TOPSPIN

Users Guide

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Chapter 2

The TOPSPIN Interface

2.1 The Topspin Window

The TOPSPIN window consist of several areas, bars, fields and buttons. The main part is a split pane which consists of the data area and the browser. Note that the browser can be inactive [hit ***Ctrl***+***d***] or displayed as a separate window.

Fig. 2.1 shows the Topspin window with two data windows in the data area and the browser as an integral part.

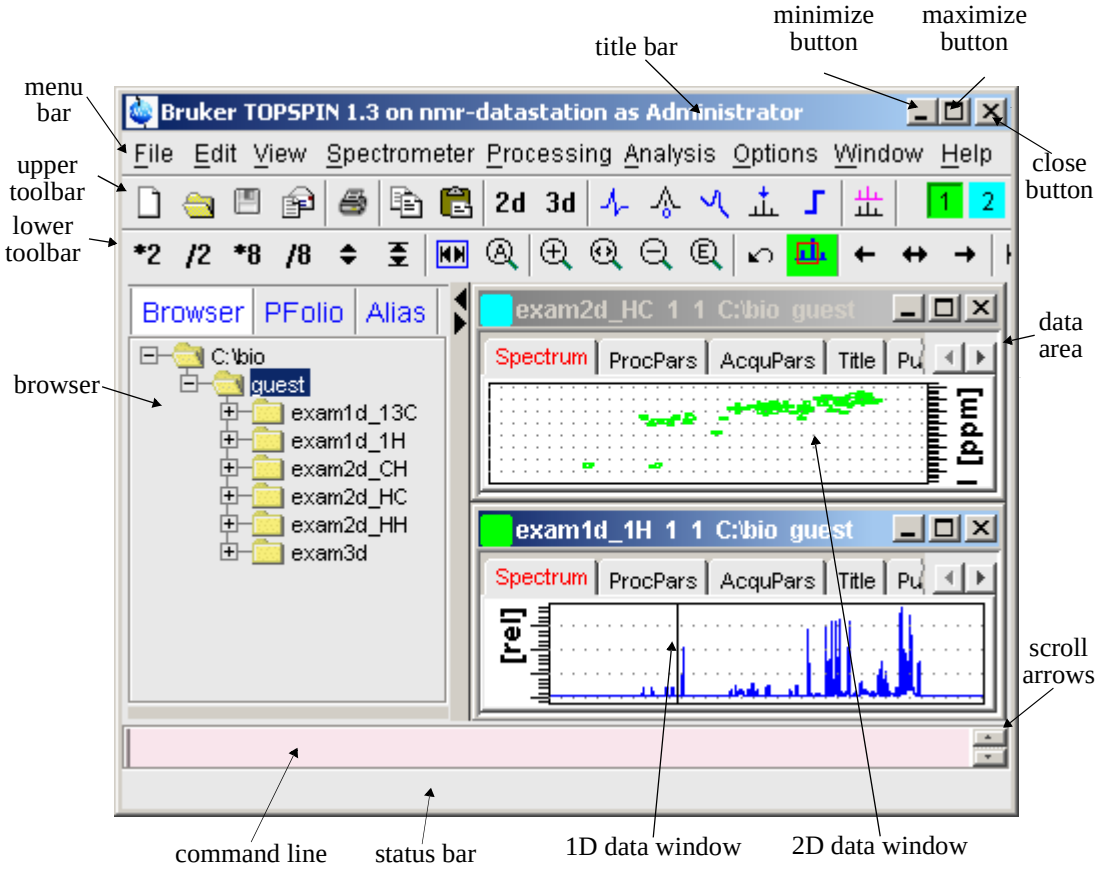


Figure 2.1

Note that the menus and toolbars depend on the data dimensionality. The descriptions below hold for 1D data. For 2D and 3D data, the menus and toolbars are similar and will be discussed in the chapters 9, 10 and 12, respectively.

How to Use Multiple Data Windows

TOPSPIN allows you to use multiple data windows. Data windows can be opened from the browser or from the ***Window*** menu. They can contain the same of different datasets. Data windows can be arranged from the ***Window*** menu. One of them is the active (current) data window. The active window:

- can be selected by clicking inside the window or hitting F6 repeatedly.
- has a highlighted title bar
- has the mouse focus
- is affected by menu, toolbar and command line commands

A cursor line (1D) or crosshair (2D) is displayed in all data windows at the same position. Moving the mouse affects the cursor in all data windows.

How to Use the Title bar

In the title bar you can:

- Left-click-hold & drag to move the window
- Double-click to maximize the window
- Right-click to open the title bar menu.
- Access the minimize, maximize and close buttons at the right
- Access the title bar menu button at the left

How to Use the Menu bar

The menu bar contains the following menus:

- ***File*** : performing data/file handling tasks
- ***Edit*** : copy & paste data and finding data
- ***View*** : display properties, browser on/off, notebook
- ***Spectrometer*** : data acquisition and acquisition related tasks
- ***Processing*** : data processing
- ***Analysis*** : data analysis
- ***Options*** : setting various options, preferences and configurations
- ***Window*** : data window handling/arrangement
- ***Help*** : access various manuals.

Experienced users will usually work with keyboard commands rather than menu commands. Note that the main keyboard commands are displayed in square brackets [] behind the corresponding menu entries. Furthermore, right-clicking any menu entry will show the corresponding command.

How to Use the Upper Toolbar

The upper toolbar contains buttons for data handling, switching to interactive modes, display settings, and starting acquisition.

Buttons for data handling:

The functions of the individual buttons are:

- Create a new dataset[***Ctrl***+***n***, ***new***]
- Open a dataset [***Ctrl***+***o***, ***open***]
- Save the current dataset [***Ctrl***+***s***, ***sav***]
- Email the current dataset[***smail***]
- Print the current dataset [***Ctrl***+***p***, ***print***]
- Copy the data path of the active data window to the clipboard [***copy***]
- Paste the data path on the clipboard to the active data window [***paste***]
- 2d Switch to the last 2D dataset [***.2d***]
- 3d Switch to the last 3D dataset [***.3d***]

For more information on dataset handling, please refer to chapter 4.3.

Buttons for interactive manipulation

The functions of the individual buttons are:

- Switch to phase correction mode
- Switch to calibration mode
- Switch to baseline correction mode

 Switch to peak picking mode

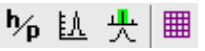
 Switch to integration mode

 Switch to multiple display mode

 Switch to distance measurement mode

For more information on interactive manipulation, refer to chapter 11 and 12.

Buttons for display options



The functions of the individual buttons are:

 Toggle between Hz and ppm axis units

 Switch the y-axis display between abs/rel/off

 Switch the overview spectrum on/off

 Toggle grid between fixed/axis/off

For more information on display options, please refer to chapter 8.5 and 9.5.

How to Use the Lower Toolbar

The lower toolbar contains buttons for display manipulations.

Buttons for vertical scaling (intensity manipulation)

 Increase the intensity by a factor of 2 [***2***]

 Decrease the intensity by a factor of 2 [***/2***]

 Increase the intensity by a factor of 8 [***8***]

 Decrease the intensity by a factor of 8 [***/8***]

Increase/decrease the intensity smoothly

Reset the intensity [***.vr***]

Buttons for horizontal scaling (zooming):

Reset zooming (horizontal scaling) to full spectrum [***.hr***]

Reset zooming (horizontal scaling) and intensity (vert. scaling) [***.all***]

Zoom in (increase horizontal scaling) [***.zi***]

Zoom in/out smoothly

Zoom out (decrease horizontal scaling) [***.zo***]

Exact zoom via dialog box[***.zx***]

Retrieve previous zoom [***.zl***]

Retain horizontal and vertical scaling when modifying dataset or changing to different dataset. Global button for all data windows [***.keep***]

Buttons for horizontal shifting

Shift to the left, half of the displayed region [***.sl***]

Smoothly shift to the left or to the right

Shift to the right, half of the displayed region [***.sr***]

Shift to the extreme left, showing the last data point [***.sl0***]

Shift to the extreme right, showing the first data point [***.sr0***]

Buttons for vertical shifting

Shift the spectrum baseline to the middle of the data field [***.su***]

Smoothly shift the spectrum baseline up or down.

Shift the spectrum baseline to the bottom of the data field [***.sd***]

2.2 Command Line Usage

How to Put the Focus in the Command Line

In order to enter a command on the command line, the focus must be there. Note that, for example, selecting a dataset from the browser, puts the focus in the browser. To put the focus on the command line:

☞ Hit the ***Esc*** key

or

☞ Click inside the command line

How to Retrieve Previously Entered Commands

All commands that have been entered on the command line since TOPSPIN was started are stored and can be retrieved. To do that:

☞ Hit the ↑ (***Up-Arrow***) key on the keyboard

By hitting this key repeatedly, you can go back as far as you want in retrieving previously entered commands. After that you can go forward to more recently entered commands as follows:

☞ Hit the ↓ (***Down-Arrow***) key on the keyboard

How to Change Previously Entered Commands

1. Hit the ← (***Left-Arrow***) or → (***Right-Arrow***) key to move the cursor
2. Add characters or hit the ***Backspace*** key to remove characters
3. Mark characters and use ***Backspace*** or ***Delete*** to delete them, ***Ctrl***+***c***

to copy them, or ***Ctrl*+*v*** to paste them.

In combination with the arrow-up/down keys, you can edit previously entered commands.

How to Enter a Series of Commands

If you want to execute a series of commands on a dataset, you can enter the commands on the command line separated by semicolons, e.g.:

```
em;ft;apk
```

If you intend to use the series regularly, you can store it in a macro as follows:

☞ right-click in the command line and choose ***Save as macro***.

2.3 Command Line History

TOPSPIN allows you to easily view and reuse all commands, which were previously entered on the command line. To open a command history control window; click ***View*** → ***Command Line History***, or right-click in the command line and choose ***Command Line History***, or enter the command ***cmdhist*** (see Fig. 2.2).

It shows all commands that have been entered on the command line since TOPSPIN was started. You can select one or more commands and apply one of the following functions:

Execute

Execute the selected command(s).

Append

Append the (first) selected command to the command line. The appended command can be edited and executed. Useful for commands with many arguments such as ***re***.

Save as..

The selected command(s) are stored as a macro. You will be prompted for the macro name. To edit this macro, enter ***edmac <macro-name>***. To execute it, just enter its name on the command line.

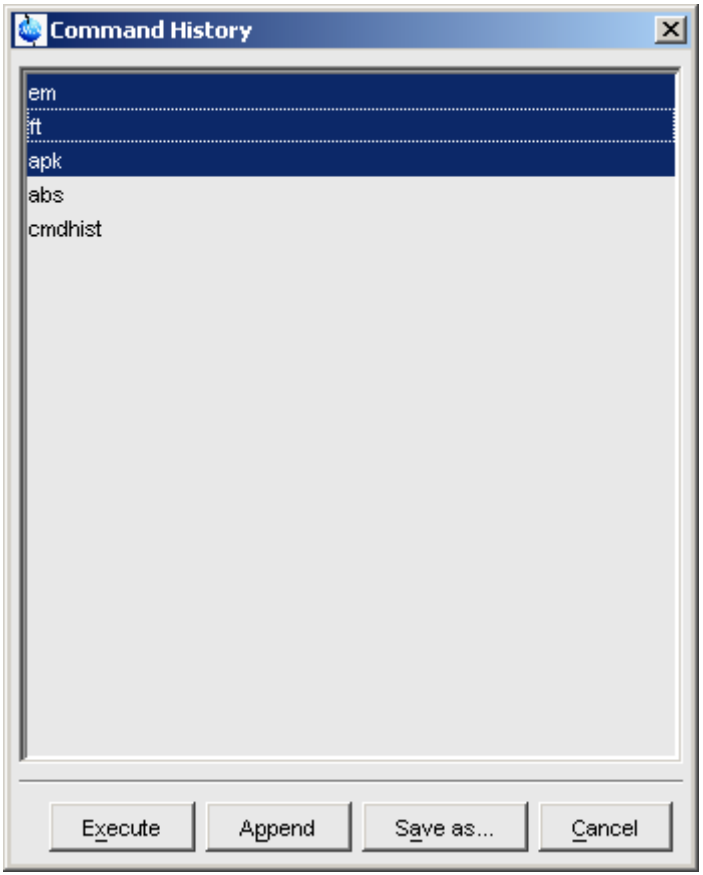


Figure 2.2

2.4 Starting TOPSPIN commands from a Command Prompt

TOPSPIN commands can be executed from a Windows Command Prompt or Linux Shell. To do that:

1. Open a Windows Command Prompt or Linux Shell
2. Enter a TOPSPIN command in the following format:

   ```
   <tshome>\prog\bin\sendgui <topspincommand>
   ```

   where <tshome> is the TOPSPIN installation directory.

Examples:

C:\ts1.3\prog\bin\sendgui re exam1d_1H 1 1 C:/bio joe

reads the dataset C:/bio/joe/nmr/exam1d_13C/1/pdata/1.

C:\ts1.3\prog\bin\sendgui ft

executes a 1D Fourier transform.

Commands are executed on the currently active data window.

2.5 Function Keys and Control Keys

For several TOPSPIN commands or tasks, you can use a control-key or function-key short cut.

Focus anywhere in TOPSPIN

Esc	Put the focus in the command line
Shift+Esc	Display menu bar and toolbars (if hidden)
F2	Put the focus in the browser / portfolio
F1	Search for string in command help or NMR Guide [***help***]
F6	Select the next window in the data area
Alt*+*F4	Terminate TOPSPIN [***exit***]
Ctrl*+*d	Switch the browser/portfolio on/off
Ctrl*+*o	Open data [***open***]
Ctrl*+*f	Find data [***find***]
Ctrl*+*n	New data [***new***]
Ctrl*+*p	Print current data [***print***]
Ctrl*+*s	Save current data [***sav***]
Ctrl*+*w	Close active window [***close***]
Ctrl*+*c	Copy a text that you selected/highlighted in an error box, dialog box, pulse program, title etc., to the clipboard
Ctrl*+*v	Paste text from the clipboard into any editable field.

Focus in the Command Line

Ctrl*+*Backspace	Kill current input
Ctrl*+*Delete	Kill current input
UpArrow	Select previous command (if available).
DownArrow	Select next command (if available).

Focus in the Browser/Portfolio

UpArrow	Select previous dataset
DownArrow	Select next dataset
Enter	In the Browser: expand selected node
Enter	In the Portfolio: display selected data

Focus anywhere in TOPSPIN

Scaling Data	
Alt*+*PageUp	Scale up the data by a factor of 2 [****2***]
Alt*+*PageDown	Scale down the data by a factor 2 [***/2***]
Ctrl*+*Alt*+*PageUp	Scale up by a factor of 2, in all data windows
Ctrl*+*Alt*+*PageDown	Scale down by a factor of 2, in all data windows
Alt*+*Enter	Perform a vertical reset
Ctrl*+*Alt*+*Enter	Perform a vertical reset in all data windows
Zooming data	
Alt*+*Plus	Zoom in [***.zi***]
Alt*+*Minus	Zoom out [***.zo***]
Ctrl*+*Alt*+*Plus	Zoom in, in all data windows
Ctrl*+*Alt*+*Minus	Zoom out, in all data windows
Shifting Data	
Alt*+*UpArrow	Shift spectrum up [***.su***]
Alt*+*DownArrow	Shift spectrum down [***.sd***]
Alt*+*LeftArrow	Shift spectrum to the left [***.sl***]
Alt*+*RightArrow	Shift spectrum to the right [***.sr***]
Ctrl*+*Alt*+*UpArrow	Shift spectrum up, in all data windows
Ctrl*+*Alt*+*DownArrow	Shift spectrum down, in all data windows
Ctrl*+*Alt*+*LeftArrow	Shift spectrum to the left, in all data windows
Ctrl*+*Alt*+*RightArrow	Shift spectrum to the right, in all data windows

Focus in a Table (e.g. peaks, integrals, nuclei, solvents)

delete	Delete the selected entries
home	Select the first entry
end	Select the last entry
Shift*+*Home	Select the current and first entry and all in between
Shift*+*End	Select the current and last entry and all in between
DownArrow	Select next entry
UpArrow	Select previous entry
Ctrl*+*a	Select all entries
Ctrl*+*c	Copy the selected entries to the clipboard
Ctrl*+*z	Undo last action
Ctrl*+*y	Redo last undo action

Focus in a Plot Editor

F1	Open the Plot Editor Manual
F5	Refresh
ctrl+F6	Display next layout
ctrl*+*Shift*+*F6	Display previous layout
Ctrl*+*tab	Display next layout
delete	Delete the selected objects
Ctrl*+*a	Select all objects
Ctrl*+*i	Open TOPSPIN Interface
Ctrl*+*c	Copy the selected object from the Clipboard
Ctrl*+*l	Lower the selected object
Ctrl*+*s	Save the current layout
Ctrl*+*m	Unselect all objects
Ctrl*+*n	Open a new layout
Ctrl*+*o	Open an existing layout
Ctrl*+*p	Print the current layout
Ctrl*+*r	Raise the selected object
Ctrl*+*t	Reset X and Y scaling of all marked objects
Ctrl*+*v	Paste the object from the Clipboard
Ctrl*+*w	Open the attributes dialog window.
Ctrl*+*x	Cut the selected object and place it on the Clipboard
Ctrl*+*z	Undo the last action

Note that the function of function keys can be changed as described in chapter 2.7.

2.6 Help in Topspin

TOPSPIN offers help in various ways like online manuals, command help and tooltips.

How to Open Online Help documents

The online help manuals can be opened from the ***Help*** menu. For example, to open the manual that you are reading now:

☞ Click ***Help*** → ***User's Guide***

To open the Avance Beginners Guide guide:

☞ Click ***Help*** → ***Avance Beginners Guide***

To open the Processing Reference guide:

☞ Click ***Help*** → ***Processing Reference Manual***

Note that most manuals are stored in the directory:

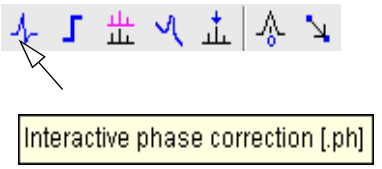
<tshome>/prog/docu/english/xwinproc/pdf

The most recent versions can be downloaded from:

`www.bruker-biospin.de`

How to Get Tooltips

If you hold the cursor over a button of the toolbar, a tooltip will pop up. This is a short explanation of the buttons function. For example, if you hold the cursor over the interactive phase correction button, you will see the following:



The corresponding command line command, in this case ***.ph***, is indicated between square brackets.

Note that the tooltip also appears in the status bar at the bottom of the TOPSPIN window.

How to Get Help on Individual Commands

To get help on an individual command, for example ***ft***:

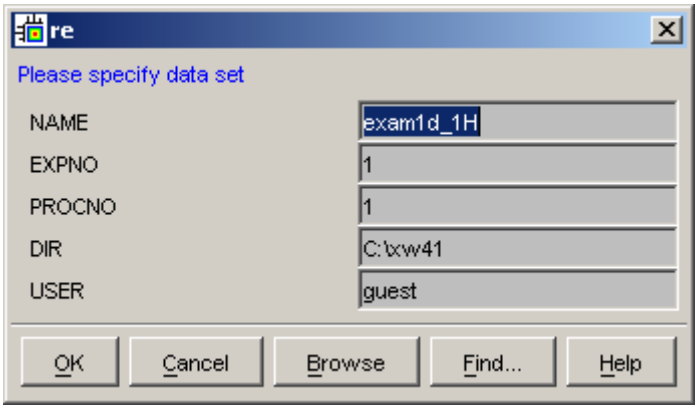
☞ Enter ***ft?***

or

☞ Enter ***help ft***

In both cases, the HTML page with a description of the command will be opened.

Note that some commands open a dialog box with a ***Help*** button. Clicking this button will show the same description as using the ***help*** command. For example, entering ***re*** and clicking the ***Help*** button in the appearing dialog box



opens the same HTML file as entering ***help re*** or ***re?***.

How to Use the Command Index

To open the TOPSPIN command index:

☞ Enter ***cmdindex***

or

☞ Click ***Help*** → ***Command Index***

From there you can click any command and jump to the corresponding help page.

2.7 User Defined Functions Keys

The default assignment of functions keys is described in chapter 2.5 and in the document:

☞ ***Help → Control and function keys***

You may assign your own commands to functions keys. Here is an example of how to do that:

1. Open the file `cmdtab_user.prop`, located in the subdirectory `userdefined` of the user properties directory (to locate this directory, enter ***hist*** and look for the entry "User properties directory="). The file `cmdtab_user.prop` is initially empty and can be filled with your own command definitions.
2. Insert e.g. the following lines into the file:

```
_f3=$em
_f3ctrl=$ft
_f3alt=$pk
_f5=$halt
_f5ctrl=$reb
_f5alt=$popt
```

3. Restart TOPSPIN

Now, when you hit the ***F3*** key, the command ***em*** will be executed. In the same way, ***Ctrl***+***F3***, ***Alt***+***F3***, ***F5***, ***Ctrl***+***F5*** and ***Alt***+***F5*** will execute the commands ***ft***, ***pk***, ***halt***, ***reb*** and ***popt***, respectively. You can assign any command, macro, AU program or Python program to any function keys. Only the keys ***Alt***+***F4***, ***F6***, ***Ctrl***+***F6***, and ***Alt***+***F6*** are currently fixed. Their function cannot be changed.

2.8 How to Open Multiple TOPSPIN Interfaces

TOPSPIN allows you to open multiple User Interfaces. This is, for example, useful to run an acquisition in one interface and process data in another. To open an addition interface, enter the command ***newtop*** on the command line or click ***Window → New Topspin***. To open yet another interface, enter ***newtop*** in the first or in the second interface. The display in each interface is completely independent from the others. As such, you can display different datasets or different aspects of the same

dataset, e.g. raw/processed, regions, scalings etc. When the dataset is (re)processed in one interface, its display is automatically updated in all TOPSPIN interfaces.

The command ***exit*** closes the current Topspin interface. Interfaces that were opened from this interface remain open. Entering ***exit*** in the last open TOPSPIN interface, finishes the entire TOPSPIN session. The position and geometry of each TOPSPIN interface is saved and restored after restart.

Chapter 4

Dataset Handling

4.1 The Topspin Browser and Portfolio

TOPSPIN offers a data browser/portfolio from which you can browse, select, and open data. Furthermore it allows you to define and list alias names for data. The browser appears at the left of the TOPSPIN window and can be controlled from the ***View*** menu.

The browser is similar to the Windows Explorer. It shows data directory trees and allows you to expand/collapse their elements. Figure 4.1 shows a TOPSPIN browser with one top level data directory and one dataset fully expanded.

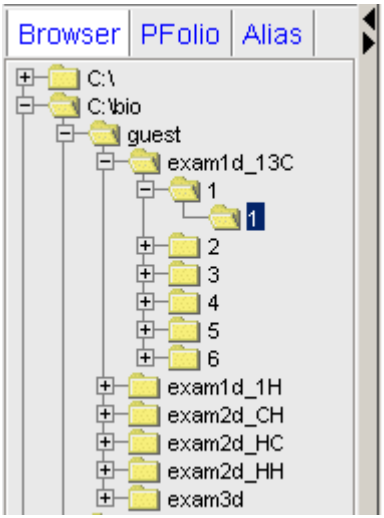


Figure 4.1

The TOPSPIN portfolio shows the list of datasets that has been opened so far by the current user. Each dataset that you open, is automatically added to the current portfolio. A portfolio with five datasets look like this:

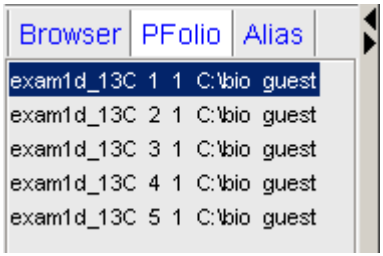


Figure 4.2

Each line displays one dataset showing its *name*, *expno*, *procno*, *top level directory* and *user*.

The TOPSPIN Alias list show a list of alias names for datasets. Just right-click any

entry to define, remove or interpret alias names.

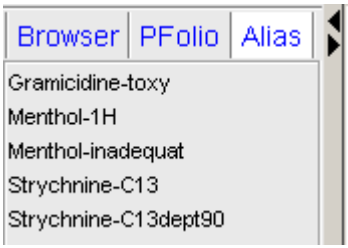


Figure 4.3

How to Open the Browser/Portfolio

☞ Click ***View*** → ***Browser Panel On/Off*** [**`Ctrl`**+**`d`**]

The browser or portfolio will appear depending on which one was used last.

How to Open the Browser/Portfolio in a separate window

The browser or portfolio can be opened in a separate window as follows:

☞ Click ***Options*** → ***Preferences*** [**`set`**], click ***Window settings*** and check ***Display dataset browser in a separate window***.

You must restart TOPSPIN for the change to take effect.

How to Put the Focus in the Browser/Portfolio

☞ Hit the ***F2*** key

or

☞ Click inside the browser or portfolio

How to Select Folders in the Browser

To select a particular folder:

☞ Left-click the folder button

or

☞ Hit the arrow-up/down keys while the focus is in the browser

To select multiple folders:

☞ Hold the ***Ctrl*** key and left-click multiple folders to select them

or

☞ Hold the ***Shift*** key and left-click two folders to select these two and all in between.

How to Expand/Collapse a Folder in the Browser

To expand a collapsed folder:

☞ Click the + button to the left of the folder button

or Double-click the folder button

or Hit the ***Right-Arrow*** key while the folder is highlighted

or Right-click the folder button and choose ***Expand fully*** from the popup menu to fully expand the folder

To collapse an expanded folder:

☞ Click the - button to the left of the folder button

or Double-click the folder button

or Hit the ***Left-Arrow*** key while the folder is highlighted

How to Expand a Folder showing Pulse program and Title

☞ Right-click the data name folder button and choose ***Expand fully & show PULPROG /Title*** from the popup menu

Fig. 4.4 shows an example of an expanded dataset showing the pulse program and title.

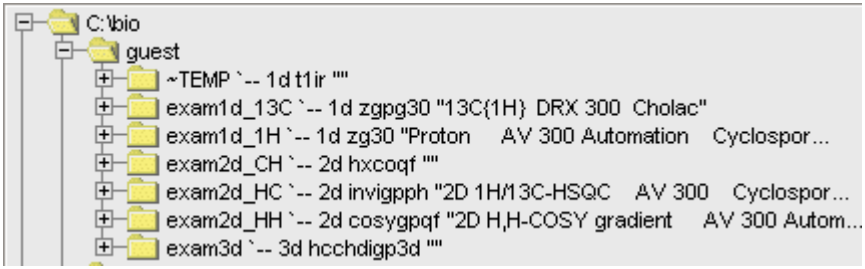


Figure 4.4

Note that collapsing the data name folder will deselect the display of the pulse program and title.

How to Add/Remove a Top Level Data Directory

To add a new top level data directory, local or remote, to the browser:

1. Right-click any position in the browser
2. Choose ***Add new data dir...*** from the popup menu (see Fig. 4.5)
3. Enter the top level directory in the dialog box and click ***OK***

To remove an existing top level directory from the browser:

1. Right-click the folder button of the top level directory
2. Choose ***Remove selected data dir...*** from the popup menu (see Fig. 4.5)

Figure 4.5

3. Click ***OK*** to confirm the appearing message

By default, the browser shows the TOPSPIN installation directory with the Bruker example datasets. To suppress this feature click ***Options*** → ***Preferences*** [`set`], click ***Program startup actions*** and uncheck ***Show TOPSPIN default data directory in data browser***.

How to Open a New Portfolio

1. Right-click inside the portfolio

2. Choose ***Open portfolio...*** from the appearing popup menu (see Fig. 4.6)
3. Navigate to the folder that contains the portfolio files
4. Select the desired portfolio file (extension `.prop`)
5. Click ***Open***

How to Save the current Portfolio

1. Right-click inside the portfolio.
2. Choose ***Save portfolio...*** from the appearing popup menu (see Fig. 4.6).
3. Specify a folder and filename in the appearing dialog box. The filename must have the extension `.prop`.
4. Click ***Save***.

How to Remove Datasets from the Portfolio

To remove a single dataset from the portfolio:

1. Right-click the dataset.
2. Choose ***Remove from portfolio...***from the popup menu (see Fig. 4.6).
3. Click ***OK*** in the appearing alert box.

To remove multiple datasets from the portfolio:

1. Hold the ***`Ctrl`*** key and left-click several datasets to select them or hold the ***`Shift`*** key and left-click two datasets to select these two and all in between.
2. Right-click any of the selected datasets.
3. Choose ***Remove from portfolio...***from the popup menu (see Fig. 4.6).
4. Click ***OK*** in the appearing alert box.

How to Find Data and Add them to the Portfolio

1. Click ***Edit*** → ***Find data*** [***`Ctrl+f`*** | ***`find`***].
2. Specify the search criteria and click ***OK***.
3. Select dataset(s) and click ***Add to portfolio***.

How to Sort Data in the Portfolio

1. Right-click inside the portfolio

2. Choose ***Sort mode*** from the popup menu (see Fig. 4.6).
3. Click ***Alphabetical*** to sort data in alphabetical order

   or

   Click ***Recent first*** to sort data by date of last open.

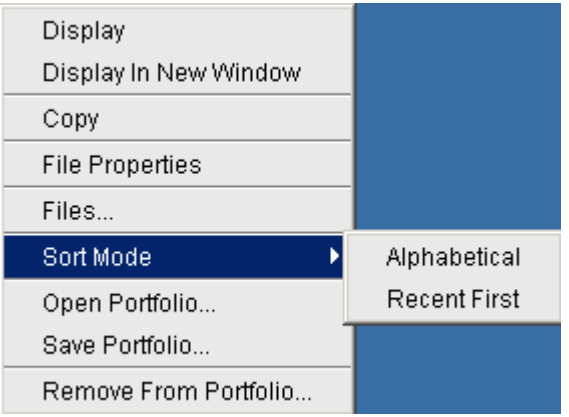


Figure 4.6

How to Add, Remove or Interpret Alias Names

To add an alias name:

1. Click the ***Alias*** tab in the browser.

2. Right-click in the Alias table to open the popup menu (see Fig. 4.7).

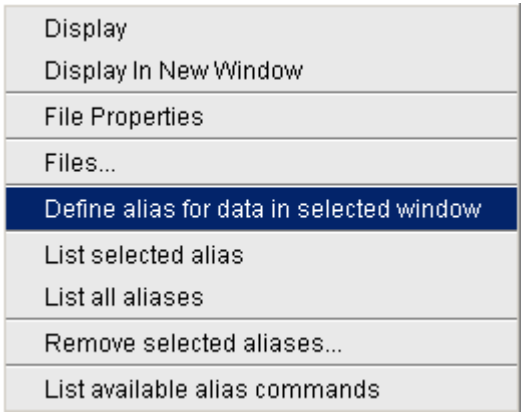


Figure 4.7

3. Click ***Define alias names for data in selected window.***
4. Enter an alias name in the appearing dialog box and click ***OK***. Note that alias names must begin with a letter.

To remove an alias name:

1. Right-click the ***alias name***
2. Click ***Remove selected aliases...*** from the popup menu (see Fig. 4.7)

Furthermore, the popup menu offers entries to display the dataset, list its properties and print the full dataset specification.

4.2 Creating Data

How to Create a New Dataset

1. Click ***File*** → ***New*** [**`new`**, **`Ctrl`**+**`n`**]

   or

   Click the button  in the upper toolbar.

2. Specify the dataset *name*, *expno*, *procno*, *dir*, and *user* in the appearing dialog box. If one or more datasets are open, the fields are initialized with the current dataset (see Fig. 4.8).

3. Click the down-arrow of the ***Solvent*** box and choose a solvent from the list, or type a solvent name.
4. Click the down-arrow of the ***Experiment*** box and choose a parameter set from the list, or type a parameter set name.
5. Type the dataset title in the ***TITLE*** box.
6. Click ***OK***.

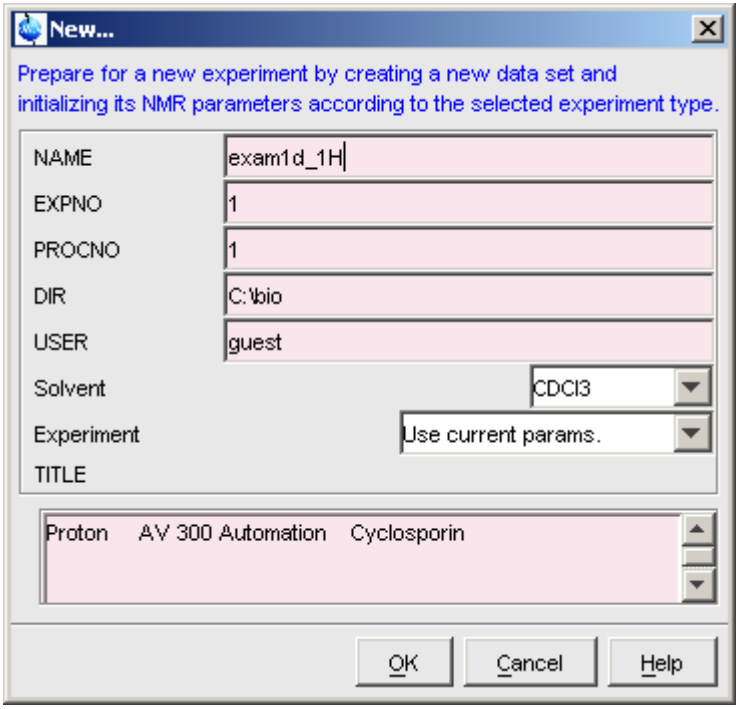


Figure 4.8

A dataset will be created and initialized with the parameters of the chosen experiment. No fid or spectrum are available yet. They can be created by data acquisition and data processing, respectively.

4.3 Opening Data

TOPSPIN allows you to open data in several ways, from the browser, the menu, the

Explorer or the command line. Furthermore, data can be opened:

- in an existing data window replacing the current dataset.
- in a data window which is in multiple display mode, being superimposed on the current spectra.
- in a new data window which becomes the active window.

Note that if a dataset is already displayed in one window and it is opened in a second existing window, it still replaces the dataset in the latter one. As a result, the same dataset will be displayed in two windows (see also command ***reopen***).

How to Open Data Windows Cascaded

By default, a new data window appears maximized, filling the entire data field and covering possibly existing window. You can, however, configure TOPSPIN to open new windows cascaded. This is convenient if you want to open several data windows and then select one.

To open new windows cascaded:

1. Click ***Options*** → ***Preferences*** [***set***]
2. Click ***Window Setting*** in the left part of the dialog box.
   The right part of the dialog box shows the window settings (see Fig. 4.9).

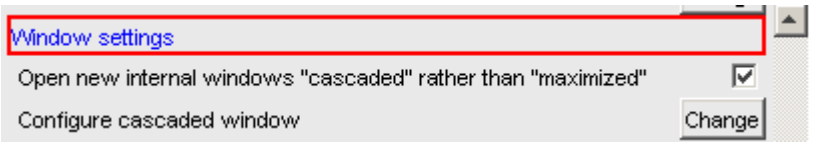


Figure 4.9

3. Check *Open new internal windows 'cascaded' rather than 'max'*.
4. Optionally you can configure the cascaded windows by clicking the respective ***Change*** button. This will open the dialog box shown in Fig. 4.10.

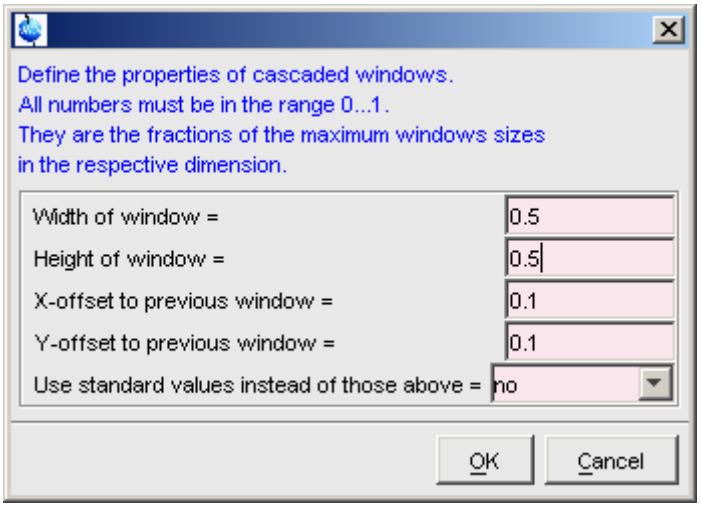


Figure 4.10

5. Here you can specify the data window sizes and offsets as fractions of the maximum window sizes.
6. Click ***OK*** to close the dialog box.

How to Open Data from the Browser

In the browser:

☞ Left-click-hold a data *name*, *expno* or *procno* and drag it into the data area. The data will be displayed in a new data window.

or Left-click-hold a data *name*, *expno* or *procno* and drag it into an open data window. The data will replace the currently displayed data.

or Left-click-hold a data *name*, *expno* or *procno* and drag it into an empty data window created with ***Alt+w n***.

or Left-click-hold a data *name*, *expno* or *procno* and drag it into a multiple display data window. The data will be superimposed on the currently displayed data.

or Right-click a data *name*, *expno* or *procno* and choose ***Display*** from the pop-up menu; the data will be displayed in the current data window.

or Right-click a data *name*, *expno* or *procno* and choose ***Display in new win-***

dow from the popup menu; the dataset will be displayed in a new data window.

or Hold the ***Ctrl*** key and left-click several datasets to select them or hold the ***Shift*** key and left-click two datasets to select these two and all in between. Then right-click one of the selected datasets and choose ***Display*** from the popup menu. A new window will be opened showing the selected datasets in multiple display mode. However, if the current window was already in multiple display mode, the selected spectra will be superimposed on the currently displayed spectra.

How to Open Data from the Portfolio

The portfolio offers the same possibilities to open a dataset as the browser. Additional options are:

☞ Hit the ***Enter*** key to display the highlighted dataset in the current window.

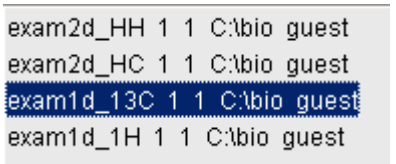


Figure 4.11

☞ Double-click a dataset to display it in the current window.

How to Automatically Select the first *expno*/*procno* of a dataset

If you open a dataset from the Browser by clicking a data *name*, there might be more that one *expno* and/or *procno* available. By default, TOPSPIN then opens a dialog box from which you can select the desired *expno/procno* combination (see Fig. 4.12). You can, however configure TOPSPIN to automatically open the first available *expno*/*procno* combination. To do that:

1. Click ***Options*** → ***Preferences*** [***set***].
2. Click ***Miscellaneous*** in the left part of the dialog box.
3. Uncheck the item *Display expno/procno list when opening data.*
4. Click ***OK*** to close the dialog box.

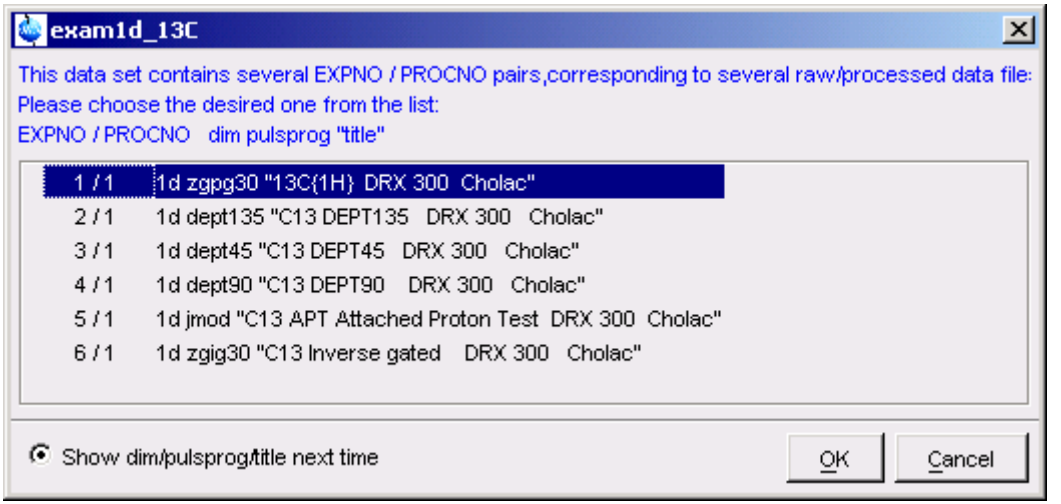


Figure 4.12

How to Open Data from the Topspin menu

1. To open a dataset:

   ☞ Click the  button in the upper toolbar.

   or

   ☞ Click ***File*** → ***Open*** [**`open`**, **`Ctrl`**+**`o`**] (see Fig. 4.13).

Figure 4.13

2. In the appearing dialog box (see Fig. 4.14)

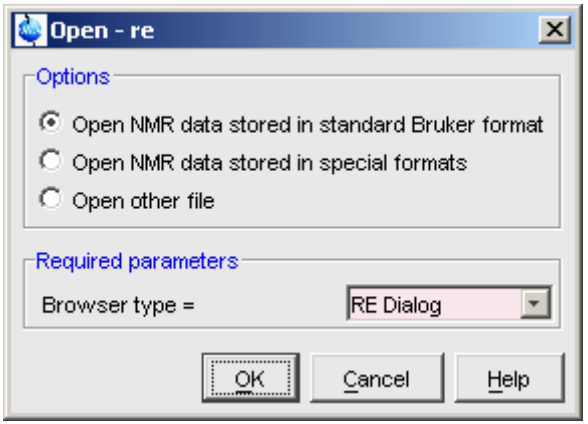


Figure 4.14

a) Select the option ***Open NMR data stored in standard Bruker format***.

b) Select the browser type ***RE Dialog***.

c) Click ***OK***.

3. In the appearing dialog box (see Fig. 4.15).

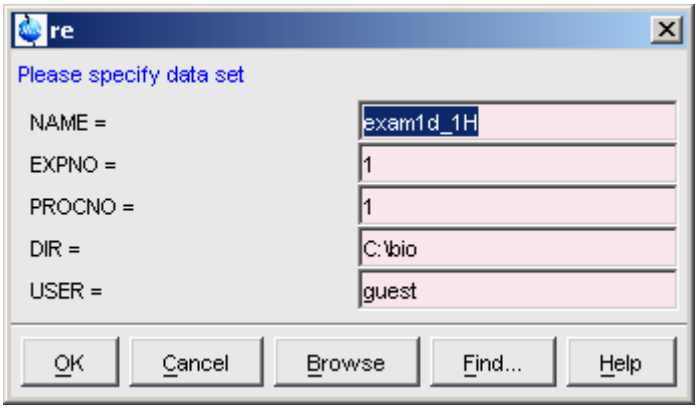


Figure 4.15

a) Specify the dataset *name*, *expno* etc.

b) Click ***OK***.

Note that the dataset specification consists of the five variable parts of the data directory tree, in this case:

C:\bio\data**guest**\nmr**exam1d_1H\1**\pdata**1**

The text boxes are initialized with the dataset in the current data window.

How to Open Data from the Explorer, Konqueror or Nautilus

You can open a dataset from the Windows Explorer as follows:

1. Open the Windows Explorer. You can do that in two different ways:

   ☞ from the Windows ***Start*** button. Navigate to the data *name*, *expno* or *procno*.

   or

   ☞ by entering the command ***expl*** in TOPSPIN. The Explorer shows the contents of the current dataset *procno* directory. Navigate to the desired data *name*, *expno* or *procno*. ***expl*** can also be used with the argument ***top*** to open the TOPSPIN installation directory, ***home*** to open user home directory or with an absolute pathname to open that directory.

2. Now you can open a dataset with:

☞ **drag & drop**: click-hold a dataset *name* or any of its sub-folders or files and drag it into the TOPSPIN data area or data window.

or

☞ **copy & paste**: right-click a dataset and choose ***copy*** from the popup menu. In TOPSPIN, click ***Edit*** → ***Paste*** [**`paste`**] (see Fig. 4.16).

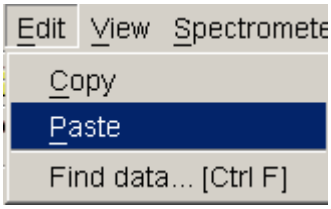


Figure 4.16

Likewise, a dataset can be opened from the Windows Search window or Internet Browser.

