker file :



2. Peaks

This menu is used to read, write, to create a new annotation layer and to get information about the selected annotation. There is no peak-picking facility in Cindy. The Peaks format file is simple and peak files from other software can be converted to Cindy Peaks Files.

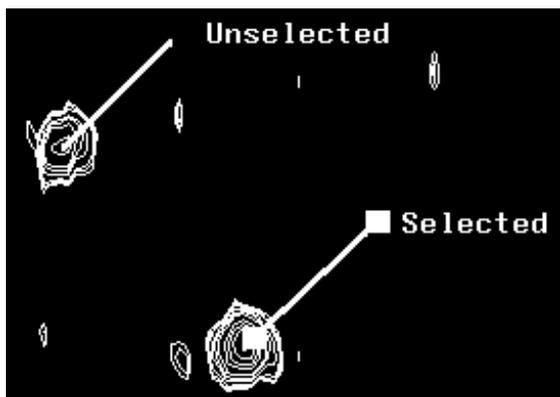
Example of conversion from Pronto Peak file to Cindy file:

Using Unix awk with the following format specifier:

```
{printf("%8.3f%8.3f%8.3f%8.3f 255 255 255 1 1 0%s\n",-$2,-$3,(-$2+0.01),(-$3+0.01),
$6$7$8$9)}
```

This just prints four real number using columns 2 and 3 from the input file; since the Pronto format just give the peak coordinates the end of the line is assumed to be at x+0.01 and y+0.01 ppm. The peak label is done by gluing together the fields 6 to 9 from the input pronto file.

Cindy Peaks are just visualized by lines starting from the center of a cross peak. A label can be added to a line. The next picture shows two lines, one selected and the other not selected.



It is possible to draw other things (not just lines) like rectangles and circles, but this is really not useful to annotate contours.

NOTE : Assignments for 2D NMR (essentially NOEs) must follow the syntax :

```
ATM_1(RES_1)ATM_2(RES_2)
```

Where : ATM_1 is the spin's name in dimension 1 (vertical)

RES_1 is the residue number in dimension 1

ATM_2 is the spin's name in dimension 2 (horizontal scale)

RES_2 is the residue number in dimension 2

Example : sequential alpha-NH NOE between residues 12 and 13

```
HA(12)HN(13)
```

Example : long range NOE between residues 12 and 44

```
HD2(12)HG1(44)
```

In the case of NOEs it is useful to set the line width according to the cross peak class (small, medium and big NOE)

Line Width	Upper Bound	When
1	4.8	really small peaks (spin diffusion ?)
2	4.4	small peaks
3	3.6	medium
4	2.8	big NOE peaks
5	2.4	Those found in beta sheets (sequential HA-HN)

2.1. Open

Shows the ``File Selection Dialogs''. Refer to section 1.1 for details.

2.2. New

Create a new annotation layer. The user is asked to give a name to this layer. This name is used to set the file name as well. Note that no file is created at this point.



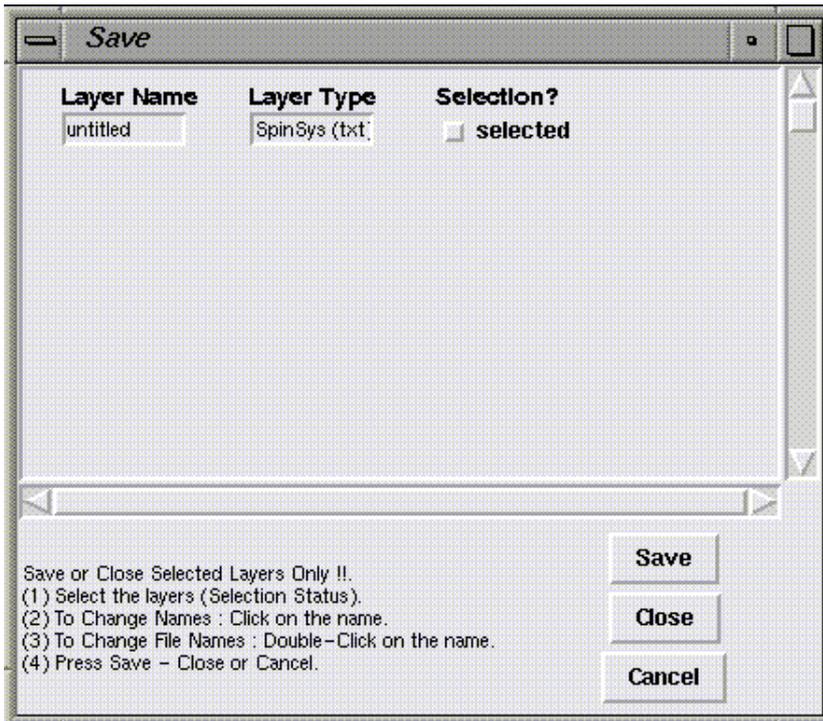
You must enter a layer name. This name will be the file name as well.



2.3. Save & Close

Shows the ``Save Selection Dialogs''. First select the layer(s) then choose the “close” or “save” option. Refer to section 1.2 for details.

NB : If you want to change the file name, just double-click on the Layer Name.



2.4. Undo move

Undo only the last displacement for selected annotations.

2.5. Copy

Copy ppm values of the last selected annotations to the textual clipboard.

2.6. Paste

Paste the selected annotations. It makes a Copy of the annotations from previously copied ones.

2.7. Cut

This is equivalent to Copy first and then Clear the selected annotations.

2.8. Clear

Really remove selected annotations. There is no way to retrieve them;

2.9. Select all

Select all annotations from the actual selected layer. If more than one layer is selected, this applies to the last used layer.

2.10. Unselect all

Remove selection status.

