Processing Commands and Parameters

Reference for TopSpin 2.1
Version 2.1.1

Bruker BioSpin

TopSpin 2.1

Version 2.1.1

Processing Commands and Parameters

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Chapter 1

Introduction

1.1 About this manual

This manual is a reference to TOPSPIN processing commands and parameters. Every command is described on a separate page with its syntax and function as well and its main input/output files and input/output parameters. Most of them are processing commands in the sense that they manipulate the data. The manual, however, also includes several commands that analyse data or send information to the screen or printer.

1.2 Conventions

Font conventions

abs - commands to be entered on the command line are in courier bold italic

ProcPars - commands to be clicked are in times bold italic

`fid` - filenames are in courier

name - any name which is not a filename is in times italic

File/directory conventions

<tshome> - the TOPSPIN home directory (default C\:Bruker\topspin[1] under Windows and /opt/topspin under LINUX)

<userhome> - the user home directory

Header conventions

SYNTAX - only included if the command described requires arguments.

USED IN AU PROGRAMS - only included if an AU macro exist for the command described

1.3 About directions

TOPSPIN can process data up to 8-dimension. TOPSPIN 2.1 has been tested for data up to dimension 6. The directions of a dataset are indicated with the terms F6, F5, F4, F3, F2 and F1 which are used as follows:

1D data

F1 - first and only direction

2D data

F2 - first direction (acquisition or direct direction)
F1 - second direction (indirect direction)

Commands like ***xf2*** and ***abs2*** work in the F2 direction. ***xf1***, ***abs1*** etc. work in F1. ***xfb***, ***xtrf*** etc. work in both F2 and F1.

3D data

F3 - first direction (acquisition or direct direction)
F2 - second direction (indirect direction)
F1 - third direction (indirect direction)

4D data

F4 - first direction (acquisition or direct direction)
F3 - second direction (indirect direction)
F2 - third direction (indirect direction)

[1] If C if the default drive.

F1 - fourth direction (indirect direction)

Commands like ***tf3*** and ***tabs3*** work in F3. ***tf2***, ***tabs2*** etc. work in F2. ***tf1***, ***tabs1*** etc. work in F1.

Data with dimension > 3, can be processed with the command ***ftnd***.

1.4 About time and frequency domain data

The result of an acquisition is a representation of intensity values versus acquisition time (seconds); the data are in the time domain. The result of a Fourier transform is a representation of intensity values versus frequency (Hz or ppm); the data are in the frequency domain.

Examples of time domain data are:

- raw data (1D, 2D, and 3D)
- 1D data processed with ***bc***, ***em*** or ***gm***
- 2D data processed with ***xf2*** (time domain in F1)
- 3D data processed with ***tf3*** (time domain in F2 and F1)

Examples of frequency domain data are:

- 1D data processed with ***ft***, ***ef***, ***gf***, ***efp***, ***gfp***, ***trf****
- 2D data processed with ***xfb***, ***xf2***, ***xf1***, ***xtrf****
- 3D data processed ***tf3***, ***tf2***, ***tf1***

Be aware: the commands ***trf**** and ***xtrf**** only perform a Fourier transform if the processing parameter FT_mod (type ***edp***) is set (see ***trf***).

Time and frequency domain data can usually be distinguished by the data type (FID versus spectrum) and axis labelling (Hz or ppm versus sec). The only unequivocal way to distinguish them, however, is the processing parameter FT_mod (type ***dpp***):

- FT_mod = no : no FT was done and the data are still in the time domain
- FT_mod = f* : FT was done and the data are in the frequency domain
- FT_mod = i* : FT and IFT was done and the data are again in the time domain

1.5 About raw and processed data

The result of an acquisition are raw data. Raw data are data which have not been processed in any way. They are stored in:

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data
`ser` - 2D or 3D raw data

The result of processing are processed data. They are stored in:

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

`1r`, `1i` - 1D processed data
`2rr`, `2ir`, `2ri`, `2ii` - 2D processed data
`3rrr`, `3irr`, `3rir`, `3rri` - 3D processed data

Concerning their input data, processing commands can be divided into:

- commands which only work on raw data
- commands which only work on processed data
- commands which work on raw or processed data

1.5.1 Commands that only work on raw data

The following commands only work on raw data. If no raw data exist, they stop with an error message.