How to Open Data from the Command Line

To open a dataset from the command line:

1. Enter **`re`**
2. Specify a dataset in the appearing dialog box (see Fig. 4.15).
3. Click ***OK***

To open a new *procno* of the current dataset:

1. Enter **`rep`**
2. Specify a *procno* in the appearing dialog box.
3. Click ***OK***

To open a dataset in a new window:

1. Enter **`rew`**
2. Specify a dataset in the appearing dialog box.
3. Click ***OK***

To open a new *procno* of the current dataset in a new window:

1. Enter **`repw`**

2. Specify a *procno* in the appearing dialog box.
3. Click ***OK***

To open a data browser and read a dataset from there:

1. Enter ***reb***
2. Select a dataset from the appearing dialog box.
3. Click ***Display***

Note that ***re***, ***rep*** and ***reb***:

- Replace the data in the currently selected data window.
- Open the data in a new window when they are used after typing ***Alt***+***w n***
- Add the data in the currently selected window if this is in multiple display mode.

whereas ***rew*** and ***repw*** :

- Always open the dataset in a new window.

How to Open Special Format Data

Apart from the standard Bruker data format, TOPSPIN is able to read and display various other formats. To do this:

☞ Click ***File*** → ***Open*** [***open***, ***Ctrl***+***o***]

select the option ***Open NMR data stored in special formats***, select the desired file type (see Fig. 4.17) and click ***OK***..

A dialog will appear which depends on the chosen file type. Just follow the instructions on the screen.

The following file types are supported:

- JCAMP-DX - Bruker TOPSPIN[1] data stored in JCAMP-DX format
- Zipped TOPSPIN - Bruker TOPSPIN data stored in ZIP format
- WINNMR - Bruker WINNMR data
- A3000 - Bruker Aspect 3000 data

1. Note that the TOPSPIN data format is identical to the XWIN-NMR data format.

- VNMR - data acquired on a Varian spectrometer
- JNMR - data acquired on a Jeol spectrometer
- Felix - 1D data, FID or spectrum, which are stored in FELIX format.

Note that in all cases, the data are stored in a single data file which is unpacked/converted to standard Bruker format, i.e. to a data directory tree.

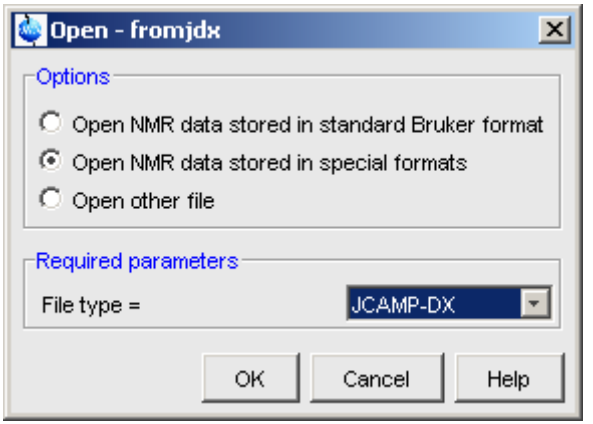


Figure 4.17

How to Open a ZIP or JCAMP-DX file from the Windows Explorer

Data stored in ZIP or JCAMP-DX format can also be opened directly from the Windows Explorer. You can do that as follows:

☞ **drag & drop**: click-hold a file with the extension `.dx` or `.zip` and drag it into the TOPSPIN data area or data window.

☞ **copy & paste**: right-click a file with the extension `.dx` or `.zip` and choose ***copy*** from the popup menu. In TOPSPIN, click ***Edit*** → ***Paste*** [***paste***].

4.4 Saving/Copying Data

How to Save or Copy Data

You can save the current dataset as follows:

1. Click ***File*** → ***Save*** [***Ctrl***+***s***].

   This will open a dialog box (see Fig. 4.18).

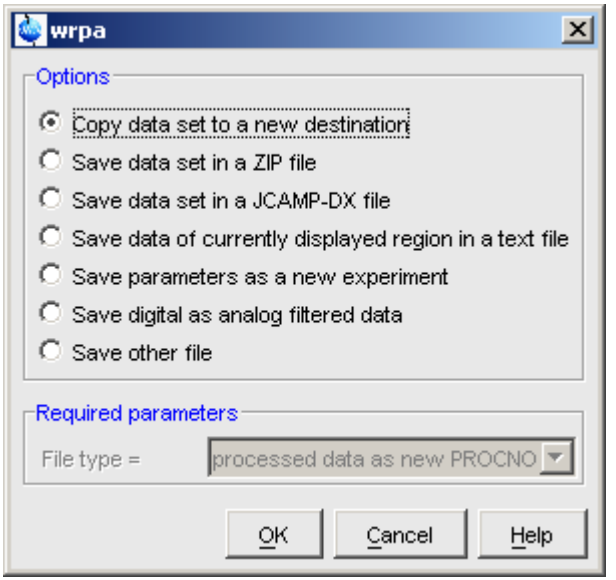


Figure 4.18

2. Select an option and, if applicable, a file type.
3. Click ***OK*** to execute the option.

The six options correspond to the following command line commands:

- ***wrpa*** - copies the current data to a new data *name* or *expno*
- ***tozip*** - convert a dataset of any dimension to ZIP format
- ***tojdx*** - convert a 1D or 2D dataset to JCAMP-DX format
- ***totxt*** - convert a 1D or 2D dataset text format
- ***wpar*** - write parameter set
- ***convdta*** - save digitally filtered data as analog filtered data
- ***wrp***, ***wra***, ***genfid***, ***wmisc*** - write various files

How to Save an Entire Dataset

1. Click ***File*** → ***Save*** [***Ctrl***+***s***].

2. Select the option ***Copy dataset to a new destination*** [**`wrpa`**] and click ***OK***
3. Specify the dataset variables and click ***OK***

How to Save Processed Data

1. Click ***File*** → ***Save*** [**`Ctrl`**+**`s`**].
2. Select the option ***Save other file***
3. Select File type ***Processed data as new procno*** [**`wrp`**] and click ***OK***
4. Enter a processing number (*procno*) and click ***OK***

How to Save Acquisition Data

1. Click ***File*** → ***Save*** [**`Ctrl`**+**`s`**].
2. Select the option ***Save other file***
3. Select File type ***Acqu. data as new expno*** [**`wra`**] and click ***OK***
4. Enter a experiment number (*expno*) and click ***OK***

How to Save Processed Data as Pseudo Raw Data

1. Click ***File*** → ***Save*** [**`Ctrl`**+**`s`**]
2. Select the option ***Save other file***
3. Select File type ***1r/1i as fid*** [**`genfid`**] or ***2rr/2ii as ser*** [**`genser`**]
4. Click ***OK***
5. Enter a destination *expno.*

   (optionally, you can specify further data path specifications)
6. Click ***OK***

4.5 Deleting Data

How to Delete a Specific Dataset

☞ Right-click the data *name*, *expno* or *procno* in the browser, then click ***Delete...***

In each case, a delete dialog will appear. The dialog box for a data expno, for an is shown in Fig. 4.19.

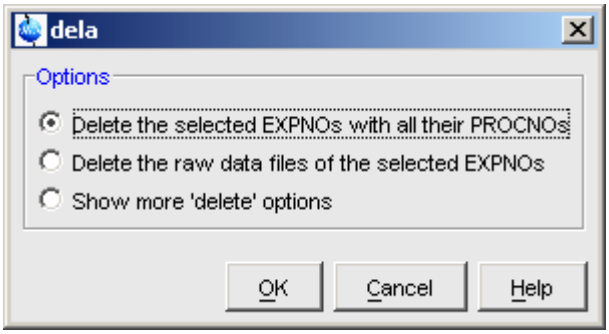


Figure 4.19

You can choose to delete just the raw data, delete the entire expno with all procnos or open further delete options. In the later case, the dialog box shown in Fig. 4.20 will appear.

How to Delete Types of Datasets

To delete certain types of data like 1D raw data, 2D processed data etc.:

☞ Click ***File*** → ***Delete...***

or

☞ Enter ***`delete`*** on the command line.

The dialog window shown in Fig. 4.20 will appear. Here you can select the data type and selection criteria.

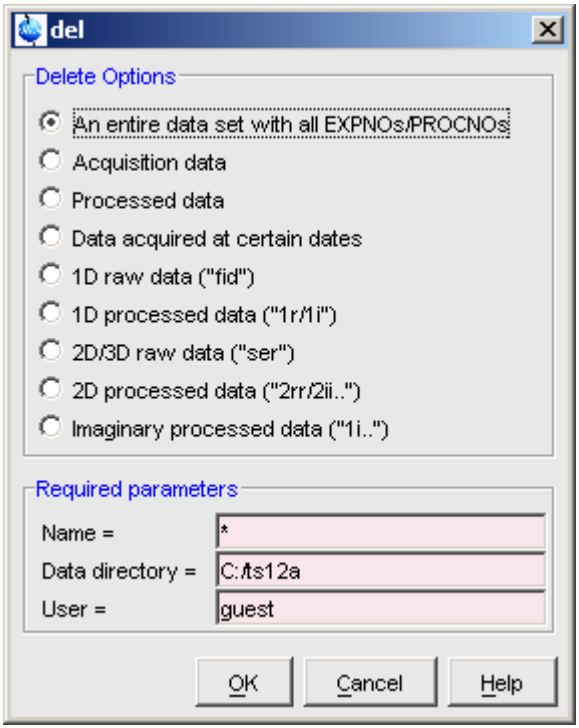


Figure 4.20

1. Select a data type option

   For each option, the corresponding command appears in the title of the dialog box. These commands can also be used to delete data from the command line.

2. Specify the ***Required parameters***

   Note that you can use the wildcards:

   - Asterix (*) for any character and any number of characters.
   - Question mark (?) for any single character.

3. Click ***OK***

A dialog box will appear showing the matching datasets. For example, if you select the option ***An entire dataset ...*** :

1. Select dataset entries for deletion (selected entries are highlighted).

To select multiple entries: click them holding the ***Shift*** or ***Ctrl*** key.

2. Click ***Delete*** to delete the entire data directory.

If you select the option ***Acquisition data*** or ***Processed data***, you can choose between deleting the data files only and deleting the entire *expno* or *procno* directory, respectively (see Fig. 4.21).

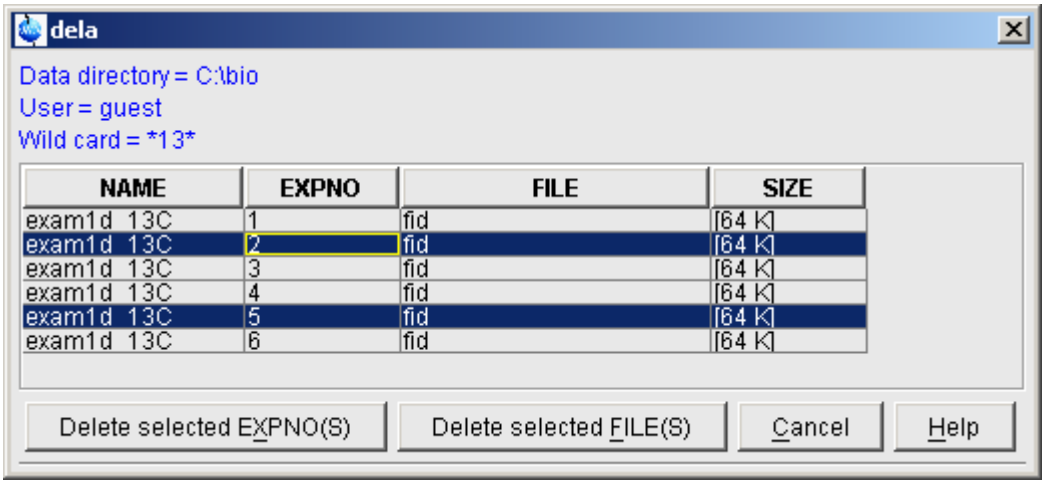


Figure 4.21

4.6 Searching/Finding Data

How to Find Data

You can find TOPSPIN data according to various criteria. To start searching do the following:

1. Click ***Edit*** → ***Find data*** [***Ctrl+f*** | ***find***]
to open the *Find data* window (see Fig. 4.22).

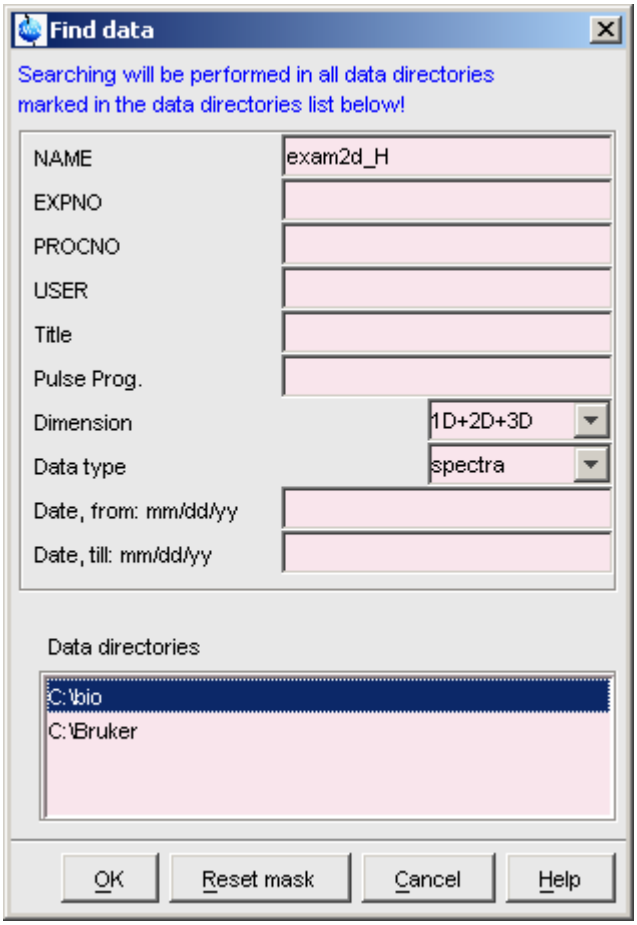


Figure 4.22

2. Specify the search criteria. Note that:
   - Dataset variables are searched that contain the specified string.
   - Search is restricted to data created between the specified dates. Note that the acquisition date is evaluated.

   The ***Reset mask*** button resets the default criteria.
3. Click ***OK***
   to get a list of data that fulfil these criteria (see Fig. 4.23).

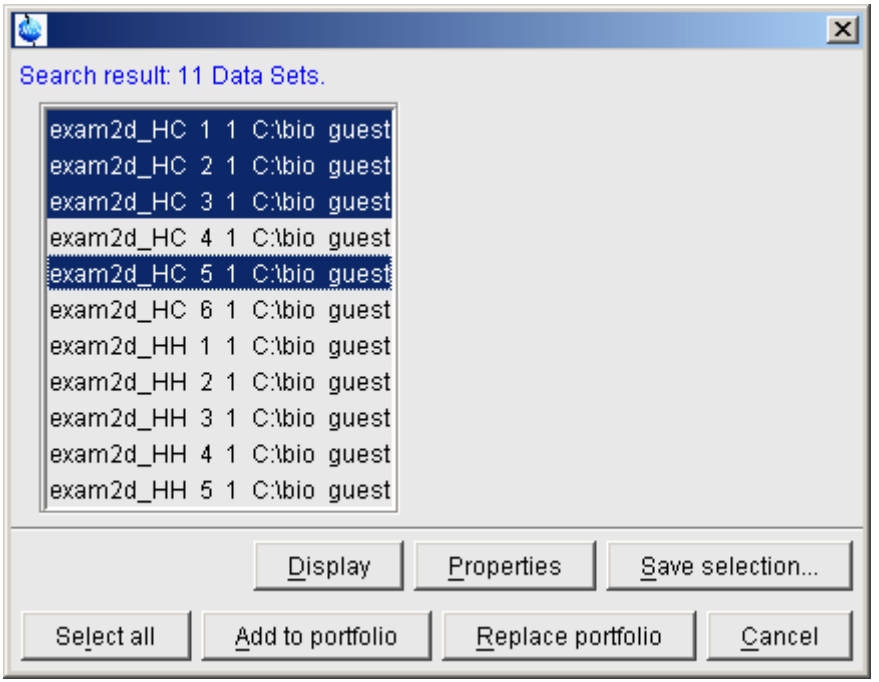


Figure 4.23

Note that the current search criteria are preserved until you exit TOPSPIN.

How to Display one of the Found Datasets

In the search result window (see Fig. 4.23):

1. Click one dataset to select it.

   Optionally: click ***Properties*** to view the datasets properties.

2. Click ***Display***
   to display the selected dataset in the current data window.

Note that if the search result consist of only one dataset, this is automatically selected and you can skip step 1.

How to Select Data from the Found Datasets

In the search result window (see Fig. 4.23):

☞ Hold the ***Ctrl*** key and left-click several datasets to select these datasets.

or

☞ Hold the ***Shift*** key and left-click two datasets to select these datasets and all datasets in between.

or

☞ Click ***Select all*** to select all datasets in the search result.

How to Add Selected Datasets to the Portfolio

1. Select the desired dataset(s) as described above.
2. To add them to the portfolio:

   ☞ Click ***Add to portfolio*** to extend the current portfolio.

   or

   ☞ Click ***Replace portfolio*** to replace the current portfolio.

How to Save Selected Datasets to a List

1. Select the desired dataset(s) as described above.
2. Click ***Save selection***...
3. In the appearing browser:
   a) Navigate to the desired list directory.
   b) Enter or select the list filename.
   c) Click ***OK***

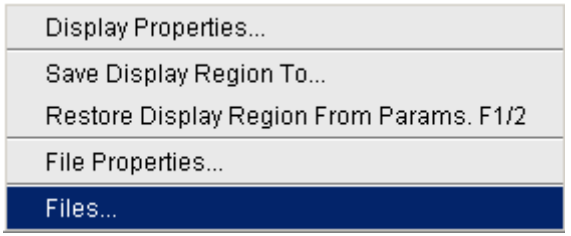
Dataset lists can be used by the acquisition or by serial processing (command ***serial***).

4.7 Handling Data Files

How to List/Open the Current Dataset Files

A Bruker dataset is represented by a directory tree which contains files in the *expno* and *procno* subdirectories. These files contain the actual data, parameters, lists etc.

☞ Right-click inside the data window and choose ***Files*** from the popup menu.



If the spectrum is displayed, the files in the *procno* subdirectory are shown. If the **Fid** is displayed, the files in the *expno* subdirectory are shown.

☞ Select a file and click ***Open*** to view its contents.

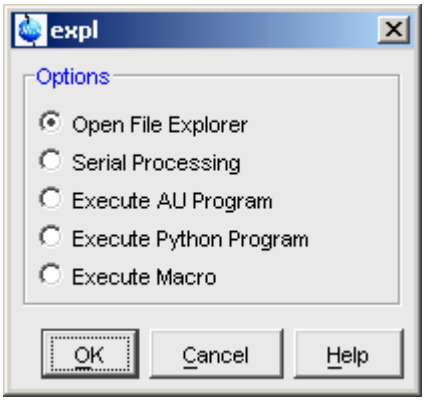
Note that this only makes sense for ascii files.

How to List/Open the current Dataset Files in the Windows Explorer

To list the current dataset files in the Windows Explorer:

1. Click ***Files*** → ***Run...***
2. Select ***Open file explorer*** [***expl***] in the appearing dialog box
3. Click ***OK***

Alternatively, you can enter the command ***expl*** on the command line. The Win-



dows Explorer will be opened showing the processed data files (the files in the *procno* directory) of the current dataset. Under Linux a Web browser like KDE

Konqueror or Gnome Mozilla will be opened.

To open a file:

☞ Double-click the file or right-click the folder icon and choose ***Open***

If TOPSPIN data area contains no datasets, the ***expl*** command opens the Explorer showing the users home directory. When entered on the command line, ***expl*** can also be used with the argument ***top*** to open the TOPSPIN installation directory, ***home*** to open user home directory or with an absolute pathname to open that directory.

4.8 Data Consistency Check

TOPSPIN maintains audit trail files for compliance with GLP, GMP and FDA requirements.

The processing command that creates processed data from the raw data, e.g. ***em***, creates the processing audit trail file `auditp.txt` and inserts the first entry. Any processing command that modifies/updates the processed data, e.g. ***ft***, makes an additional entry. Furthermore, any command that changes one or more processing status parameters makes an additional entry. The audit trail can be checked with the command ***audit***. This command opens a dialog box (see Fig. 4.24).

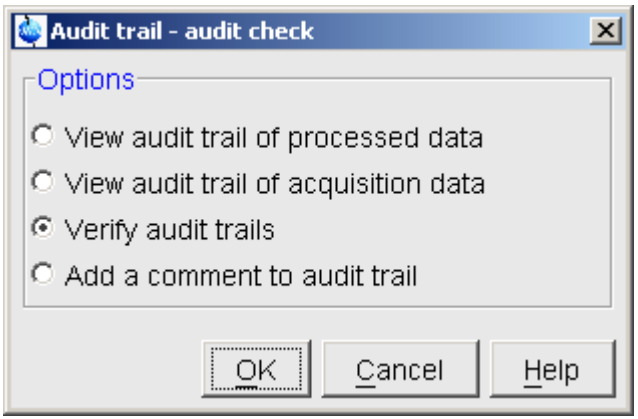


Figure 4.24

The first two entries allow you to view the audit trail files. The third entry performs an audit trail check, i.e. a data consistency check. If both raw and processed

data are consistent, you will get the message shown in Fig. 4.25).

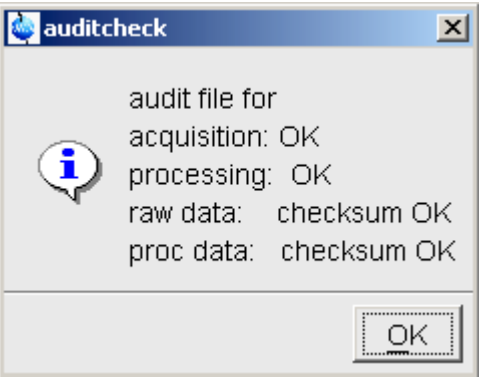


Figure 4.25

If the data have been manipulated outside of TOPSPIN, e.g. with third party software, the checksum will be inconsistent. Fig. 4.26 shows the message for inconsistent processed data.

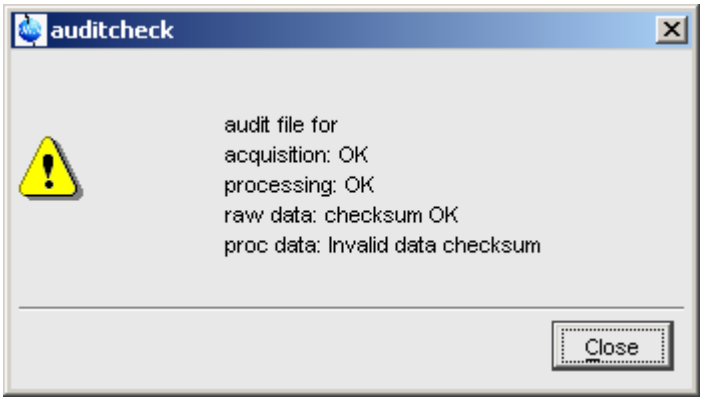


Figure 4.26

The fourth entry in Fig. 4.24 allows you to add a comment to one of the audit trail files (raw or processed).

Chapter 5

Parameter Handling

5.1 Processing Parameters

Processing parameters can be set/changed in three different ways:

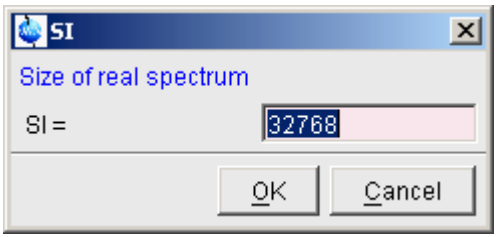
- from the parameter editor: click the ***ProcPars*** tab or enter ***edp***
- from the command line: e.g. enter ***si***
- from a command dialog box: e.g. ***wm***

How to Set a Processing Parameter from the Command Line

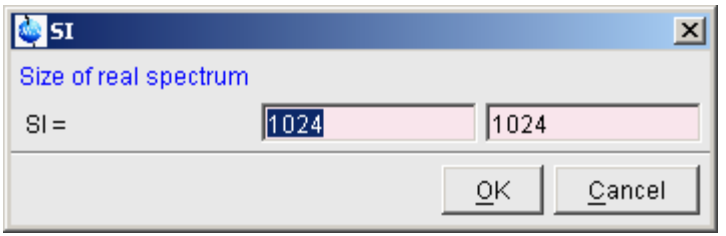
Enter the parameter name on the command line. For example to set the size:

1. Enter ***si***

   for 1D data, the following dialog box will appear:



for 2D data, the following dialog box will appear:



2. Specify the desired value(s), e.g. `32768` or `32k`
3. Click ***OK***

How to Set Processing Parameters from the Parameter Editor

To open the processing parameter editor:

☞ Click the ***ProcPars*** tab in the Tab bar of the data window.

or

☞ Enter ***edp*** on the command line.

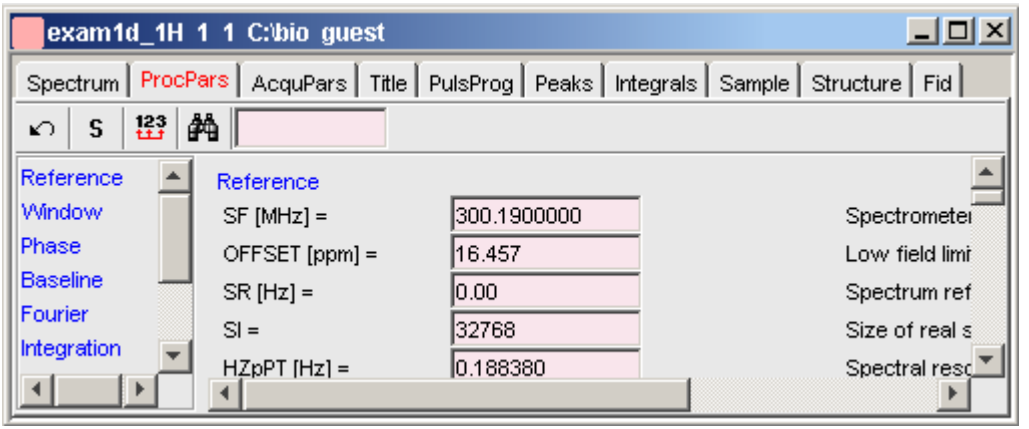


Figure 5.1

At the left of the parameter editor window you will see a list of parameter sections.

The processing parameter editor supports the following functions:

☞ Enter (part of) a parameter name in the search field and click  .

☞ Click a parameter section, e.g. Phase at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.

☞ Click in a parameter field, e.g. PHC0, to set the parameter value.

☞ Hit the ***Tab*** key to jump to the next parameter field.

☞ Hit ***Shift***+***Tab*** to jump to the previous parameter field.

☞ Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

How to Undo the Last Processing Parameter Change

☞ Click the following button:

 Undo last parameter change.

How to Display Processing Status Parameters

☞ Click the following button:

 Show processing status parameters.

Note that the command ***dpp*** opens the parameter editor and automatically shows the status parameters.

How to Change Processed Data Dimensionality

☞ Click the following button:

 Change data dimensionality.

This changes the number of parameter columns and value of the processing parameter PPARMOD.

The parameter editor does not allow you to modify status parameters. Processing status parameters reflect the status of the processed data and are used for further processing, display or plotting. Changing them can make the dataset inconsistent. In rare cases, however, it can be useful to change a status parameter and TOPSPIN allows you to do that from the command line. If, for instance, you want to change the F1 status parameter MC2 of a 2D dataset, you have to enter:

```
s mc2
```

Note that the command ***s*** is used for 1D, 2D and 3D dataset. TOPSPIN automatically recognizes the dimensionality of the data and displays the parameter in all relevant dimensions. Note that, for example, the parameter MC2 only exists in F1.

5.2 Acquisition Parameters

How to Set Acquisition Parameters

Acquisition parameters can be set/changed as follows:

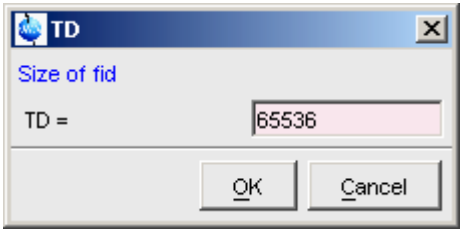
- from the parameter editor: click the ***AcquPars*** tab or enter ***eda***
- from the command line: e.g. enter ***td***
- from the interactive parameter adjustment window (enter ***gs***)

How to Set an Acquisition Parameter from the Command Line

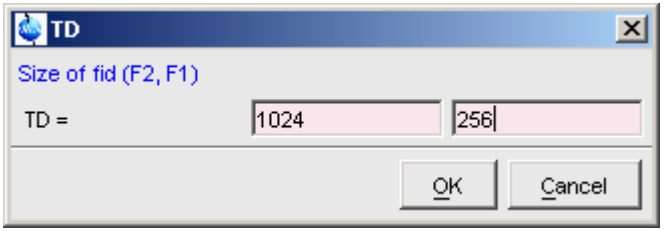
Enter the parameter name on the command line. For example to set the time domain size:

1. Enter ***td***

   for 1D data, the following dialog box will appear:



   for 2D data, the following dialog box will appear:



2. Specify the desired value(s), e.g. **`65536`** or **`64k`**
3. Click ***OK***

How to Set Acquisition Parameters from the Parameter Editor

To open the acquisition parameter editor:

☞ Click the ***AcquPars*** tab in the Tab bar of the data window.

or

☞ Enter ***`eda`*** on the command line.

Fig. 5.2 shows an example of the acquisition parameter editor with the Experiment parameters displayed.

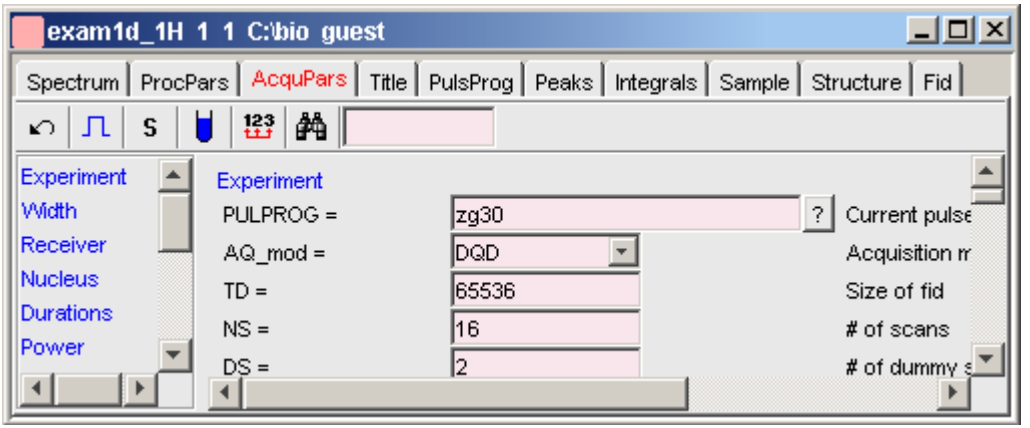


Figure 5.2

The processing parameter editor supports the following functions:

☞ Enter (part of) a parameter name in the search field and click .

☞ Click a parameter section, e.g. Experiment at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.

☞ Click in a parameter field, e.g. TD, to set the parameter value.

☞ Hit the ***`Tab`*** key to jump to the next parameter field.

☞ Hit ***`Shift`***+***`Tab`*** to jump to the previous parameter field.

☞ Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

How to Undo the Last Acquisition Parameter Change

☞ Click the following button:

 Undo last acquisition parameter change.

How to Set Pulse Program Parameters

☞ Click the following button:

 Show pulse program parameters [***ased***]

The button will change to . To make this the default setting:

Click ***Options*** → ***Preferences***, click ***Miscellaneous***, check the entry "*Show reduced parameter set (ased)*" and click ***OK***.

How to Display Acquisition Status Parameters

☞ Click the following button:

 Show acquisition status parameters.

Note that the command ***dpa*** opens the acquisition parameter editor and automatically shows the status parameters.

How to Get Probehead/Solvent dependent Parameters

☞ Click the following button:

 Set probehead/solvent dependant parameters [***getprosol***].

Probehead and solvent dependant parameters can be set up with the command ***edprosol***.

How to Change Acquisition Data Dimensionality

☞ Click the following button:

 Change data dimensionality.

This changes the number of parameter columns and value of the acquisition parameter PARMODE.

How to Set Lock Parameters

Enter the command ***edlock*** and set the lock parameters in the appearing dialog box. For a detailed description of ***edlock***, please refer to the Acquisition Reference manual or enter ***edlock?*** on the command line.

How to Set Routing Parameters

Enter the command ***edasp*** and set the routing parameters in the appearing dialog box. For a detailed description of ***edasp***, please refer to the Acquisition Reference manual or enter ***edasp?*** on the command line.

Chapter 6

Data Processing

6.1 Interactive Processing

Interactive processing allows full control over the processing sequence. However, it requires detailed knowledge about the required parameters (see chapter 5.1) and commands. Therefore, it is only suitable for the advanced user. New or intermediate users are recommended to use the Processing Guide for semi-automatic processing (see chapter 6.2).

How to Process Data with Single Commands

Data can be processed by entering single commands on the command line. A typical 1D processing sequence would be:

- ***em*** : exponential window multiplication
- ***ft*** : Fourier transform
- ***apk*** : automatic phase correction
- ***sref*** : automatic calibration (referencing)
- ***abs*** : automatic baseline correction

This allows you full control over each individual processing step.

How to Process data with Composite Commands

Data can also be processed with so called composite commands. These are combinations of single processing commands. The following composite commands are available.

- ***ef*** : Exponential multiplication + Fourier transform
- ***efp*** : Exponential multiplication + Fourier transform + phase correction
- ***fmc*** : Fourier transform + magnitude calculation
- ***fp*** : Fourier transform +phase correction
- ***gf*** : Gaussian multiplication + Fourier transform
- ***gfp*** : Gaussian multiplication + Fourier transform + phase correction

They can be entered on the command line or clicked from the menu. For the latter option:

☞ Click ***Processing*** → ***More transforms*** → ***Shortcuts***

Just like single commands, composite commands can be used in Macros, AU programs and Python programs.

6.2 Semi-automatic Processing

How to Use the Processing Guide in *Automatic* mode

The Processing Guide in automatic mode guides you through the entire processing sequence of data selection, processing, printing and archiving with minimum user interaction.

1. Click ***Processing*** → ***Processing Guide***

   The Processing Guide window will appear as an integral part of the current data window (see Fig. 6.1).

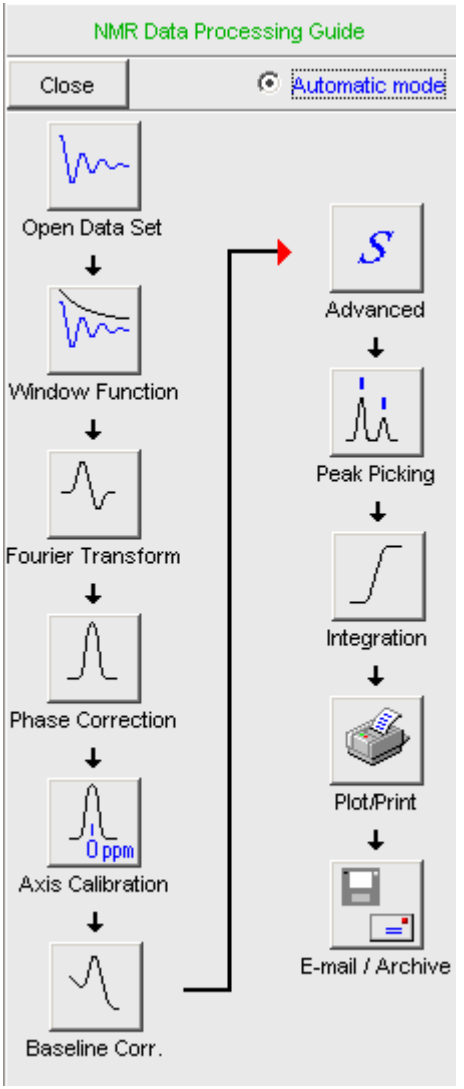


Figure 6.1

2. In the Processing Guide window:

a) Check ***Automatic mode***

b) Click ***Open data set*** and click ***OK*** to open a dataset manually, e.g. from the browser or click ***Browse*** to open the File Chooser.

c) Click ***Window function → Fourier Transform → etc.***

Each processing step will be executed without user interaction.

How to Use the Processing Guide in *Interactive* mode

The Processing Guide in interactive mode guides you through the entire processing sequence of data selection, processing, printing and archiving requiring some user interaction.

1. Click ***Processing → Processing Guide***

   The Processing Guide window will appear as an integral part of the current data window.

2. In the Processing Guide window:

   a) Uncheck ***Automatic mode***

   b) Click ***Open data set*** and click ***OK*** to open a dataset manually, e.g. from the browser or click ***Browse*** to open the File Chooser.

   c) Click ***Window function → Fourier Transform → etc.***

For each step a dialog box will appear where you can enter options, parameters etc. For details on these items, please refer to the corresponding commands in the Processing Reference Guide.

6.3 Processing Data with AU programs

Data processing can be performed by using AU programs. An AU program is actually a C-program which contains TOPSPIN commands (macros) and/or C-language statements. Various standard AU programs are delivered with TOPSPIN. A typical 1D processing AU program is ***proc_1d***. A simplified version of this AU program is:

```
EF
APK
SREF
ABS
AUTOPLOT
QUIT
```

It executes the commands ***ef***, ***apk***, ***sref***, ***abs*** and ***autoplot***. To run this AU

program, just enter ***proc_1d*** on the command line [1]. You can create your own AU programs with the command ***edau***. Note that an AU program must end with QUIT or QUITMSG("your message"), and that all statements must be specified in capital letters. For more information on AU programs, please refer to the AU program reference manual:

Click ***Help → Programming → AU programming***

As an alternative to AU programs, you can also write Python programs, which allow you to use TOPSPIN commands, User Interface functions and Graphic functions. For more information:

☞ Click ***Help → Programming → Python Programming***

6.4 Serial Processing using Python programs

TOPSPIN allows you to process a series of datasets using serial scripts. The dataset list and command(s) to be used can be easily setup from the TOPSPIN interface as follows. Enter the command ***serial*** on the command line. This will open the

1. Before you can use any Bruker AU program, ***expinstall*** must have been executed once.

dialog window shown in Fig. 6.2.

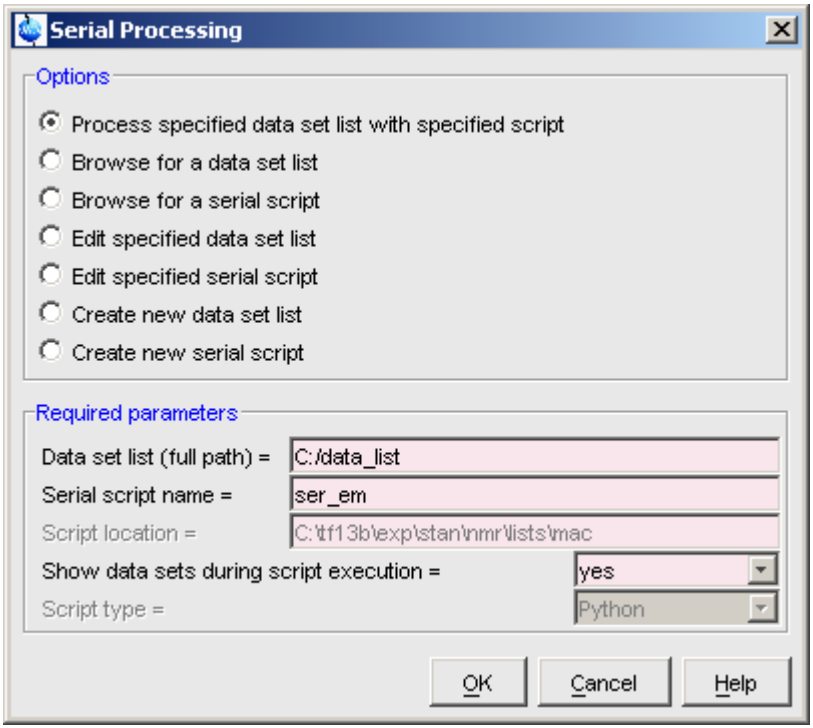


Figure 6.2

Here you can set up and start data processing of a series of datasets using scripts, which can be TOPSPIN macros or Python programs.

The dialog offers you the following options:

Process specified data set list with specified script

Process the data in the specified dataset list using the specified serial script. The flag ***Show data sets during script execution*** allows you to either display the currently processed dataset or remain on the current dataset.

Browse for a dataset list

Browse for an existing dataset list, starting in the users home directory.

Browse for a serial script

Browse for existing serial script. Depending on the parameter ***Script type***, the browser opens the ../exp/stan/nmr/py for ***Script type*** Python or ../exp/stan/nmr/lists/mac ***Script type*** macro. TOPSPIN, by default, searches for for files named `ser_*`.

Edit specified data set list

View or edit the list specified in the field ***Data Set List***.

Edit specified serial script

View or edit the script specified in the field ***Serial script name***

Create new data set list

Opens a dialog box for finding datasets. Proceed as follows:

1. Specify all search criteria and click ***OK***
2. In the appearing Search result box:
   a) Select the desired datasets.
   b) Click ***Save selection..***
3. In the appearing browser:
   a) Navigate to the desired list directory.
   b) Enter or select the list filename.
   c) Click ***OK***

Alternatively, you can create a dataset list manually.The format of a list entry is:

<name> <expno> <procno> <dir> <user>

An example of a dataset list is:

```
exam1d_13C 1 1 C:/bio guest
exam1d_13C 2 1 C:/bio guest
exam1d_13C 3 1 C:/bio guest
```

Create new serial script

Opens the appropriate editor to create a new script. For ***Script type*** Python, ***edpy*** is executed, for ***Script type*** macro, ***edmac*** is executed. The name of a serial script (macro of Python) must start with `ser_`. Python scripts must have the extension `.py`. A standard example is the python script `ser_efp.py`.

An example of a simple processing sequence is exponential window multiplication, Fourier transform and automatic phase correction of a 1D dataset. A TOPSPIN macro performing this task would be:

```
ef

apk
```

A Python programs performing the same task would be:

```
EF()
APK()
```

Note that Python programs are much more versatile than macros. Details on Python programming can be found under:

Help → Programming → Python programming

Note that serial processing can also be started as follows:

- Click ***Processing → Serial Processing...***

or

- Click ***File → Run***, select ***Execute Serial script on Data set list*** and click ***OK***

Chapter 7

Printing/Exporting Data

7.1 Printing/plotting Data

How to Print/Plot from the Menu

The current data window can be printed as follows:

1. From the TOPSPIN menu:

☞ Click the button  in the upper toolbar

or Click ***File*** → ***Print***

or Enter ***`print`*** or ***`Ctrl+p`***

All these actions are equivalent; they open the Print dialog box (see Fig. 7.1).

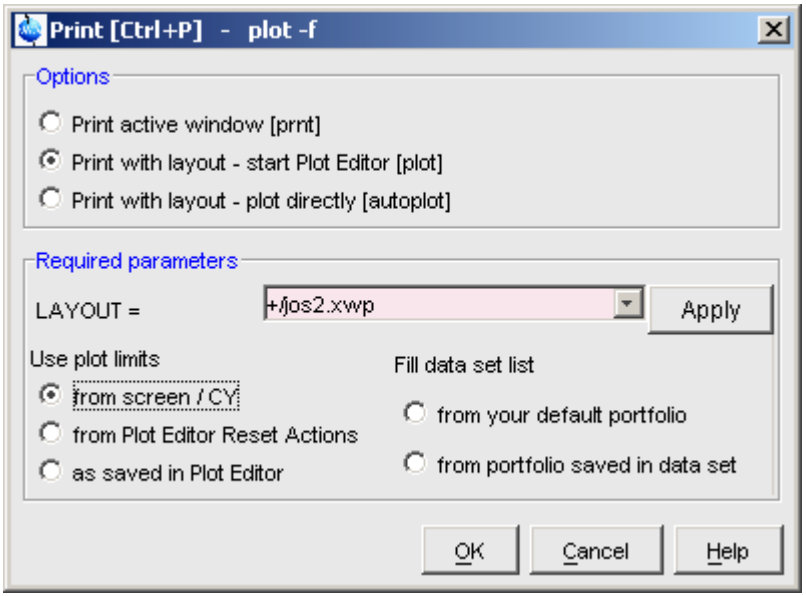


Figure 7.1

2. In the Print dialog box:

   a) Select ***Print active window*** [**`prnt`**]

   b) Click ***OK***

   Before printing starts, the operating system print dialog box will appear. Here you can, for example, select the printer name and the printer properties.