2.11. Group

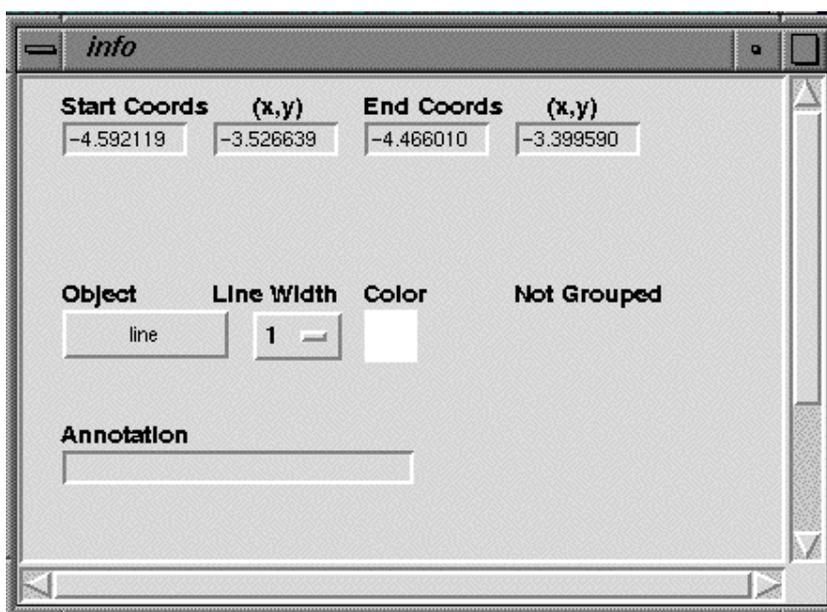
Make a group from the selected annotations. The group name can be set using the “Peaks Info” menu.

2.12. Ungroup

Remove the group and revert to individual annotations.

2.13. Info

Shows the Info window to display parameters of the selected annotation. All parameters can be modified in this dialog box. The top line correspond to (x,y) coordinates of the beginning and the end of the annotation (line), or the lower-left, upper-right corner of a rectangle.



NOTE : if the peak annotation belong to a group then the Group name can be edited, otherwise the it is called “Not Grouped”.

2.14. Build SpinSys

This menu builds a group of annotations (vertical and horizontal grid) starting from a previously ensemble of selected annotations. This is useful to test if they belong to a spin system, since cross peaks are expected to occur at each corner in the grid.

2.15. Assign

Not implemented in the new version

3. SpinSys

This menu is used to read, write, to create a new spin system layer, to edit, to display and to build Spin Systems.

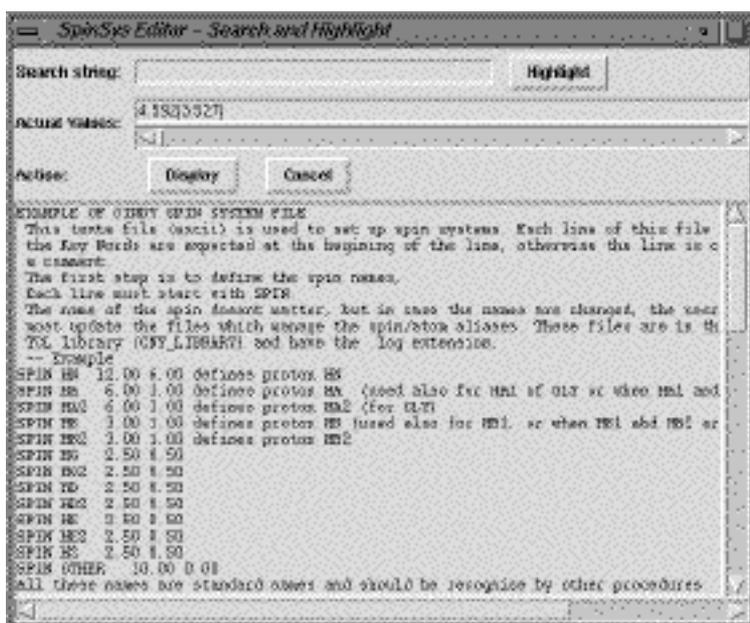
3.1. Open

Shows the "File Selection Dialogs" to open the spin system file. Refer to section 1.1 for details.

3.2. New

Create a new spin system layer with the default name "SpinSys" and a default file name "new_spin_systems". Note that no file is created at this stage.

The spin system editor should look like this:



NOTE : The spin system layer which is created by default has no NOE fields in it. This is to keep the line length short enough. Other SPIN fields can be added. Refer to section 3.4 for details.

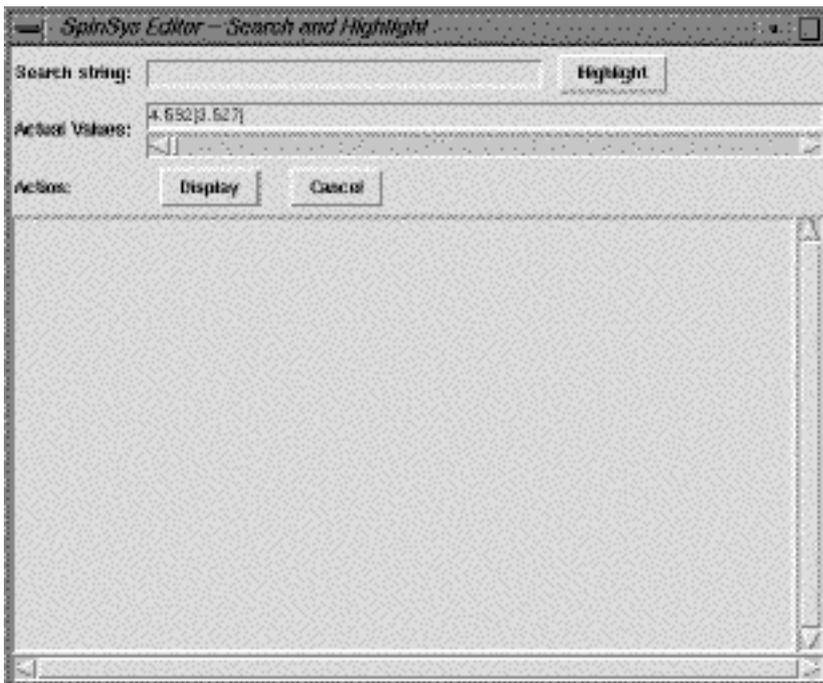
3.3. Save

Shows the "Save Selection Dialogs". First select the layer(s) then choose the "close" or "save" option. Refer to section 1.2 for details.