- 1D commands ***bc***, ***trf***, ***addfid***, ***convdta***
- 2D commands ***xtrf***, ***xtrf2***, ***addser***, ***convdta***
- 3D commands ***tf3***, ***convdta***

1.5.2 Commands that work on raw data or processed data

The following processing commands work on raw or processed 1D data:

em, ***gm***, ***sinm***, ***qsin***, ***sinc***, ***qsinc***, ***tm***, ***traf***, ***trafs***,
ft, ***ef***, ***gf***, ***efp***, ***gfp***

They work on raw data if one of the following is true:

- no processed data exist (file `1r` and/or `1i` do not exist)
- processed data exist but they are already Fourier transformed

They work on processed data if the following is true:

- processed data exist but they are not Fourier transformed

add, ***addc***, ***and***, ***div***, ***filt***, ***ls***, ***mul***, ***mulc***, ***or***, ***rs***, ***rv***, ***xor***, ***zf***, ***zp***

They work on raw data if the parameter DATMOD = raw

They work on processed data if the parameter DATMOD = processed

The following processing commands work on raw or processed 2D data:

xfb, ***xf2***, ***xf1***

They work on raw data if one of the following is true:

- the option *raw* is added, e.g. ***xfb raw***
- no processed data (i.e. the file `2rr`) exist
- the processing status parameter files `procs` or `proc2s` do not exist or are not readable
- for ***xf2***: data are already Fourier transformed in F2
- for ***xf1***: data are already Fourier transformed in F1
- for ***xfb***: data are already Fourier transformed in both F2 and F1
- the processing status parameter PH_mod is set to *ps* (power spectrum) or *mc* (magnitude spectrum) in F2 and/or F1

They work on processed data if one of the following is true:

- the option *processed* is used, e.g. ***xfb processed***
- none of the conditions for using raw data is fulfilled

1.5.3 Commands that always work on processed data

Several processing commands can, by definition, only work on processed data. If no processed data exist, they stop with an error message.

On 1D data:

abs, ***absf***, ***absd***, ***apk***, ***apk0***, ***apk1***, ***apks***, ***bcm***, ***sab***, ***trfp***, ***ift***, ***ht***, ***genfid***, ***filt***

On 2D data:

abs2, ***abs1***, ***abst2***, ***abst1***, ***sub2***, ***sub1***, ***sub1d2***, ***sub1d1***, ***bcm2***, ***bcm1***, ***xf2p***, ***xf1p***, ***xfbp***, ***xf2m***, ***xf1m***, ***xfbm***, ***xf2ps***, ***xf1ps***, ***xfbps***, ***sym***, ***syma***, ***symj***, ***tilt***, ***ptilt***, ***ptilt1***, ***rev2***, ***rev1***, ***xif2***, ***xif1***, ***xht2***, ***xht1***, ***xtrfp***, ***xtrfp2***, ***xtrfp1***, ***add2d***, ***genser***

On 3D data:

tf2, ***tf1***, ***tht3***, ***tht2***, ***tht1***,***tf3p***, ***tf2p***, ***tf1p***,***tabs3***, ***tabs2***, ***tabs1***

1.6 About digitally filtered Avance data

The first points of the raw data measured on an Avance spectrometer are called group delay. These points represent the delay caused by the digital filter and do not contain spectral information. The first points of the group delay are always zero. The group delay only exists if digital filtering is actually used, i.e. if the acquisition parameter DIGMOD is set to digital.

1.7 Usage of processing commands in AU programs

Many processing commands described in this manual can also be used in AU programs. The description of these commands contains an entry USAGE IN AU PROGRAMS. This means an AU macro is available which is usually the name of the command in capitalized letters. If the entry USAGE IN AU PROGRAMS is missing, no AU macro is available. Usually, such a command requires user interaction and it would not make sense to put it in an AU program. However, if you still want to use such a command in AU, you can use the XCMD macro which takes a TOPSPIN command as argument. Examples are:

```
XCMD("edp")
XCMD("setdef ackn no")
```

AU programs can be set up with the command ***edau***.

Most TOPSPIN commands can also be used in a TOPSPIN macro (see ***edmac***) or Python program (see ***edpy***).

1.8 Clicking commands from the TOPSPIN menu

This manuals describes all processing commands as they can be entered on the command line. However, they can also be clicked from the TOPSPIN popup menus. Most commands can be found under the ***Processing*** or ***Analysis*** menu. The corresponding command line commands are specified in square brackets or appears on right-clicking the menu item.