The Print dialog box (see Fig. 7.1) contains two further options:

- ***Print with layout - start Plot Editor*** [**`plot`**]
  If you select this option and click ***OK***, the Plot Editor will be started. This option is equivalent to entering **`plot`** on the TOPSPIN command line.
- ***Print with layout - plot directly*** [**`autoplot`**]
  Selecting this option activates the Plot Editor layout list box. Select the desired layout and click ***OK*** to print. Standard layouts are delivered with TOPSPIN. They use the Windows default printer. User defined layouts use the printer defined in the Plot Editor. On a 1D dataset, only 1D layouts are listed, on a 2D dataset only 2D layouts are listed etc.

For the last two options, the following Required Parameters are available:

Use plot limits:

- ***from screen/ CY***
  The plot limits and maximum intensity are used as they are on the screen (processing parameter F1P, F2P and CY, respectively).
- ***from Plot Editor Reset Actions***
  The plot limits and maximum intensity are set according to the Plot Editor Reset Actions (right-click inside the Plot Editor data field and choose ***Automation*** to set the Reset Actions).
- ***as saved in Plot Editor***
  The plot limits and maximum intensity are set in the specified layout

Fill dataset list:

- ***from your default portfolio***
  The portfolio contains the current TOPSPIN dataset plus the data from the default Plot Editor portfolio.
- ***from port folio saved in dataset***
  The portfolio contains the current TOPSPIN dataset plus the data from the portfolio stored in this dataset.

How to Plot Data from the Processing guide

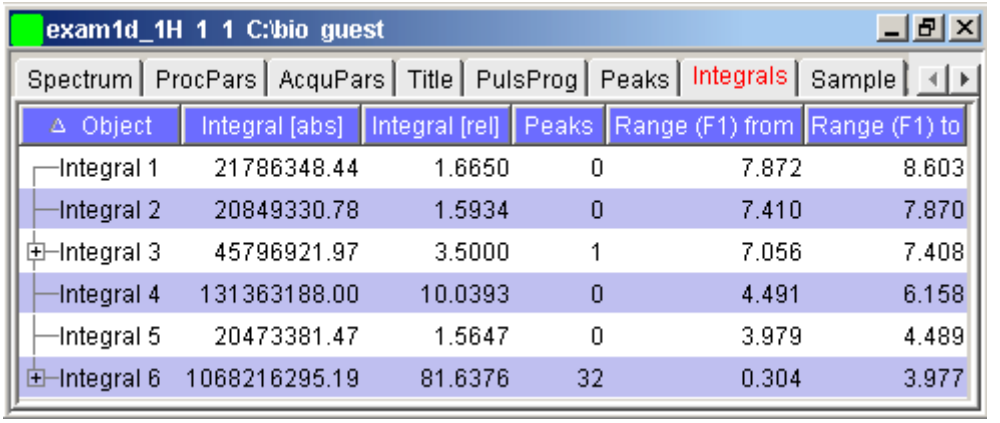
Printing/plotting data can be done from the Processing guide by clicking the ***Plot/Print*** button. If ***Automatic mode*** is checked, the active data window will be printed as it appears in the screen. If ***Automatic mode*** is unchecked, you will get the dialog box as displayed in Fig. 7.1.

How to Plot Data with the Plot Editor

The Plot Editor can be started from the Plot Editor or from the command line (command ***plot***). The Plot Editor allows you to create layouts and plot data. The complete functionality is described in the online manual, which can be opened from the Plot Editor ***Help*** menu.

How to Print the Integral list

1. Click the ***Integrals*** tab of the data window (see Fig. 7.2).
2. Enter ***print*** or ***Ctrl***+***p*** to print it.

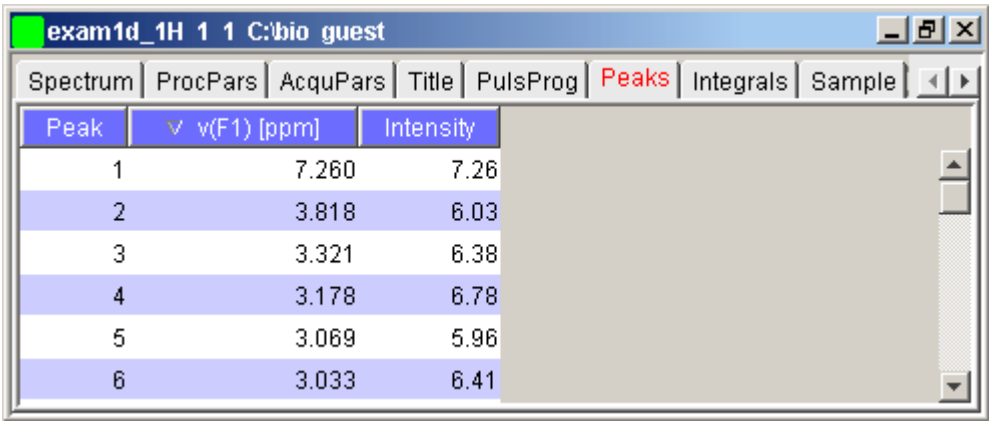


Object	Integral [abs]	Integral [rel]	Peaks	Range (F1) from	Range (F1) to
Integral 1	21786348.44	1.6650	0	7.872	8.603
Integral 2	20849330.78	1.5934	0	7.410	7.870
Integral 3	45796921.97	3.5000	1	7.056	7.408
Integral 4	131363188.00	10.0393	0	4.491	6.158
Integral 5	20473381.47	1.5647	0	3.979	4.489
Integral 6	1068216295.19	81.6376	32	0.304	3.977

Figure 7.2

How to Print the Peak list

1. Click the ***Peaks*** tab of the data window (see Fig. 7.3).
2. Enter ***`print`*** or ***`Ctrl`***+***`p`***



Peak	ν(F1) [ppm]	Intensity
1	7.260	7.26
2	3.818	6.03
3	3.321	6.38
4	3.178	6.78
5	3.069	5.96
6	3.033	6.41

Figure 7.3

7.2 Exporting Data

How to Copy data to Other Applications

Under MS Windows, you can easily copy the data window contents to other applications. To do that:

☞ Click ***Edit*** → ***Copy*** [***copy***].

This will copy the data window contents to:

- the clipboard. After that you can paste the clipboard contents to any Windows application.
- the Windows Metafile file `screenDump.wmf` in the user properties directory (enter ***hist*** to locate this directory). The Windows Metafile can be imported by other applications or send to a different computer.

Please note:

Some programs, when importing spectra from the clipboard or metafile, do not display the contained information correctly. Particularly when you resize the imported graphics, sections of the text, the spectrum, or the axis sometimes have disappeared. Usually this is only a display problem. When you print the respective page, the representation is correct.

How to Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TOPSPIN allows you to save the contents of a data window in a graphics file of selectable type, e.g. `.png`, `.tif`, `.wmf` etc. To do that:

1. Click ***File*** → ***Export***.... [***exportfile***].
2. Navigate to the storage folder.
3. Enter the destination filename and extension.
4. Click ***Export***

The resolution of such a *screen dump* equals the resolution of your screen.When you import a graphics file into an other program, you may loose information when resizing the graphics.

Chapter 8

1D Display

8.1 The 1D Data Window

The 1D data window consists of a data field, a title bar, a Tab bar and buttons. Fig. 8.1 shows a data window with a 1D spectrum.

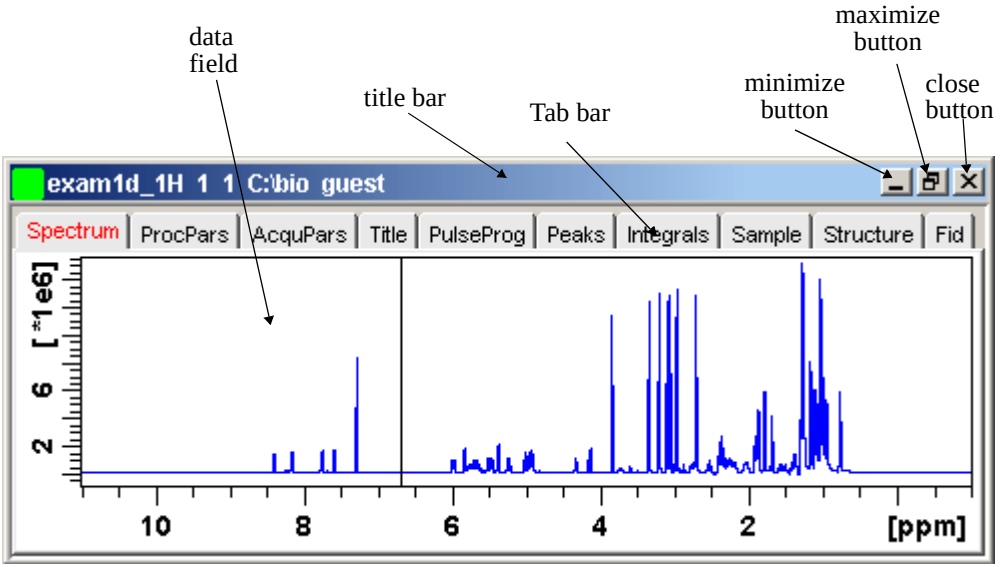


Figure 8.1

8.2 Displaying one Dataset in Multiple windows

TOPSPIN allows you to display one dataset in multiple data windows. This is, for example, convenient to view various regions or various objects (spectrum, fid, parameters etc.) of the same dataset.

How to Reopen a Dataset in a Second/Third etc. Window

1. Select (activate) the desired dataset.
2. Click ***File*** → ***Reopen*** [**`reopen`**].

Multiple data windows with the same dataset are indicated with a number in square brackets, e.g. [1], in the title bar (see Fig. 8.2).

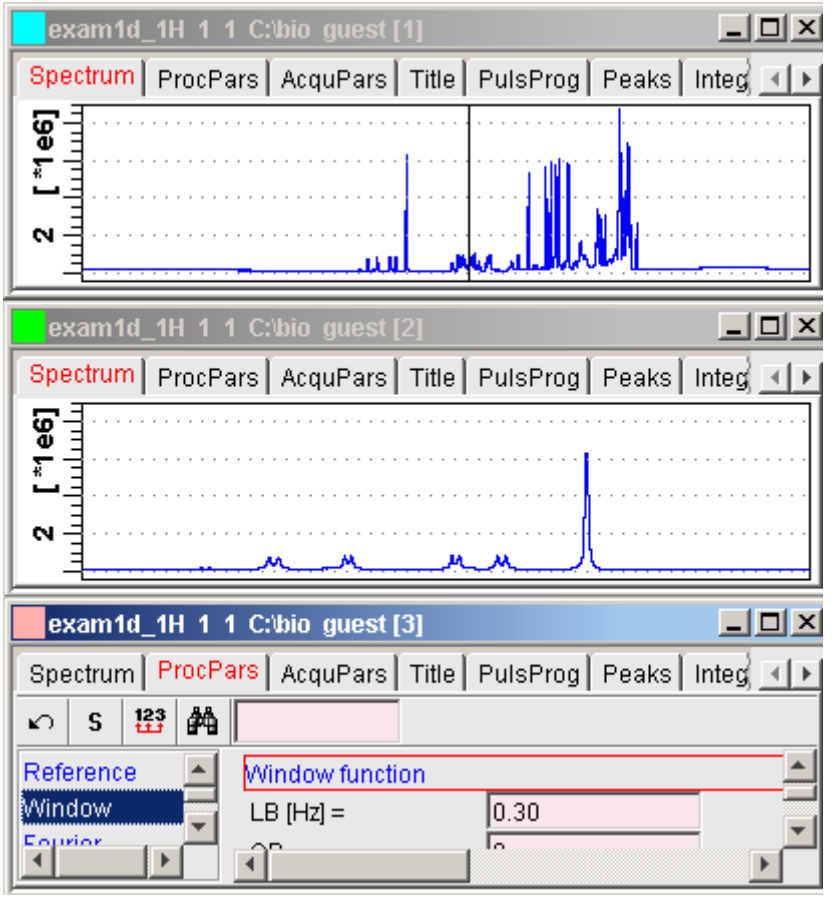


Figure 8.2

How to Rescale or Shift one Dataset in Multiple windows

Display manipulation buttons like *2 and ⤒ only work on the active data window. The same counts for the keys ***Alt***+***PageUP*** and ***Alt***+***PageDown***. However, when used with the control key, they work on all windows, for example:

☞ Hit ***Ctrl***+ *2 , ***Ctrl***+***Alt***+***PageUp*** or ***Ctrl***+***Alt***+***PageDown***

8.3 Changing the Display of a 1D Spectrum or FID

TOPSPIN offers buttons to scale or shift the spectrum vertically and horizontally.

How to Change the Vertical Scaling of the FID or Spectrum

☞ Hit one of the following the keys:

- ***Alt***+***PageUp*** : Increase the intensity by a factor of 2.
- ***Alt***+***PageDown*** : Decrease the intensity by a factor of 2.
- ***Alt***+***Enter*** : Reset the intensity.

or

☞ Click-hold the button and move the mouse:

 Change the intensity smoothly.

or

☞ Click one of the following buttons:

 Increase the intensity by a factor of 2 [****2***].

 Increase the intensity by a factor of 8 [****8***].

 Decrease the intensity by a factor of 2 [***/2***].

 Decrease the intensity by a factor of 8 [***/8***].

 Reset the intensity [***.vr***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all data windows, press the ***Ctrl*** key while clicking one of the above buttons.

How to Change the Horizontal Scaling of the FID or Spectrum

☞ Click-hold the button and move the mouse:

 Zoom in/out smoothly.

or

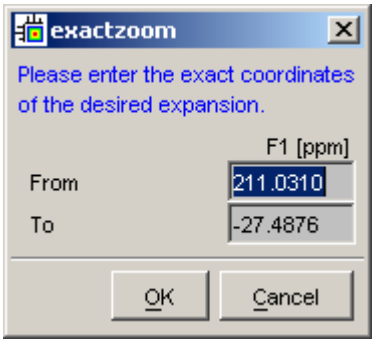
☞ Click one of the following buttons:

Zoom in (increase horizontal scaling) [***.zi***].

Zoom out (decrease horizontal scaling) [***.zo***].

Perform an exact zoom via a dialog box [***.zx***].

a) Enter the coordinates of the desired region in the dialog box:



b) Click ***OK***

Retrieve previous zoom [***.zl***].

Reset zooming (horizontal scaling) to full spectrum [***.hr***].

Reset horizontal (zooming) and vertical (intensity) scaling [***.all***].

Retain horizontal and vertical scaling when modifying dataset or changing to different dataset [***.keep***]. Effects all data windows.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift a Spectral Region to the Left or to the Right

☞ Click-hold the following button and move the mouse:

Smoothly shift to left or right.

or

☞ Click one of the following buttons:

- Shift to the left, half of the displayed region [***.sl***].
- Shift to the right, half of the displayed region [***.sr***].
- Shift to the extreme left, showing the last data point [***.sl0***].
- Shift to the extreme right, showing the first data point [***.sr0***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift the Spectrum Up or Down

To shift the FID or spectrum display up or down:

☞ Click-hold the button and move the mouse:

- Smoothly shift the spectrum baseline up/down.

or

☞ Click one of the following buttons:

- Shift the spectrum baseline to the middle of the data field [***.su***].
- Shift the spectrum baseline to the bottom of the data field [***.sd***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

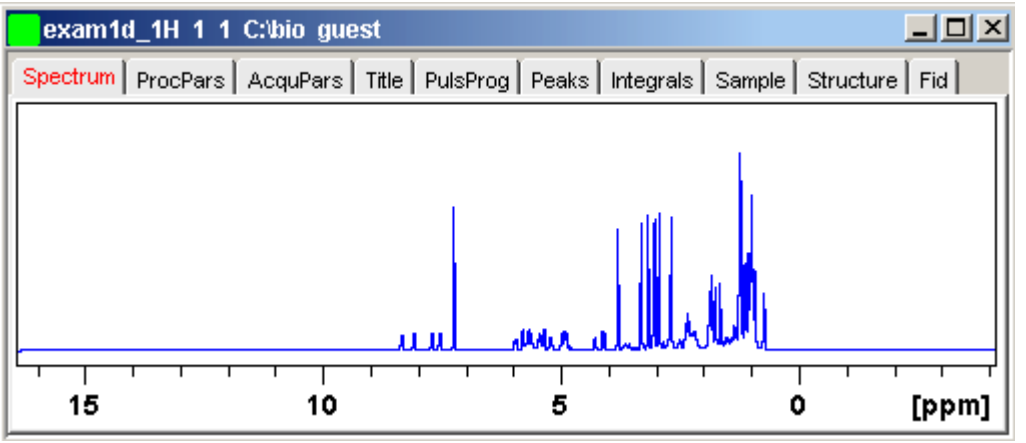
8.4 Using the Tab bar

Tabs of the data window can be activated by clicking them or by entering the corresponding commands, as specified between square brackets, on the command line. Note that command line commands always work on the currently selected (active) data window.

The Tab bar can be configured from the User Preference box (command ***set***).

How to Display the Spectrum

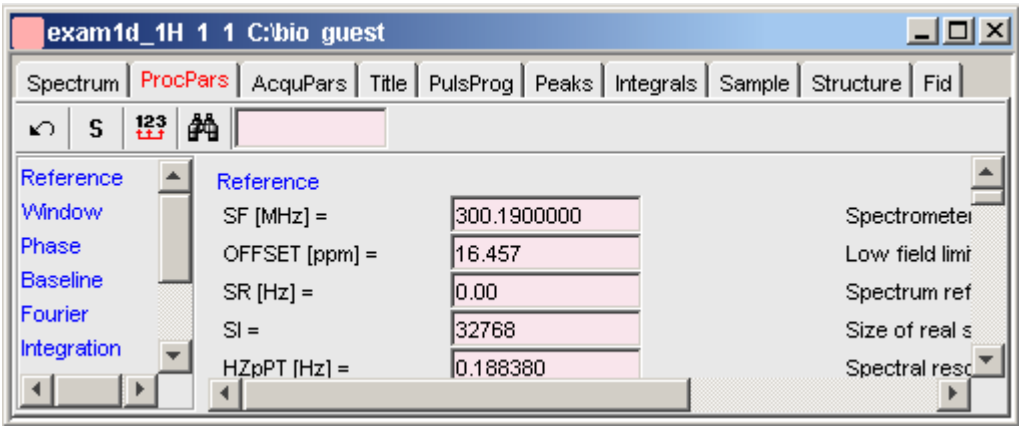
☞ Click the ***Spectrum*** tab [**`spec`**]



This displays the processed data. If these do not exist, the text '*No processed data available*' appears.

How to Set Processing Parameters

☞ Click the ***ProcPars*** tab [**`edp`**]



This opens the processing parameter editor (see also chapter 5.1). The following extra buttons are available:

↶ Undo last value change. Can be used to undo multiple changes.

S Status parameter display. The button turns green when activated [***dpp***].

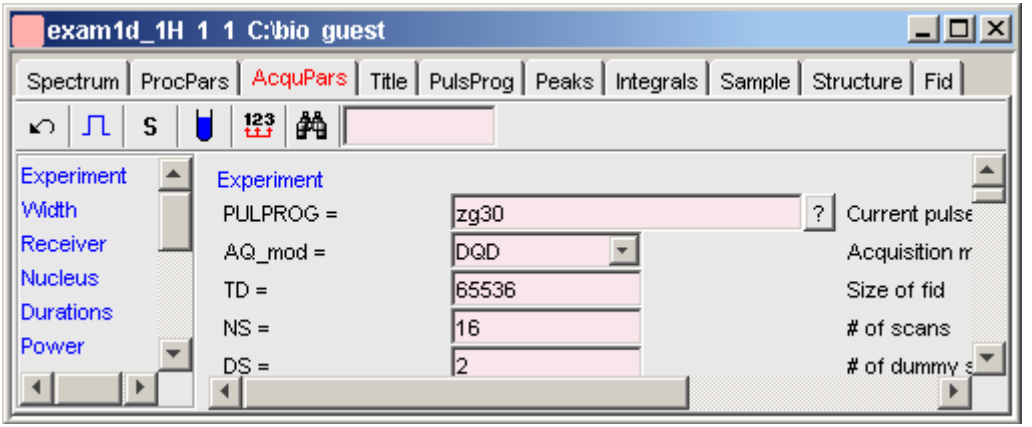
123 Change processed dataset dimensionality (parameter PPARMOD).

Search for specified parameter.

Changed parameters are automatically saved.

How to Set Acquisition Parameters

☞ Click the ***AcquPars*** tab [***eda***]



This opens the acquisition parameter editor (see also chapter 5.1)). The following extra buttons are available:

Undo last value change. Can be used to undo multiple changes.

Show pulse program parameters [***ased***].

S Status parameter display. The button turns green when activated [***dpa***].

Set probehead/solvent dependant parameters [***getprosol***].

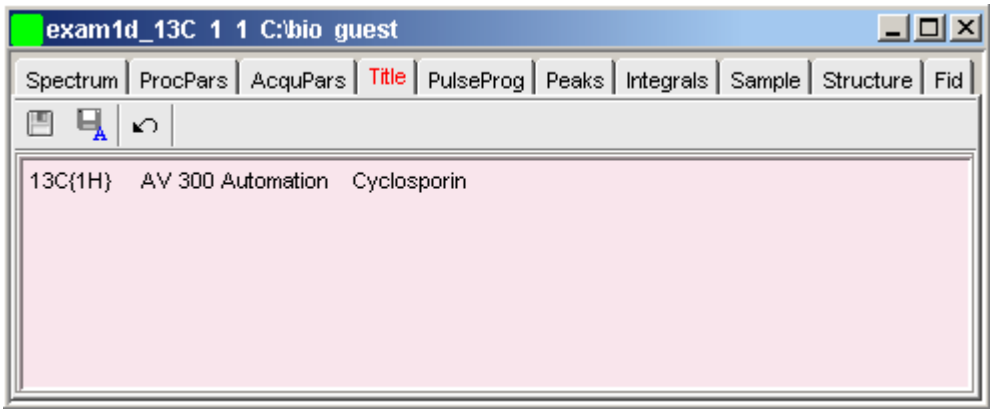
123 Change raw dataset dimensionality (parameter PARMODE).

Search for specified parameter.

Changed parameters are automatically saved.

How to Edit the Title

Click the ***Title*** tab [***edti***]



This allows you to edit the title that appears in the data window and on the plot.

Save the title file under its current name.

Save the title file under a new name.

Reload the title file. Undo modifications since the last save.

How to Edit the Pulse Program

☞ Click the ***PulsProg*** tab [***edcpul***]

This allows you to edit the current pulse program. The following extra buttons are available here:

- Save the pulse program under its current name.
- Save the pulse program under a new name.
- Reload the pulse program. Undo modifications since the last save.
- S Switch to status pulse program.
- E Show the pulse program in an external editor.
- Start the graphical pulse program display [***nmrsim***].

How to Display the Peak list

Click the ***Peaks*** tab

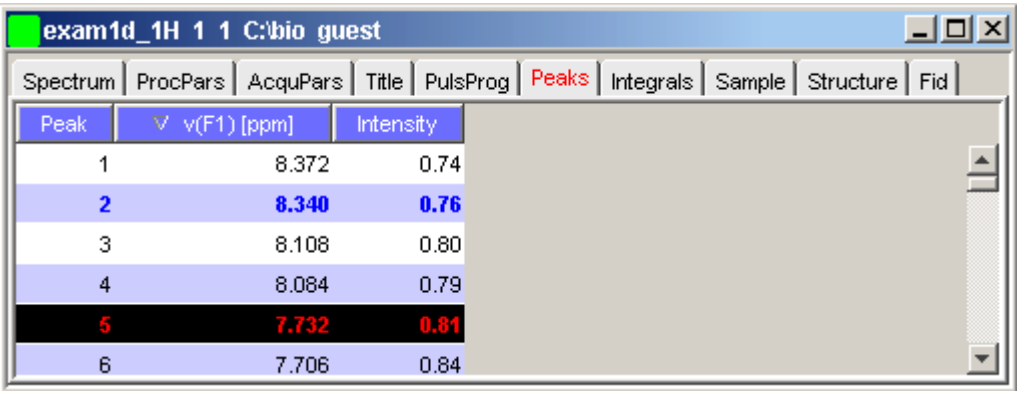


Figure 8.3

This displays the peak list. By default, the peak list shows the following entries:

Peak : the peak number

v(F1) [ppm] : the chemical shift

Intensity: the peak intensity

Display the spectral region around a peak

☞ Right-click the desired peak

this will open the popup menu shown in Fig. 8.4.

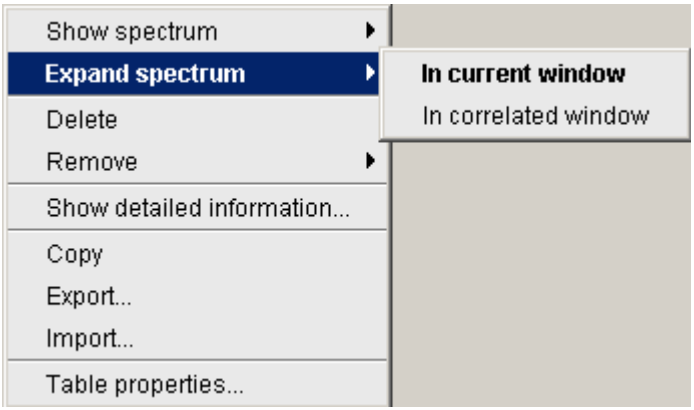


Figure 8.4

Here you can choose from the following options:

☞ ***Show spectrum → In correlated window***
to open a new data window showing the full correlated spectrum

☞ ***Expand spectrum → In current window***
to change the current data window to spectrum display, showing the region around the selected peak

☞ ***Expand spectrum → In correlated window***
to open a new data window showing the region around the selected peak

Export entries of the peak list

Entries of the peak list can easily be exported to Excel or any other program as follows:

1. For multiple peaks:

   Select the desired entries while pressing the ***Ctrl*** or ***Shift*** key
2. Right-click an entry to open the popup menu (see Fig. 8.4)
3. Click one of the following menu items:
   - ***Copy***
     Copy the selected peak(s) entry to the Clipboard. Equivalent to clicking ***Edit → Copy*** or hitting ***Ctrl+c***. Copied peaks can easily be pasted in any other application such as Excel.

- **Export...**
  Export selected peaks. Opens a dialog box where you can specify the export file (`.cvs`, `.txt` or `.xml`). Check the box in the lower-left corner to export the selected peaks only or uncheck it to export the entire list. Then click ***Export***.

Import a peak List

A peak list from a different dataset can be imported as follows:

1. Right-click an entry to open the popup menu (see Fig. 8.4)
2. Click **Import...**
3. In the appearing dialog box, navigate to the directory where the list resides and select the peak list (`.xml` or `.txt`).

As such you can import a peak list from a different dataset or a previously exported list from the current dataset. Note that peak picking commands store the peak list in the processed data directory under the name `peak.txt`.

Delete/remove peaks from the peak list

To delete one peak:

☞ Right-click the peak and choose ***Delete*** from the popup menu

To delete multiple peaks:

1. Select the peaks while pressing the ***`Ctrl`*** or ***`Shift`*** key
2. Right-click one of the peaks and choose ***Delete*** from the popup menu

To remove possible duplicate peaks:

☞ Right-click any entry and choose ***Remove*** → ***Duplicate peaks***

To remove possible peaks outside of the spectrum:

☞ Right-click any entry and choose ***Remove*** → ***Peaks positioned outside of the spectrum***

Shortcuts

Double-click a peak : zoom into spectrum, i.e. show region around that peak

`Enter` key : zoom into spectrum, i.e. show region around selected peak(s))

`Delete` key : delete the selected peak(s) from the peak list

Ctrl*+*c : copy selected peaks to the Clipboard.

Ctrl*+*a : select all peaks.

Home : select the first peak

End : select the last peak.

Shift*+*Home : select current and first peak and all in between.

Shift*+*End : select current and last peak and all in between.

Note that these keys only work when the cursor focus is in the data window.

More features

The right-click popup menu has the following entries (see Fig. 8.4):

Table properties
Set the shown columns and specify their decimal places.

Show detailed information
Show peak information, dataset information and peak picking parameters.

When you move the cursor over the peak list, the active peak will be highlighted in blue (see peak 3 in Fig. 8.5). If the correlated spectrum is also displayed, a vertical line moves along, showing corresponding position in the spectrum (see Fig. 8.5)

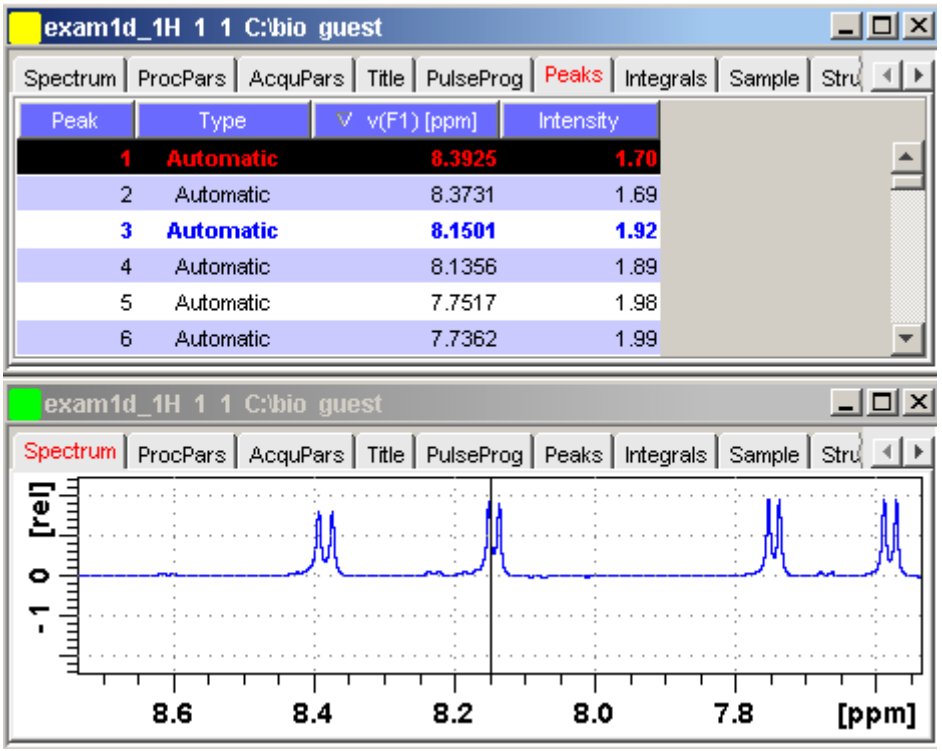


Figure 8.5

As soon as you click a peak, it is selected and displayed in red (see peak 1 in Fig. 8.5). Note that this peak remains selected, i.e. is used by ***Enter*** and ***Delete***, until a different peak is selected.

To extend the peak list with *Regions*, *Type* and *Index* entries, right-click any part of the header bar.

To sort the peaks according to peak number, ppm value or intensity, click the header of the respective entry.

Note that when you delete peaks from the peak list, they are automatically removed from the corresponding file. You cannot undo a delete action.

Peaks are only available if peak picking has been done (command ***pp***). The peak list can be printed with ***print*** [***Ctrl***+***p***]. List items can be selected with the mouse, copied with ***Ctrl***+***c*** and pasted to other applications, e.g. a text editor.

How to Display the Integral list

☞ Click the ***Integrals*** tab **[*li, lipp, lippf*]**

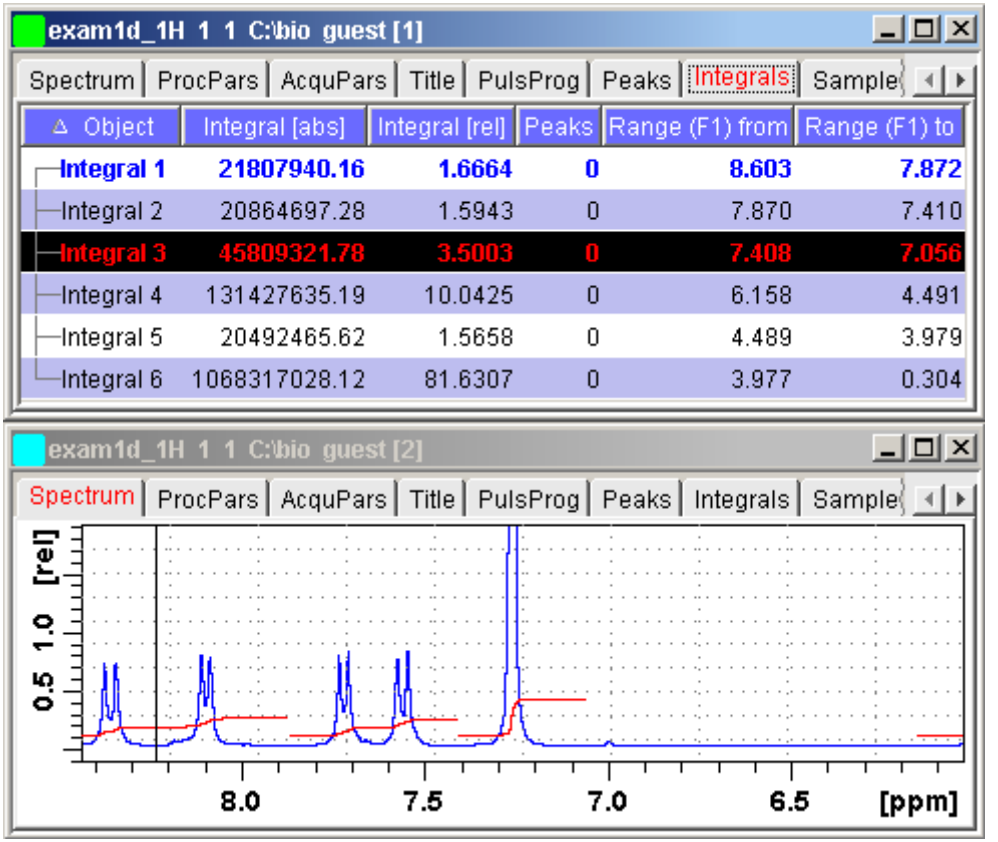


Figure 8.6

This displays the integral list (upper part of Fig. 8.6). By default, this shows the following items:

Object : the integral number

Integral [abs] : the absolute integral value

Integral [rel] : the relative integral value

Peaks : the number of peaks within the integral range

Range (F1) from : the left edge of the integral range

Range (F1) to : the right edge of the integral range

Please note the difference between the following items:

- **selected integral**: the entry that has been clicked last (Integral 3 in Fig. 8.6). If you right-click an entry, it is selected and you can execute one of the commands from the popup menu (see Fig. 8.7) The keys **`Enter`** and **`Delete`** work on the selected entry.
- **active integral**: the entry on which cursor resides (Integral 1 in Fig. 8.6). The active integral is also marked in the correlated spectrum by a black vertical line (see lower part of Fig. 8.6 and description below). When you move the cursor over the integral list, the vertical line in the correlated spectrum moves along with it and vice versa.

Display the spectral region around an integral

To display the spectral region around a particular integral:

☞ Right-click the desired integral

This will open the popup menu shown in Fig. 8.7.

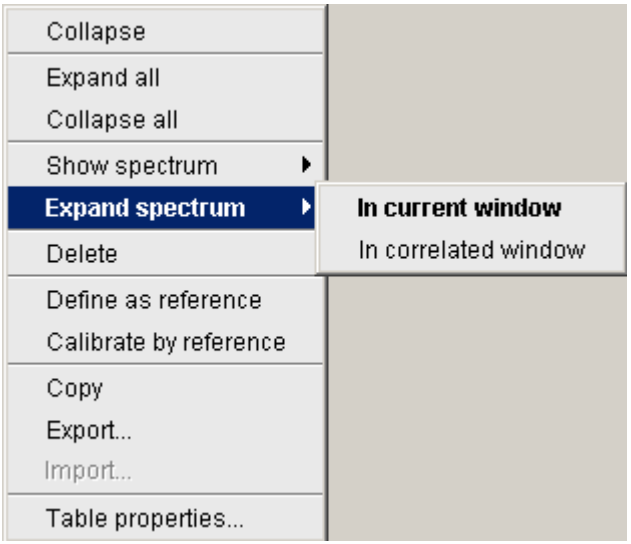


Figure 8.7

Here you can choose from the following options:

☞ ***Show spectrum → In correlated spectrum***

to open a new data window showing the full correlated spectrum

☞ ***Expand spectrum → In current window***
to change the current data window to spectrum display, showing the region around the selected integral

☞ ***Expand spectrum → In correlated window***
to open a new data window showing the region around the selected integral (lower part of Fig. 8.6)

Note that clicking the marked entry in the right-click popup menu is equivalent to pressing of the ***Enter*** key.

Export/Import Entries of the Integral List

Entries of the integral list can easily be exported to Excel or any other program as follows:

1. For multiple integrals:

   Select the desired entries while pressing the ***Ctrl*** or ***Shift*** key
2. Right-click an entry to open the popup menu (see Fig. 8.7)
3. Click one of the following menu items:
   - ***Copy***
     Copy the selected integral(s) entry to the Clipboard. Equivalent to clicking ***Edit → Copy*** or hitting ***Ctrl+c***. Copied integrals can easily be pasted in any other application such as Excel.
   - **Export...**
     Export selected integrals. Check the box in the lower-left corner to export the selected integrals only or uncheck it to export the entire list. Then click ***Export***.

TOPSPIN 1.3 supports exporting 1D integrals in `.csv` format. Future version will also 1D exporting integrals in `.txt` format and importing 1D integrals. These features are already supported for 2D and 3D integrals.

Calibrate Integrals to Compare Spectra

Integrals from the current and other spectra can be calibrated with respect to a reference integral. To do that:

1. Right-click the reference integral and choose **Define as reference** from the popup menu. This will determine the calibration constant.

2. Right-click any integral and choose ***Calibrate by reference***
   This will divide all integrals by the calibration constant, setting the reference integral to 1.0.

Now you can read any other spectrum, and calibrate its integrals with respect to the reference integral defined above. To do that:

1. Read the spectrum
2. Enter ***int*** to define the integral ranges (if this has not been done yet)
3. Click the ***Integrals*** tab
4. Right-click any integral in the list and choose ***Calibrate by reference*** from the popup menu.

Note that the calibration constant is lost when TOPSPIN is restarted.

Display the integral list with peaks

The integral list in Fig. 8.6 shows only integrals. However, if peak picking has been done, the integral list also shows the peaks within each integral range (see Fig. 8.8).

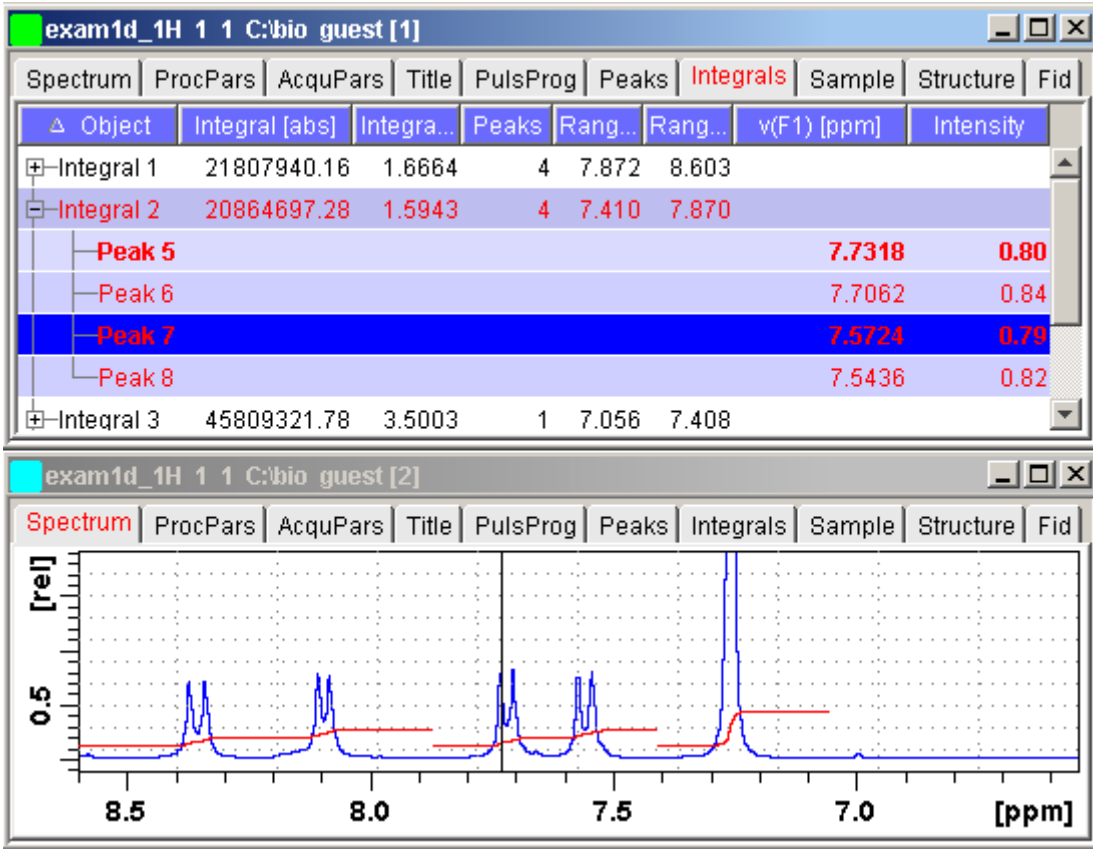


Figure 8.8

Note that the integral entries can be collapsed, (hiding the peaks) or expanded (showing the peaks). As soon as one or more integrals entries are expanded, two extra columns appear showing:

ν(F1) [ppm] : the chemical shift of the peak

Intensity: the peak intensity

Depending on whether or not integrals are expanded, the right-click popup menu contains the following extra items:

- ***Expand***
  Expand the current integral showing all peaks within it.

- ***Expand all***
  Expand all integrals showing all peaks within them.
- ***Collapse all***
  Collapse all integrals hiding all peaks within them.

In addition to the integral entry, an individual peak within an integral can be activated (by placing the cursor on it) or selected (by clicking it). In Fig. 8.8, peak 7 is selected and the correlated spectrum is displayed. Peak 5 is active which is also shown by the vertical line in the correlated spectrum.

Delete an Integral from the Integral List

To delete one integral:

☞ Right-click the integral and choose ***Delete*** from the popup menu

To delete multiple integrals:

1. Select the integrals while pressing the ***Ctrl*** or ***Shift*** key
2. Right-click one of the integrals and choose ***Delete*** from the popup menu

Shortcuts

Enter key : zoom into spectrum, i.e. show region around selected integral(s))

Delete key : delete the selected integral(s) from the integral list

Ctrl+c : copy selected integrals to the Clipboard.

Ctrl+***a*** : select all peaks.

Home : select the first peak

End : select the last peak

Shift+***Home*** : select current and first peak and all in between

Shift+***End*** : select current and last peak and all in between

Double-clicking an integral will show the peaks within the integral region if they exist. It they do not exist, it will zoom into spectrum showing the integral region.

Note that these keys only work when the cursor focus is in the data window.