3.4 Edit

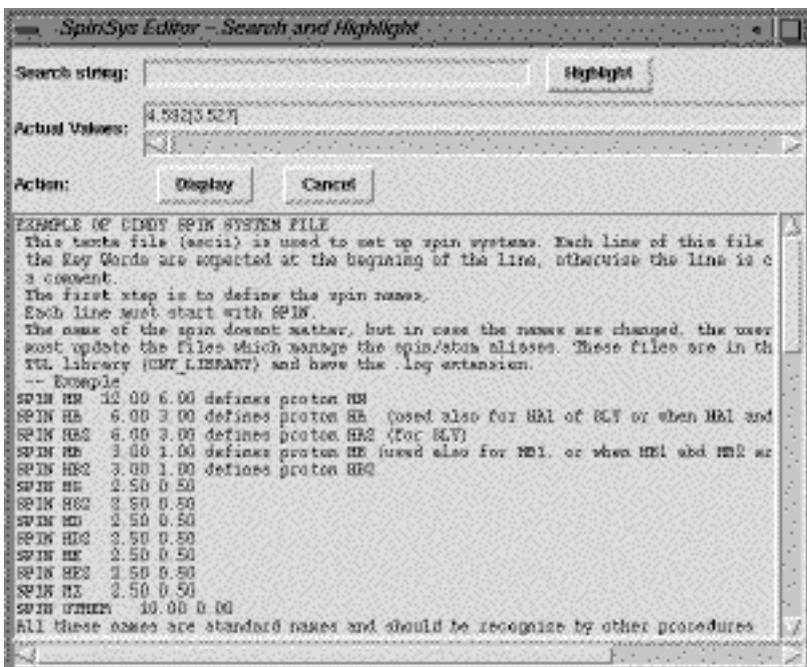
Open the spin system editor. This is a text editor with the spin systems arranged by columns. The search string allows for highlighting the occurrences of a given string in all the text. Can be used to search all occurrences of an amino-acid ... The Actual Values field displays the content of the textual clipboard. These values are those of selected annotations which have been previously Copied or Cut. These ppm values can also be accessed by a right-click in the text window. To update the change, click the "Display" button.

Just the ppm values from a peak (using the Peaks Copy menu).



There is nothing in the text window if no spin system file was previously read or created using the "SpinSys New" menu.

After SpinSys new the SpinSys Editor Window should look like this :



The syntax rules applied to the text is done according to the following list of KEY words (in capital letters). Recognized Key Words :

SPIN, COLOR, NOE, SEQUENCE, WORDS, SET, END, RESIDU, NUMBER, DISPLAY, LABEL, NEXT, FIND.

The first step involves the definition of the spin names which is done by a line starting with the key word SPIN.

This is shown in the next example which defines something called HN which is expected to occur between 12 and 5 ppm.

SPIN HN 12.00 5.00 defines proton HN (12.00 and 5.00 specify the ppm range allowed for NH)

Other examples are

SPIN HA 6.00 2.50 defines proton HA (used also for HA1 of GLY or when HA1 and HA2 are superimposed)

SPIN HA2 5.00 3.00 defines proton HA2 (for GLY)

SPIN HB 4.00 1.00 defines proton HB (used also for HB1, or when HB1 and HB2 are superimposed)

SPIN HB2 4.00 1.00 defines proton HB2

Colors are defined by a line starting with the key word COLOR. The white color is default, i.e. if a color is not defined but is still used then the program takes by default the white color. The next line shows how to define the red color, its name is "red" and 255 0 0 numbers is the corresponding RGB code.

COLOR red 255 0 0 defines red color

Other examples

COLOR green 0 255 0 defines green color

COLOR blue 0 0 255 defines blue color

COLOR cyan 0 255 255 defines cyan color

NOEs are defined when the line starts with the key word NOE. The first argument is the name to be used to define the NOE. The second and third arguments are the names of the two spins which are involved in the NOE. These two spins must have been previously defined with a SPIN definition. The last argument is a number which corresponds to the position in the stack (in case of multiple possible assignments). For example defining a sequential alpha to NH NOE, and asking to select the closest in ppm (first position corresponding to the best fit in ppm) is done by the line:

key word noe name 1st spin 2nd spin position in the list

NOE dan HA HN 1

Other Examples

NOE dbn HB HN 1 defines sequential noe dbn (id)

NOE dnn HN HN 1 defines sequential noe dnn (id)

NOE dan1 HA HN 2 defines sequential noe dan (the second possibility)

NOE dnn1 HN HN 2 defines sequential noe dnn (id)

Definition of the sequence is done in one or several lines. Each line must start with the key word SEQUENCE. Each of the words after the key word SEQUENCE are added to the sequence array and are supposed to correspond to the names which will be found in the RESIDU column.

SEQUENCE ALA ALA

The sequence continues in the next line

SEQUENCE GLY ASP LEU ARG ASN PHE

The total sequence will be (ALA ALA GLY ASP LEU ARG ASN PHE)

The start of the real data block (i.e. spin systems) is done when the line starts with WORDS. Then the program expects ONLY !!! key words on this line with the following Rules !!

Generic KEY words must be present as well as all SPIN names and all NOE names. This is shown in the following line :

WORDS RESIDU NUMBER HN HA HA2 HB HB2 DISPLAY LABEL COLOR dan dbn dnn an1 dnn1 NEXT

Note that ALL PREVIOUSLY DEFINED SPINS AND NOES MUST APPEAR ON THE WORDS LINE" IN ANY ORDER.

Then each spin system is defined by a line which must start with the SET key word otherwise it will not be processed. Key Words within each column for a given spin system have the following code :

RESIDU	NUMBER	DISPLAY	LABEL	COLOR	NEXT
ANY	ANY	ANY/CROSS	1+2	USER	FIND
STRING	STRING	BOXES	1 or 2	DEFINED	ANY

NOTE: ANY means that any string may be used. If the decoder expect a key word and if it is not recognized then no action will be taken. For example if the user does not use CROSS or BOXES in the DISPLAY field then the corresponding SET will not be displayed on the screen.

Key words 1+2, 1 and 2 in the LABEL column are used to display spin systems names according to what is found in the RESIDU and NUMBER columns. The Key word FIND in the NEXT column tells the program for searching NOEs when the "cy_spin connect" command is selected from the menu (See SpinSys Connect di-peptide Menu).