1.9 Userspecific handling of Source Directories

1.9.1 Source Directory Handling - Introduction

The following paragraphe describes the fundamental handling how TopSpin 2.1 and newer is searching for information like pulse programs, parameter sets, AU programs, lists like VD-list and files like intrng-files (see listing below, paragraphe 1.9.3). The information where to find these files is stored in the definition of ***Source Directories*** in TopSpin. There each TopSpin user can add/remove directories and change the order of directories. The order of the directories defines the priority for TopSpin when searching for a file.

This function is complemented now with the function called ***Manage Source Directories***. There all user preferences regarding Directory Handling can be defined and are keeped.

TopSpin 2.1 does not use the database anymore, which has been used in TopSpin 2.0.

1.9.2 Examples of use

In order to describe the new userspecific handling of Source Directories in TopSpin 2.1 more considerable you can find two examples of use in the following:

1. Shelter of own files
   With the new userspecific handling of Source Directories all userspecific files can be protected. If e.g. all user-files are stored in the own "Home"-Directory nobody else than the actual user can read or modifiy any file, because this directory is read- and write protected.This

protection for example can be important for pulse program development.

2. Simple and secure working in laboratories with various spectrometers
All TopSpin installations that provide the basis for spectormeter control, can be configured in TopSpin 2.1 to be got from the same directories. With this use of ***Manage Source Directories*** for example Pulse Programs can be taken from one common directory so that all modifications and improvements can be used from all spectrometer in the laboratory immediately. Along this way Source directory handling becomes much more comfortable and much fewer failures will arrive.

1.9.3 Source Directories

In TopSpin 2.1 users can specify individual directories for:

- Pulse Programs
- CPD Programs
- Shape Files
- Gradient Files
- Parameter Sets
- Macros
- Python Programs
- AU Programs
- VD Delay lists
- VP Loup Cont lists
- VC lists
- VA Amplitude lists
- VT Temperature lists
- F1 Frequency lists
- SP Shape lists
- DS Data Set lists
- Solvent Region Files
- Phase Program lists

- ’intrng’ files
- ’peakrng’ files
- ’baslpnts’ files
- ’base_info’ files
- ’peaklist’ files
- ’clevels’ files
- ’reg’ files
- ’int2drng’ files
- Structure files

1.9.4 Default directories

The default paths for directories, e.g. Pulse Programs, are:
Bruker files in: *.../exp/stan/nmr/lists/p*p
User files in: *.../exp/stan/nmr/lists/pp/user*

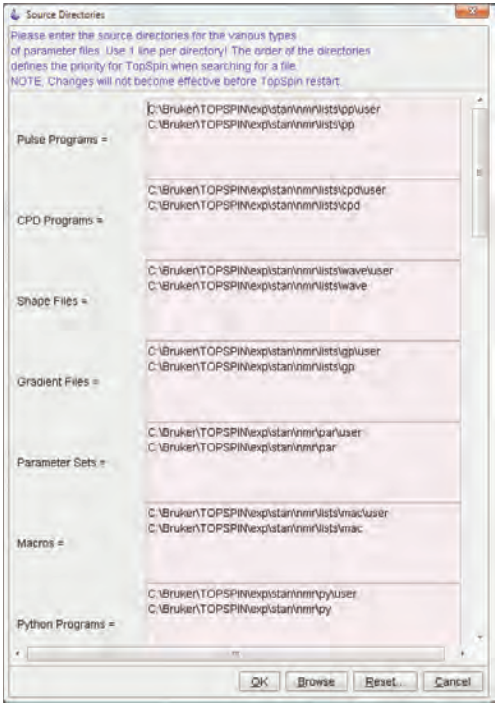
The default path for lists, e.g. VD lists, is
Bruker/User files in:*.../exp/stan/nmr/lists/vd*

1.9.5 How to define userspecific directories

With TopSpin 2.1 and newer the directory/file structure enables all users to define individual directories. The userspecific path definition of Source Directories can be reached from the menu bar by

Options → ***Preferences*** → ***Directories*** → ***Manage Source Directories*** → ***Change***.
This way leads to a list of all Source Directories, where the userspecific paths can be specified (see Figure 1.1). With this structure each user can define his own directories in an unlimited number.

This window enables the user to define the individual directories for all files as Pulse Programs, AU Programs etc. (for the complete list of Source Directories see paragraphe 1.9.3).
The order of the directories defines the priority for TopSpin when searching for a file.
Please note that changes will not become effective before TopSpin restart.