More features

The right-click popup menu has the following extra entry:

Table properties
to set the shown columns and specify their decimal places

How to view Sample Information

☞ Click the ***Sample*** tab

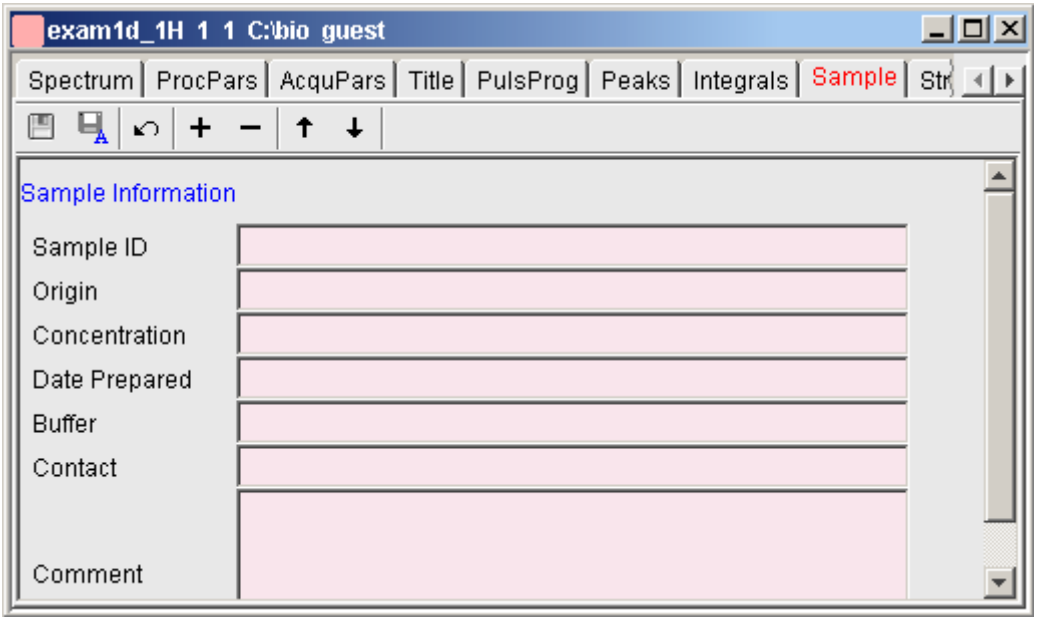


Figure 8.9

This table can be used to fill out any sample information you want to store with the dataset. The table can easily be modified or extended with the following functions:

To select an item: double-click it!

Save the sample information table with the dataset.

Save the sample information table as default.

Reload the original table discarding any changes

+ Add a new item to the table. You will be prompted for an identification name and the desired number of lines

– Remove the selected item from the table

↑ Move the selected item one place up in the table

↓ Move the selected item one place down in the table

How to Open the Jmol Molecule Structure Viewer

☞ Click the ***Structure*** tab [***jmol***]:

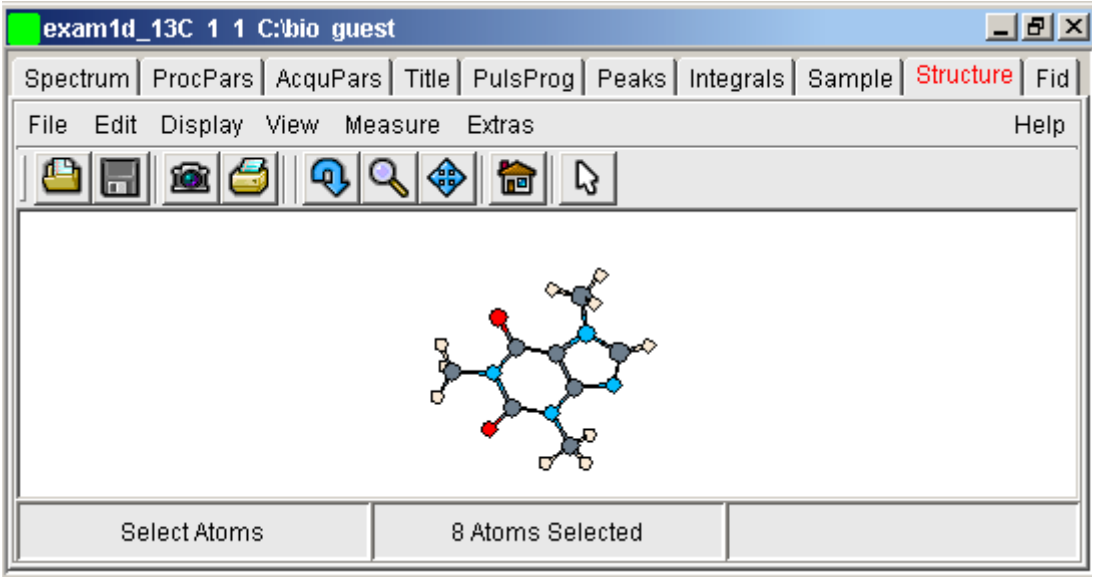


Figure 8.10

opens the *Jmol* molecule structure viewer. TOPSPIN 1.3 contains Jmol version 10. This has the following features:

- The viewer displays the structure file that resides in the *expno* of the current dataset. If this does not exist, the structure file defined by the acquisition parameter CHEMSTR is displayed. CHEMSTR can define a full pathname or a filename. In the latter case, the file is searched for in the directory defined in the User Preferences. To set this directory, click ***Options*** → ***Preferences***, select ***Directory pathnames***, enter a directory and click ***OK***. If no structure file is found, you can open one by clicking ***File*** → ***Open*** in the Molecule Viewer

- The following structure file types are supported: `.xyz`, `.mol`, `.pdb`, `.cml`, `.out`, `.mmlgp`, `.res`, `.cif`, `.gpr`, `.hin`, `.nwo`.
- Secondary structure elements of proteins (backbone, cartoons, ribbons, ...) can be displayed in selectable sizes and colors.
- Mouse button effects:

  Rotate a molecule around the x- and y-axis by pressing the left mouse button, and moving the mouse left/right or up/down, respectively.

  Rotate a molecule around the z-axis by pressing the middle mouse button and moving the mouse left/right .

  Zoom in or out a molecule by pressing the middle mouse button, and moving the mouse up or down.
- RASmol command scripts are supported. To send a RASmol command to the currently displayed molecule enter:

  ☞***jmol <RASmol command>***

  Here are some example:

  ☞***jmol zoom 400***

  ☞***jmol ribbon 200***

  ☞***jmol color ribbon yellow***

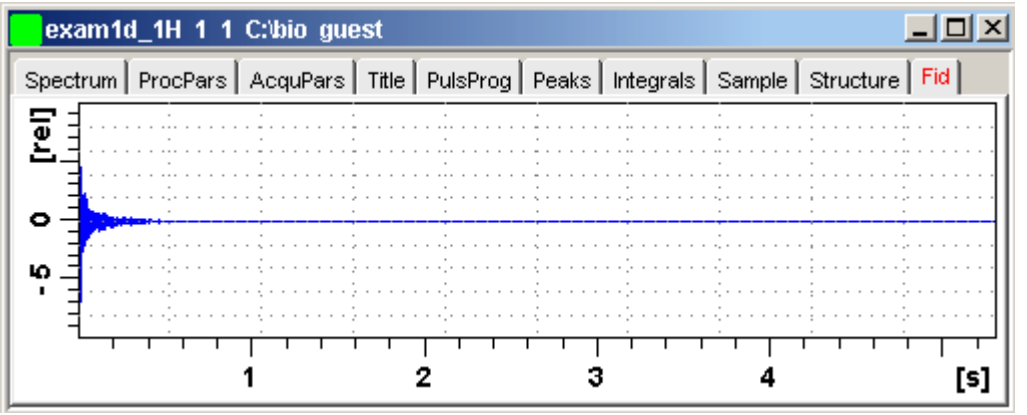
  You may create TOPSPIN macros containing RASmol commands. Just enter ***edmac*** on the TOPSPIN command line and insert the RASmol commands in the appearing editor. Here is an example:

  ```
  jmol load /mystructures/alphahelix.pdb # load a structure
  jmol backbone 0.7 # display its backbone with 0.7 Angstrom size
  jmol color backbone yellow # change backbone color
  jmol background green # change background color
  jmol zoom 200 # zoom structure
  ```

  The available RASmol commands are described in the ***Jmol*** Help menu.
- Multiple molecules (or multiple aspects of one molecule) can be displayed simultaneously. To do that just open multiple data sets or open the same dataset in multiple data windows and click on the ***Structure*** Tab in each window.

How to Display the FID

☞ Click the ***Fid*** tab [***fid***]



displays the raw data. If these do not exist, the text '*No raw data available*' appears. The following additional buttons appear at the right of the lower toolbar:

Show FID in shuffled mode

Show FID in unshuffled mode

If you open a new dataset, the ***Spectrum*** tab is activated, no matter which tab was selected before. If you switch to any interactive manipulation mode, for example to phase correction mode, the Tab bar is replaced by a toolbar for that mode.

8.5 1D Display Options

How to Toggle between Hertz and ppm Axis Units

Click the following toggle button in the upper toolbar:

Toggle between Hz and ppm axis units [***.hz***]

How to Switch on/off the Spectrum Overview display

The spectrum overview shows the entire spectrum at the top of the data window. It is useful when only a certain region of the spectrum is displayed. In the overview, the displayed region is marked as a green area. To switch on the spectrum overview, click the following toggle button in the upper toolbar:

Switch the spectrum overview display on/off [**.ov**]

To shift the displayed region, simply click-hold the green area in the overview spectrum and move the mouse (see Fig. 8.11).

How to Switch Y-axis Display

Click the following toggle button in the upper toolbar:

Switch the y-axis display between abs/rel/off [**.y**]

Fig. 8.11 shows a data window with the spectrum overview on, ppm axis units, and absolute y-axis display.

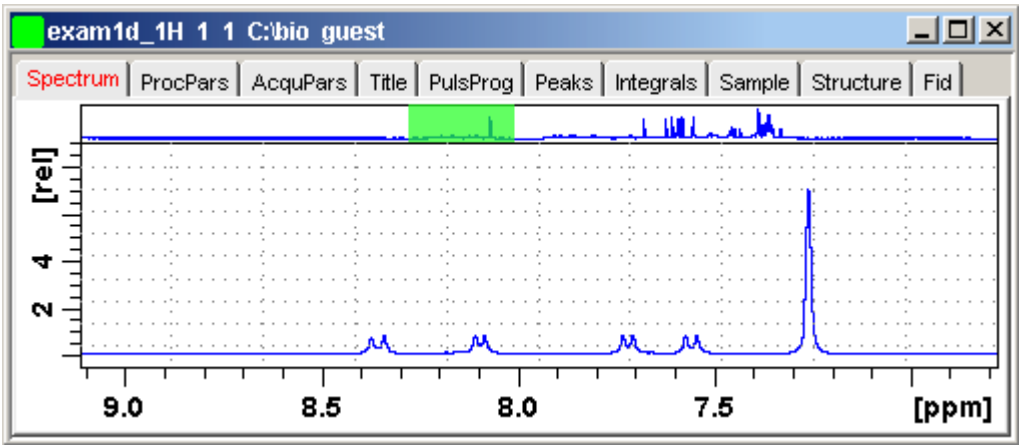


Figure 8.11

8.6 Show Display Properties/Regions/Files

If you right-click inside the data window, the following popup menu will appear:

If you choose ***Display Properties...***, a dialog box (see Fig. 8.12) will appear.

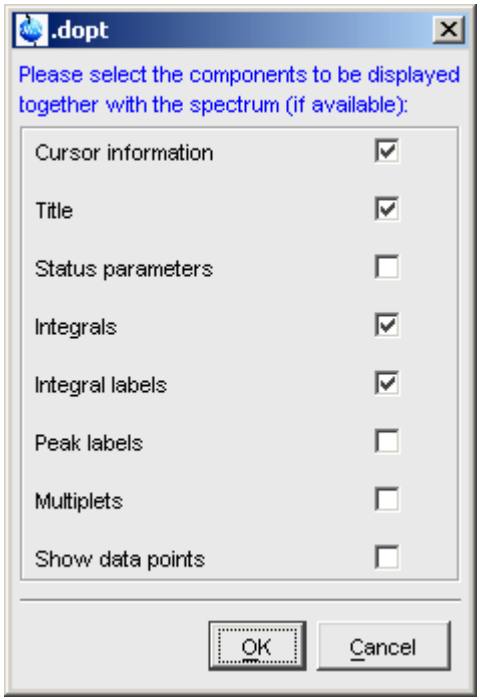


Figure 8.12

Here you can check or uncheck the spectrum components that you want to be displayed in the data window.

you the ***Display Properties...*** dialog box can also be opened from the ***View*** menu.

How to Superimpose the Cursor Information

To superimpose the cursor information on the spectrum:

1. Right-click in the data window and choose ***Display Properties*** [**`.dopt`**]
2. Check ***Cursor information*** in the appearing dialog box and click ***OK***

How to Superimpose the Title on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Title*** in the appearing dialog box and click ***OK***

How to Superimpose the main Status Parameters on the Spectrum [1]

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Status parameters*** in the appearing dialog box and click ***OK***

How to Superimpose the Integral Trails/Labels on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Integrals*** and, if desired, ***Integral labels*** in the appearing dialog box
3. Click ***OK***

If no integrals appear, the integral regions have not been determined yet. This can be done with the **`int`** command.

How to Superimpose Peak Labels on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Peak list*** in the appearing dialog box and click ***OK***

If no peak labels appear, peak picking has not been done yet. This can be done with the **`pp`** command.

How to Show Individual Data Points of the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Show data points*** in the appearing dialog box and click ***OK***
3. Expand the spectral region where you want to see individual points.

---

1. These are the status parameters that also appear on the plot.

How to Display the Main Dataset Properties

☞ Right-click inside the data window and choose ***File Properties***

An information box as displayed in Fig. 8.13 will appear.

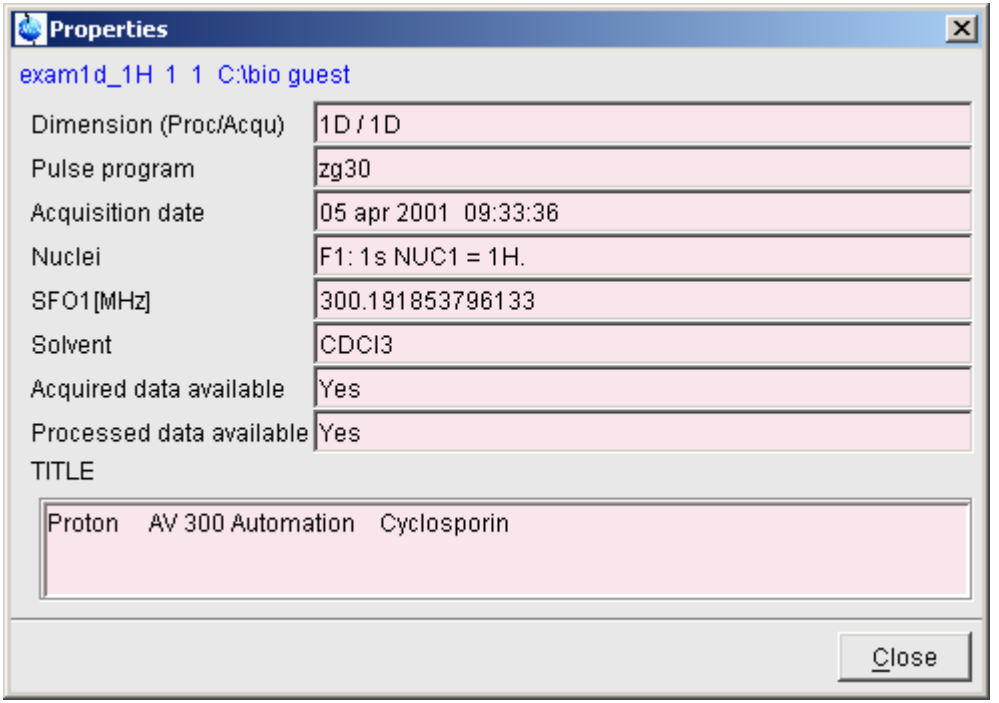


Figure 8.13

Note that this is status information which cannot be changed.

How to Display a List of Files of a Dataset

☞ Right-click inside the data window choose ***Files***

Fig. 8.14 shows the file list when the ***Fid*** tab is active, i.e. when the raw data are displayed. It is the contents of the *expno* directory.

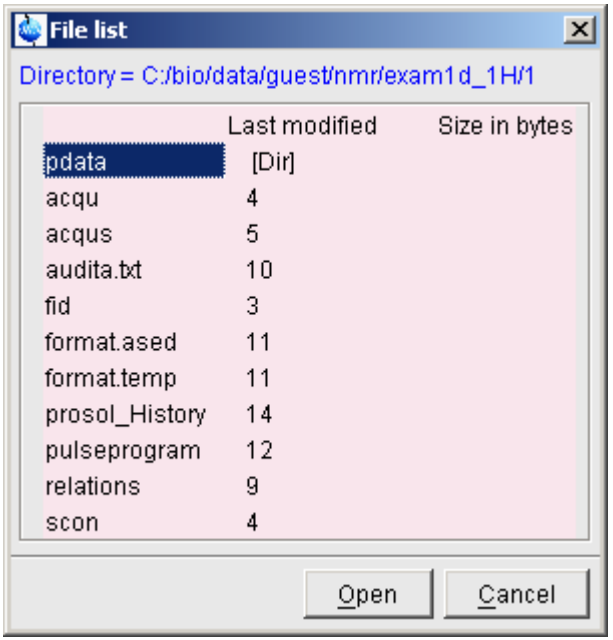


Figure 8.14

Fig. 8.15 shows the file list that appears when the ***Spectrum*** tab is active, i.e. when the processed data are displayed. It is the contents of the *procno* directory.

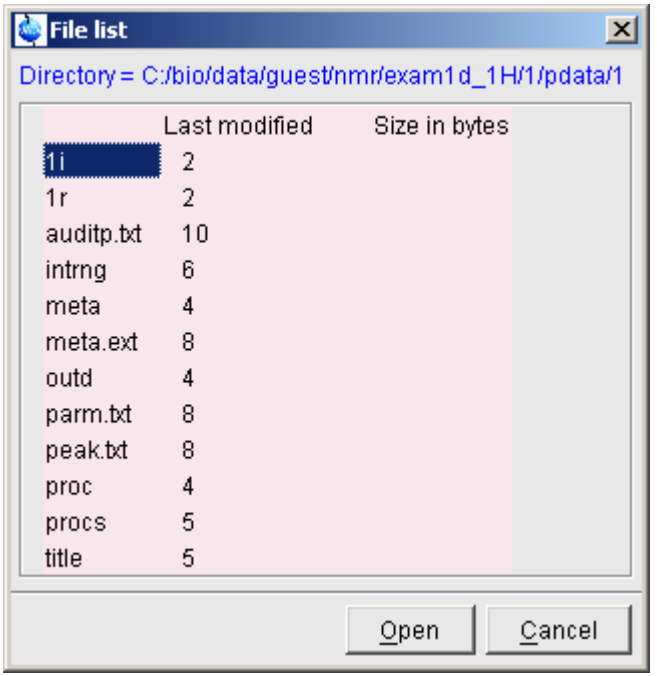


Figure 8.15

The contents of any file in the list can be displayed as follows:

1. Select a filename (it will be highlighted)
2. Click ***Open***

Note that this only makes sense for ascii files, e.g. `acqu*`, `proc*` or files with the extension `.txt`.

Dataset files can also be displayed/opened with the command ***`expl`***. This opens the Windows Explorer, or under Linux, the Konqueror or Mozilla, showing the contents of the *procno* directory.

8.7 Saving Display Region

The currently displayed spectral region can be stored as follows:

☞ Right-click in the data window and choose ***Save Display Region To...***

This will open the dialog box shown in Fig. 8.16.

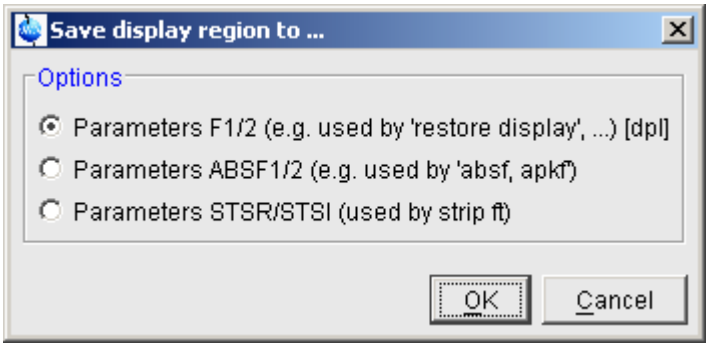


Figure 8.16

How to Save the Display Region for Re-display

☞ Click **Parameters F1/2** [***dpl***]

The saved region can be restored as follows:

☞ Right-click in the data window and choose

Restore Display Region from Params F1/2

How to Save the Display Region for Baseline or Phase Correction

☞ Click **Parameters ABSF1/2**

The region will be stored in the processing parameters ABSF1 and ABSF2. These are used by the commands ***absf*** and ***apkf***.

How to Save the Display Region for Strip FT

☞ Click **Parameters STSR/STSI**

The region will be stored in the processing parameters STSR and STSI. These are used for Fourier Transform commands like ***ft*** and ***trf*** to perform strip FT.

Chapter 9

2D Display

9.1 The 2D Data Window

The 2D data window consists of a data field, a title bar, a Tab bar and buttons. Fig. 9.1 shows a data window with a 2D spectrum.

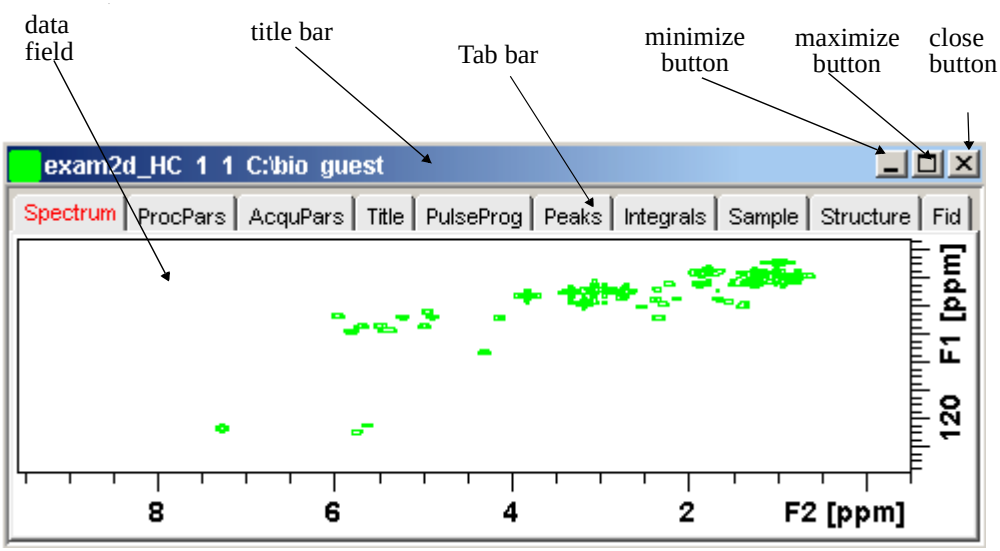


Figure 9.1

9.2 Changing the Display of a 2D spectrum

TOPSPIN offers various buttons to scale or shift a 2D spectrum both vertically and horizontally.

How to Change the Intensity Scaling

☞ Click the button:

Change the intensity scaling (contour levels) [***edlev***]

or

☞ Hit one of the keys:

- ***Alt***+***PageUp*** : Increase the intensity by a factor of 2.
- ***Alt***+***PageDown*** : Decrease the intensity by a factor of 2.
- ***Alt***+***Enter*** : Reset the intensity.

or

☞ Click-hold the button and move the mouse:

Increase/decrease the intensity smoothly.

or

☞ Click one of the following buttons:

*2 Increase the intensity (decrease the levels) by 2 [****2***].

*8 Increase the intensity (decrease the levels) by 8 [****8***].

/2 Decrease the intensity (increase the levels) by 2 [***/2***].

/8 Decrease the intensity (increase the levels) by 8 [***/8***].

Reset the intensity to the last saved intensity (contour levels) [***.vr***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all data windows, press the ***Ctrl*** key while clicking one of the above buttons.

How to Switch on/off Square 2D layout

Right-click inside the data field and click ***Square Layout On/Off***

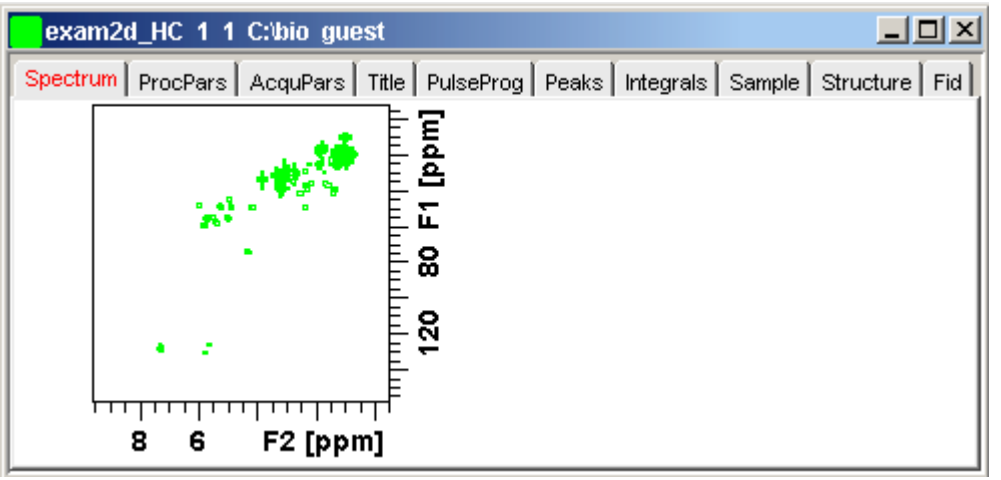


Figure 9.2

The F2 scaling will be adjusted to reach a square display.

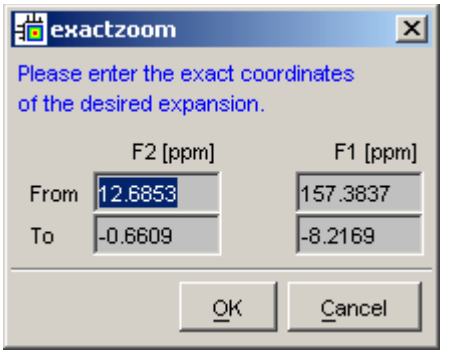
How to Zoom a 2D spectrum in/out

☞ Click one of the following buttons:

Zoom in [***.zi***].

Zoom out [***.zo***].

Perform an exact zoom via a dialog box [***.zx***].



a) Enter the coordinates of the desired region in the dialog box.

b) Click ***OK***

 Retrieve previous zoom [***.zl***].

 Reset F2 direction zooming to full spectrum [***.f2r***].

 Reset F1 direction zooming to full spectrum [***.f1r***].

 Reset F2- and F1-zooming to full spectrum [***.all***].

 Retain horizontal and vertical scaling when modifying dataset or changing to different dataset. Effects all data windows [***.keep***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift a Spectral Region in the F2 direction (left/right)

☞ Click one of the following buttons:

 Shift to the left, half of the displayed region [***.sl***].

 Shift to the right, half of the displayed region [***.sr***].

or

☞ Click-hold the button and move the mouse:

 Smoothly shift up/down and left/right.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift a Spectral Region in the F1 direction (up/down)

☞ Click one of the following buttons:

 Shift the spectrum up, half of the displayed region [***.su***].

 Shift the spectrum down, half of the displayed region [***.sd***].

or

☞ Click-hold the button and move the mouse:

 Smoothly shift up/down and left/right.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

9.3 Show Display Properties/Regions/Files

If you right-click inside the data window, the popup menu shown in Fig. 9.3 will appear.

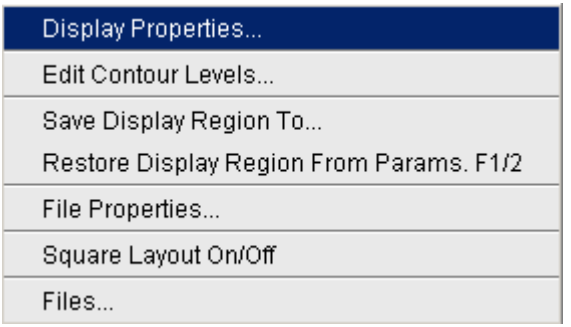


Figure 9.3

Here you can select various display properties, region setting and file properties. If you choose ***Display Properties...***, a dialog box (see Fig. 9.4) will appear.

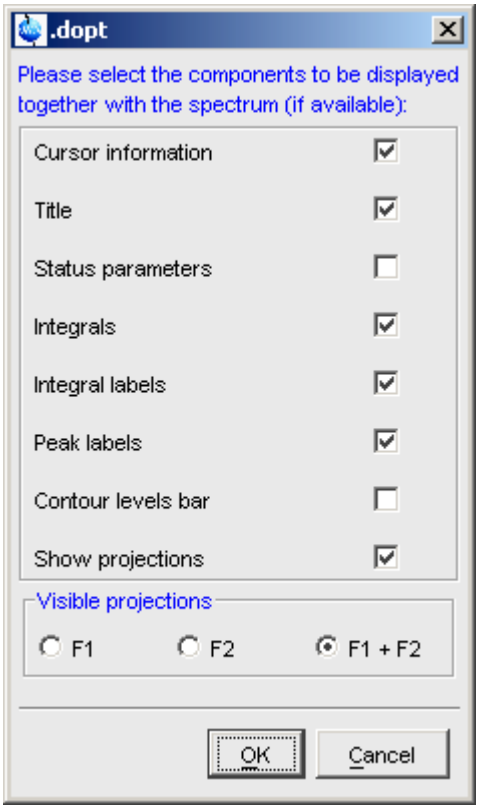


Figure 9.4

Here you can set various display options including parameter, integrals, peaks, contours and projections.

9.4 Using the Tab bar

The 2D data window is a tabbed pane. This means its contents depends on the currently active tab in the Tab bar. The individual tabs are basically the same as for 1D display (see chapter 8.4). There are, however, some differences, which are discussed below.

How to Set Processing Parameters

☞ Click the ***ProcPars*** tab [**`edp`**]

The 2D processing parameter editor contains a column for each of the two dimensions F2 and F1. Note that not all parameters exist in both dimensions (see Fig. 9.5).

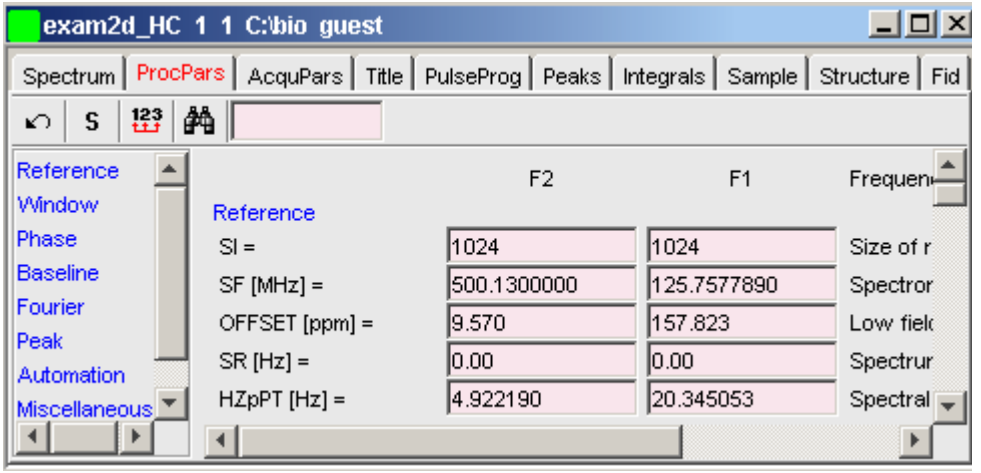


Figure 9.5

How to Set Acquisition Parameters

☞ Click the ***AcquPars*** tab [**`eda`**]

The 2D acquisition parameter editor contains a column for each of the two dimensions F2 and F1. Note that not all parameters exist in both dimensions (see Fig. 9.6).

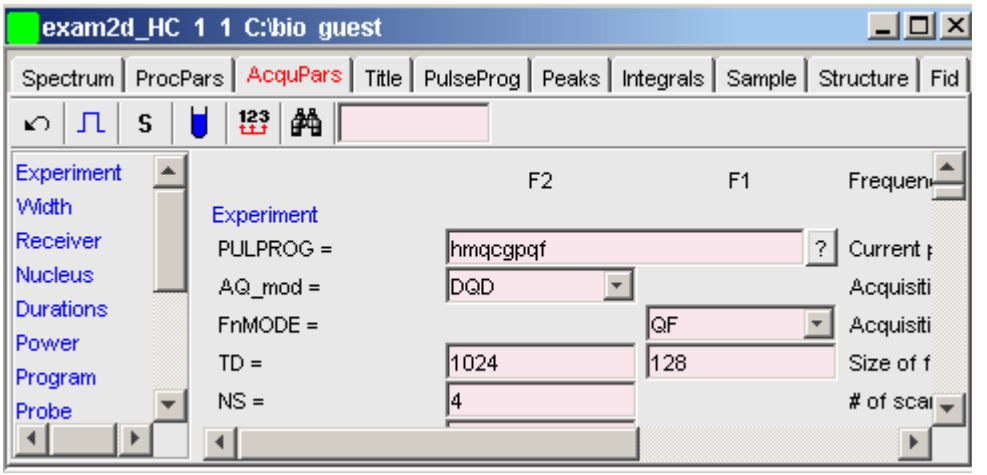


Figure 9.6

How to Display the Peak list

☞ Click the ***Peaks*** tab

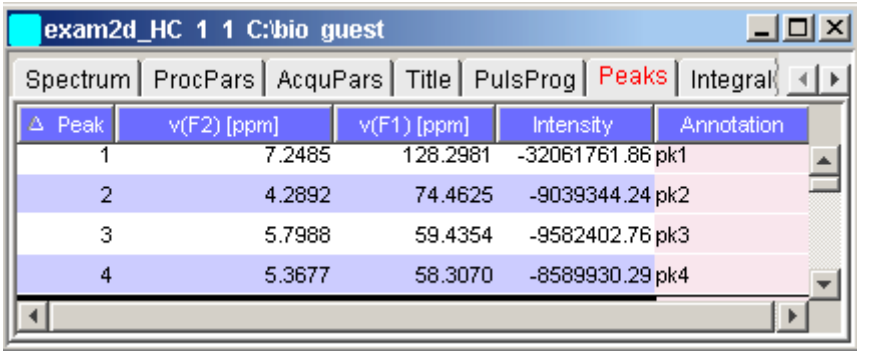


Figure 9.7

This displays list of peaks if these have been calculated (command ***pp***). The list is basically the same as for 1D spectra. The only difference is that there are two columns for the two dimensions now and an extra column for peak annotations:

v(F2) [ppm] : the chemical shift in the F2 direction

v(F1) [ppm] : the chemical shift in the F1 direction

Annotation: the peak annotation

To specify or edit an annotation, click inside the *Annotation* field and enter a character string. The peak annotations are shown in the correlated spectrum (see Fig. 9.8)

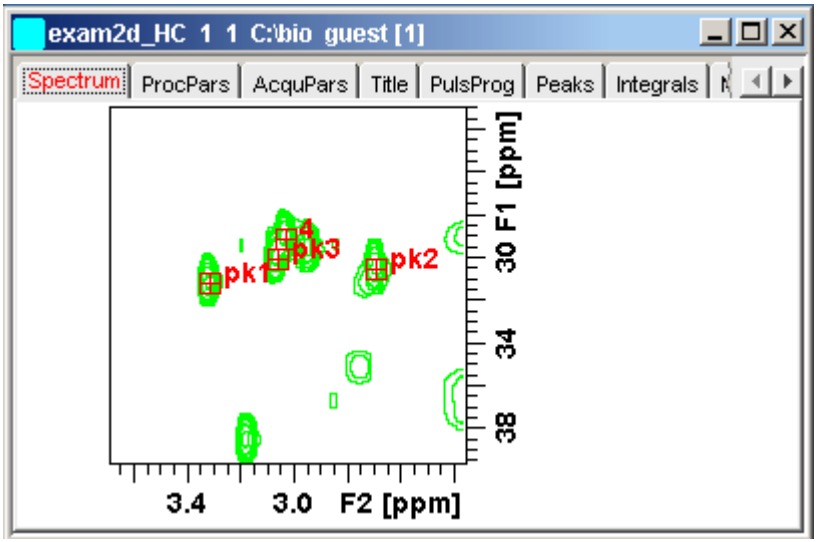


Figure 9.8

How to Display the Integral list

☞ Click the ***Integrals*** tab

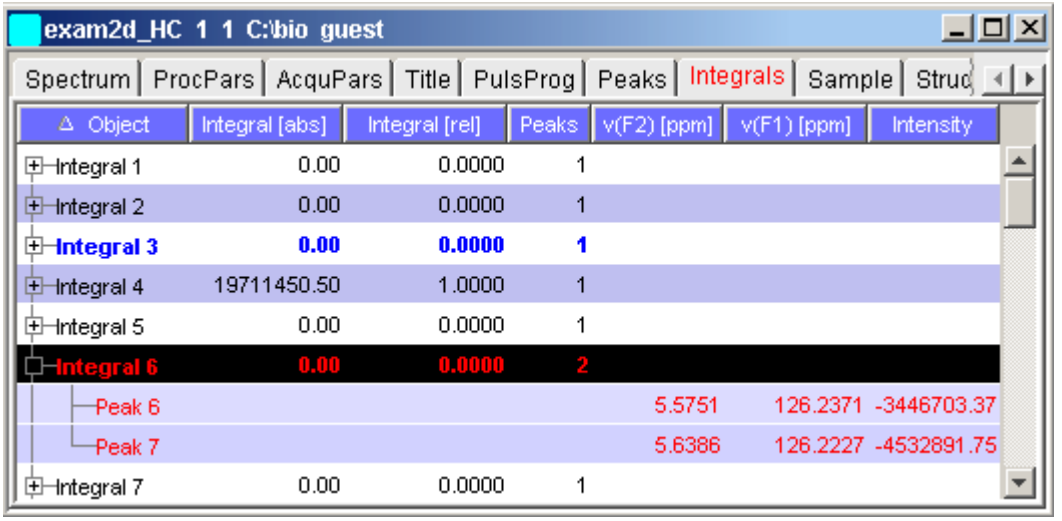


Figure 9.9

This displays list of integrals if these have been calculated (command ***int***). The list is basically the same as for 1D spectra. The only difference is that, when peaks are shown, there are two columns for the chemical shift:

v(F2) [ppm] : the chemical shift in the F2 direction

v(F1) [ppm] : the chemical shift in the F1 direction

Furthermore, a stored or exported 2D integral list can be imported as follows:

1. Right-click an entry to open the popup menu
2. Click **Import...**
3. In the appearing dialog box, navigate to the directory where the list resides and select the integral list.

As such you can import an integral list from a different dataset or a previously exported list from the current dataset. Note that integration commands store the integral list in the processed data directory under the name `integrals.txt`. Exported integrals are stored in the files `<name>.txt` and `<name>.reg`, where `<name>` is the name specified by the user.

How to Display the FID

☞ Click the ***Fid*** tab [***fid***]

2D raw data consist of a series of FIDs which are displayed in a row. Individual FIDs can be displayed by zooming out. To do that, click repeatedly. Now you can shift and zoom in/out the data to display different FIDs (see Fig. 9.10)

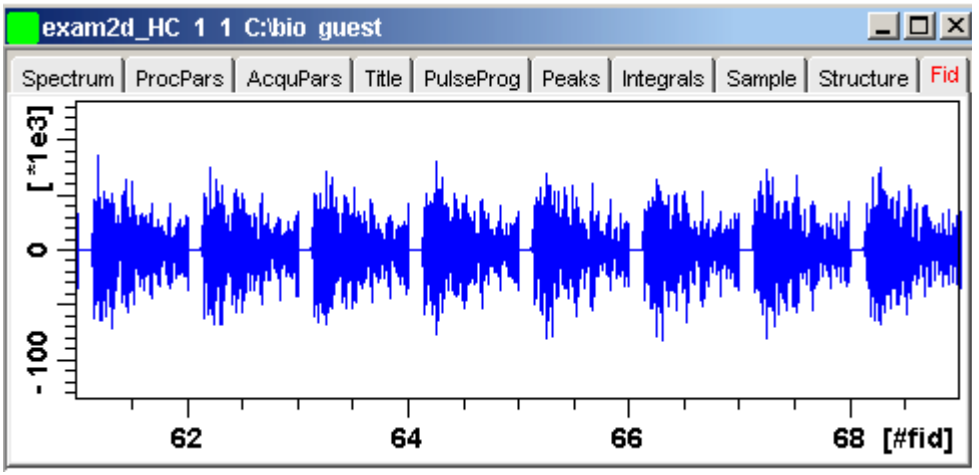


Figure 9.10

9.5 2D Display Options

How to Switch between Hertz and ppm Axis Units in F2 and F1

☞ Click the following multi-state button in the upper toolbar:

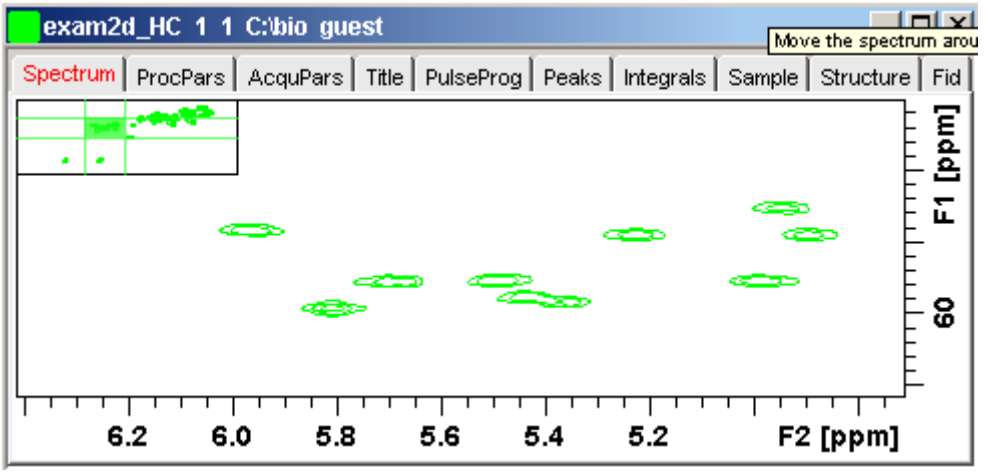
Switch between Hz and ppm axis units in F2 and F1 [***.hz***]

How to Switch on/off the Spectrum Overview display

☞ Click the following toggle button in the upper toolbar:

Switch the spectrum overview display on/off [***.ov***]

With the spectrum overview on, the data window will, for example, look like this:

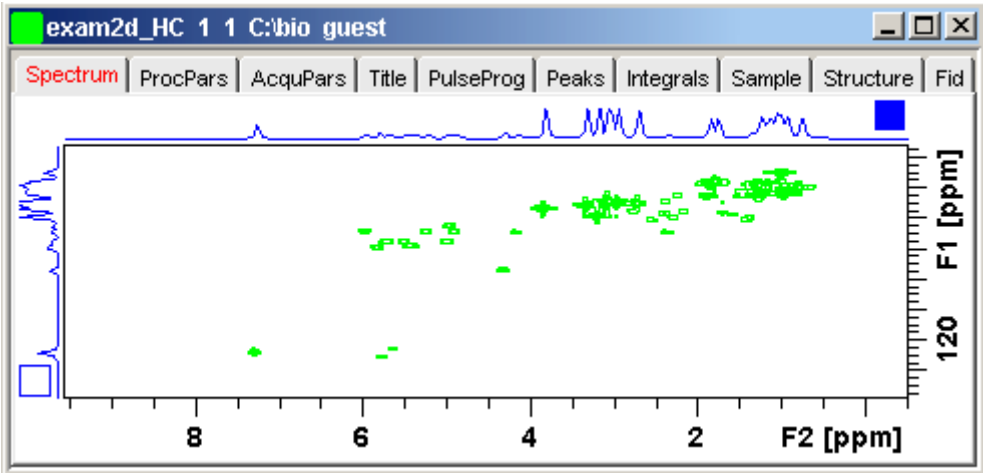


How to Switch on/off the Projection display

☞ Click the following toggle button in the upper toolbar:

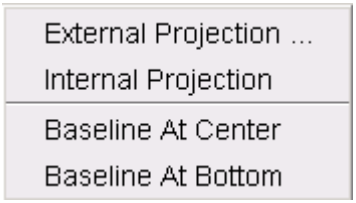
Switch the projection display on/off [***.pr***]

With the projections displayed, a 2D dataset looks like this:



In this example, the F1 projection is selected as indicated by the filled blue square

whereas the F2 projection is not selected. A selected projection can be rescaled using the toolbar rescale buttons of function keys. If you right-click inside the projection area of the data window, the following popup menu appears:



Clicking ***External Projection*** opens the a dialog box where you can specify or search for a 1D dataset and display this as a projection of the current 2D dataset.