The program stops processing when the key word END is found. This key word is optional and is useful only when a fragment of the text needs to be processed. This is mainly the case when several experimental conditions are used and thus spin systems exist in multiple copies within the same file.

A simple example of SET lines is shown below :

WORDS	RESIDU	NUMBER	HN	HA	HA2	HB	HB2	DISPLAY	LABEL	COLOR	dan	bn	dnn	dan1	dnn1	NEXT
SET	ALA	1	10.22	4.30	----	1.40	----	CROSS	OFF	white	---	---	---	---	---	FIND
SET	ALA	2	9.22	4.20	----	1.50	----	BOXES	1+2	red	---	---	---	---	---	---

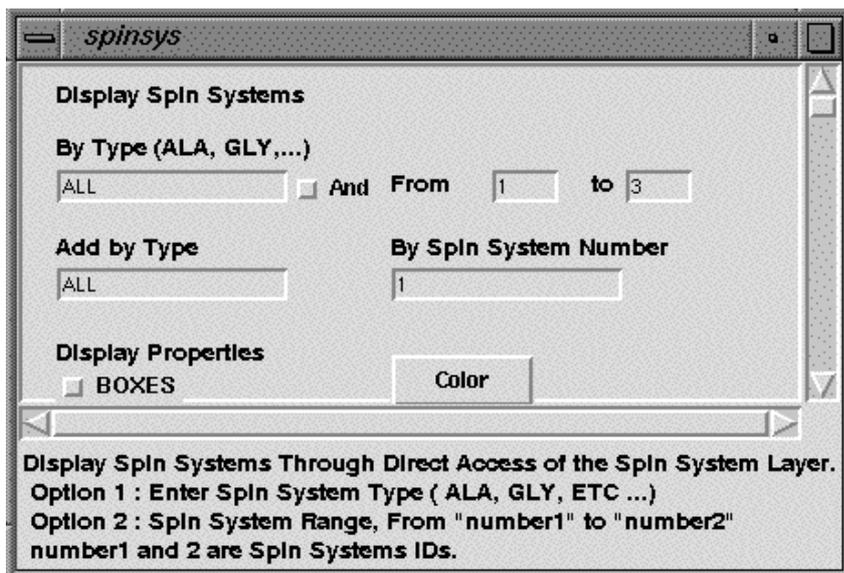
With this three lines two spin systems will be displayed. The first one, named ALA 1, will appear on the screen in white color crosses without labels. The second spin system named ALA 2 will be displayed with red lines and labels will be present at the intercepts of each line. Issuing the "cy_spin connect" command (or using the SpinSys connect di-peptide menu) will search for dan, dbn, dnn, dan1 and dnn1 NOEs for the first spin system. See "cy_spin connect" topic for more details or refer to section 3.7.

3.5 Show

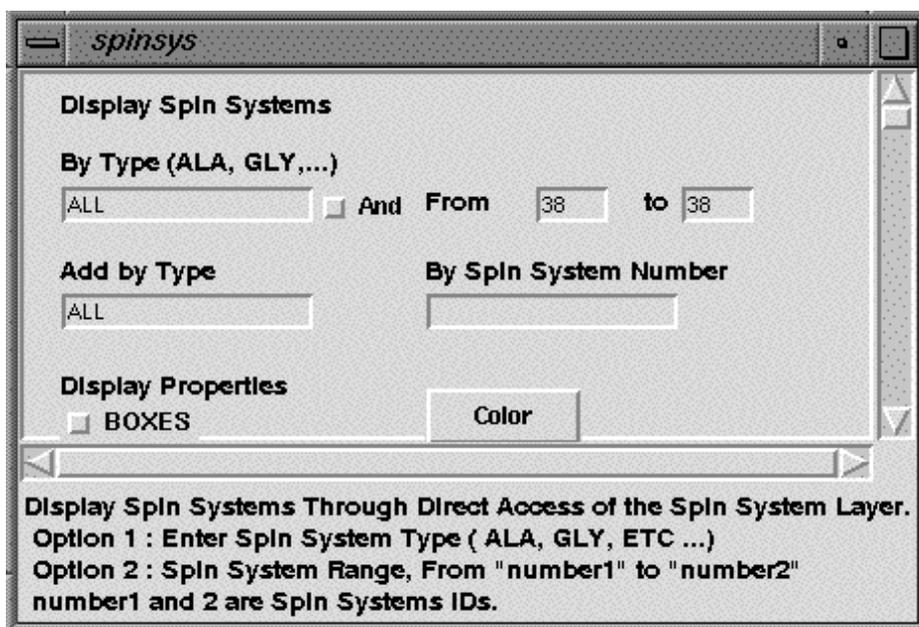
Shows the spin system selection window. It is used to display one or more spin systems, and change the color and display options.

Before using SpinSys Show, you must first edit and display the spin systems using the SpinSys Edit menu and click the Display button.

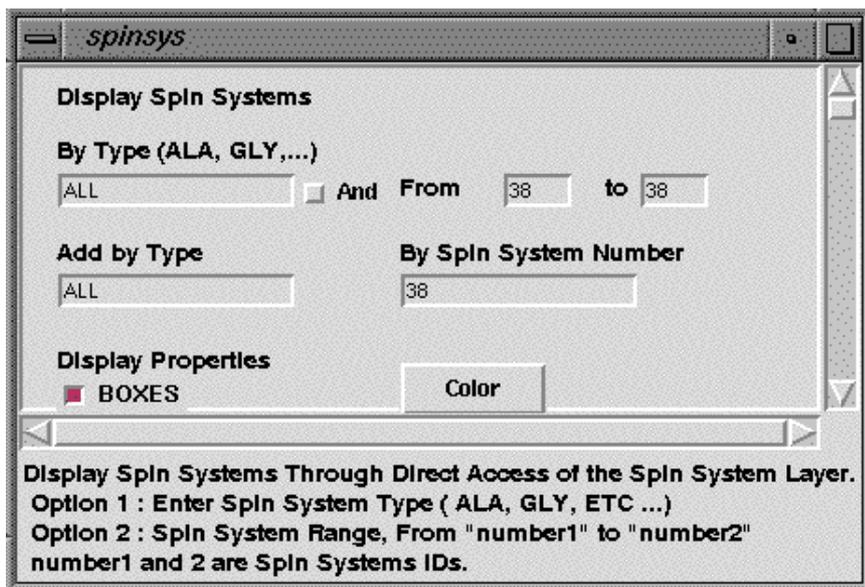
Within this window opened by the SpinSys Show menu the changes are not updated to the spin system layer. They are volatile. This allows fast display changes without editing the spin systems themselves.