Clicking ***Internal Projection*** calculates and displays the positive projection and displays it along with the 2D spectrum.

Clicking ***Baseline at Bottom*** or ***Baseline at Center*** allows you to put the projection baseline at the respective positions.

Various other projection features are available. To access them:

click ***Processing*** → ***Calculate projections*** [***proj***]

This will open the dialog box shown in Fig. 9.11.

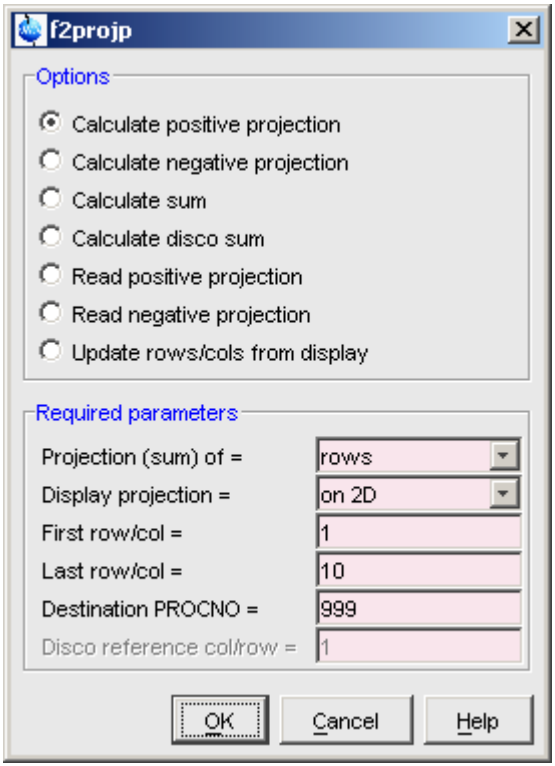


Figure 9.11

From here, you can calculate positive, negative, sum and disco projections and either show them with the 2D spectrum or display them in separate data window as a 1D data. For more details on the corresponding commands (as shown in the header of the dialog box), please refer to the Processing Reference Manual.

How to Switch on/off the Grid display

☞ Click the following multi-state button in the upper toolbar:

Switch between 'no grid', 'axis aligned grid' and 'fixed grid' [***.gr***]

Fig. 9.12 shows an example of axis aligned grid display.

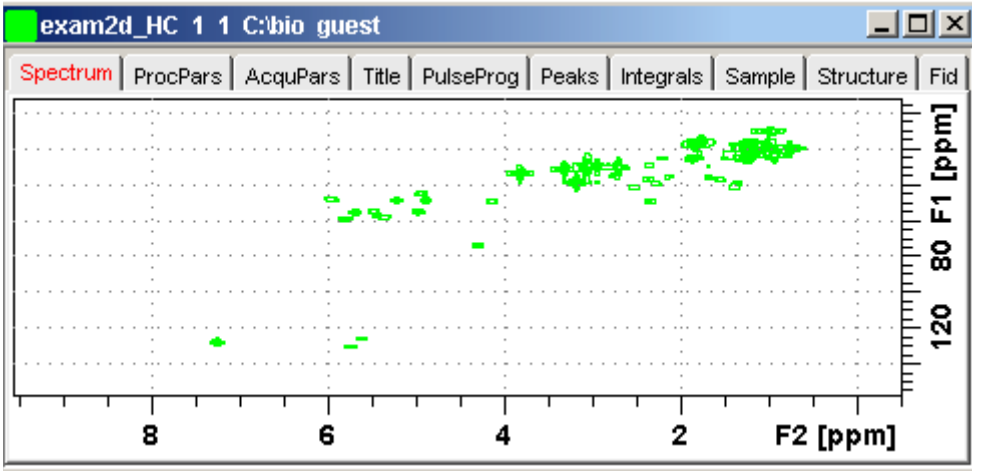


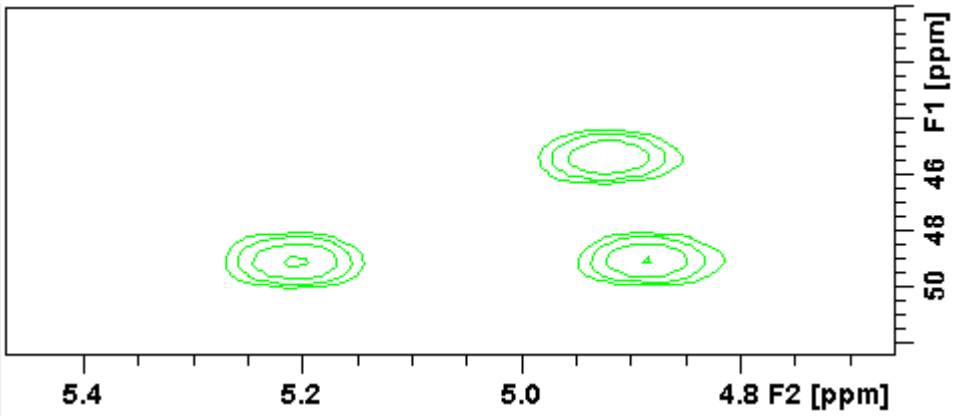
Figure 9.12 Axis aligned grid display

How to Display a 2D Spectrum in Contour Mode

☞ Click the following button in the upper toolbar:

Switch to contour display mode [**.co**]

In contour mode, a spectral region looks like this:



How to Set the 2D Contour Levels

☞ Click the following button in the lower toolbar

 Edit contour levels [***edlev***, ***.lv***]

This will open the following dialog box shown in Fig. 9.13. Contour levels can be entered manually or they can be calculated.

Manual setup

This allows you to create an arbitrary sequence of levels

1. Enter the level values in the fields 1, 2, ... at the top of the dialog box.
2. Click ***Apply*** to update the display or ***OK*** to store the levels, update the display and close the dialog box.

Calculation

This allows you to easily create a geometric or equidistant sequence of levels.

1. Click one of the following items:
   - ***Multiply with increment***
     to create a geometric sequence of levels.
   - ***Add increment***
     to create a equidistant sequence of levels.
2. Enter the desired *Base level*, *Level increment* and *Number of levels.*
3. Click ***Fill*** to display and activate the sequence.
4. Click ***Apply*** to update the display or ***OK*** to store the levels, update the display and close the dialog box.

The Contour level sign allows you to select positive levels, negative levels or both.

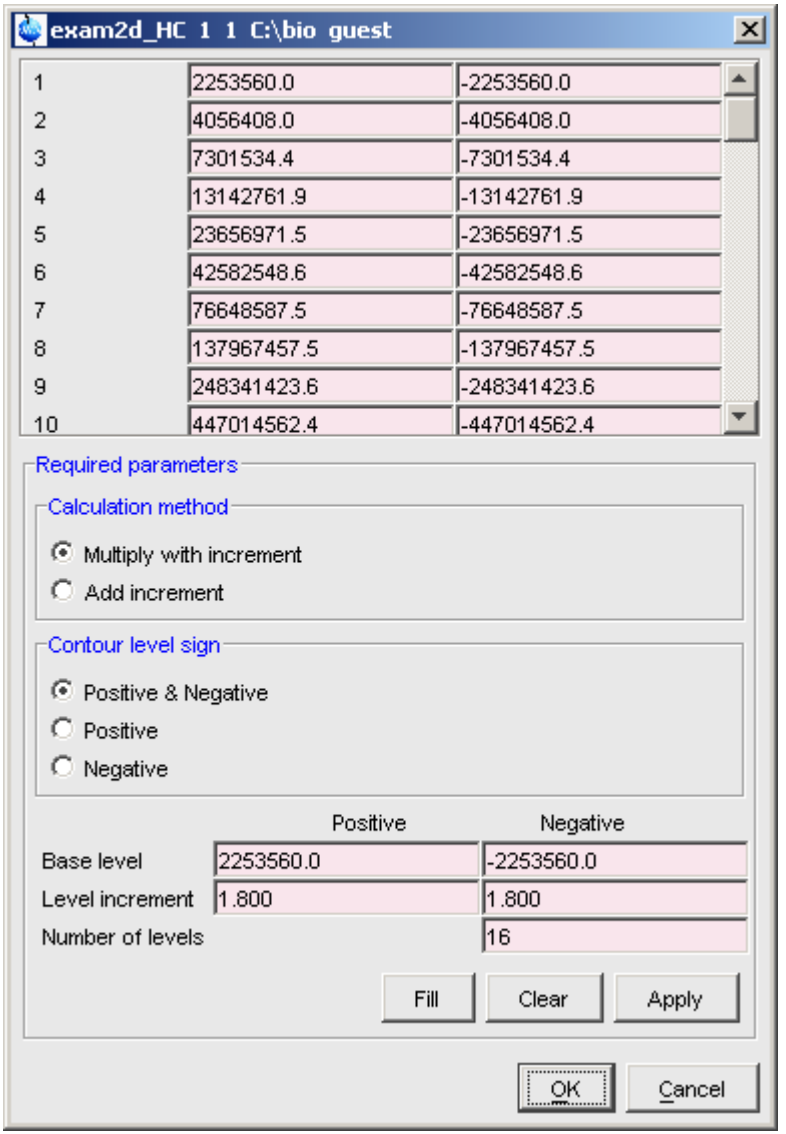


Figure 9.13

How to Store interactively set Contour Levels

To store contour levels that were set interactively, for example by clicking *2 or

pressing ***Alt***+***PageUp***:

☞ Click the following button in the lower toolbar:


Store contour levels [***.ls***]

The levels are stored in the file:

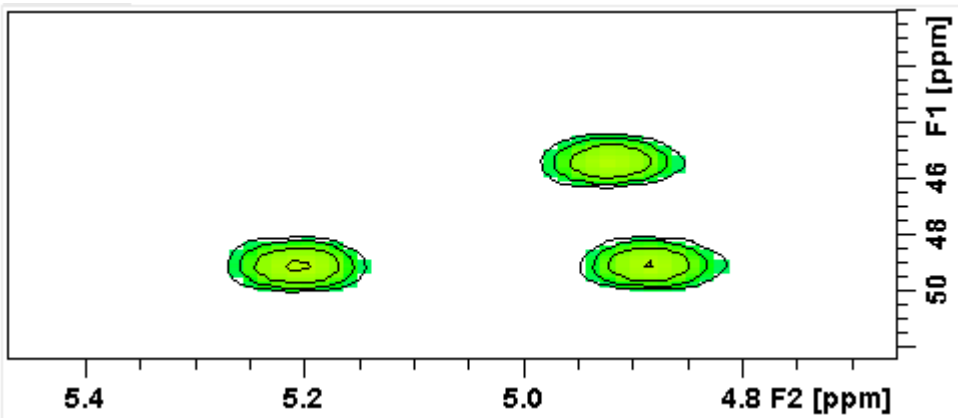
/<*dir*>/data/<*user*>/nmr/<*name*>/<*expno*>/pdata/<*procno*>/clevels

How to Display a 2D spectrum in Image Mode

☞ Click the following button in the upper toolbar:


Switch to image color display mode [***.im***]

In image mode, a spectral region looks like this:



Note that in image mode, the contours are superimposed, in black, on the image.

How to Display a 2D Spectrum in Oblique Mode

☞ Click the following button in the upper toolbar


Switch to oblique display mode [***.st***]

In oblique mode, a spectral region looks like in Fig. 9.14.

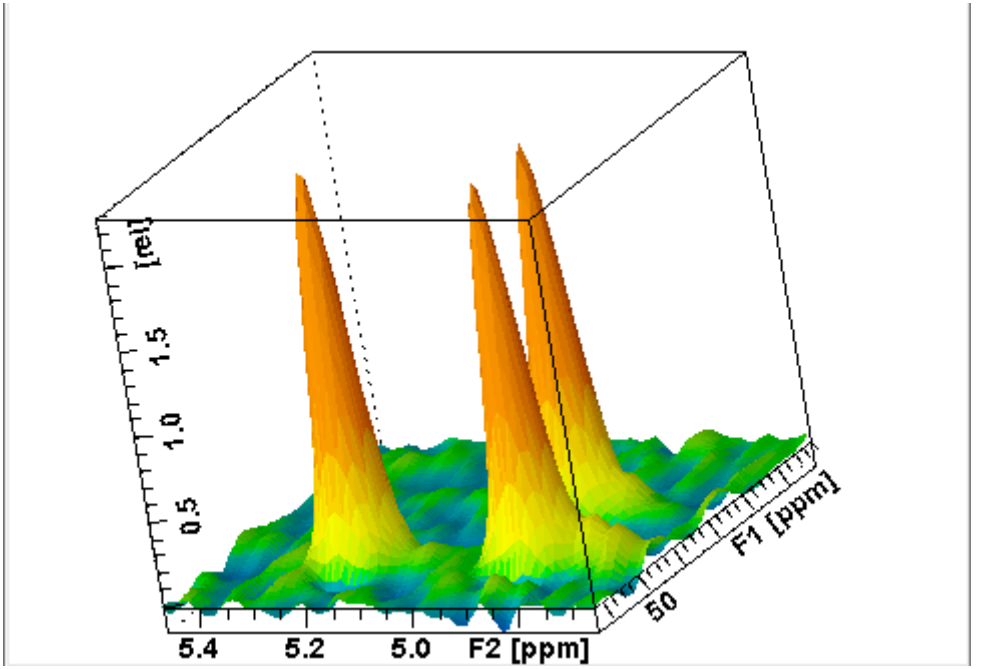


Figure 9.14

In this mode you can manipulate the display in various ways. Just right-click inside the data window and choose one of the options from the appearing popup menu (see Fig. 9.15)

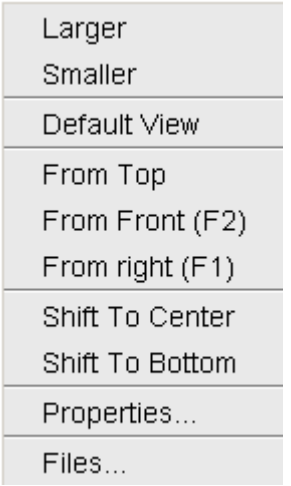


Figure 9.15

How to Rotate a 2D Spectrum in Oblique Mode

Click-hold one of the following button and move the mouse up/down:

- Rotate around x-axis.
- Rotate around y-axis.

How to Switch between Displaying Positive and Negative levels

Click the following multi-state button in the lower toolbar:

- Switch between *positive*, *negative* and *both* contours [**`.lt`**].

Chapter 10

3D Display

10.1 Plane Display Mode

3D data can be displayed as 2D planes or as a 3D cube. By default, the first F3-F1 plane is displayed (see Fig. 10.1) The plane orientation and number is shown. The cube in the lower left corner graphically indicates which plane is displayed. The full 2D display functionality is available (see chapter 9).

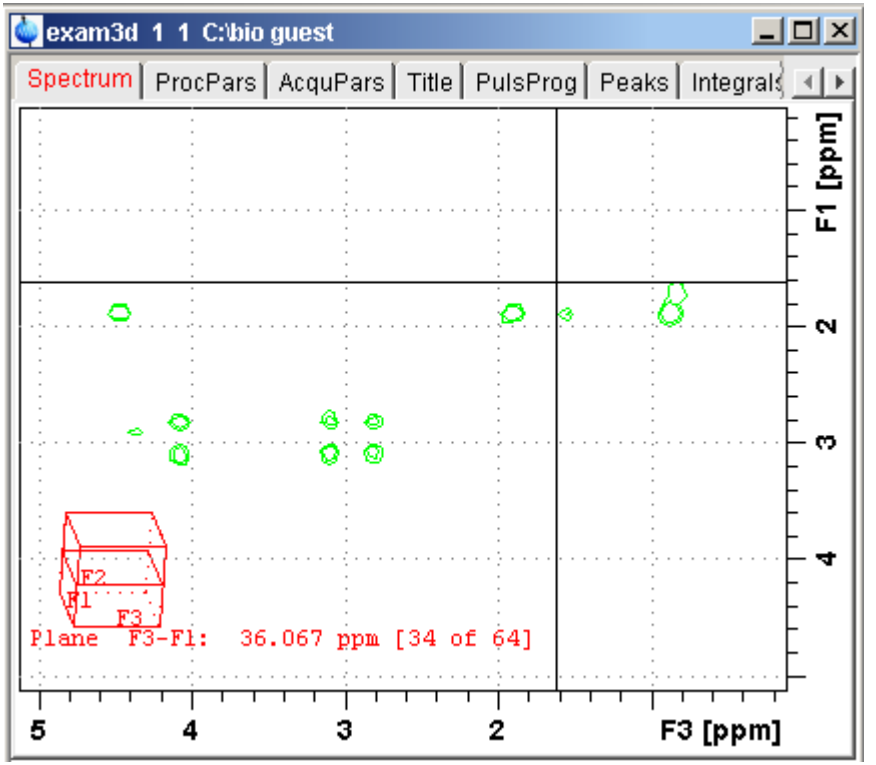


Figure 10.1

How to Switch to 2D Plane Display

If the 3D cube is displayed you can switch to 2D plane display by clicking one of the following buttons:

- Switch to 2D contour display.
- Switch to 2D image display.
- Switch to 2D oblique display.

How to Display various Plane Orientations

Click one of the following buttons:

- 12 Show F1-F2 planes.

23 Show F2-F3 planes.

31 Show F3-F1 planes.

How to Display various Plane Positions (numbers)

Click one of the following buttons:

+ Show the next plane.

− Show the previous plane.

↕ Scan planes smoothly.

E Enter the exact plane number.

10.2 Cube Display Mode

How to Display the 3D Cube

Click the following button:

Show 3d cube (see Fig. 10.2).

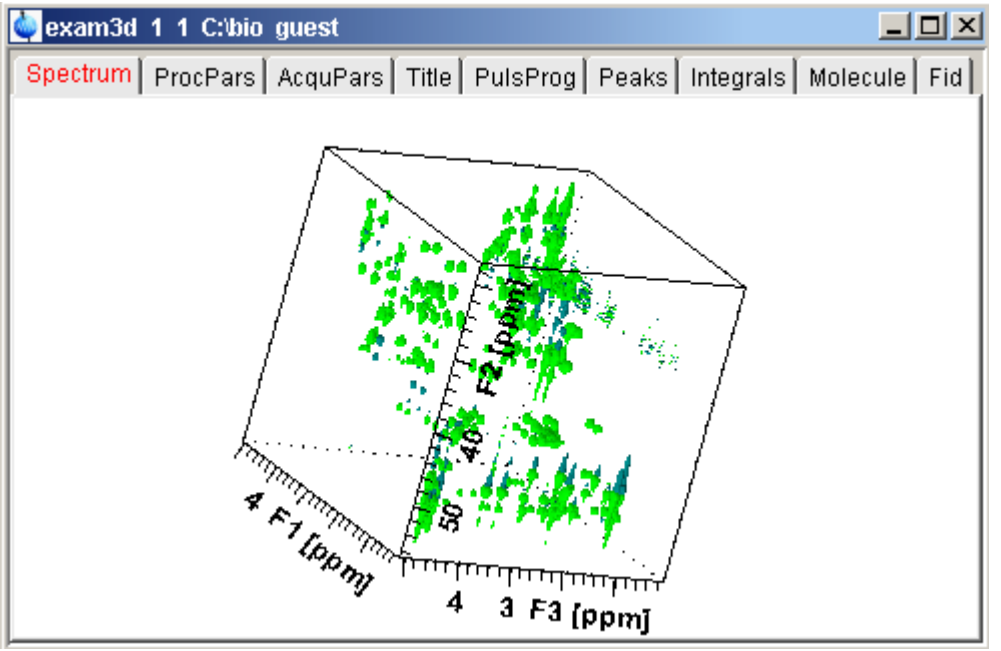


Figure 10.2

How to Rotate the 3D Cube

Click-hold one the following buttons and move the mouse up/down:

- Rotate cube around x-axis.
- Rotate cube around y-axis.
- Rotate cube around z-axis.

How to Scale Up/Down the 3D Cube

1. Right-click inside the data window.
2. Choose ***Larger*** or ***Smaller*** from the popup menu (see Fig. 10.3).

How to Reset the Cube Size and Orientation

Click the following button:

- **R** Reset to default size and orientation.

How to Switch Depth Cueing on/off

1. Right-click inside the data window
2. Choose ***Depth Cueing On/off*** (see Fig. 10.3)

Depth cueing makes data points which are closer to the viewer appear brighter and those that are further away appear dimmer. This increases the depth effect of the 3D image.

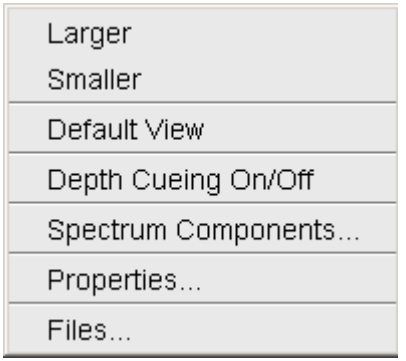


Figure 10.3

How to Display a Cube Front or Side view

Click one the following buttons:

12 Show F1-F2 plane.

23 Show F2-F3 plane.

31 Show F3-F1 plane.

10.3 Using the Tab bar

The 3D data window is a tabbed pane. This means its contents depends on the currently active tab in the Tab bar. The individual tabs are basically the same as for 1D and 2D display (see chapter 8.4). When you click the ***ProcPars*** or ***AcquPars*** tab, you will find a parameters column for each of the three dimensions F3, F2 and F1. The ***Fid*** tab allows you to display the 3D raw data as a series of 1D FIDs. The ***Peaks*** tab will display the 3D peak list with a column for the chemical shift in each of the three dimensions. Similarly, the ***Integrals***

tab will display the 3D integral list. Peaks and integrals only appear if they have been calculated (commands ***pp*** and ***int***, respectively).When the integral list shows peaks, with a column for the chemical shift in each of the three dimensions appears. Like in 2D, a stored or exported 3D integral list can be imported (see Fig. 9.4).

Chapter 11

1D Interactive Manipulation

The upper toolbar of the 1D menu offers various buttons for interactive manipulation. If you click such a button, the active data window will switch to the corresponding mode. An interactive manipulation mode is data window specific, i.e. it only applies to the active window.

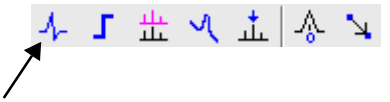
11.1 1D Interactive Phase Correction

Manually acquired spectra can be phased corrected automatically, with commands like ***apk*** or ***apks*** or, interactively, in phase correction mode.

11.1.1 1D Interactive Phase Correction Procedure

How to Switch to Phase Correction Mode

Click the indicated button in the upper toolbar:



or enter ***.ph*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig.

11.1:)

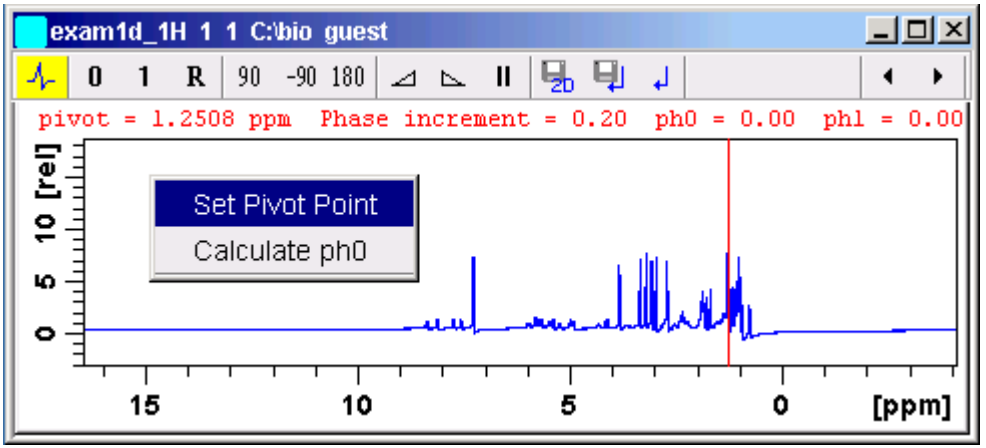


Figure 11.1 Data window in phase correction mode

The yellow button indicates that you are in phase correction mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

How to Perform a Typical 1D Interactive Phase Correction

For a typical 1D phase correction, take the following steps:

1. Click-hold the button **0** and move the mouse until the until the reference peak is exactly in absorption mode.
2. Click-hold the button **1** and move the mouse until the entire spectrum is exactly in absorption mode.
3. Click the button to save and execute the phase correction and return.

11.1.2 1D Interactive Phase Correction Details

How to Set the Phase Pivot Point

By default, the phase pivot point is set to the biggest magnitude intensity of the displayed region of the spectrum. To change the pivot point:

1. Right-click on the desired pivot point position
2. Choose ***Set pivot point*** from the popup menu (see Fig. 11.1)

How to Perform Default Zero Order Phase Correction

1. Right-click in the data window
2. Choose ***Calculate ph0*** in the popup menu (see Fig. 11.1)

The spectrum will automatically be corrected according to the calculated value.

How to Perform Interactive Zero Order Phase Correction

1. Click-hold the following button (button turns green):

   0 Zero order phase correction (parameter PHC0).

2. Move the mouse until the reference peak is exactly in absorption mode.
3. Release the mouse (button turns grey).

How to Perform Interactive First Order Phase Correction

1. Click-hold the following button (button turns green):

   1 First order phase correction (parameter PHC1).

2. Move the mouse until the entire spectrum is exactly in absorption mode.
3. Release the mouse (button turns grey).

How to Perform 90, -90 or 180° Zero Order Phase Correction

☞ Click one of the following buttons:

90 Perform 90 zero order phase correction [***.ph90***].

-90 Perform -90° zero order phase correction [***.phm90***].

180 Perform 180° zero order phase correction [***.ph180***].

How to Reset the Phase to the Original Values

☞ Click the following button:

R Reset zero and first order phase values [***.phr***].

How to Change the Mouse Sensitivity

☞ Click one of the following buttons:

 Increase (double) the mouse sensitivity [***.inc***].

 Decrease (halve) the mouse sensitivity [***.dec***].

 Reset the mouse sensitivity.

How to Return from Phase Correction Mode with/without Save

To return while saving the phase correction to the current dataset:

☞ Click the following button:

 Save, execute and return [***.sret***].

This will perform the following tasks:

- Execute phase correction (command ***pk***).
- Save the current phase correction values.
- Leave the phase correction mode.

To return without save:

☞ Click the following button:

 Return, discarding any changes [***.ret***].

To return while saving the phase correction to the source 2D dataset:

☞ Click the following button:

 Save to 2D [***.s2d***].

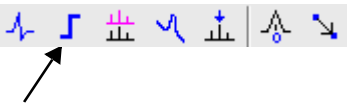
This is only applicable on rows or columns extracted from 2D data. The phase values will be saved to the 2D dataset from which the current 1D dataset was extracted.

11.2 1D Interactive Integration

Integration of 1D data can be done automatically, with the commands ***abs*** and ***li*** or, interactively, as described in this paragraph.

How to Switch to Integration Mode

☞ Click the indicated button in the upper toolbar:



or enter ***.int*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.2).

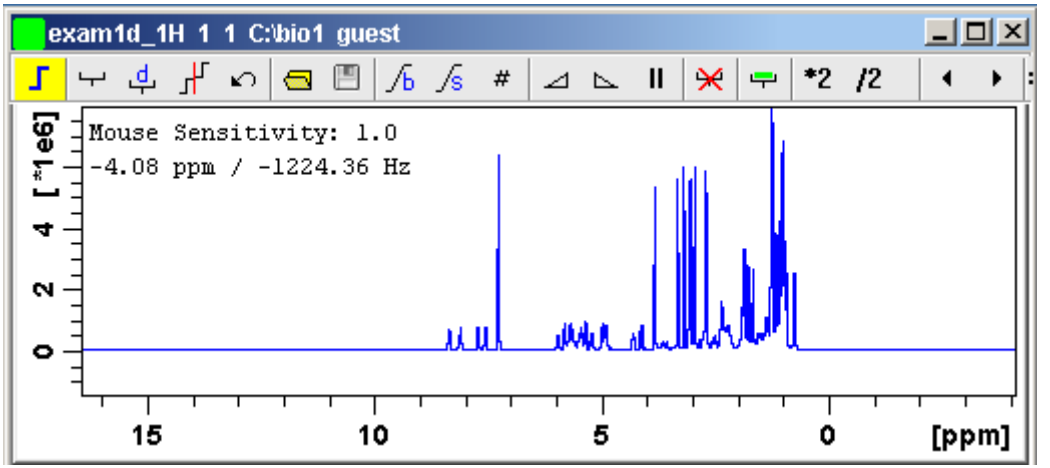


Figure 11.2 Data window in integration mode

The yellow button indicates that the data window is in integration mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

If integral regions have already been determined, for example with ***abs*** or with a previous interactive integration, these regions are displayed in the data window, along with the integral values. You can remove them, change them or add to them, as described below.

How to Define Integral Regions

To define integral regions interactively:

1. Click the following button (button turns green):

   Define integral region interactively.

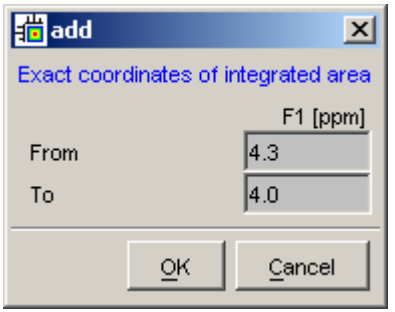
2. Put the red cursor line at one edge of a peak or multiplet.
3. Left-click-hold and drag the cursor line to the other edge of the peak or multiplet.
4. Do step 2 and 3 for all regions to be defined.
5. Click the green button to leave the "define region" mode (button turns grey).

To define integral regions via a dialog box:

1. Click the following button:

   Define region via dialog.

2. In the appearing dialog box:



   Enter the exact values for the region limits.

3. Click ***OK*** to define the selected region.

How to Select/Deselect Integral Regions

To select/deselect <u>all displayed</u> integral regions:

☞ Click the following button:

Select/Deselect all regions.

To select a single integral region:

1. Right-click in the integral region.
2. Choose ***Select/Deselect*** from the popup menu.

Selected integral regions are indicated by a color filled integral label. In the Fig. 11.3, the two left most regions have already been selected, the right most region is currently being selected.

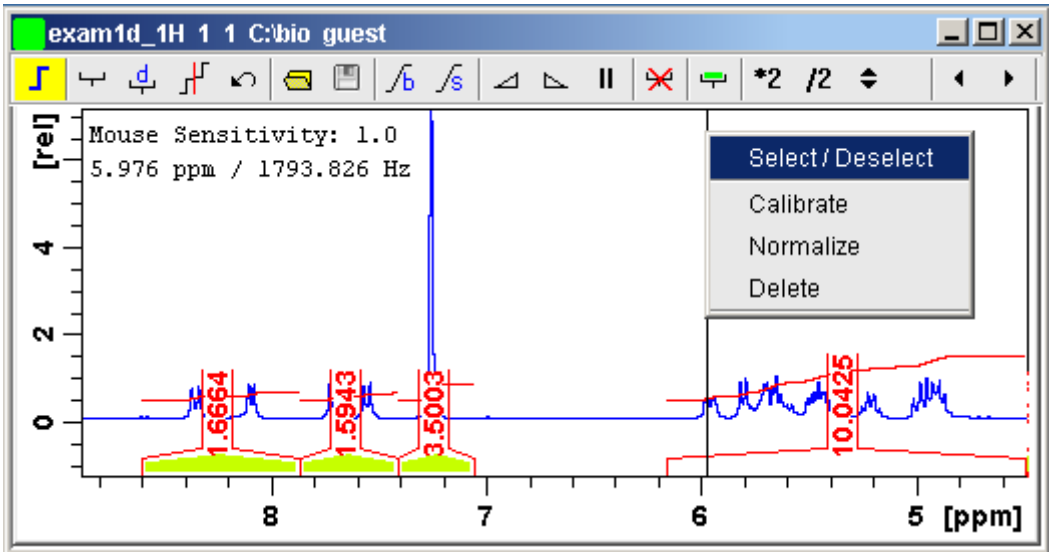


Figure 11.3

How to Read Integral Regions from Disk

You can read integrals regions from disk which have been stored by automatic integration (command ***abs***) or by a previous interactive integration.

To read integrals:

1. Click the following button:

   Read integral regions.

   The following popup menu will appear:

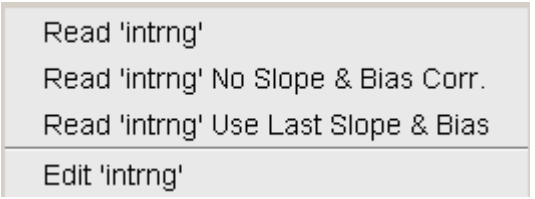


Figure 11.4

2. From the popup menu, choose one of the following entries:
   - ***Read 'intrng'***
     to read the last saved integral regions and apply the saved slope and bias correction values.
   - ***Read 'intrng' no slope & bias corr.***
     to read the last saved integral regions but do not apply the saved slope and bias correction values.
   - ***Read 'intrng' use last slope & bias***
     to read the last saved integral regions applying the last slope and bias correction values.
   - ***Edit 'intrng'***
     to edit the file (`intrng`) that contains the integral regions and slope and bias correction values. Changes in this file are automatically shown on the screen.

How to Perform Interactive Bias and Slope Correction

To perform interactive bias correction:

1. Select the integral(s) that you want to correct (right-click in the region).

   If no integral is selected, bias correction will work on all integrals.

2. Click-hold the following button (it turns green) and move the mouse,

   Integral bias correction.

   until the integral bias is correct.

3. Release the mouse (button turns grey).

To perform interactive slope correction:

1. Select the integral(s) that you want to correct (right-click in the region).

If no integral is selected, slope correction will work on all integrals.

2. Click-hold the following button (it turns green) and move the mouse,

   Integral slope correction.

   until the integral slope is correct.

3. Release the mouse (button turns grey).

How to Set the Limit for Bias Determination

☞ Click the following button:

Limit for bias determination.

How to Change the Mouse Sensitivity

☞ Click one of the following buttons:

Increase (double) the mouse sensitivity [***.inc***].

Decrease (halve) the mouse sensitivity [***.dec***].

Reset the mouse sensitivity.

How to Calibrate/Normalize Integrals

Calibrating integrals means setting the value of a reference integral and adjusting all other integrals accordingly. To do that:

1. Right-click in the reference integral region.
2. Choose **Calibrate** from the popup menu (see Fig. 11.5).
3. Enter the desired value for the reference integral and click ***OK***

Normalizing integrals means setting the sum of all integrals and adjusting individual integral values accordingly. To do that:

1. Right-click in the reference integral region.
2. Choose **Normalize** from the popup menu (see Fig. 11.5).

3. Enter the desired sum of all integrals and click ***OK***

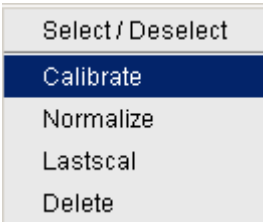


Figure 11.5

Calibrating and normalizing only effects the current dataset. To scale integrals with respect to a reference dataset, choose ***lastscal*** from the right/click popup menu (see below).

How to Scale Integrals with respect to Different Spectra

Integrals can be scaled with respect to the last spectrum that was integrated interactively. To do that:

1. Right-click in the reference integral region.
2. Choose ***Lastscal*** from the popup menu (see Fig. 11.5).

As such, you can compare integrals of different spectra. Note that this only make sense for spectra which have been acquired under the same experimental conditions. The scaling factor is stored in the file:

```
<tshome>/prog/curdir/<user>/intscale
```

How to Delete Integral Regions from the Display

To delete the selected integral regions from the display:

☞ Click the following button:

Delete selected integral regions from the display.

To delete a single integral region from the display:

1. Right-click in the integral region.
2. Choose **Delete** from the popup menu (see Fig. 11.5)

To delete all integral regions from the display:

☞ Click the following buttons:

Select all integral regions.

Delete selected integral regions from the display.

Note that regions are only deleted from the screen. Regions which are saved on disk (in the `intrng` file) are not affected.

How to Scale Selected Integrals

Integral scaling only manipulates selected integrals. However, if no integrals are selected, it works on all integrals.

☞ Click one of the following buttons:

*2 Scale up selected integrals by a factor of 2.

/2 Scale down selected integrals by a factor of 2.

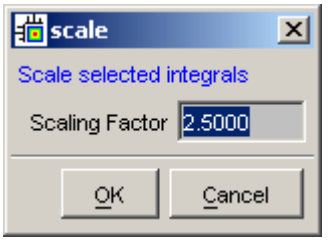
Scale selected integrals up/down smoothly.

To scale up/down integrals by a factor entered via a dialog:

1. Click the following button:

   *x Scale integrals via a dialog.

2. Enter a scaling factor, e.g. 2.5. in the appearing dialog.



3. Click ***OK*** to apply this factor.

To scale all integrals to the same height:

☞ Click the following button:

= Scale/unscale all integrals to the same height.

The individual scaling factor for each region is displayed above the integral. Clicking this button again rescales all integrals to their original height.

How to Move the Integral Trails Up/Down

To move the integrals (selected and unselected) up or down:

☞ Click one of the following buttons:

The left edge of the lowest integral is put just above the baseline.

The right edge of the highest integral is put at 3/4 of the window height.

Shift all integral trails up/down smoothly.

How to Cut Integral Regions

1. Click the following button (button turns green):

   Cut integral region.

2. Move the red cursor line into an integral region to the position where it must be cut and click the left mouse button.
3. Do step 2 for each integral region that must be cut.
4. Click the (green) button to leave the *cut integral* mode (button turns grey).

How to Save Integral Regions

1. Click the following button:

   Save integral regions.

   The following popup menu will appear:

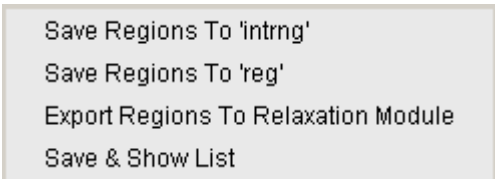


Figure 11.6

2. Choose one of the following entries:

   - ***Save regions to 'intrng'***
     Save the currently displayed integral regions including the slope and bias correction values.

- ***Save Regions to 'reg'***
  Save the integral regions to the file `reg`.
- ***Save & show list***
  Save the currently displayed integral regions including the slope and bias correction values and show the integrals on the screen.

How to Undo the Last Region Operation

☞ Click the following button:


Undo the last region operation.

How to Return from the Integration Mode with/without Save

To return and save the integrals to the current dataset:

☞ Click the following button:


Save integrals and return [***.sret***].

As such, you will:

- save the integral regions and corresponding slope and bias corrections to the file `intrng`.
- save the integral regions, slope and bias corrections and integral values to the file `integrals.txt`. This file is displayed when you click the ***Integrals*** Tab.
- leave the integration mode.

To return without save:

☞ Click the following button:

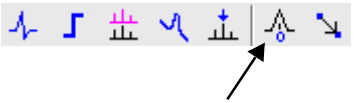

Return, discarding any changes [***.ret***].

11.3 1D Interactive Calibration

A 1D spectrum can be calibrated (referenced), automatically, with the command ***sref*** or, interactively, as described below.

How to Switch to Calibration Mode

☞ Click the indicated button in the upper toolbar



or enter ***.cal*** on the command line. The Tab bar of the active data window will be replaced by a toolbar.

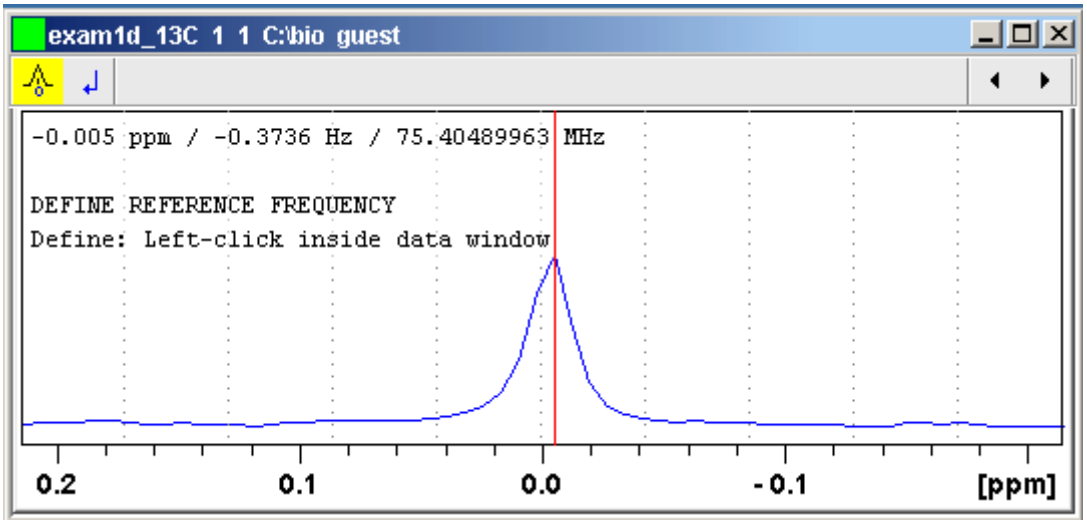


Figure 11.7 Data window in calibration mode

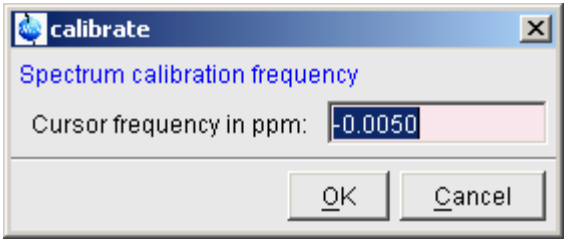
The yellow button indicates that the data window is in calibration mode.

How to Calibrate a Spectrum Interactively

In calibration mode:

1. Position the red cursor line at the reference peak.
2. Left-click at that position.

The following dialog box will appear:



Note that the units (Hz or ppm) correspond to the axis units of the display.

3. Enter the frequency you want to assign to the reference peak.
4. Click ***OK***

The spectrum will be calibrated and re-displayed. TOPSPIN will automatically leave calibration mode.

11.4 1D Multiple Display

The multiple display mode allows you to display multiple superimposed spectra.The spectra will be ppm aligned or Hz aligned, according to the selected axis unit. Each spectrum can be individually shifted and scaled allowing exact alignment of corresponding peaks in different spectra. The number of superimposed spectra is unlimited.

Although multiple display is normally used for spectra with matching nuclei, it allows you to superimposed spectra with non-matching nuclei. You will get a warning that the nuclei do not match. Just just click ***OK*** to continue.

How Switch to Multiple Display Mode and Read Multiple Spectra

One way to superimpose data in multiple display is to read one dataset, switch to multiple display mode and add other datasets:

1. Read a 1D dataset.
2. Click the button in the upper toolbar or type ***.md*** on the command line.

   The data window will switch to multiple display mode.
3. Add a dataset as follows:

   ☞ Left-click-hold the dataset in the browser and drag it into the data win-

dow.

or

☞ Right-click the dataset in the browser and choose ***Display*** from the popup menu.

or

☞ Enter ***re*** and specify the additional dataset in the appearing dialog box.

Another way to superimpose data in multiple display is to read multiple datasets simultaneously:

1. In the browser or portfolio:

☞ Hold down the ***Ctrl*** key and click multiple datasets to select them.

or

☞ Hold down the ***Shift*** key and click two datasets to select these two and all datasets in between.

2. Right-click any of the selected data:

☞ Choose ***Display*** from the popup menu.
This will show the data in the active data window if that is in multiple display mode or, otherwise, show the data in a new window.

or

☞ Choose ***Display in new window*** from the popup menu.
This will show the data in a new window.

In multiple display mode, the Tab bar of the active data window is replaced by a toolbar. Fig. 11.8 shows three comparable 1D spectra and the sum of all three.