I want just to see residue 38.

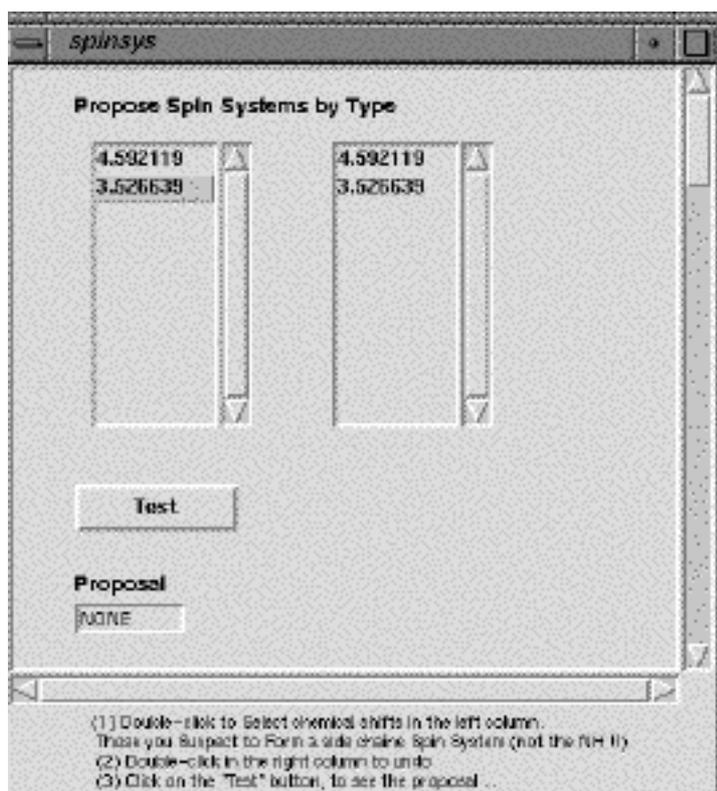


I want to see lines connecting chemical shifts for the spin system of residue 38.

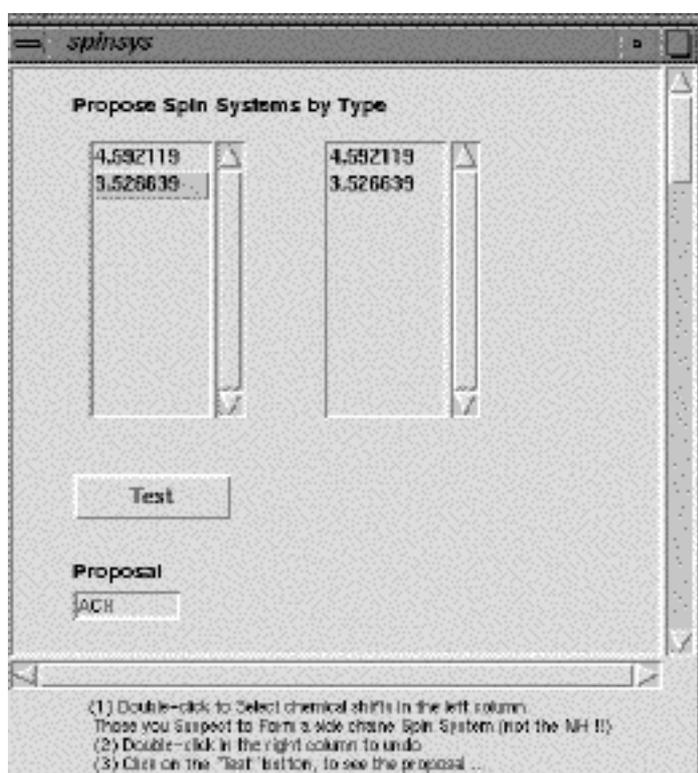


3.6. Test

Shows a double column window. The left column has the chemical shifts of all selected annotations. Mouse clicks allows selection/deselection of the side-chain chemical shifts starting from the Calpha chemical shift as the root chemical shift. Selected chemical shift values appear in the right column. The first chemical shift must be the Calpha; the next ones must correspond to the side-chain. Pressing the TEST button compare the list of chemical shifts to standard ones and outputs the most probable type of spin system 's amino-acid.



Pressing the Test Button gives :



The proposal is ACX which means Ser or Cys residues. The scores are given in the terminal window.

```
score(AMX) = 1.64173185743
score(ACX) = 5.67968793087
score(ARO) = 4.09119186734
score(ILV) = 8.59851329529
score(ALA) = 8.59233040968
score(THR) = 8.97453812576
score(LNG) = 8.434267830186
score(GLX) = 8.29379335154
```

Spin system types: AMX (Asp, Asn, etc ...), ACX (probably Ser or Cys), ARO (aromatics), ILV (Ile, Leu, Val), ALA (Ala), THR (Thr), LNG (Lys, Met, Arg), GLX (Glu, Gln)

3.7. Connect

This menu is used to get proposals for the sequential assignments. Two functions are used: the “connect di-peptide” and the “connect sequence”. They both rely on definitions found in the spin system layer file. Three fields must be defined in this file: the SPIN, the NOE and the SEQUENCE. See the example file or create a new spin system layer and edit using the “SpinSys Edit” menu, to see default definitions, however NOEs should be defined and the NEXT field must be present. Refer to the file example.spin in the EXAMPLE directory. Connect di-peptide needs as input a selected layer with annotations (labeled or not) which are assumed to indicate NOE peaks. For each spin system (with the NEXT field set to FIND) the first atom defined in the NOE is taken as root. The chemical shifts of each root atom in each spin system found in the SpinSys layer are compared to ppm coordinates of each annotation. If they match within the tolerance (given by `cny_spin_tolerance`) and if the second coordinate is within the range defined by the SPIN definition then the field corresponding to the NOE label (giving the name of the sequential NOE) is filled with this chemical shift. Searching for sequential connections may also be entered at the terminal using the command `cy_spin connect` and giving a tolerance value “real number”.

There is no automatic selection to determine what would be the best candidate for the sequential NH. The NOE columns (assuming that they correspond to sequential NOE definitions, `dNN`, `daN`, `dbN`) just give proposals which may help the user to decide which is the next NH chemical shift. This chemical shift must be given in the NEXT field (hand edited) before using the “Spinsys connect sequence” menu.

The “connect to sequence” menu uses the chemical shifts given in the NEXT column for each spin system, and compare this value with NH chemical shifts for all spin systems. Then the spin system names (assuming that they correspond to amino-acids names) are compared to the sequence given in the SEQUENCE field, and the program outputs at the terminal possible sequential connectivities. Since this process only uses NH chemical shifts many ambiguities are still present in the output. The ppm tolerance can be changed using the full command :

```
> cy_spin sequence tolerance(real)
```

4. Analysis

This menu related commands, include file in/out, formats (PDB, ...), NOE Tool and assignments.

4.1. NoesyCalc

This menu is used to display NOEs computed from distance information of atom coordinates given in a PDB file. A new layer called "NoesyCalc" is created to handle calculated NOEs. Each NOE is shown by a circle of radius proportional to $1/d^6$. So short distances give a really big circle, and long distances (in the 5 angstroms range) give just a small circle. Click on a given NOE circle to display information about the involved atoms. The first thing to do is to load a PDB file, then to rename atoms according to spin system atom names (See "Analysis PDB rename" menu), and to use the command "Analysis AddppmInfo" which adds ppm values found in the spin system layer to the PDB layer. At that stage each atom in the PDB layer has an equivalent name which correspond to its spin name (in the spin system layer) and has also a chemical shift assigned. In the NoesyCalc's window there is a button to select a spectral area. First of all click on this button and then define the area you want NOEs to be calculated in the spectrum window using the mouse. The other button labeled "Show NOE" can now be used to display the calculated NOEs in this area. The spectral area is defined using the rubber icon. So before using it be sure that no contour layer has been selected, otherwise contours within this area could be deleted very easily.

4.2. Assign

Not used in the new version

4.1. AddppmInfo

This moves chemical shift information from the spin systems to the PDB layer. The destination PDB layer must be selected first.

4.3. PDB

Open : file selection dialog to open PDB file. Refer to section 1.1.

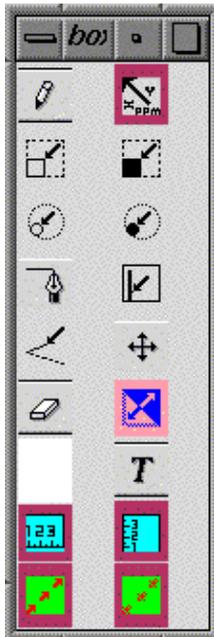
Save & Close : selection dialog window to select layers to save or close. Refer to section 1.2.

Rename : adds equivalence between the original atom names found in the PDB layer and those found in the spin system layer. This is done using one of the macro files rename_Xplor.log or rename_Dyana.log. Both files use spin names defined in the standard spin system file and apply to PDB files generated by X-plor or Dyana, respectively.

5. Display

5.1. Tools

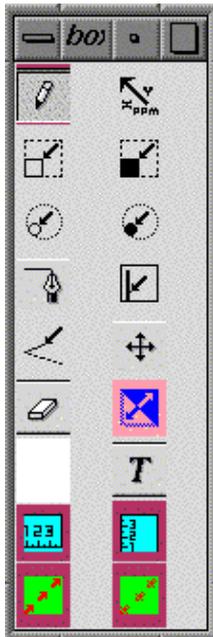
Displays the tool panel. The first upper-left icon is for drawing lines, the next to the right is the default cursor used for selecting annotations and gives ppm infos. The other icons are used to draw rectangles and circles. There is an icon for the rubber. Next to it there is an icon to erase the temporary buffer, another to change the color settings, enter text for annotations, display x and y scales. The last icons are used to increase/decrease the translation and scaling speeds.



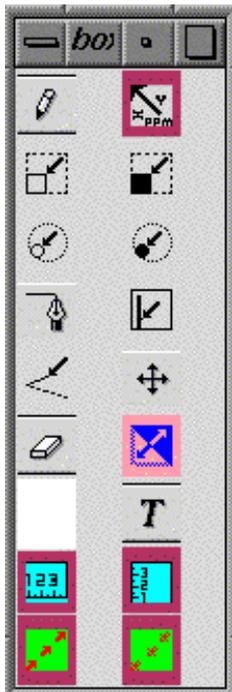
Icons description :

- 1 st row : line drawing, selection cursor
- 2 nd row : rectangle, filed rectangle
- 3 rd row : circle, filed circle
- 4 th row : horizontal buffer line, vertical buffer line
- 5 th row : modify already existing annotation, draw a cross in buffer
- 6 th row : rubber, erase buffer
- 7 th row : change color, add a label to the selected peak annotation
- 8 th row : x scale (ppms), y scale (ppms)
- 9 th row : speed up mouse, slow down mouse.

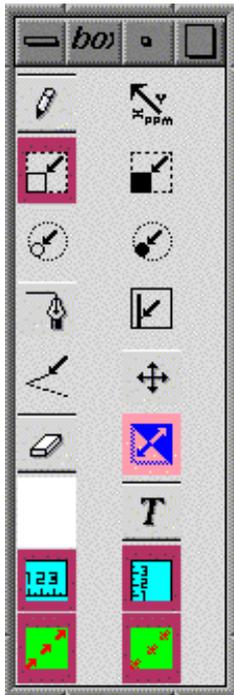
To draw a simple line, click the pencil icon and draw it in the main window



To select a peak annotation (line) click the xppm icon and click on an already existing annotation in the main window. Click in an empty area gives chemical shifts values.