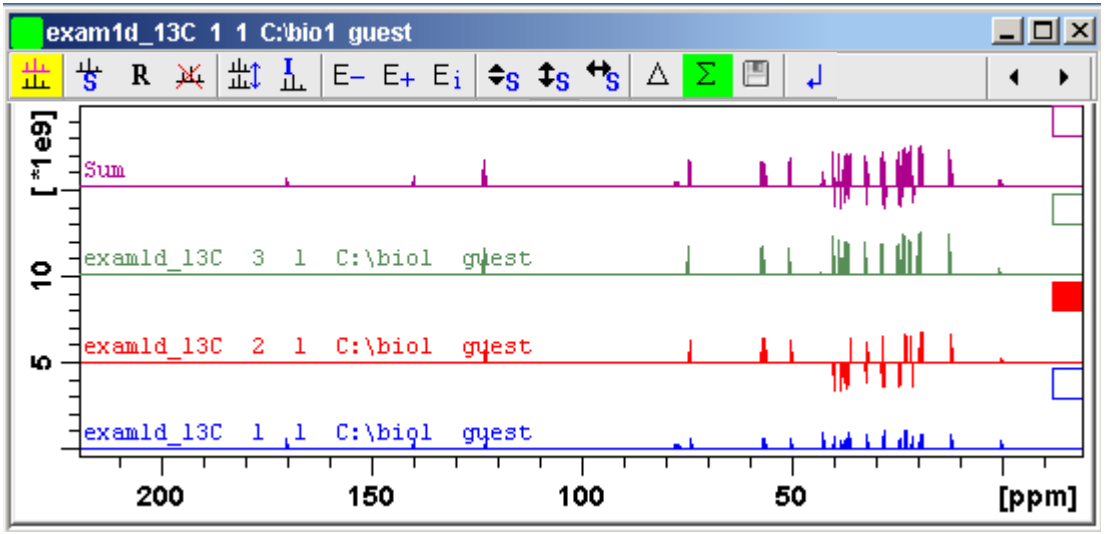


Figure 11.8 Data window in multiple display mode

The yellow button indicates that the data window is in multiple display mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

Furthermore, the browser/portfolio is split in two parts as shown in Fig. 11.9.

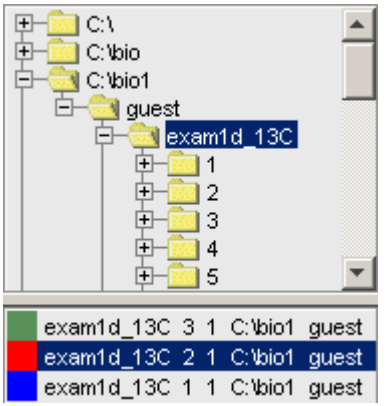


Figure 11.9

The additional lower part shows:

- which datasets are displayed in the active data window.
- which datasets are selected (these are highlighted).

How to Select/Deselect Datasets

To select a dataset:

☞ Click in the corresponding area in the data window.

or Click the small square at the upper right of the spectrum.

or Click the corresponding entry in the lower part of the browser/portfolio.

In the lower part of the browser/portfolio, you can:

☞ Click one dataset to select it.

or Hold down the ***Ctrl*** key and click multiple datasets to select them.

or Hold down the ***Shift*** key and click two datasets to select these two and all datasets in between.

When you select a dataset, the corresponding small square is filled (see Fig. 11.8) and its entry in the lower part of the browser is highlighted (see Fig. 11.9).

Note that:

- no spectrum selected = all spectra selected
- scale/shift buttons of the data window toolbar only work on selected spectra

To deselect a dataset:

☞ Select a different dataset.

To deselect all datasets:

☞ Click the following button:

 Deselect all datasets.

How to Remove a Dataset from Multiple Display

1. Select the dataset(s) you want to remove.
2. Click the following button:

Remove selected data from the screen.

Note that the data on disk are not affected. Furthermore, the first spectrum cannot be removed from the screen.

How to Display the Sum or Difference Spectra

☞ Click one of the following button (button turns green):

Show the difference between the first and the sum of the other datasets.

Show the sum of all datasets in the multiple display window.

How to Save the Sum or Difference Spectra

1. Click the following button:

   Save the displayed sum or difference spectrum.

2. In the appearing dialog box, specify the destination *procno*.

How to Display the Next/Previous Name/Expno

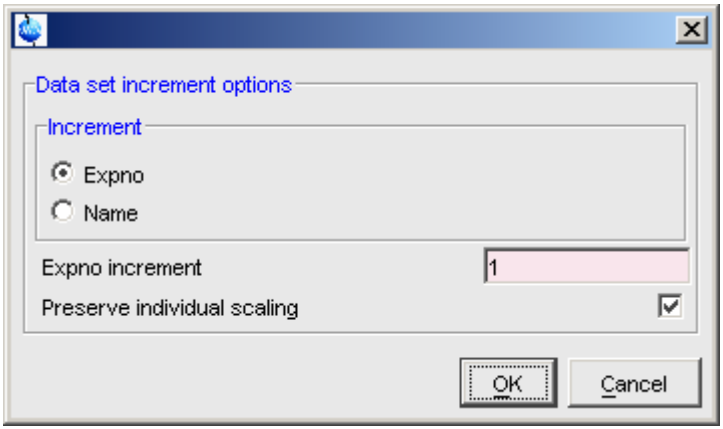
To compare a series of spectra you can interactively increment or decrement the dataset name or expno. A dataset name is incremented according to the ICON-NMR naming convention of increasing extensions, e.g. name.001, name.002 etc.

☞ Click one of the following button (button turns green):

Show the previous name/expno.

Show the previous name/expno.

Set the increment options. Clicking this button will open the following dialog:



Here you can choose to increment the expno or name, set the expno increment and switch individual scaling on/off.

How to Toggle between Superimposed and Stacked Display

☞ Click the following button:

Toggle between superimposed and stacked display.

How to Shift and Scale Individual Spectra

To compare the intensity and chemical shift of corresponding peaks, you can shift and scale individual spectra. To do this:

1. Display the spectra in multiple display mode as described above.
2. Expand the spectra to display the desired region or peak.
3. Select one of the spectra (e.g. by clicking it in the lower part of the browser).
4. Click-hold the S button and move the mouse to align the intensities.
5. Click-hold the S button and move the mouse to align the peak positions.

The alignment can be facilitated by showing the difference spectrum (△ button) and minimize that. Clicking the R button resets individual scaling and shifting.

The performed scaling and shifting are displayed in the data window (see Fig. 11.10 and 11.11).

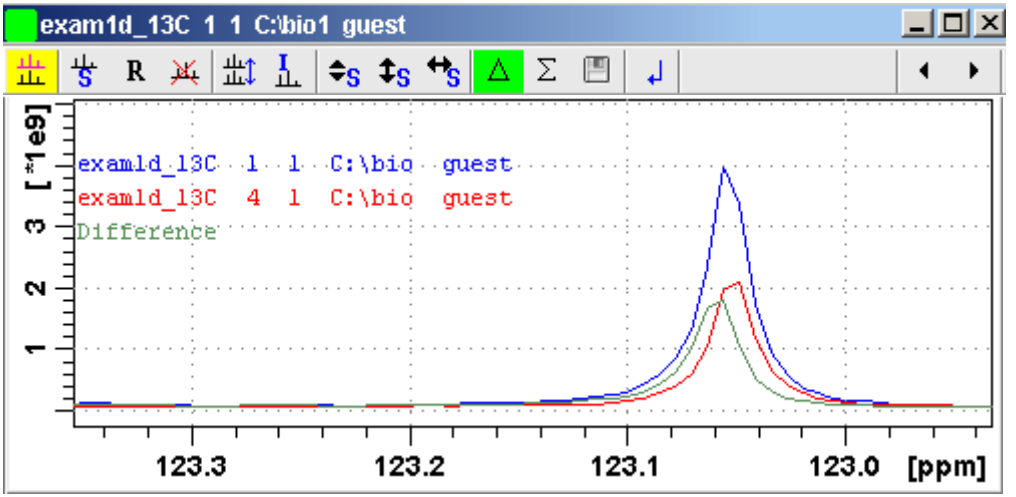


Figure 11.10

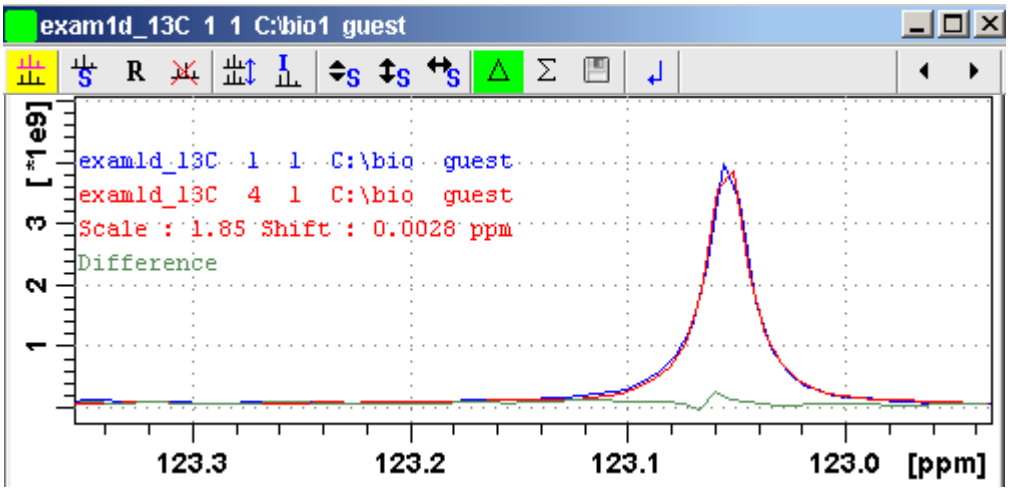


Figure 11.11

How to Switch on/off the Display of Datapaths and Scaling Factors

☞ Click the following button:

Switch on/off display of datapaths and scaling factors.

How to Return from Multiple Display mode

☞ Click the following button:

Return from multiple display mode [**`.ret`**].

How to Set the Colors of the 1st, 2nd, .. Dataset

The colors of the different datasets in the multiple display mode can be set in the *User preferences* dialog box. To set, for example, the color of the second spectrum:

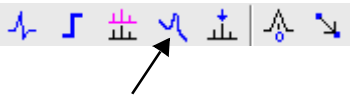
☞ Click ***Options*** → ***Preferences*** and click the ***Change*** button for the item *Color of 2nd 1D spectrum*.

11.5 1D Interactive Baseline Correction

Baseline correction can be performed with commands like **`abs`** or **`absd`** or, interactively, as described below.

How to Switch to Baseline Correction Mode

☞ Click the indicated button in the upper toolbar:



or enter **`.basl`** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.12).

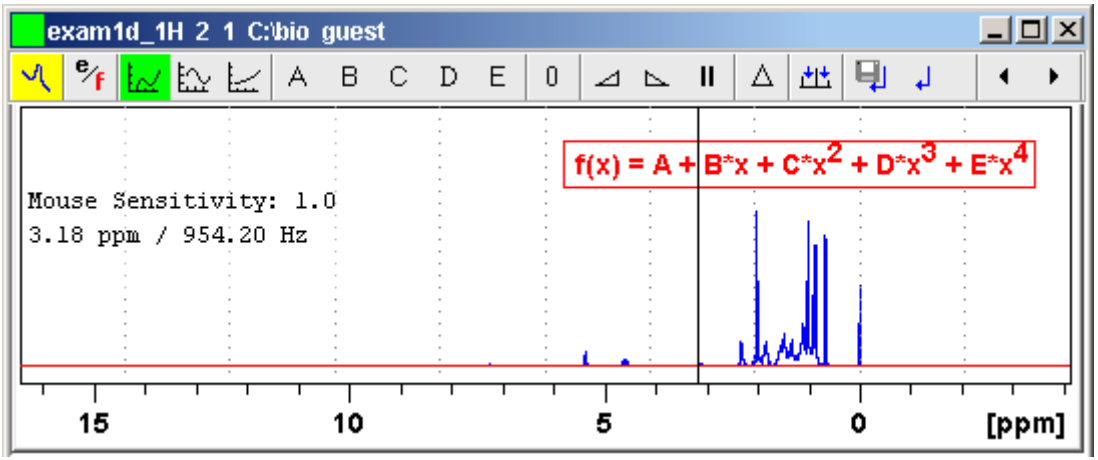


Figure 11.12 Data window in baseline correction mode

The yellow button indicates that the data window is in baseline correction mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

How to Perform Polynomial Baseline Correction

1. Click the following button (button turns green):

   Perform polynomial baseline correction.

   In the data window, a red horizontal line will appear as well as the equation that describes the polynomial function:

   $$f(x) = A + B*x + C*x^2 + D*x^3 + E*x^4$$

2. Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
3. Repeat step 2 with the buttons **B**, **C**, **D** and **E** until the red line coincides with the entire baseline of the spectrum.

How to Perform Sine Baseline Correction

1. Click the following button (button turns green):

 Perform sine baseline correction.

A red horizontal line will appear as well as the equation describing the sine function:

$$f(x) = A + B*\sin(C*x + D)$$

2. Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
3. Repeat step 2 with the buttons **B**, **C** and **D** until the red line coincides with the entire baseline of the spectrum.

How to Perform Exponential Baseline Correction

1. Click the following button (button turns green):

    Perform exponential baseline correction.

   A red horizontal line will appear as well as the equation describing the exponential function:

$$f(x) = A + B*\exp(C*x)$$

2. Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
3. Repeat step 2 with the buttons **B** and **C** until the red line coincides with the entire baseline of the spectrum.

How to Preview the Baseline Corrected Spectrum

Before actually performing the baseline correction, you can preview the result by displaying the difference between the uncorrected spectrum and the red correction line.

To do that:

1. Click the following button (button turns green):

    Preview corrected spectrum (show difference).

   The corrected spectrum will be displayed in red.

2. If the baseline is correct, click the  button to save the correction. If further correction is needed, click the  button to show the original spectrum and the red correction line.

How to Reset the Baseline Correction Line

1. Click the following button:

   Reset the red correction line to zero.

   If the difference spectrum is displayed (the button is active), clicking the reset button will restore the original spectrum.

How to Change the Mouse Sensitivity

☞ Click one of the following buttons:

Increase (double) the Mouse Sensitivity [***.inc***].

Decrease (halve) the Mouse Sensitivity [***.dec***].

Reset the Mouse Sensitivity.

How to Save the Baseline Correction and/or Return

To return while saving the baseline correction:

☞ Click the following button:

Save baseline correction and Return [***.sret***]

This will perform the following tasks:

- Execute the baseline correction [***bcm***].
- Save the baseline correction values **A**, **B**, **C**, **D** and **E.**
- Leave the baseline correction mode.

To return while discarding any changes:

Click the following button:

Return, Discarding any changes [***.ret***].

How to Perform Cubic Spline Baseline correction

☞ Click the following button:

Define points for cubic spline baseline correction.

The toolbar of the data window will change as shown in Fig. 11.13.

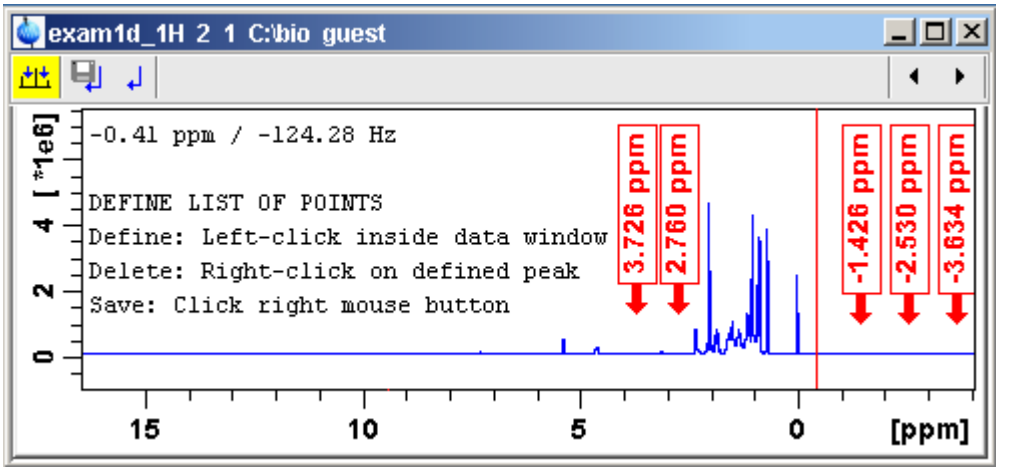


Figure 11.13 Data window in spline baseline correction mode

The cursor line in the data window turns red. If a list of baseline points already exists, you are prompted to overwrite or append to these points. If you choose ***Append***, the labels of the existing points are displayed on the screen. If you choose ***Overwrite***, no labels are displayed. Nevertheless, the existing points are only overwritten when you define and save new points.

To define new baseline points:

1. Move the cursor line to a baseline point and left-click at that position.
2. Do this for at least five baseline points.

Fig. 11.13 shows a spectrum with five defined baseline points. Note that here the points have been chosen at the right part of the spectrum for display reasons only.

How to Delete Spline Baseline Points from the screen

To delete one baseline point:

1. Right-click the baseline point position in the data window.
2. Choose ***Delete Current*** from the popup menu (see Fig. 11.14).

Figure 11.14

To delete all baseline points:

1. Right-click any position in the data window.
2. Choose ***Delete All*** from the popup menu (see Fig. 11.14).

How to Return from Cubic Spline Baseline mode with/without Save

To return while saving the baseline points:

☞ Click the following button:

Save baseline points and Return [***.retsab***].

To return while discarding any changes:

☞ Click the following button:

Return, Discarding any changes [***.ret***].

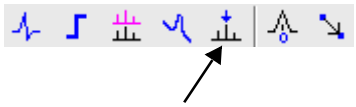
Alternatively, you can right-click in the data window and choose ***Save & Quit*** or ***Quit***, respectively.

11.6 1D Interactive Peak Picking

Peak picking can be performed, automatically, with the commands ***pps*** or, interactively, in the peak picking mode.

How to Switch to Peak Picking Mode

☞ Click the indicated button in the upper toolbar:



or enter ***.pp*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.15).

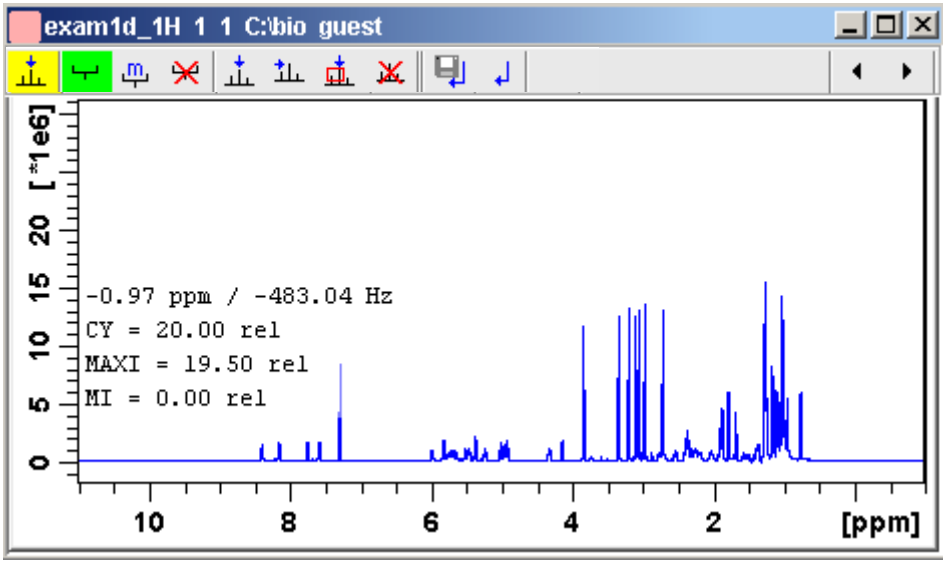


Figure 11.15 Data window in peak picking mode

The yellow button indicates that you are in peak picking mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

Note that the  button is automatically activated, i.e. you are in *Define peak picking range* mode

How to Define New Peak Picking Ranges

1. Put the cursor at the upper-left corner of a peak picking range.

2. Left-click-hold and drag the mouse to the lower-right corner of the range.

   The peak picking range will be marked green. The minimum and maximum intensity are set and the peaks in the range are picked and displayed.

3. Repeat step 1 and 2 for each peak picking range to be defined.
4. Click the green button to leave the "Define peak picking range" mode.

Note that the parameters MI and MAXI are set to the lowest minimum and the highest maximum intensity, respectively, of all ranges.

How to Change Peak Picking Ranges

1. Click the following button (button turns green):

    Change peak picking ranges.

2. Put the cursor on one of the edges of the peak picking range.

   The cursor turns into a double-headed arrow.

3. Left-click-hold and drag the peak range edge to its new position.
4. Optionally: repeat step 2 and 3 for the other edge and for other peak ranges.
5. Click the green button to leave the "Change peak picking range" mode.

How to Pick Peaks in Peak Picking Ranges only

Peaks in a peak range are automatically picked when the range is defined.If peaks have been deleted from a rang, they can be picked again as follows:

1. Right-click in the data field.
2. Choose ***Pick Peaks On Ranges*** from the popup menu.

Alternatively, you can enter ***ppl*** on the command line. This command can be entered in Interactive peak picking mode or in the normal display mode.

How to Delete all Peak Picking Ranges

☞ Click the  button in the data window toolbar.

or

☞ Right-click in the data field and click ***Delete All Ranges*** in the popup menu.

How to Define Peaks Manually

1. Click the following button (button turns green):

    Define peaks manually.

   A red vertical line will appear in the data window.
2. Put the red cursor line at the desired peak and click the left mouse button. The peak label will appear at the top of the data window.
3. Repeat step 2 for each peak to be defined.
4. Click the green button to leave the "Define peaks" mode.

How to Pick Peaks Semi-Automatically

1. Click the following button (button turns green):

    Define peaks semi-automatically.
2. Move the cursor into the data window.
3. Put the cursor line near the desired peak.
4. Left-click to pick forward

   or

   Right-click to pick backward (see Fig. 11.16).

   A red cursor line will appear at the nearest peak whose intensity is between MI and MAXI.
5. Right-click to add the selected peak to the peak list (see Fig. 11.16).

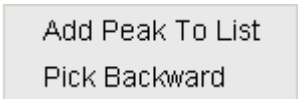


Figure 11.16

   The peak label will appear at the top of the data window.
6. Click the green button to leave the "define peaks semi-automatically" mode.

How to Delete Peaks from the Peak List

To delete a specific peak:

1. Right-click on a defined peak.

2. Choose ***Delete peak under cursor*** from the popup menu (see Fig. 11.17).

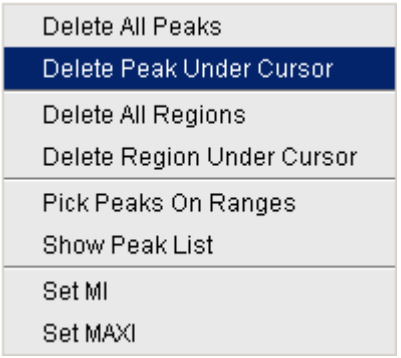


Figure 11.17

To delete all peaks:

☞ Click the button in the data window toolbar.

or

☞ Right-click in the data field and click ***Delete All Peaks*** in the popup menu.

How to Return from Peak Picking Mode with/without Save

To return while saving the peak list and peak ranges:

☞ Click the following button:

Save the Peak Region and Peak List and Return [***.sret***].

This will:

- Save the peak list to the file `peak.txt` and the peak ranges to the file `peakrng`.
- Leave the peak picking mode.

To return while discarding any changes:

☞ Click the following button:

Return, discarding any changes [***.ret***].

Chapter 12

2D Interactive Manipulation

The upper toolbar of the 2D menu offers various buttons for interactive manipulation. If you click such a button, the active data window will switch to the corresponding mode. An interactive manipulation mode is data window specific, i.e. it only applies to the active window.

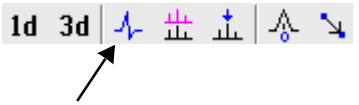
12.1 2D Interactive Phase Correction

2D spectra can be phase corrected interactively in both the F2 and F1 direction by selecting certain rows and/or columns and phase correct them.

12.1.1 2D Interactive Phase Correction Procedure

How to Switch to 2D Interactive Phase Correction

Click the corresponding button in the upper toolbar as indicated below:



or enter ***.ph*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar. Fig. 12.1

shows an example of an unphased 2D inverse spectrum.

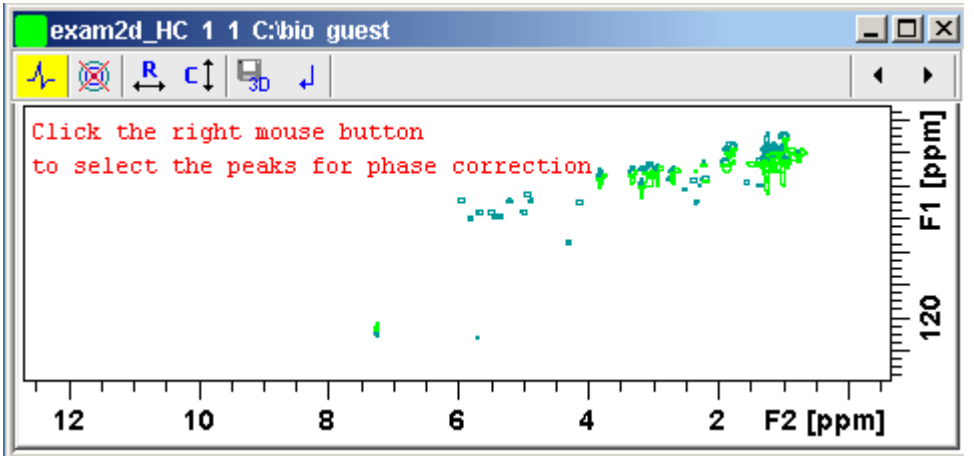


Figure 12.1 Data window in phase correction mode


The yellow button indicates that you are in phase correction mode.


Toggle the contour display on/off.


Switch to *phase row* mode to display rows of selected peaks.


Switch to *phase columns* mode to display columns of selected peaks.


Save the phase values to the 3D data from which this 2D was extracted.


Return.

How to Perform a Typical 2D Interactive Phase Correction

In this example we will perform F1 phase correction (columns) only. Take the following steps:

1. Select two or more peaks in different parts of the spectrum. To do that:
   a) Zoom in on a peak by drawing a box around it. To do that, click-hold the left mouse button and move the mouse (see Fig. 12.2).
   b) Right-click at the peak position and choose ***Add*** from the popup menu.

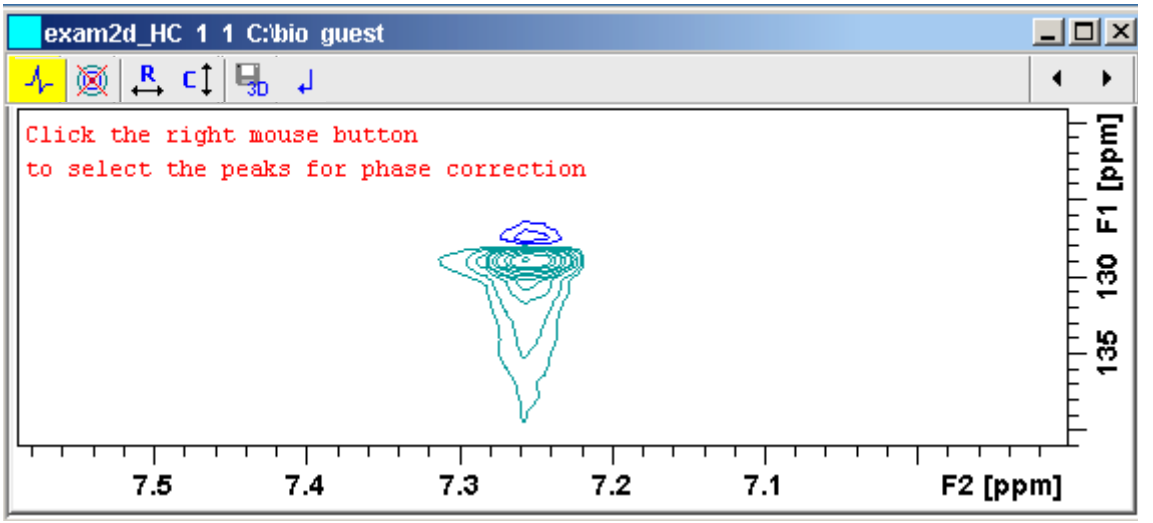


Figure 12.2

c) Click the button to display the full spectrum.

d) Zoom in on the next peak and add in the same way as the first one.

e) Zoom in on the next peak etc.

Fig. 12.3 shows an example of three selected peaks.

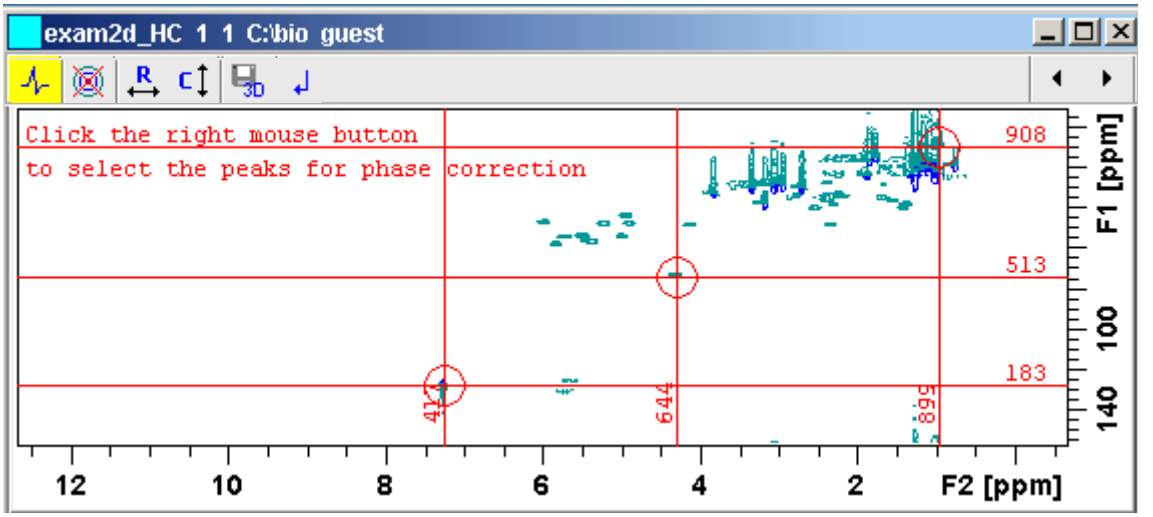


Figure 12.3

2. Click the button to phase correct the columns (F1).

A new data window called *Phase 2D* will appear showing the columns of the selected peaks (see Fig. 12.4).

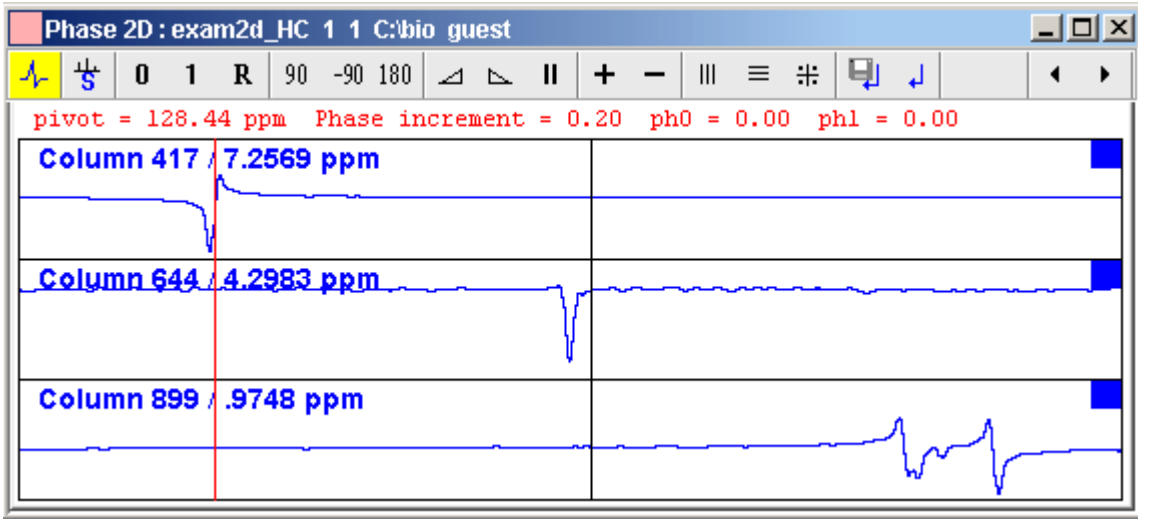


Figure 12.4

Note that the toolbar and the right-click popup menu offer the full 1D phase correction functions.

By default, all columns are selected as indicated by the filled blue squares ■. The red vertical line indicates the default pivot point in the upper column.

3. A typical way to perform phase correction is:
   - Click-hold the **0** button for zero order correction and move the mouse until the reference peak of the first column is exactly in absorption mode.
   - Click-hold the **1** button for first order correction and move the mouse until the reference peak in other column is exactly in absorption mode.
   - Click the button to execute, save and return (see Fig. 12.5).

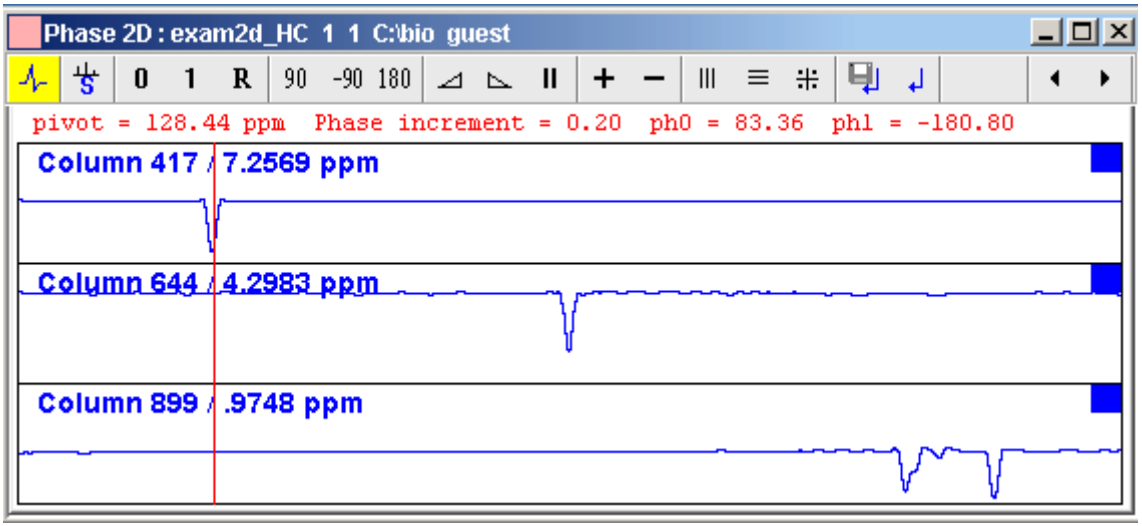


Figure 12.5

12.1.2 2D Interactive Phase Correction Details

How to Scale or Shift Individual Rows/Columns

To select one row or column:

☞ Click in the corresponding part of the data window.

The selected row/column will be marked with a filled blue square ■ whereas unselected rows/columns will be marked with an unfilled blue square □. Selecting

a single row /column allows you to shift and scale it separately from the other rows/columns as shown in Fig. 12.6.

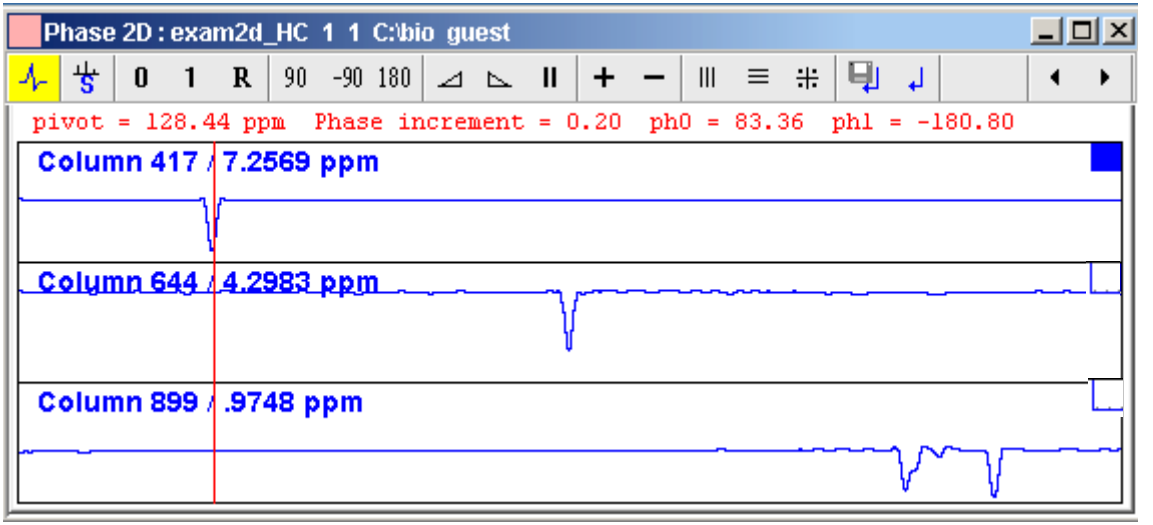


Figure 12.6

To select all rows or columns,

☞ Click the following button:

Select all rows or columns.

How to Perform Smooth Phase Correction

To perform zero order phase correction:

1. Click-hold the following button (it turns green) and move the mouse:

   0 Zero order phase correction.

   until the reference peak of the first row/column is exactly in absorption mode.
2. Release the mouse (button turns grey).

The parameter PHC0 will be set accordingly.

To perform first order phase correction:

1. Click-hold the following button (it turns green) and move the mouse:

   1 First order phase correction.

until the reference peak of the second and further rows/columns is exactly in absorption mode.

2. Release the mouse (button turns grey).

The parameter PHC1 will be set accordingly.

How to Perform 90, -90 or 180° Zero Order Phase Correction

Click one of the following buttons:

90° zero order phase correction.

-90° zero order phase correction.

180° zero order phase correction.

How to Reset the Phase to the Original Values

Click the following button:

Reset zero and first order phase.

How to Change the Mouse Sensitivity

Click one of the following buttons:


Increase (double) the mouse sensitivity [***.inc***].


Decrease (halve) the mouse sensitivity [***.dec***].


Reset the mouse sensitivity to 1.0.

How to Show the Next/Previous Row or Column

To show the next row/column, click the following button:


Show next row/column.

Note that only the selected row/column is increased. If all rows/columns are selected, only the first one is increased.

To show the previous row/column, click the following button:

Show previous row/column.

Note that only the selected row/column is decreased. If all rows/columns are selected, only the first one is decreased.

How to Arrange Rows or Columns

Click one of the following buttons:

 Arrange rows/columns horizontally.

 Arrange rows/columns vertically (see Fig. 12.6).

 Arrange rows/columns vertically in a split window.

How to Return from Multi-1D Phase to 2D Phase Display

Click the following button:

 to save, execute and return.

This will perform the following tasks:

- Execute phase correction.
- Save the current phase correction values.
- Leave the multi-1D phase mode.

Click the following button:

 to return to the 2D phase display without save.

How to Return from 2D Phase Mode

Click the following button:

 Return.

12.2 2D Multiple Display and Row/Column Handling

2D multiple display shows a 2D spectrum with an arbitrary number of 1D and/or 2D spectra superimposed.

Spectra are ppm aligned or Hz aligned, according to the selected axis unit.

A superimposed 1D spectrum is automatically displayed in the direction of the matching nucleus (for a hetero-nuclear 2D) or in the F2 direction (for a homo-

nuclear 2D).

Although multiple display is normally used for spectra with matching nuclei, it allows you to superimposed spectra with non-matching nuclei. You will get a warning that the nuclei do not match. Just just click ***OK*** to continue.

How Switch to Multiple Display mode and Read Multiple Spectra

Switching to multiple display and reading multiple spectra can be done in two different ways:

- Read a 2D dataset and click  to switch to multiple display mode. Then add 1D and/or 2D spectra, e.g. from the browser or with ***re***.

or

- Select multiple spectra in the browser, right-click one of them and click ***Display***.

For a more detailed description of reading multiple data in multiple display mode, see chapter 11.4.

In multiple display mode, the Tab bar of the active data window is replaced by a toolbar (see Fig. 12.7).

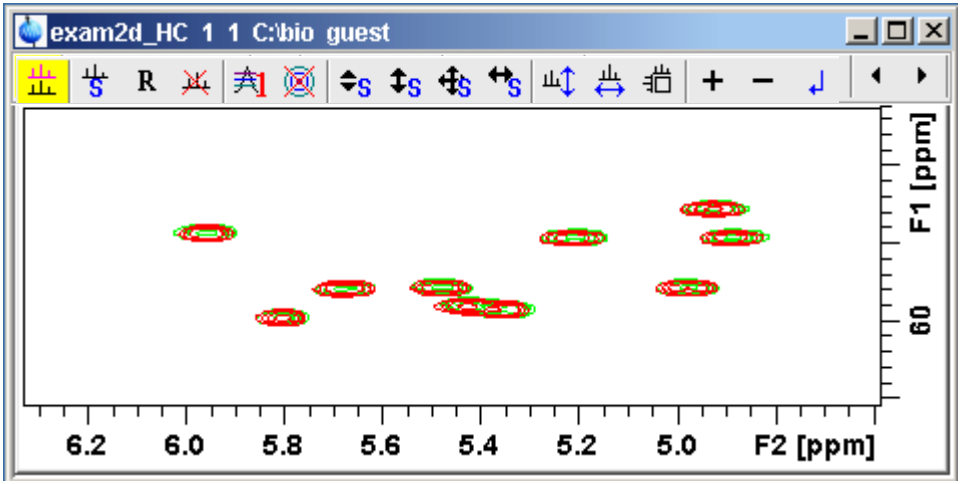


Figure 12.7 Multiple display with two 2D spectra superimposed

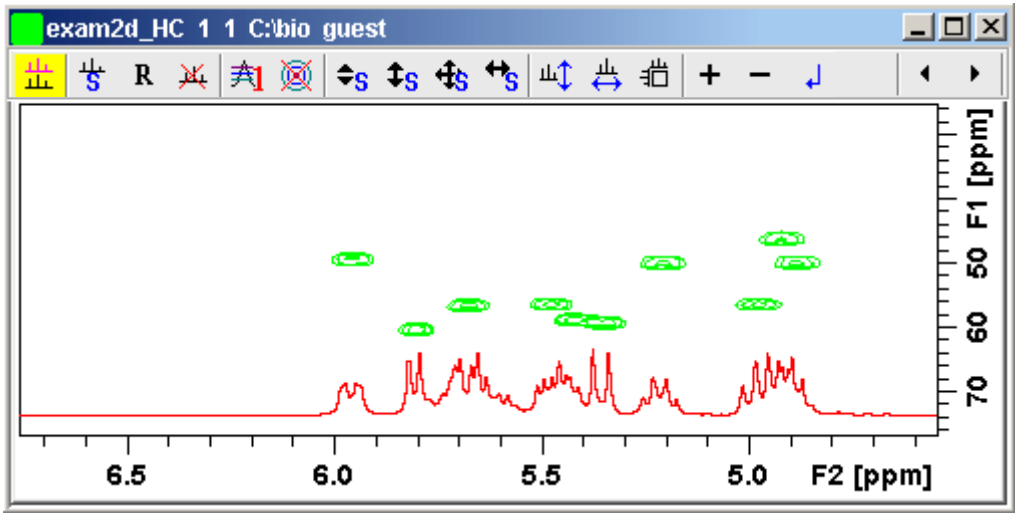


Figure 12.8 Multiple display with a 1D spectrum superimposed on a 2D spectrum

The yellow button indicates that the data window is in multiple display mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

The browser/portfolio in multiple display is split in two parts (see Fig. 12.9).The additional lower part shows:

- which datasets are displayed in the active data window
- which datasets are selected (they are highlighted)

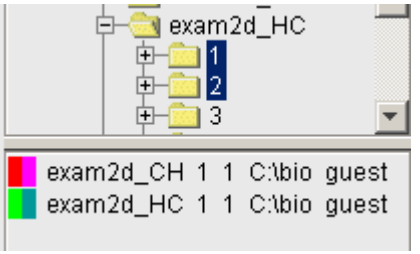


Figure 12.9

How to Align Multiple 2D Spectra

2D spectra in multiple display can be individually shifted. To do that:

1. Select one of the spectra in the lower part of the browser.
2. Click-hold the button and move the mouse.

Fig. 12.10 shows a region of two comparable 1H/13C inverse 2D datasets which are shifted relative to each other.