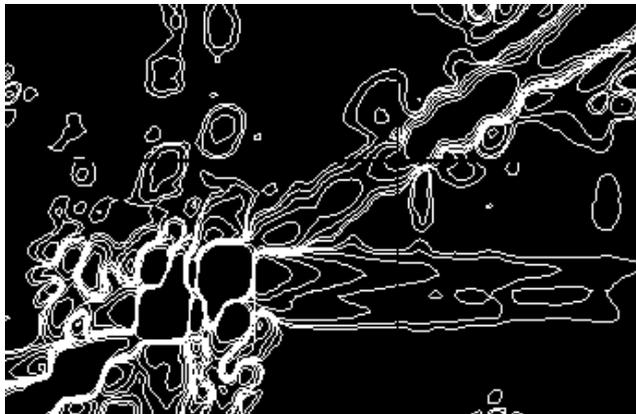


To draw a rectangle:

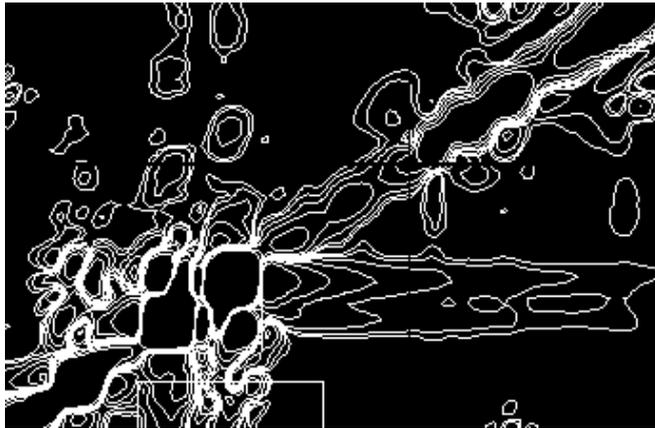


To erase contours, first select a 2D contour layer using the Layer Info Menu (see section 6.1), then select the rubber in the “Tools” window and use the left mouse button to define the area to be deleted.

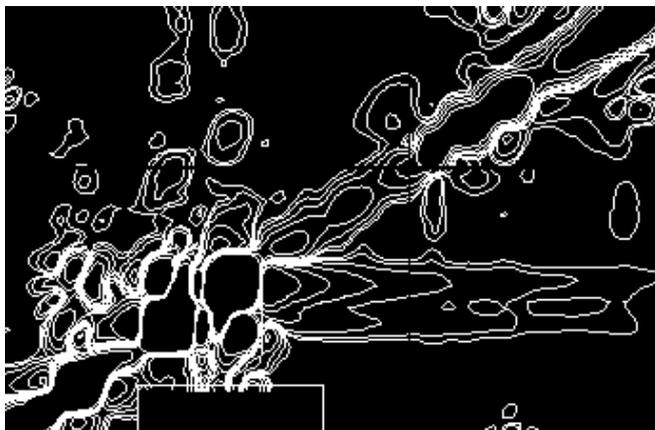
Initial contour :



Defining the area in the bottom of this view :



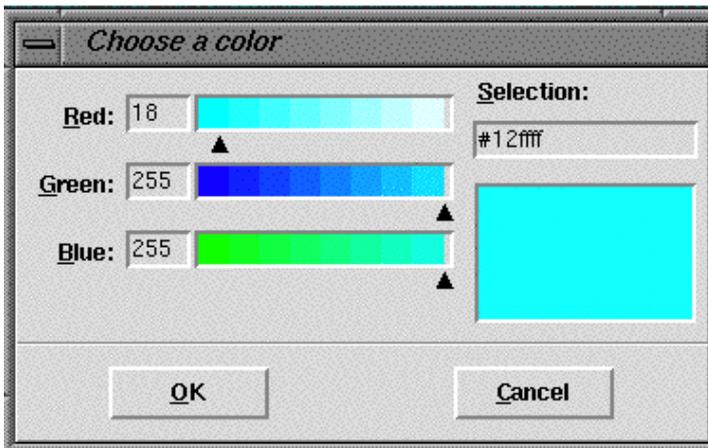
Contours within this region are removed



NOTE : erasing contour can be done to remove the water signal and t1 noise. This is only useful to keep small size of contour files, and so you must write the new contours.