Clicking the R button resets individual scaling and shifting.

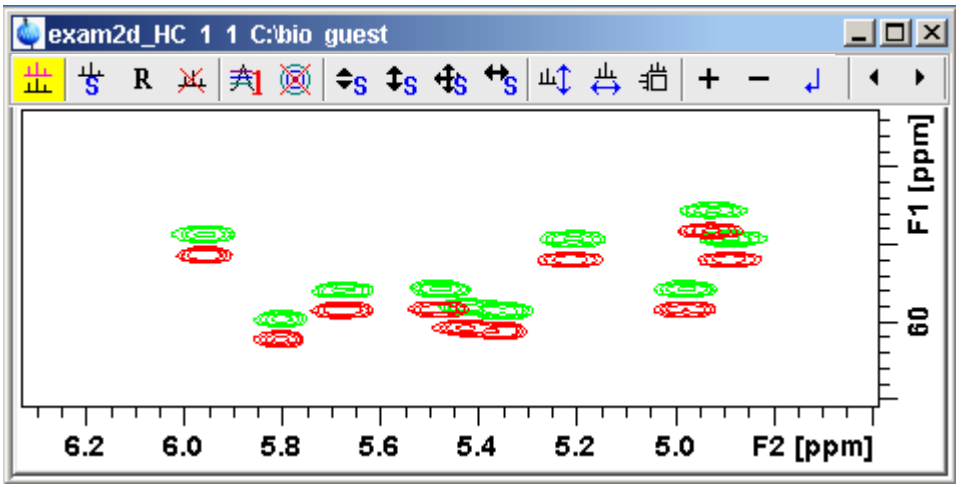


Figure 12.10

How to Scan Rows/Columns

Click the following button (it turns green) and move the mouse in the data field:

to scan rows in the 2D spectrum.

Click the following button (it turns green) and move the mouse in the data field:

to scan columns in the 2D spectrum.

To scale up the displayed row/column:

☞ Click the left mouse button or turn the mouse wheel up.

To scale down the displayed row/column:

☞ Click the middle mouse button or turn the mouse wheel down.

How to Grab a Row/Column

You can grab a row or column, i.e. keep it displayed in the data window as follows:

1. Scan rows or columns as described above and hold at the desired position.
2. Right-click in the data window.
3. Choose ***Grab Row/Column*** from the popup menu (see Fig. 12.11).

Note that a grabbed row/column appears in the lower apart of the browser. It can be selected there and individually scaled or shifted.

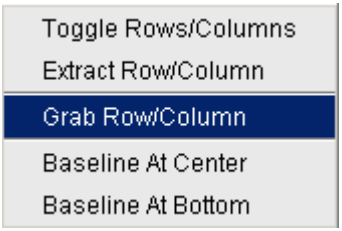


Figure 12.11

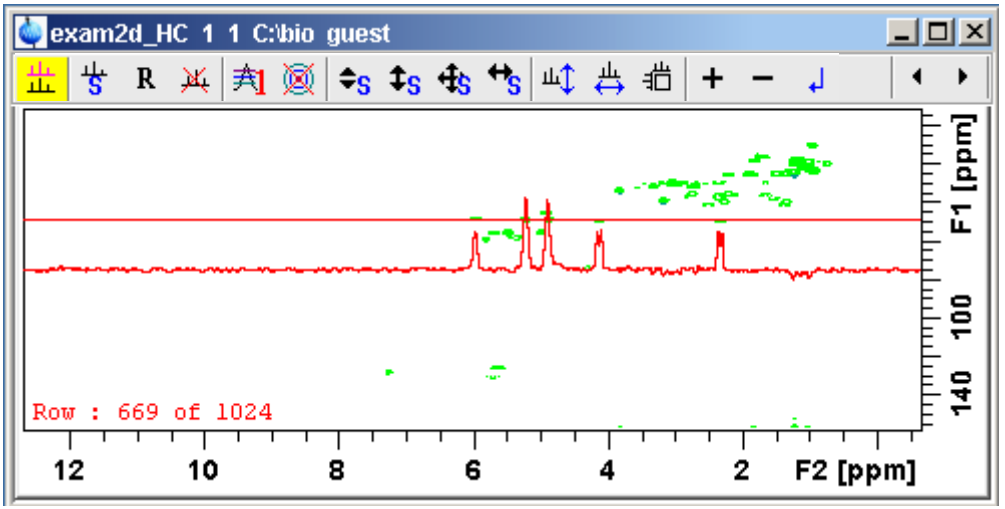


Figure 12.12

Fig. 12.12 shows row 669 with the 1D baseline at the center of the data window.

How to Extract a Row/Column

1. Scan rows or columns as described above and hold at the desired position.
2. Right-click in the data window and choose ***Extract Row/Column*** from the popup menu (see Fig. 12.11).
3. Specify the row/column number and output *procno* in the dialog box. Note that the ROW/COLUMN field is initialized with the grabbed row/column or, if no grabbing was done, with the current row/column.
4. Click ***OK***

The extracted row or column is stored as a 1D dataset under the specified PROCNO and displayed in a new data window. In the upper left part is this, the row number and source 2D dataset is specified (see Fig. 12.13).

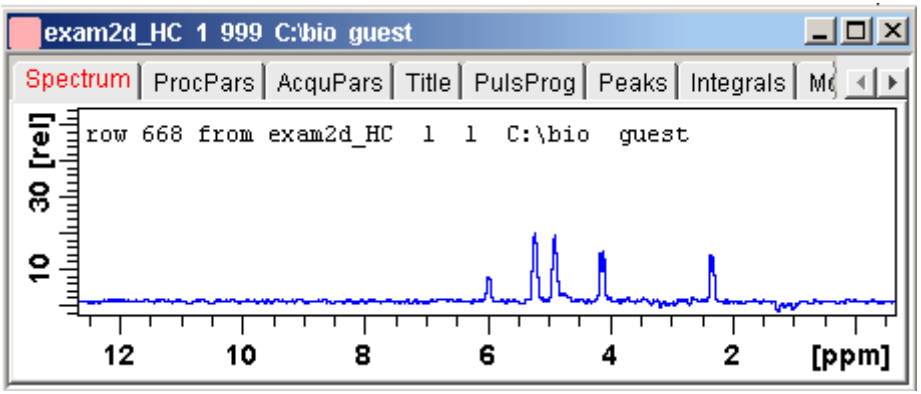


Figure 12.13

How to Copy Contour Levels from First to Other Spectra

Click the following button:

Copy contour levels from the first to the other spectra.

Note that the contour levels are only changed on screen, not on disk.

How to Switch on/off 2D contour display

Click the following button:

 Switch on/off 2D contour display.

How to Position the Baseline of the Row/Column

To put the baseline at the center of the data window:

1. Right-click in the data window.
2. Choose in ***Baseline At Center*** from the popup menu (see Fig. 12.11).

To put the baseline at the bottom of the data window:

1. Right-click in the data window.
2. Choose in ***Baseline At Bottom*** from the popup menu (see Fig. 12.11).

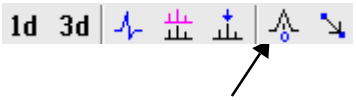
This works both in the scan submode or on a grabbed row/column.

12.3 2D Interactive Calibration

A 2D spectrum can be calibrated, automatically with the command ***sref*** or, interactively as described below.

How to Switch to 2D Calibration mode

☞ Click the corresponding button in the upper toolbar:.



The Tab bar of the active data window will be replaced by a toolbar (see Fig. 12.14).

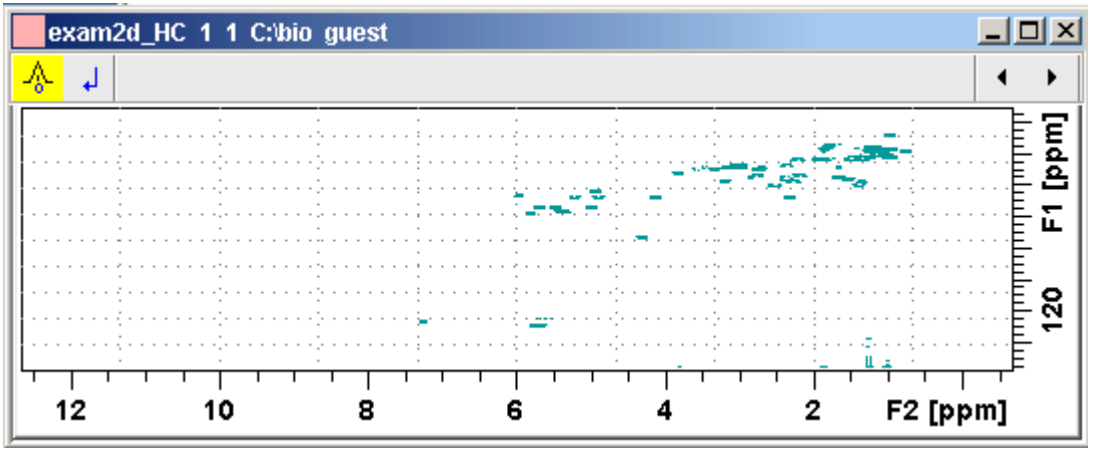


Figure 12.14 Data window in calibration mode

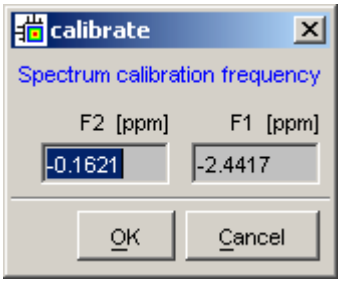
The yellow button indicates that the data window is in calibration mode.

How to Perform 2D Calibration

In calibration mode:

1. Left-click in the data window at the reference peak.

   The following dialog box will appear:



   Note that the units for F2 and F1 (Hz or ppm) correspond to the axis units of the display.

2. Enter the F2 and F1 frequency you want to assign to the reference peak.
3. Click ***OK***.

The spectrum will be calibrated and re-displayed. The calibration button will turn grey again.

12.4 2D Chemical Shift Distance Measurement

How to Measure a 2D Chemical Shift Distance

1. Click the following button (button turns green):

   Chemical shift distance measurement.

2. Click-hold the left mouse button at one peak position and drag the mouse to another peak position.

   The distance in ppm, will be displayed.

3. Right-click in the data window to quit distance mode (button turns grey).

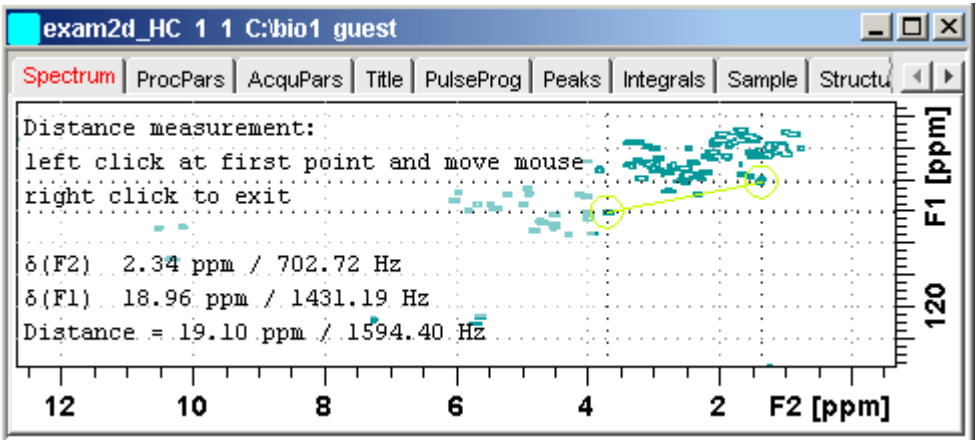


Figure 12.15 Data window in distance measurement mode

12.5 2D Integration

TOPSPIN provides automatic 2D integration. Before you do this, you must first perform peak picking using the ***pp*** command.

Automatic 2D integration can be started as follows:

☞ click ***Analysis*** → ***Integration*** [**`int`**]

This opens the following dialog box.

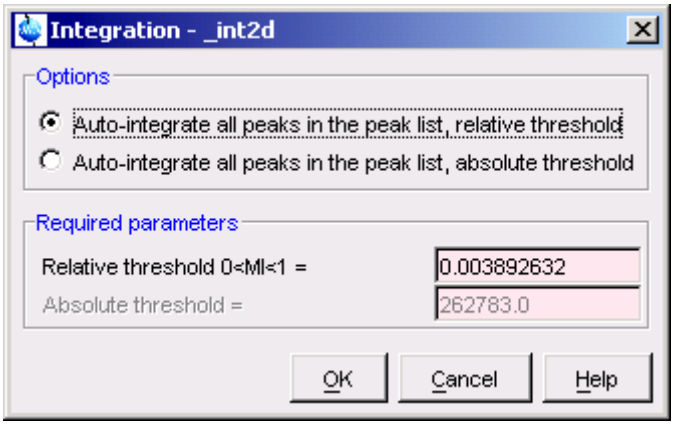


Figure 12.16

Here you can choose between integration using a relative or absolute threshold and set the required parameters. Integral regions are only determined for picked peaks. The calculated integrals will be marked in the data field with the letter **I** and can be listed by clicking the ***Integrals*** tab.

Fig. 12.17 shows a region of peaks after peak picking. Fig. 12.18 shows the same region after 2D integration. Here you can see the integral labels and areas (in this case yellow). The area color can be set in the user preferences (command **`set`**) as *Color of 3rd spectrum*.

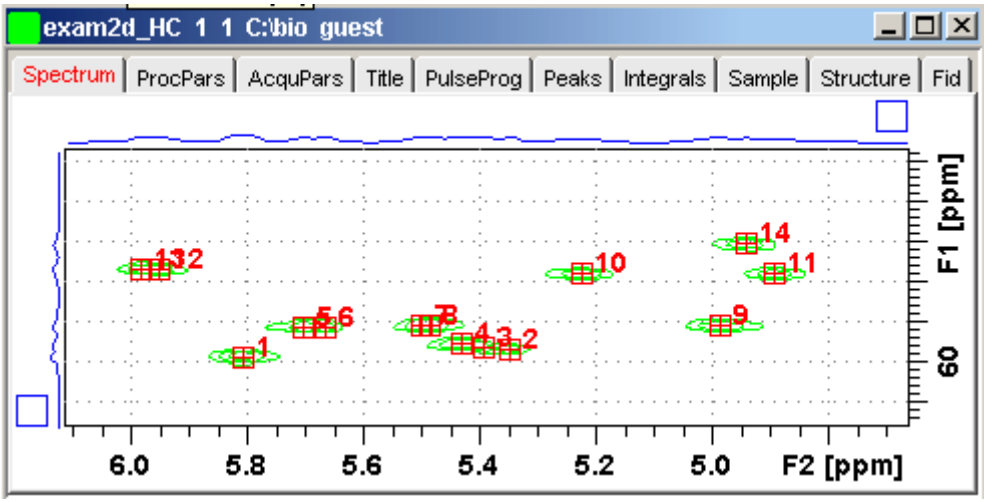


Figure 12.17

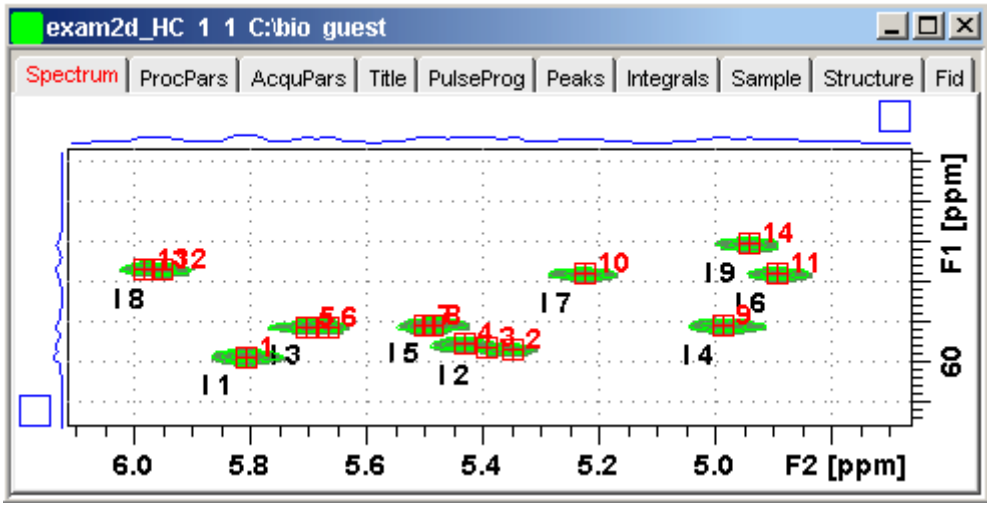


Figure 12.18

Chapter 13

Data Window Handling

13.1 Data Windows

The TOPSPIN window has a data area that may contain multiple data windows. The size of the data area depends on the overall size of the TOPSPIN window and on presence of the Browser and/or Processing Guide. Fig. 13.1 shows the TOPSPIN window with the Browser and three data windows.

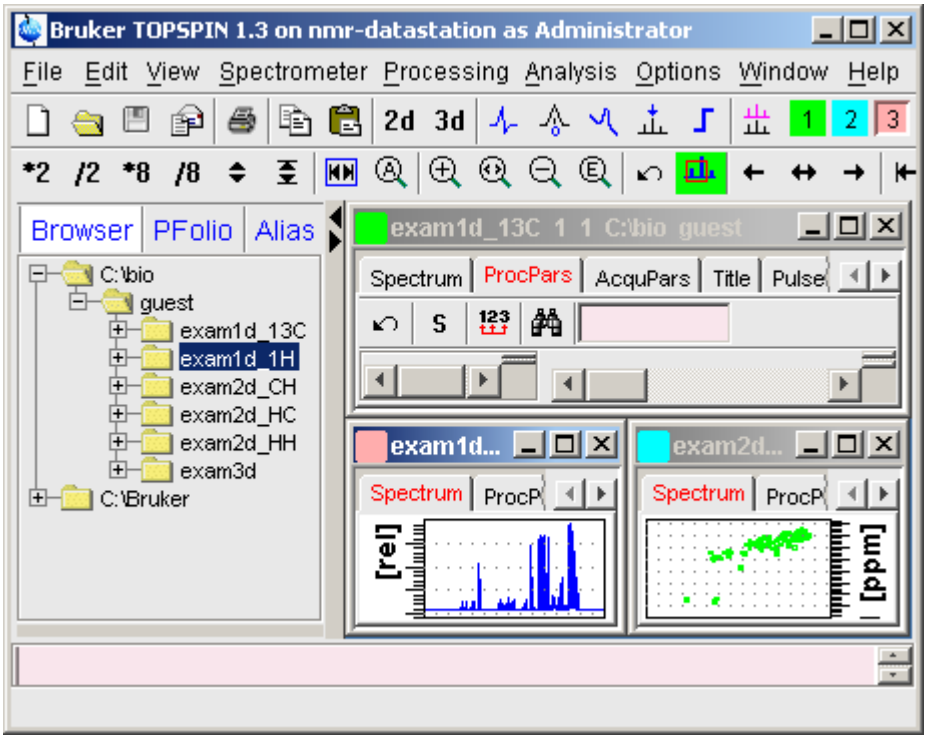


Figure 13.1

Note that the three data windows show different data objects: 1D processing parameters, a 1D spectrum and a 2D spectrum.

How to Move a Data Window

☞ Click-hold the title bar and move the mouse.

How to Resize a Data Window

1. Move the cursor to the window edge until it becomes a double-headed arrow.
2. Left-click-hold that position and move the mouse.

Depending on the position of the double-headed arrow, you can change the window height, width or both (see Fig. 13.2)

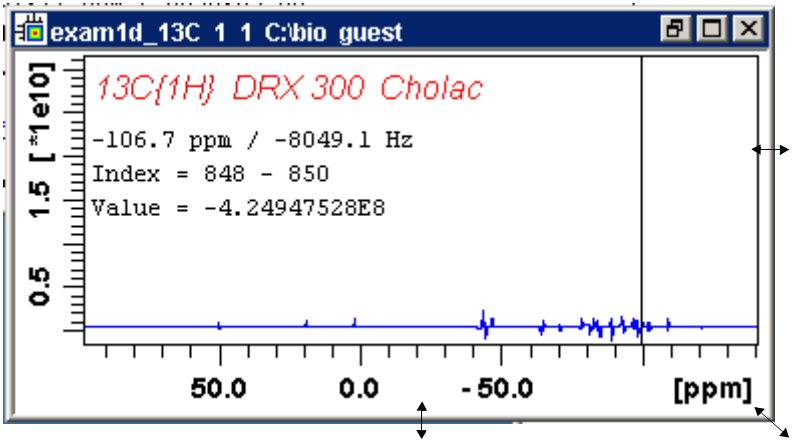


Figure 13.2

How to Select (activate) a Data Window

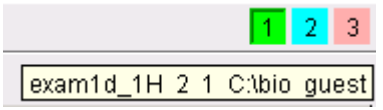
The active data window is the window of which the title bar is highlighted. The TOPSPIN menu, tool bars and command line commands correspond to and act on that window. Only one data window is active at a time.

To activate a different data window:

☞ Click in the desired data window or click its title bar.

or

☞ Click one of the colored radio buttons above the data area. The pressed radio button (the green one in the example below) corresponds to the current dataset.



If you hold the cursor over one of the buttons without clicking it and wait a few seconds, the corresponding dataset specification will be shown.

or

☞ Click ***Window*** → ***x dataname expno procno dir user***

where ***x*** is the number of the desired window and ***dataname***, ***expno***, ***procno, dir*** and ***user*** refer to the dataset displayed in that window.

or

☞ Hit the ***F6*** key to activate the next window. Repeat that until the desired window is the active window.

How to Open a New empty Data Window

☞ Click ***Window*** → ***New window [Alt+w-n]***

The new data window will become the active window and will, by default, cover the entire data area, hiding possible existing data windows. To open a dataset in the new window, drag a dataset from the browser or from the Windows Explorer into the new window or click ***File*** → ***Open*** (see also chapter 4.3).

How to Arrange Data Windows

If the data area contains multiple data windows, you can arrange them in various ways. All the arrange commands arrange the windows left to right and/or top to bottom in the order in which the windows have been active. The currently active data window will therefore be positioned at the top and/or left of the data area.

To arrange the data windows as a grid:

☞ Click ***Window*** → ***Arrange as a Grid***

Depending on the number of windows, they will be arranged vertically and/or horizontally (see Fig. 13.3).

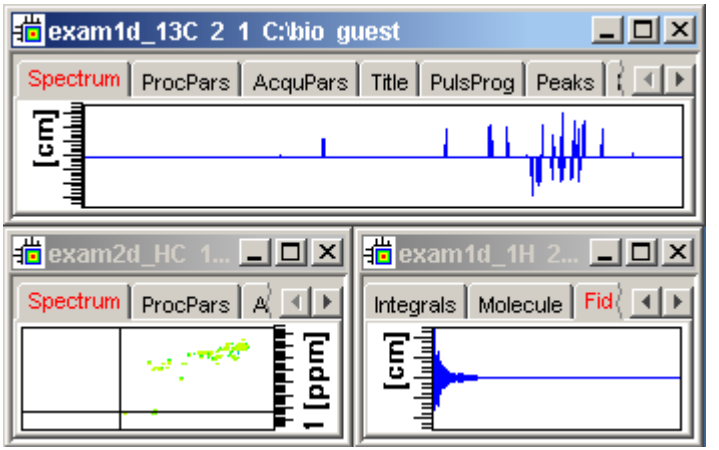


Figure 13.3

To arrange data windows in stack (see Fig. 13.4):

☞ Click ***Window*** → ***Arrange in Stack***

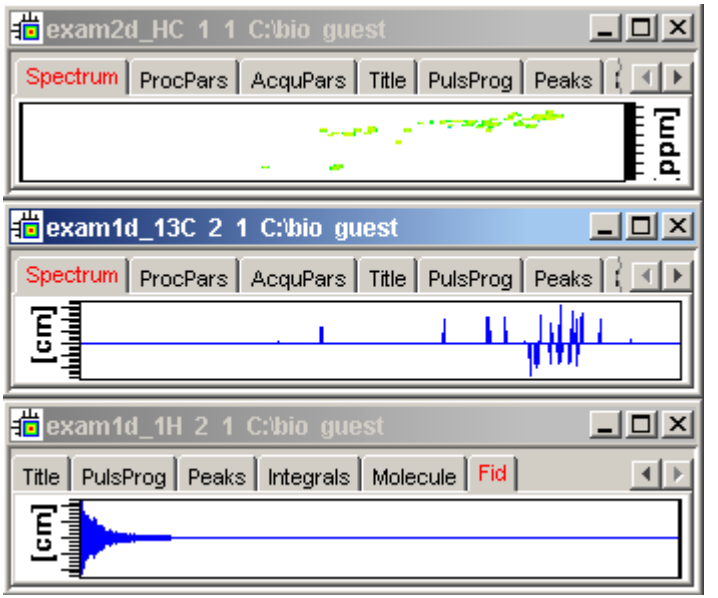


Figure 13.4

To arrange data windows side by side (see Fig. 13.5):

☞ Click ***Window*** → ***Arrange Side-by-Side***

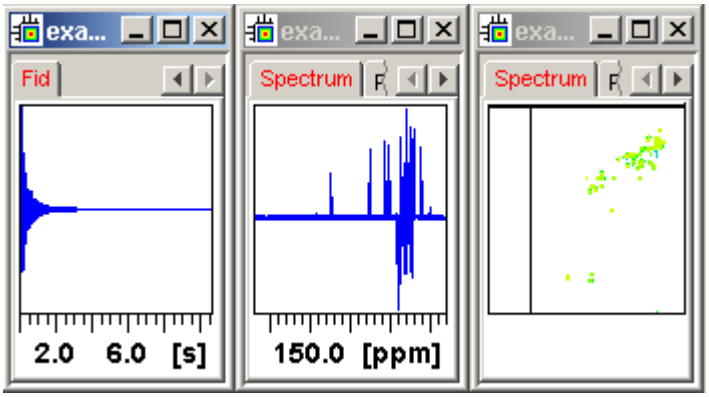


Figure 13.5

To cascade data windows (see Fig. 13.6):

☞ Click ***Window*** → ***Cascade***

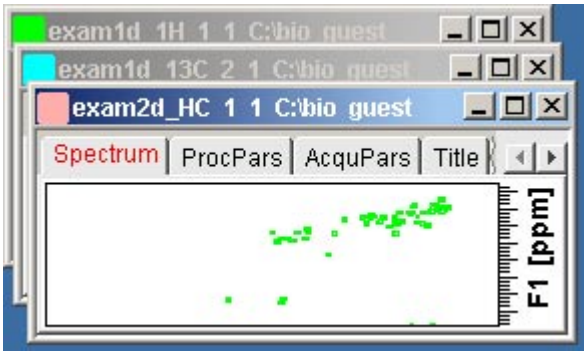


Figure 13.6

Note that you can instruct TOPSPIN to open new data windows cascaded rather than maximized as well configure cascaded windows (command ***`set`*** → ***Window settings***, see also chapter 4.3)

How to Iconify (minimize) a Data Window

☞ Click the button in the windows title bar

or

☞ Click ***Window*** → ***Iconify all*** to iconify all windows.

How to De-iconify a Data Window

☞ Click the button or double-click the title bar.

How to Maximize a Data Window

☞ Click the button or double-click the title bar.

The window will cover the entire data area. Note that a maximized window cannot be moved of resized but can be restored (in size and position), iconified or closed.

How to Restore the Size and Position of a Data Window

☞ Click the button or double-click the title bar.

Note that this is only possible if the title bar contains the button. This is only the case after the window has been maximized or iconified.

How to Close a Data Window

To close the active data window:

☞ Click ***File*** → ***Close*** [**`Crtl-w`**]

or

☞ Click the button in the windows title bar.

To close any data window:

☞ Click the button in the data windows title bar

or

☞ Click the title bar and then click ***File*** → ***Close*** [**`Crtl-w`**].

To close all data windows:

☞ Click ***File*** → ***Closeall*** [**`closeall`**]

How to Iconify all Data Windows

☞ Click ***Window*** → ***Iconify all***

How to Maximize all Data Windows

☞ Click ***Window*** → ***Maximize all***

The active window will be displayed on top, all other windows are hidden.

How to Activate the Next Data Window

☞ Click ***Window*** → ***Next window*** [***F6***].

The windows title bar will become highlighted.

13.2 Window Layouts

A data window layout defines the position, geometry and window type of one or more TOPSPIN windows. The following windows types are available:

- data windows
- lock display window
- acquisition display window
- BSMS display window
- temperature unit window

How to Save the Current Window Layout

1. Click ***Window*** → ***Save layout***
2. In the appearing dialog box:
   Specify the layout File name (extension `.prop`) and click ***Save Layout***

How to Read a Window Layout

1. Click ***Window*** → ***Read layout***
2. In the appearing dialog box:
   Specify or click the layout File name and click ***Read Layout***

Windows are arranged according to the following rules:

- Each currently displayed window type gets the position and geometry to the corresponding definition in the layout.
- If a window type is displayed but not defined in the layout, it keeps its current position and geometry.
- If a window type is defined in the layout but not displayed, the layout definition is ignored.
- Multiple *data* windows are, arbitrarily, assigned to the available data window definitions.

How to Swap Data Windows

Within a certain layout, you can easily swap two TOPSPIN windows with the command ***swin***. If the data area contains exactly two windows, ***swin*** simple swaps their position and geometry. If it contains more than two data windows, ***swin*** opens a list from which you can select any window to be swapped with the currently selected (active) window. Swapping windows can also be executed from the ***Window*** menu.

Chapter 14

Analysis

This chapter describes various TOPSPIN analysis methods including chemical shift measurement, signal to noise calculation, solids line shape analysis, T1/T2 relaxation analysis and multiplet analysis.

14.1 1D Chemical Shift Distance Measurement

How to Measure a Chemical Shift Distance

1. Click the following button (button turns green):

    Chemical shift distance measurement.

2. Left-click-hold at one peak position and drag the mouse to another peak position.

   The distance in ppm, will be displayed.

3. Right-click in the data window or move the cursor out of the data window to leave distance measurement mode (button turns grey).

14.2 1D Signal to Noise Calculation

How to Perform Interactive S/N Calculation

1. Click ***Analysis*** → ***Signal/Noise Calculation*** [**`.sino`**].

   The current signal region (parameters SIGF1-SIGF2) and noise region (parameters NOISF1-NOISF2) are displayed.

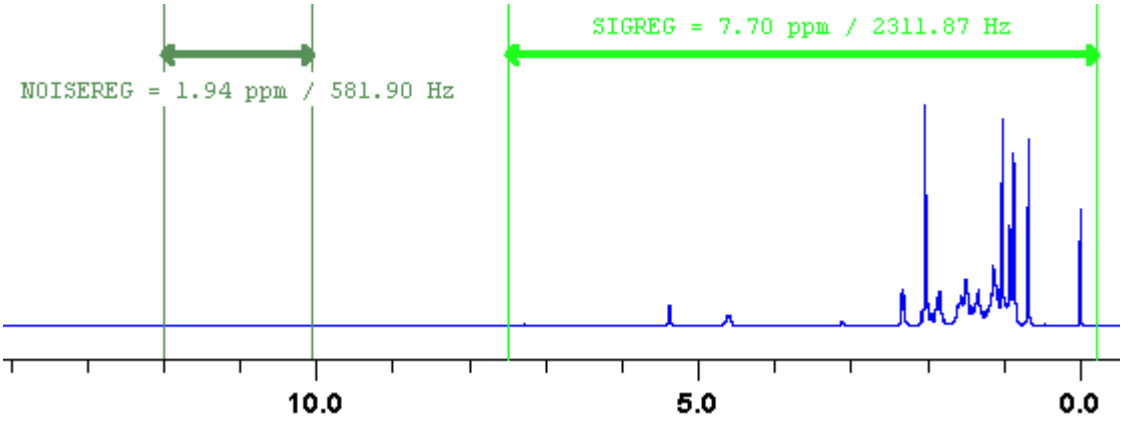


Figure 14.1 Data window in S/N measurement mode

2. Move the mouse into the data window.
3. Left-click-hold and drag the mouse from one edge of the *signal* region to the other edge.

   A horizontal double-headed arrow will indicate the signal region.
4. Left-click-hold and drag the mouse from one edge of the *noise* region to the other edge.

   A horizontal double-headed arrow will indicate the noise region.
5. Right-click any position in the data window. The popup menu as shown in Fig. 14.2 will appear.

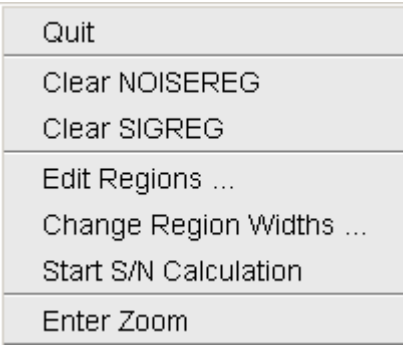


Figure 14.2

Choose ***Start S/N calculation***

The other entries allow you to redefine or clear the regions. After the noise calculation has finished, the result will appear on the screen.

How to Delete the Signal Region or Noise Region

To delete the current signal region:

1. Right-click in the data window.
2. Choose ***Clear SIGREG*** from the popup menu (see Fig. 14.2).

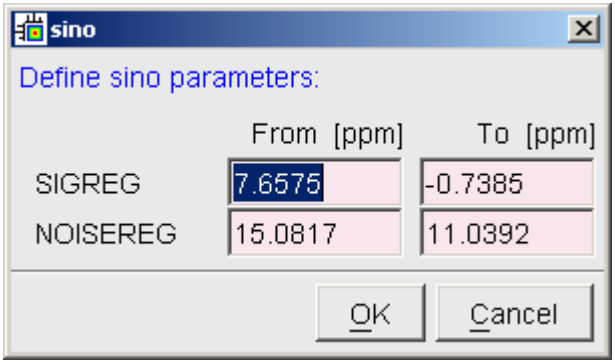
To delete the current noise region:

1. Right-click in the data window.
2. Choose ***Clear NOISEREG*** from the popup menu (see Fig. 14.2).

How to Edit the Limits of the Signal Region or Noise Region

1. Right-click in the data window.
2. Choose ***Edit regions...*** from the popup menu (see Fig. 14.2).

3. Enter new limit values in the appearing dialog box.

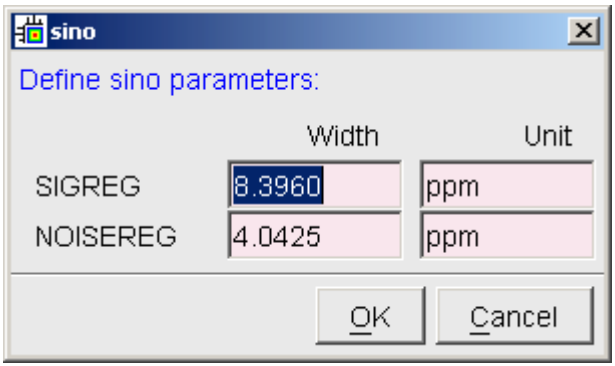


4. Click ***OK***

The S/N value is automatically recalculated and displayed.

How to Change the Width of the Signal Region or Noise Region

1. Right-click in the data window.
2. Choose ***Change region width...*** from the popup menu (see Fig. 14.2).
3. Enter new width values in the appearing dialog box.



4. Click ***OK***

Note that as you change the width, the right limit is modified correspondingly. The left limit is kept. The S/N value is automatically recalculated and displayed.

14.3 Solids Line Shape Analysis

Solids Line Shape Analysis allows you to simulate and fit calculated spectra to various experimental 1D solid NMR spectra. The following fitting models are available:

- Gauss/Lorentz
- Chemical Shift Anisotropy
- Quadrupolar Central Peak of the +/- 1/2 Transition of a Quadrupolar Nucleus
- All Quadrupolar Transitions of a Quadrupolar Nucleus
- The Combination of the Chemical Shift Anisotropy and Quadrupolar Interaction

You can simulate powder spectra of static or rotating samples at single or double axis conditions. Both rotation angles can be set. The inner and outer rotating speeds are freely adjustable. For rotating samples, a maximum of ten rotation side bands and five DOR bands can be set. You can simulate one 1D spectrum with a maximum of 25 observable nuclei, i.e. 25 sites of a nucleus. Ten other nuclei can be defined as dipolar coupling partners of the observed nucleus (Topspin 1.3 allows only one observed nucleus (site) if you define heteronuclear dipolar couplings).

Spectrum Preparation

Before starting Solids Line Shape Analysis, the 1D spectrum must be properly phase corrected and baseline corrected.

Switch to Line Shape Analysis Mode

To switch to Solids Line Shape Analysis mode:

☞ click ***Analysis*** → ***Solids Lineshape Analysis*** [**`solaguide`**]

This opens the workflow as shown in Fig. 14.3.

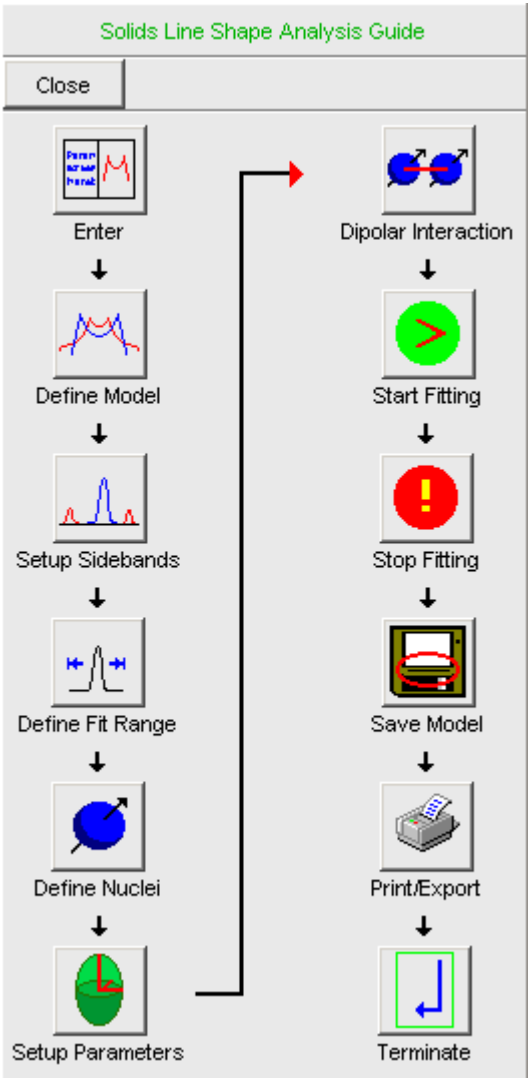


Figure 14.3

Clicking ***Enter*** here will split the data window in two. Experienced users can enter this mode directly and skip the workflow with the command ***`sola`***.

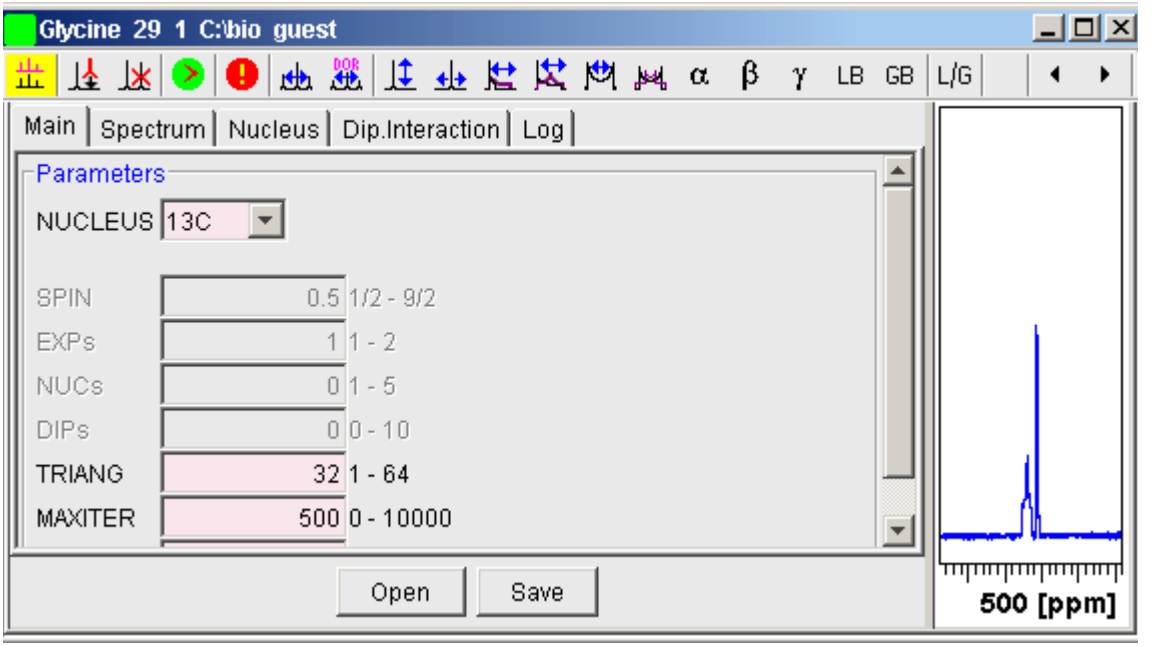


Figure 14.4

The right part of this window is the data window showing the 1D experimental and calculated spectrum. The left part is the parameter window with five panels, where the second one, the ***Main*** panel is selected by default.

The simulation procedure

The simulation procedure consists of the following steps:

Set Optional parameters

In the ***Main*** panel, you find some parameters which you can normally leave unchanged. See the section *Simulation Details* below for more information. If a simulation on the current dataset has already been done and stored, you can read this by clicking ***Open***. If not, you will start from scratch and setup the simulation as described below.

Define the Model

Click the ***Spectrum*** panel and select the ***Model*** according to your experiment. You can refine the experimental conditions by checking one of the following

boxes:

- ***All*** for all quadrupolar transitions.
- ***DOR*** for performed double rotation experiments.
- ***Sync*** for rotor synchronized experiments.

When a parameter is greyed, this means it cannot be changed for the selected model or it is related to one of the other (checked) parameters.

Define Rotation Parameters

From the ***Spectrum*** panel, set the values for:

- MASR - rotation speed of the single axis MAS (VAS) experiments or DOR outer axis speed.
- DORR - inner rotation speed in DOR experiment.

and set their checkmark if they must be optimized during the simulation.

Set the value for:

- SBands: the number of side bands on one side of the central transition.

Define the Spectral Region

Typically, non-overlapping experimental peaks are fitted in separated simulations. Before each simulation, the region to which it is applied must be defined.

1. Zoom in on the region to be simulated.
2. Right-click in the data window choosing ***Define Fitting Region Using Display Region*** or click ***DefReg*** in the panel window.

This will set the parameters F1P and F2P in the Spectrum panel. Alternatively, you can enter the values in the respective parameter fields.

Define Nuclei parameters

For each observable nucleus (site), a set of parameters (see below) must be set. To do that:

1. Click the ***Nucleus*** panel or the  button.
2. Click ***Add*** if the nucleus is not shown yet.
3. Adjust the nuclei parameters until the calculated spectrum approximately fits the experimental spectrum.You can do that as follows:

☞ Enter the values in the parameter field

or

☞ Click the radio button to the right of the parameter, click-hold the corresponding toolbar button (colored green) and move the mouse horizontally.

Note that the calculated spectrum in the data field is automatically updated as you adjust a parameter (see Fig. 14.5).