5.2. Colors

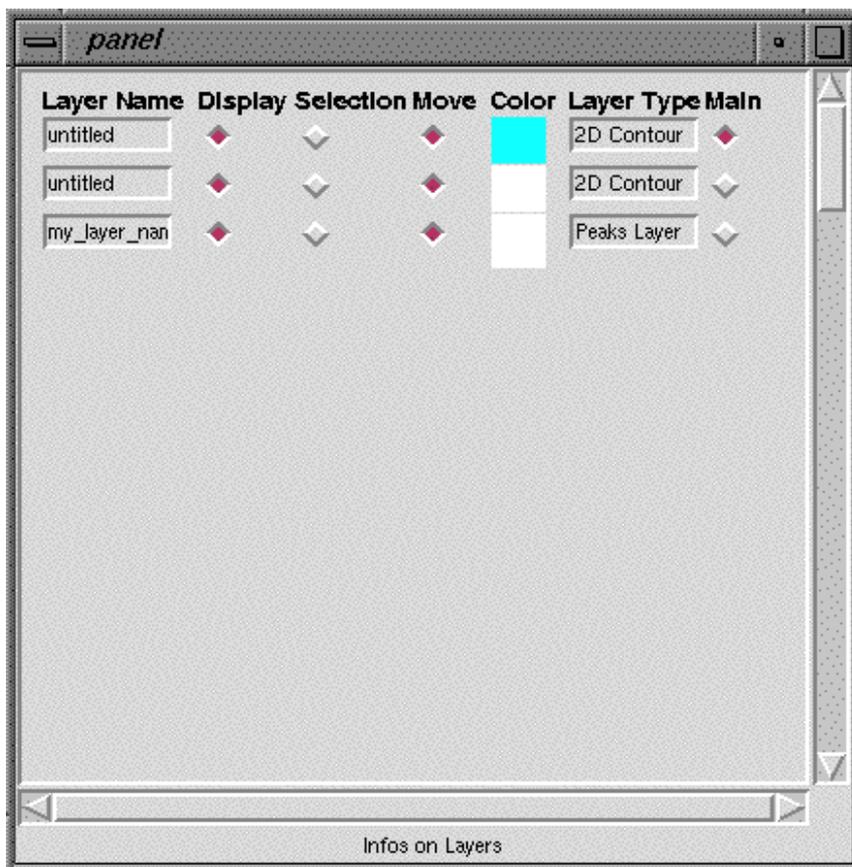
Used to select colors



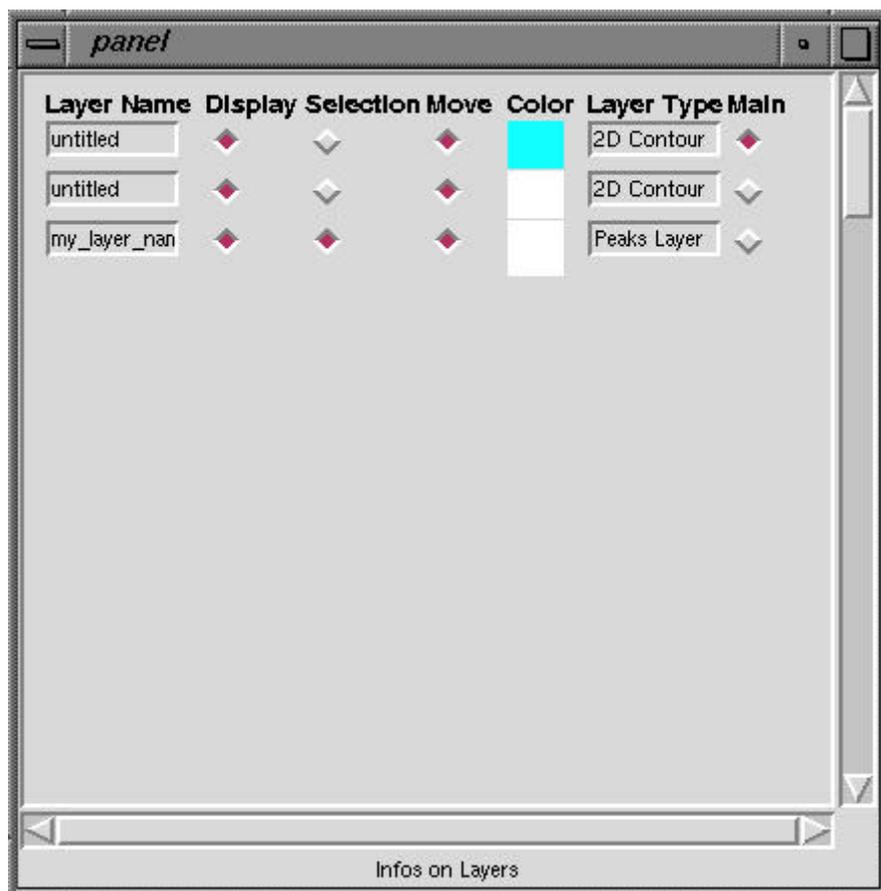
6. Layers

6.1. Info

This window gives a table of loaded layers, with the following information: Layer Name, Display (status), Selection (status), Move (status), Color, Layer Type, Main (status).



Changing the selection status of the Peaks Layer (last on in the stack) allows selection and addition of new annotations to it.



6.2. *Reset*

Reset the display area centered at $x=0$ ppm and $y=0$ ppm.

6.3. *Link*

Reset all layers (scales and translations) according to the main layer.

6.4. *Zoom In*

Make a zoom using an area defined by one selected annotation. If the annotation is a rectangle then the edges of the display area is the rectangle itself. If it is a simple line then it defines the lower-left / upper-right points of the zoom area.

6.5. *Select All*

Set the Selection status of all layers to ON.

6.6. *Unselect All*

Set the selection status of all layers to OFF.

6.7. *Navigate*

Opens a scroll bar used to scroll between layers. When a succession of 2D contours sequentially extracted from a 3D are loaded, individual planes can be displayed using the scroll bar.

6.8. *Print*

This is used to create a postscript file of the main window. The file names are incremented each time the Print menu is used, starting from plot_1.ps to plot_n.ps.

7. **Constraints**

This menu includes syntax control over assignments and constraints generation.

7.1. *Labels*

Check for consistency between selected annotation labels and spin-system names. A Peaks layer must be selected first (See Section 6.1 for selecting a layer). Each peak label must follow the syntax of section 2. Spin names are extracted from the assignment label and compared to the spins declared in the spin system layer. Errors are reported in the terminal window.

7.2. *Bounds*

Generates an upper-bounds constraints file either for Dyana or Xplor. Annotation labels are used to define the NOE assignments. The annotation line-width is used to define the classes of upper-bounds (Line-width 1 corresponds to weak NOE –upper-bound 4.8, Line-width 5 corresponds to an upper-bound of 2.4). The first step is the selection of a spin system layer, the annotation layer (which must contain the NOEs labeled with the convention ATM(RESNUM_1)ATM(RESNUM_2) and a molecule layer. Refer to section 2 for more details.

The second step is to set the translation for the atom names, then to check the assignments from the annotations according to spin names (from the spin system layer) and the atom names (from the molecule layer). There is the possibility to rename atoms to pseudo-atoms. Then a constraint file can be written according to the table of conversion between Line-width and upper-bounds. This conversion table can be modified by the user.

8. **User**

This menu contains the Preferences, the Configuration and the Backup Tools.

8.1. *Backup*

Save on disk all Peaks layers, the spin system layer and the molecule layers, without prompting the user. The backup utility is activated after a period of elapsed time which can be set in the User Preferences menu. Periodically, it opens a window for saving Layers to disk. Only annotation, molecule and spin system layers are shown and are saved by pressing OK.



Click OK to save these layer.

8.2. Configuration

This is used to setup a configuration file or to read an existing one. The window is a table giving the Layer infos, selection (status), keep xy (status) and keep color (status). Included layers are those which are selected. To keep the display area the “keep xy” buttons must be set. Section 9.1. shows how to manage a configuration.

8.3. Preferences

This is used to set the time elapsed between backups, and the fonts in the different windows and in the main graphic window.

9. Help

9.1. Starting

How to set a configuration file.

9.2. Balloons

Enable / Disable balloon help.

9.3. Commands

List of commands used at the terminal.

9.4. *Menu*

This menu.

9.5. *Mouse*

How to handle the mouse & buttons, to move and scale the graphics.

9.6. *Benchmark*

A Tcl macro which automatically load several layers and test several capabilities.

10. Quit

To leave the program safely