4. Check the parameters which must be optimized during the simulation.

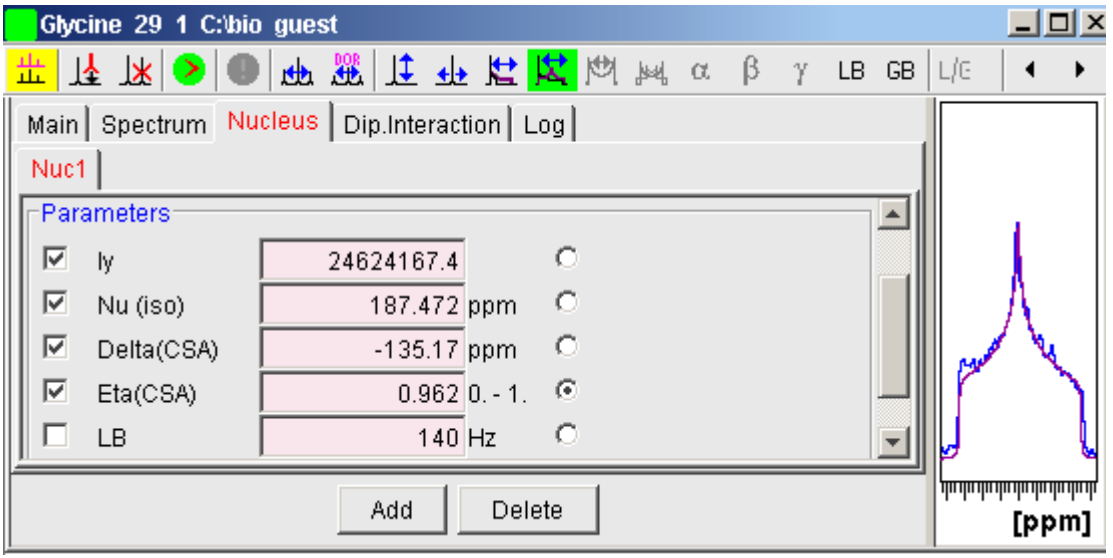


Figure 14.5

Define Dipolar coupling nuclei (if they exist)

Dipolar coupling nuclei can be defined if only one observe nucleus is defined. To set dipolar coupling parameters:

1. Click the ***Dip. Interaction*** panel.

2. Click ***Add*** if the nucleus is not shown yet.

3. Set the nuclei parameters as follows:

☞ Enter the values in the parameter field

or

☞ Click the radio button to the right of the parameter, click-hold the corresponding toolbar button (colored green) and move the mouse horizontally.

4. Check the parameters to be optimized during the simulation.

Start the Simulation

Now you can start the iterative simulation. To do that:

☞ Click the  toolbar button.

The simulated spectrum is displayed in the data window and continuously updated (see Fig. 14.6).

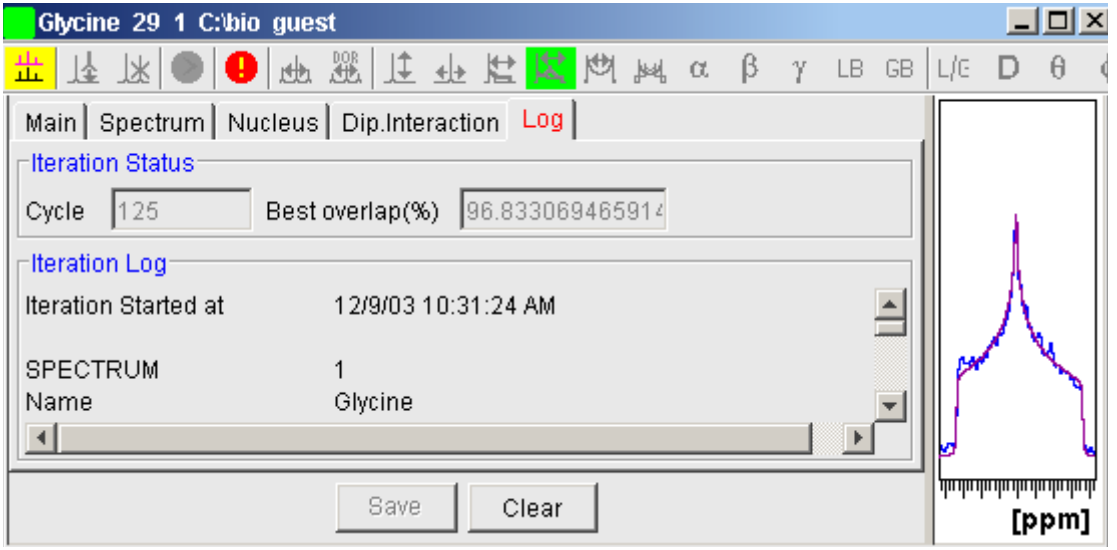


Figure 14.6

The parameter window will switch to the ***Log*** panel showing:

- *Iteration Status*, including the iteration *Cycle* and the B*est Overlap* percentage so far.
- *Iteration Log* with the starting parameters and the results of the fit. Parameters which are marked with an asterisk have been optimized dur-

ing the simulation. They are automatically updated in the respective panels.

To save the Log panel information, click the ***Save*** button.

To clear the Log panel, click the ***Clear*** button.

During the simulation process, you can freely switch to other panels to view the parameter being optimized. After the simulation has finished, the ***Nucleus*** panel will show the optimized values (see Fig. 14.7).

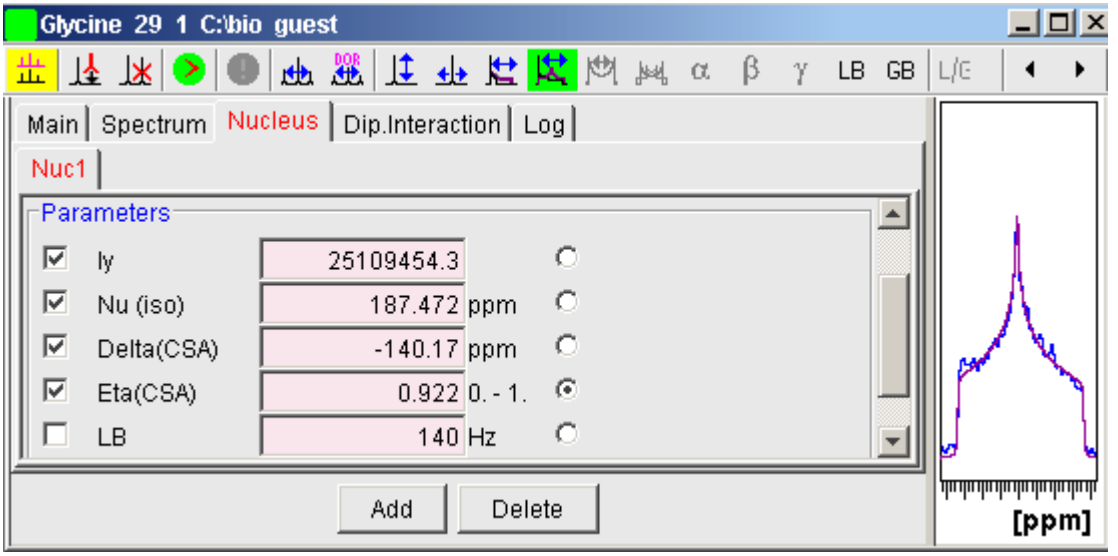


Figure 14.7

Abort the Simulation

To abort a running simulation:

☞ Click the toolbar button.

After a few seconds the iteration stops and the best spectrum will be shown in the data window.

Save the Simulation

After the simulation process is finished for all spectral regions of interest:

1. Switch to the *Main* panel.

2. Click ***Save***

to save all parameters.

Exit Solids Lineshape Analysis

To leave the solids analysis mode:

☞ Click the  toolbar button.

Simulation details

Basic parameters

The Main panel shows you a list of basic parameters:

- NUCLEUS: the observe nucleus. By default, this parameter is set to the value of the acquisition parameter NUC1.
- SPIN: spin of the observe nucleus. It is automatically set according to the selected NUCLEUS.
- EXPs: number of experimental spectra.
- NUCs: number of nuclei (sites of the observe nucleus).
- DIPs: number of dipolar coupling nuclei.
- TRIANG: number of triangles involved in powder spectrum simulation with several random oriented crystallites. The default value of 32 generally results in a good quality spectrum.
- MAXITER: maximum number of iterations.
- SSIZE: initial step size for the iterated parameters. The value represents the fraction of the initial parameter value. It ranges from 0.0 to 1.0 with a default of 0.1.

The values of NUCs and DIPs will automatically be updated when you add or delete nuclei from the ***Nucleus*** and ***Dip.Interaction*** panels.

Spectrum parameters

Spc1

TOPSPIN 1.3 supports only one experimental spectrum to be fitted.

Models

Available fitting models are: *Gauss/Lorentz, CSA, QUAD central, QUAD all*

and *QUAD & CSA.*

Experimental Spectrum

Shows the datapath variables of the experimental spectrum.

Parameters

The following parameters are available.

- MASR - rotation speed of the single axis MAS (VAS) experiments or DOR outer axis speed.
- DORR - inner rotation speed in DOR experiment.
- Angle and AngleInt - the outer and inner rotation angles.
- SBands and DORBands - number of calculated side bands.
- F1 and F2 - the left and right edge of the experimental spectrum.
- F1P and F2P - the limits of the region to be fitted. These must be within the F1-F2 range. To define F1P and F2P interactively, expand the spectrum and right-click in the data window choosing ***Define Fitting Region Using Display Region*** or click ***DefReg*** in the panel window.

The displayed parameters SI, O1P, SF, SW, SWH, LB, GB and SR are used by the fitting calculations. They are defined by the corresponding processing parameters (command ***edp***).

Nucleus Parameters

The section *Model* shows the spectrum model type, which was selected in the ***Spectrum*** panel. The section *Parameters* contains the nucleus dependent model parameters. The available parameters and the corresponding toolbar buttons are:


Iy - Signal intensity.


Nu(iso) - isotrope chemical shift given in ppm.


Delta(CSA) - Chemical shift anisotropy parameter in ppm (can be positive, negative or zero).


Eta(CSA) - Asymmetry parameter ($0 \leq Eta \leq 1$).

 CQ(Quad) - Quadrupolar coupling constant in kHz.

 Eta(Quad) - Asymmetry parameter of the quadrupolar coupling tensor. ($0 \leq Eta \leq 1$)

 Alpha Euler angle of the 'CSA & Quad' tensor.

 Beta Euler angle of the 'CSA & Quad' tensor.

 Gamma Euler angle of the 'CSA & Quad' tensor.

 Line broadening parameter (half width if GB=0).

 Gauss broadening parameter. If GB>0 then LB must be negative.

 Gauss component of the Gauss/Lorentz ratio. $0.0 \leq GL \leq 1.0$ Lorentz curve: GL=0, Gauss curve: GL=1. Used only by the *Gauss/Lorentz* model

 Dipolar coupling.

 Theta (dipolar).

 Phi (dipolar).

Dipolar nucleus parameters

TOPSPIN 1.3 supports a maximum of ten dipolar coupling partners. Note, however, that you can only simulate one observable nucleus (site) at a time if you define dipolar coupling nuclei.

- NUCLEUS - Coupling nucleus partner.
- Spin - Nucleus dependent Spin (Read only).
- D(dip) - Dipolar coupling constant.
- Angle2 - Euler angle of dipolar coupling vector.
- Angle3 - Euler angle of dipolar coupling vector.

Note that Dipolar couplings are invariant to the first Euler angle (rotation around the Z-axis), so this angle value cannot be set.

The Simplex algorithm

The Simplex iteration minimizes the least square difference of the experimental spectrum and the superimposed simulated spectra between F1P and F2P. The 'Best overlap %' value is determined as described below.

Calculate the area between the curves of the experimental and the calculated spectra.

A(dif) = Sum(Abs(Yexp(i)-Ycalc(i)))

Calculate the area of the experimental spectrum.

A(exp) = Sum(Abs(Yexp(i)))

Compare these to area values.

Overlap(%) = 100*(1-A(dif)/A(exp))

Overlap(%) = 100, if A(dif)=0. This is the theoretical maximum of the signal overlap.

Overlap(%) = 0, if the calculated spectrum is similar to the experimental one, with same area, but they do not overlap.

Overlap(%) > 0, but <100. Partial overlap.

Overlap(%) > 70-90, good agreement.

Overlap < 0. No agreement. Change the initial parameters and start a new simulation.

14.4 Relaxation Analysis

Typically, relaxation data consist of a series of 1D FIDs measured with varying delays and stored as pseudo 2D data. To analyze these data, Topspin offers an easy to use T1/T2 Relaxation Guide. Relaxation curves of various experiment types with up to six components can be fitted.

To start the Relaxation Guide:

☞ Click ***Analysis*** → ***T1/T2 Relaxation*** [**`t1guide`**].

This will open the dialog box as shown in Fig. 14.8.

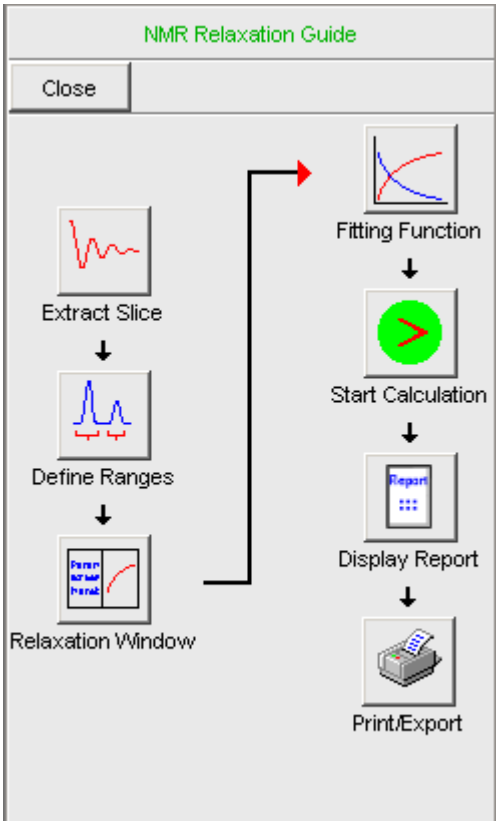


Figure 14.8

Just click the successive icons and follow the instructions on the screen. Note that holding the cursor over an icon shows the command line command that is executed when the icon is clicked. If you prefer to execute these commands from the command line, just click the ***Close*** button to close the Relaxation Guide.

Extract Slice

Prompts you for the FID or spectrum to be extracted for peak determination (see Fig. 14.9). Click ***FID*** to extract an FID or ***Spectrum*** to extract a spectrum. Note that the latter only works if the pseudo 2D data have been processed. If you click

FID, the extracted FID is automatically processed. We recommend to enter the

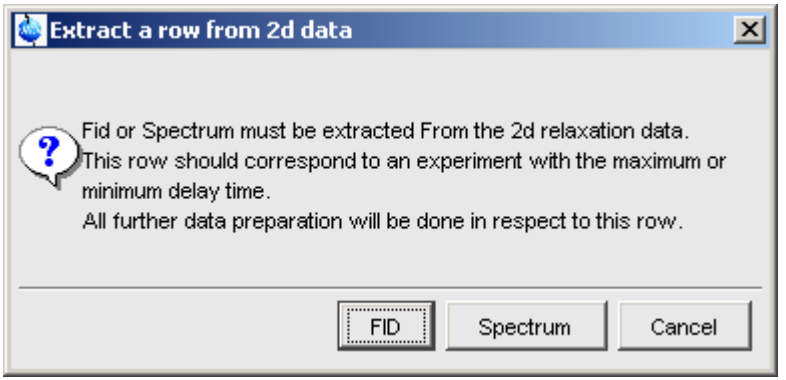


Figure 14.9

FID or spectrum number which was measured with the longest delay. It can be found in the *vdlist* file in the EXPNO data directory. A new data window will appear, showing the extracted 1D-FID.

Transform/Phase

Processes the extracted 1D FID performing exponential multiplication, Fourier transform and automatic phase correction.

Define Ranges

Switches to interactive integration mode. Here you can define the ranges for the peaks to be included in the relaxation analysis.

1. Click the button in the data window toolbar.
2. Put the red cursor line at one edge of a peak or multiplet.
3. Left-click-hold and drag the cursor line to the other edge of the peak or multiplet.
4. Do step 2 and 3 for all regions to be defined.
5. Click the button and choose ***Export Regions to Relaxation Module***
6. Click to return [**`.ret`**].

Relaxation Window

Switches the 1D data window to relaxation analysis mode (see Fig. 14.10)

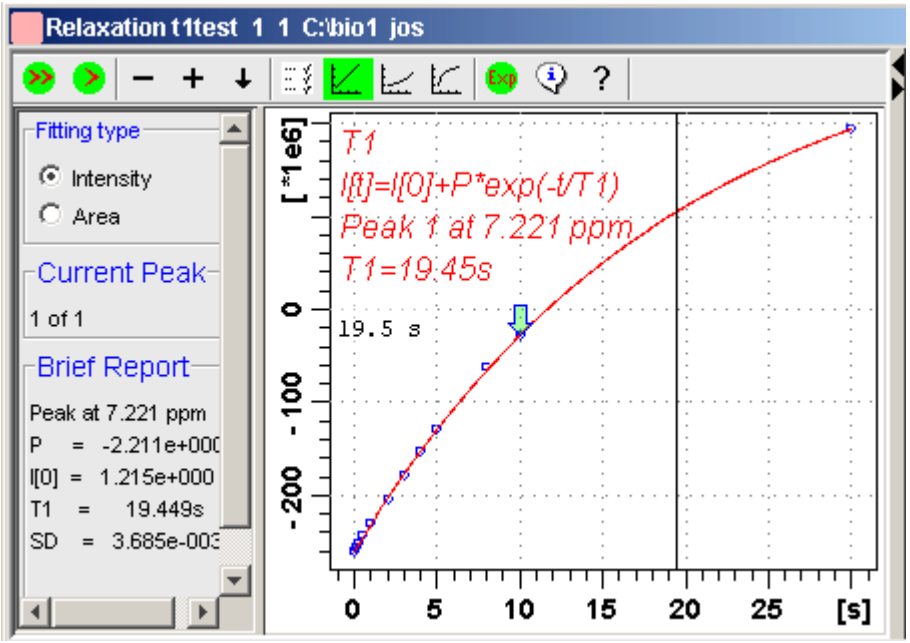


Figure 14.10

and performs a default fitting. By default, this is one-component, T1-intensity fitting (Function type *uxnmrt1*) for peak 1. If the dataset was already fitted, the previous type of fitting is performed. The fitting curve is displayed in the data section and a *Brief Report* is shown in the parameter section. If this default fitting is appropriate, you can view, interpret and print the results as described below. If not, you can perform the desired fitting as described below.

Perform Fitting and Calculate the Relaxation Time

Depending on the experiment, you can perform the appropriate fitting as follows:

1. Select a ***Fitting type***: *Intensity* or *Area*. Either every point reflects the intensity of the biggest peak in the defined integral range or the integral itself. Both of them can be used but, depending on the experiment, one of them usually give a better fitting curve.
2. Click the button to open the parameter dialog box. Select a ***Function Type*** and set the required parameters (see below). Click ***OK***.

3. Perform fitting and calculate the relaxation time:

 Fit the relaxation curve for the current peak.

 Fit the relaxation curve for all peaks.

View and interpret the results as described below.

Function Types and Parameters

The TOPSPIN relaxation routine offers functions for various relaxation experiments with up to 6 components:

uxnmrt1 for one-component T1 experiments. Set the parameter *List file name* to the list type used during the acquisition. The T1 fitting function is defined by the function:

$$I(t) = I(0) + P \times \exp\left(\frac{t}{T1}\right)$$

where *I* is Intensity or Area according to the Fitting Type. The best fit is calculated by varying I(0), P and T1 in an iterative process according to the Levenberg-Marquardt algorithm. Clicking  and  executes the commands ***ct1*** (current peak) and ***dat1*** (all peaks), respectively.

uxnmrt2 for one-component T2 experiments. Set the parameter *List file name* to the list type used during the acquisition. A T2 fitting function is defined by the function:

$$I(t) = P \times \exp\left(\frac{t}{T2}\right)$$

where *I* is Intensity or Area according to the Fitting Type. The best fit is calculated by varying P and T2 in an iterative process according to the Levenberg-Marquardt algorithm. Clicking  and  executes the commands ***ct2*** (current peak) and ***dat2*** (all peaks), respectively.

invrec, satrec, cpt1rho, expdec, gaussdec, lorgauss linear, varbigdel, varlitdel, vargrad, vardamp: these functions can be used for various experiments with up to 6 components, except for **cpt1rho** and **lorgauss** which allow only 4 and 3 components, respectively. They all use the simplex algorithm and require some parameters to be set:

- Enter the **Number of components**

- Click the ***Setup*** button to set the *Iteration Control parameters*. For each component, the initial guess (G) and step rate (S) can be set. The initial guess for I[0] must be selected such that the sum of all components does not exceed 1. If there is only one component, I[0] is usually set to 1.The step rate is usually set to about one tenth of the initial guess. If the step rate of a variable is set to zero, then this variable is not changed during the iterations.

Clicking  and  executes the commands ***simfit*** (current peak) and ***simfit all*** (all peaks), respectively.

View the Fitting Results

When the fitting procedure has finished, the fitting curve is displayed in the data section and a *Brief Report* appears in the parameter section (see Fig. 14.10). The latter consists of:

- the calculated relaxation value
- the fitted parameters
- the standard deviation SD

For further examination of the result, click one of the following buttons:

 Show the fitting result of the previous peak/area.

 Show the fitting result of the next peak/area.

 Switch x-axis to linear scaling.

 Switch x-axis to logarithmic scaling.

 Switch x-axis to quadratic scaling.

 Export integrals to dataset ~TEMP and exit.

 Show an extended report, including the fitted intensity or area distribution. This consists of the same information as the brief report plus a table with the intensity or area distribution. Example:

```
Dataset : C:/bio/data/guest/nmr/t1test/1/pdata/1

INTENSITY fit :
```

```
 I[t]=I[0]+P*exp(-t/T1)

12 points for Peak 1,  Cursor Point =  7.221 ppm

Results     Comp. 1


I[0]  =   1.215e+000
P     =   -2.211e+000
T1    =      19.449s
SD    =   3.685e-003

    tau    ppm     integral    intensity

30.000s    7.221  2.5811e+009  1.9737e+008
10.000s    7.221 -3.2898e+008 -2.9056e+007
8.000s     7.221 -7.8525e+008 -6.4616e+007
5.000s     7.221 -1.6289e+009 -1.3101e+008

...
```

Print, Export of Copy the Fitting Results

To print the fitting curve:

☞ Click ***File*** → ***Print***

To export the fitting curve as a graphics file:

☞ Click ***File*** → ***Export***

To copy the fitting curve to the Windows Clipboard:

☞ Click ***Edit*** → ***Copy***

14.5 Multiplet Analysis

TOPSPIN offers a multiplet analysis package. To start this:

☞ Click ***Analysis*** → ***Multiplet Analysis*** [***managuide***].

This will open the Multiplet Analysis Guide. This will guide you step by step through the multiplet analysis process.

Alternatively, you can enter the command ***mana*** which directly switches to Multiplet Analysis mode. The data window Tab bar will change to a multiplet analysis

toolbar. Fig. 14.11 shows a region of an ethanol spectrum.

Multiplet analysis can be performed in three different ways:

- define multiplet by region
- define multiplet manually
- define multiplet by free grid

For multi-level multiplets, the following methods are available:

- couple existing multiplets into a multi-level multiplet
- define multi-level multiplet by coupled grid

Multiplet analysis uses a maximum intensity search within a user-defined capture range (see Fig. 14.18). If peak picking has been performed (required for defining a multiplet by region), the found peaks within the capture range are used. However, only peaks with the defined minimum intensity are used (see Fig. 14.18).

The three methods are described here for the ethanol CH3, OH and CH2 group, respectively. You can use one of these methods, depending on the type of spectrum and your own preference. In this example, the chosen methods for each group is arbitrary.

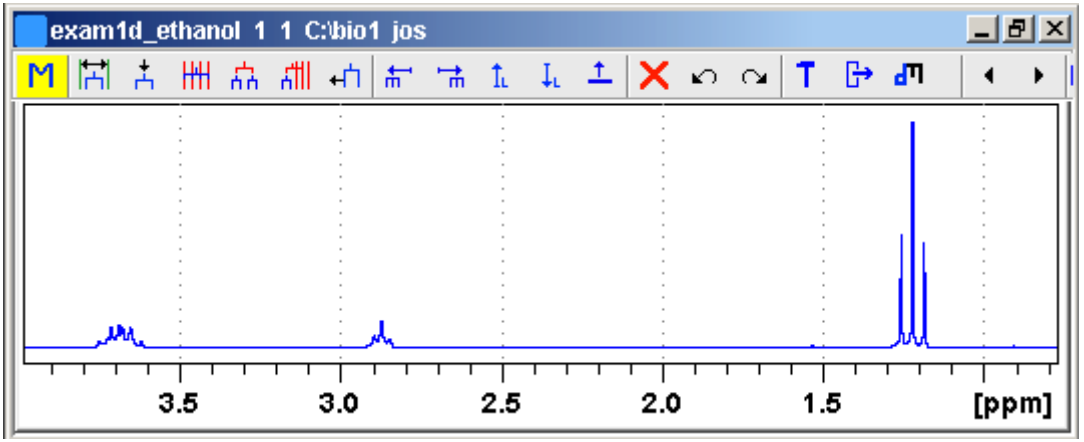


Figure 14.11

14.5.1 Define multiplet by region

In this mode, you simply define the region around the multiplet. The multiplet is

automatically defined from the peaks within the region. At least two peaks must exist in the region to be defined. To define the multiplet:

1. Click the button (it turns green).
2. Click-hold the left mouse button on one side of the multiplet region, drag the mouse and release it at the other side of the region.

   The multiplet will be displayed.
3. Click the button to leave region mode.

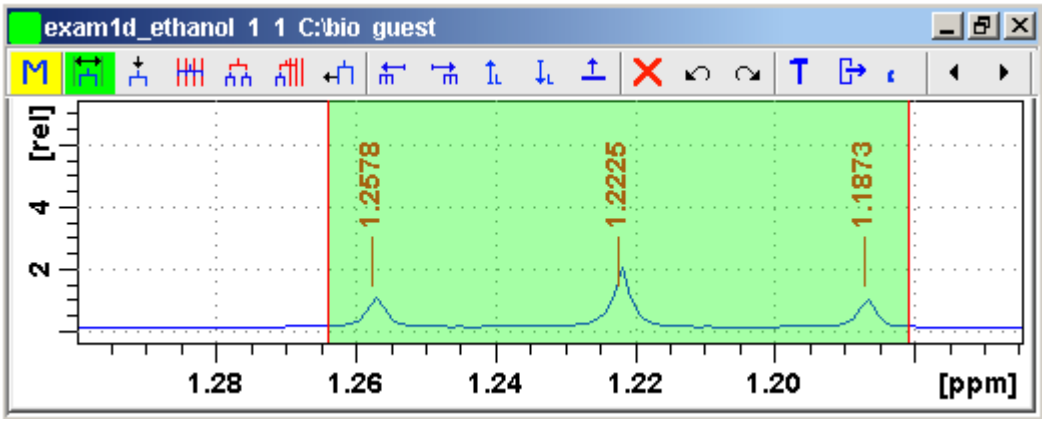


Figure 14.12

In Fig. 14.13, the triplet of the ethanol CH3-group is being defined. The marked area shows the defined region.

14.5.2 Define multiplet manually.

In this mode, you can define a multiplet by assigning individual peaks. No prior

peak picking is required. If, however, peaks have been picked, they are used.

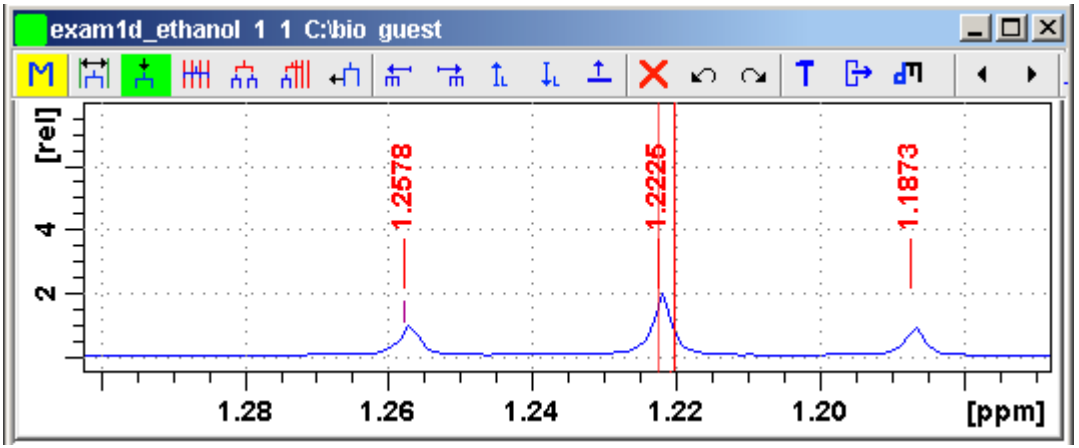


Figure 14.13

To define the multiplet:

1. Zoom in on the region around the desired multiplet.
2. Click the button (it turns green).
3. Left-click the peaks to be defined.
   (Note that left-clicking a peak again will undefine it).
4. Right-click in the data window and select ***Define Multiplet*** in the popup menu.

   The multiplet will be displayed.
5. Click the button to leave this mode.

In Fig. 14.13, the left peak is already assigned and the cursor line is within the capture range of the central peak as indicated by the faint line on the peak maximum.

Manual analysis can also be started by right-clicking in the data field and choosing ***Define Multiplet Manually***.

14.5.3 Free grid analysis

In this mode, you can define a multiplet by assigning one peak manually and all other peaks by free-grid analysis. The grid consists of a predefined number of distance lines.

To define the multiplet:

1. Zoom in on the region around the desired multiplet.
2. Click the button (it turns green).
3. Right-click in the data window and, if necessary, set the number of distance lines.
4. Left-click the central peak to be defined. For a multiplet with an even number of peaks, left-click one of the central peaks.
   The central peak will be marked. Note that clicking a marked peak again will unmark it.
5. Move the mouse to the left or right until the grid lines coincide with the remaining multiplet peaks and click the left mouse button.
   The multiplet will be displayed.
6. Click the button to leave this mode.

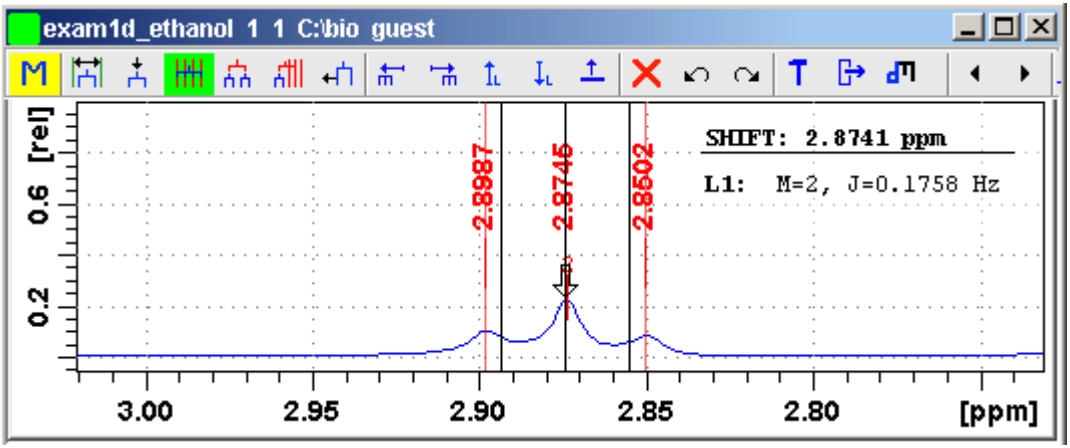


Figure 14.14

In Fig. 14.14, the triplet of the ethanol OH-group is being defined. The central peak is defined and the black grid lines are in the capture range of the other peaks as shown by the faint lines on the peak maxima.

14.5.4 Couple existing Multiplets into a Multi-level Multiplet

In this mode, you can defined a multi-level multiplet by coupling already defined multiplets. To do that:

1. Click the  button (it turns green).
2. Select all multiplets to be coupled by left-clicking them.
3. Move the mouse to the left or right until the grid lines coincide with the multiplet peaks and click the left mouse button.
4. Right-click in the data window and select ***Define Multiplet*** in the popup menu.
   The multi-level multiplet will be displayed.
5. Click the  button to leave this mode.

14.5.5 Define Multi-level Multiplet by Coupled Grid

In this mode, you can define a multi-level multiplet by defining part of the multiplet with one of the methods above and using coupled grid analysis to define the complete multi-level multiplet.

To define a multi-level multiplet:

1. Zoom in on the region around the desired multi-level multiplet.
2. Define the leftmost of rightmost multiplet using one of the methods described above.
3. Click the  button (button turns green).
4. Right-click in the data window and, if necessary, set the multiplicity to the number of multiplets in the multi-level multiplet.
5. Move the mouse to the left or right until the grid lines coincide with the multiplet peaks and click the left mouse button.
   The multiplet is defined now.

6. Click the button to leave this mode.

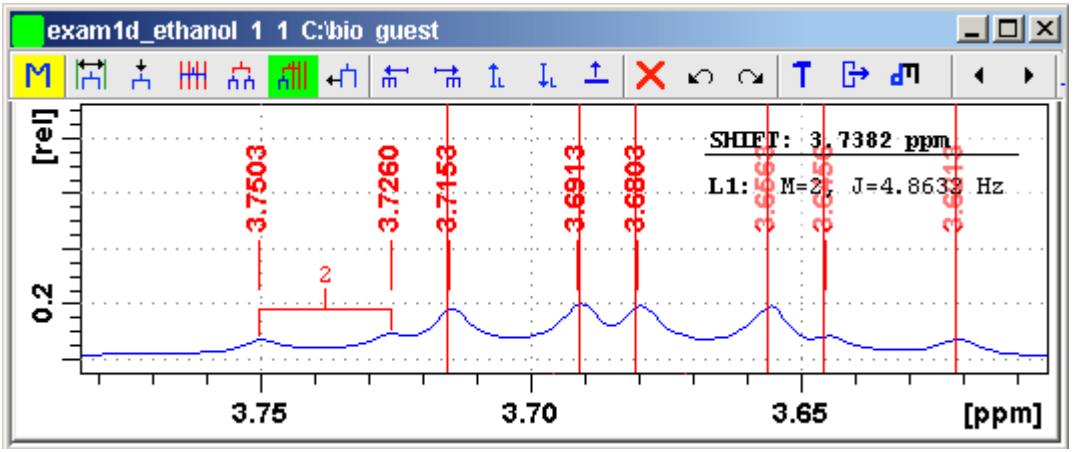


Figure 14.15

In Fig. 14.15, the multi-level multiplet of the ethanol CH2-group is being defined. The left-most doublet is already defined. The (red) lines of the coupled grid are positioned on the remaining six peaks of the multiplet.

14.5.6 Handling Defined Multiplets

Selecting a Multiplet

You can select a particular multiplet simply by clicking it in the data field. The currently selected multiplet is displayed in the color of the second spectrum (default red). Alternatively, you can select a multiplet from the toolbar as follows:

Select the previous multiplet.

Select the next multiplet.

Selecting a Level in a Multi-Level Multiplet

Multi-level multiplets can be assigned for a group which couples with multiple other groups, for example the ethanol CH2 group. Each level can be selected and designated.

Select the next level (up) of a multi-level multiplet.

Select the previous level (down) of a multi-level multiplet.

Designating a Level in Multi-Level Multiplets

A level of a multi-level multiplet can be designated to connect with another multiplet. To do that:

☞ Right-click in the multiplet and choose ***Designate Multiplet***

The designated level is displayed in the color of the fourth spectrum (default purple). Note that the selected level can be different from the designated level.

14.5.7 Define Multiplet Identifiers

To define multiplet identifiers:

1. Left-click the multiplet.
2. Right-click the multiple and select ***Define Multiplet Identifier*** in the popup menu.
3. Specify the multiplet identifier in the appearing dialog and click ***OK***

Alternatively, multiplet identifiers can be defined by clicking the button and double-clicking the respective multiplet lines in the appearing Report dialog. This will open the Identifier dialog (see Fig. 14.16). Just fill out the field **Identifier** and click ***OK***.

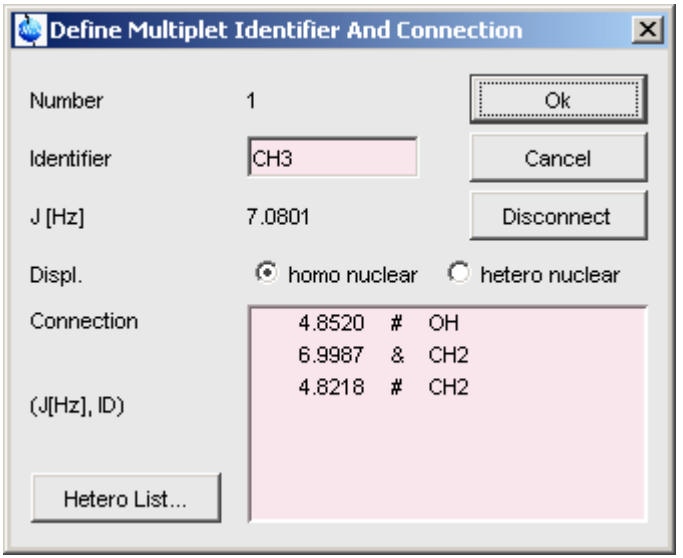


Figure 14.16

Note that the dialog also offers a button to ***Disconnect*** the current multiplet and a field *Connection* that shows all possible connections using the following flags:

& : the current connection

: a non-existing connection

! : a different existing connection

14.5.8 Define Multiplet Connections

Once the multiplets of a spectrum are defined, you can define the connections between them.

To define all connections:

1. Click the button to see the Report dialog (see Fig. 14.17).

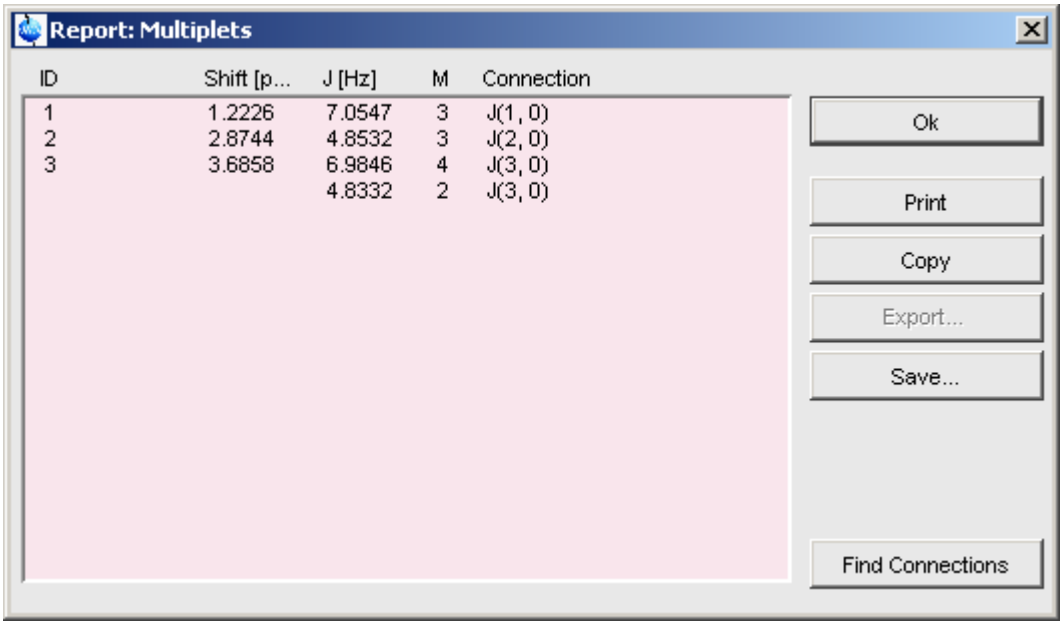


Figure 14.17

2. The multiplets appear in the order in which they have been defined.

   Newly defined multiplets appear with numbers as ID's and no multiplet connections (x,0) defined.

3. Click the button ***Find Connections*** to make the multiplet connections:

   a) Set the maximum difference between related couplings or accept the default.

   b) Set the lower limit for couplings or accept the default.

   c) Check the box ***Change already defined Connections*** if applicable.

   d) Click ***OK*** to define the connections.

Note that the Report Dialog also offer buttons for Printing the multiplet information, copying it to the clipboard and saving it to a text file.

To define individual connections:

1. Select the first multiplet. In case of a multi-level multiplet, click the  or  button to select the required level.

2. Right-click and select ***Designate Multiplet*** from popup menu.
3. Select the second multiplet. In case of a multi-level multiplet, click the  or  button to select the required level.
4. Right-click and choose the ***Connect Multiplets*** from popup menu.

To define individual connections:

To disconnect multiplets:

1. Select on of the multiplets to be disconnected.
2. Right-click and select ***Disconnect Multiplets*** from popup menu.Shifting a Multiplet Line

Alternatively, you can open disconnect a multiplet from the Identifier dialog (see Fig. 14.16)

14.5.9 Further Multiplet Functions

The Multiplet Analysis window offers several other function such as:

 Shift multiplet line. Click this button and move the vertical cursor line into the capture area of the desired line which is then marked by a faint line. The left-click-hold and move the moos to the desired position.

 Shift multiplet vertically. Click this button and move the mouse to put the horizontal line cursor above or below the multiplet tree. Then left-click to shift the multiplet to that position.

 Remove the currently selected multiplet. Clicking this button several times allows you to remove all multiplets.

 Show Daisy multiplets.

 Undo the last multiplet action.

 Redo the last multiplet action.

14.5.10 How to Set Multiplet Options

The  button opens a dialog box where you can set various multiplet options as

shown in Fig. 14.18.

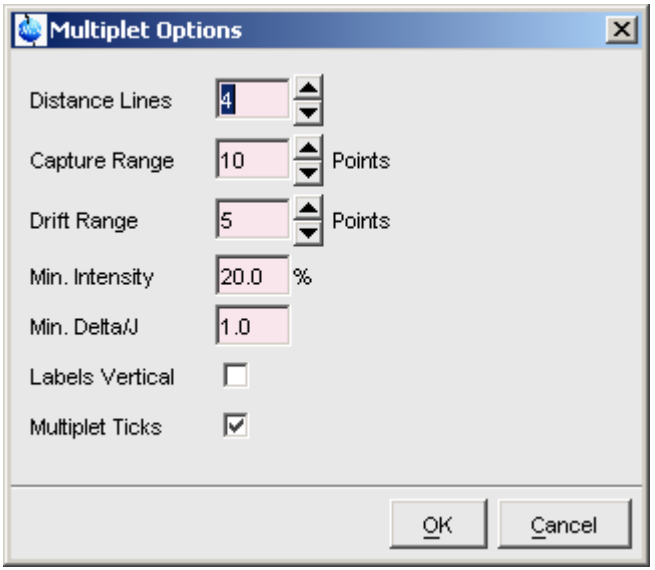


Figure 14.18

- Distance lines: the default number of distance lines in the multiplet dialogs.
- Capture range: the search range for maximum intensity of peak position in manual mode.
- Drift range: the maximum difference in data points between line distances within one multiplet
- Min. Intensity: The minimum intensity of a peak compared to the reference peak to be accepted as a multiple line.
- Min. Delta/J: the minimum ratio of the difference in chemical shift of the coupling groups and the coupling constant. Below this value, the coupling constant in the Report box is indicated with a question mark to suggest possible second order effect.
- Labels Vertical: displays multiplet labels 90° rotated.

All toolbar functions are also available from a popup menu which appears when you right-click in the data window (see Fig. 14.19).

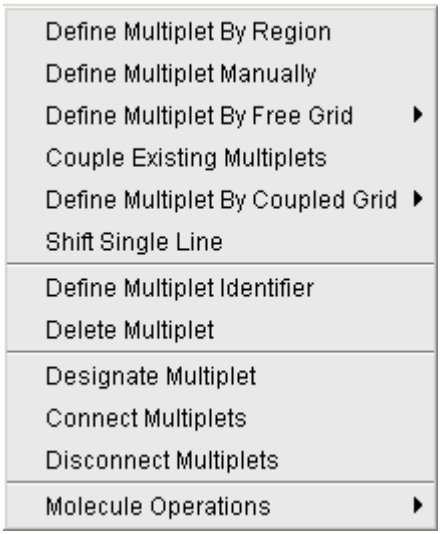


Figure 14.19

Save and close

When you have finished multiplet analysis you can save your work and exit from multiple mode as follows:

Save multiplet analysis.

Save multiplet analysis and quit.

Quit multiple analysis mode.

The multiplet analysis result is saved in the file `mult.txt` in the *procno* data directory.

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