Source Directories

Please enter the source directories for the various types
of parameter files. Use 1 line per directory! The order of the directories
defines the priority for TopSpin when searching for a file.
NOTE, Changes will not become effective before TopSpin restart.

```
Pulse Programs =     C:\Bruker\TOPSPIN\exp\stan\nmr\lists\pp\user
                     C:\Bruker\TOPSPIN\exp\stan\nmr\lists\pp
CPD Programs =       C:\Bruker\TOPSPIN\exp\stan\nmr\lists\cpd\user
                     C:\Bruker\TOPSPIN\exp\stan\nmr\lists\cpd
Shape Files =        C:\Bruker\TOPSPIN\exp\stan\nmr\lists\wave\user
                     C:\Bruker\TOPSPIN\exp\stan\nmr\lists\wave
Gradient Files =     C:\Bruker\TOPSPIN\exp\stan\nmr\lists\gp\user
                     C:\Bruker\TOPSPIN\exp\stan\nmr\lists\gp
Parameter Sets =     C:\Bruker\TOPSPIN\exp\stan\nmr\par\user
                     C:\Bruker\TOPSPIN\exp\stan\nmr\par
Macros =             C:\Bruker\TOPSPIN\exp\stan\nmr\lists\mac\user
                     C:\Bruker\TOPSPIN\exp\stan\nmr\lists\mac
Python Programs =    C:\Bruker\TOPSPIN\exp\stan\nmr\py\user
                     C:\Bruker\TOPSPIN\exp\stan\nmr\py
```

Figure 1.1

1.9.6 How to define userspecific directories with commands

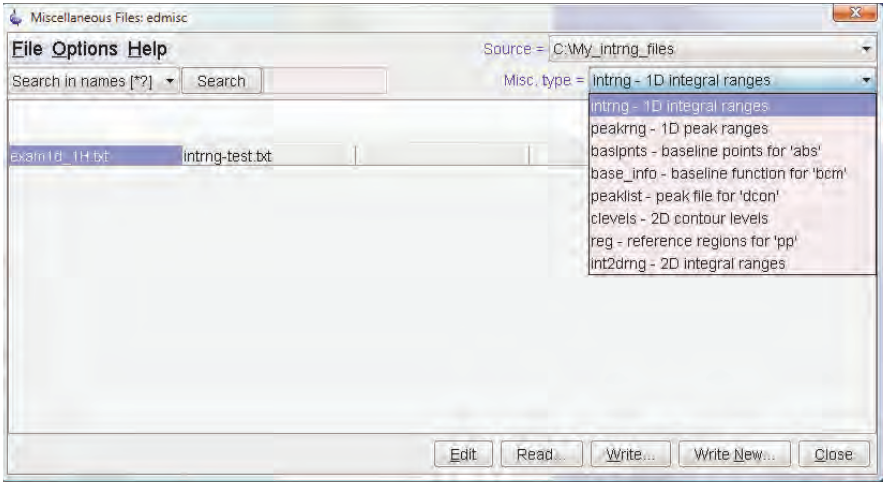
Userspecific directories can also be configured from the corresponding reading-/writing- and editing-commands for the respective information like pulse programs, parameter sets, AU programs, lists and files.

For defining special lists please enter the corresponding command in the command line:

- Pulse Programs (***edpul***)
- CPD Programs (***edcpd***)
- Shape Files (***edshape***)
- Parameter Sets (***edpar***)
- Macros (***edmac***)
- Python programs (***edpy***)

- AU Prgrams (***edau***)
- VD, VP, VC, VA, VT, F1, DS, Solvent Region Files, Phases (***edlist***)
- ’intrng’ Files, ’peakrng’ Files etc. (***edmisc***)

After entering the respective command in the command line, TopSpin will open the corresponding window in appearance like the following window. Here the example for the command ***edlist*** (see Figure 1.2).


Miscellaneous Files: edmisc

Source = C:\My_intrng_files

Misc. type = intrng - 1D integral ranges

exam1d_1H.txt

intrng-test.txt

File Options Help
Search in names [*?]
Search
intrng - 1D integral ranges
peakrng - 1D peak ranges
baslpnts - baseline points for 'abs'
base_info - baseline function for 'bcm'
peaklist - peak file for 'dcon'
clevels - 2D contour levels
reg - reference regions for 'pp'
int2drng - 2D integral ranges
Edit
Read...
Write...
Write New...
Close

Figure 1.2

On the topright of this window the sources are listed in the pull-down menu and below the file types are shown also in a pull-down menu.

All shown items can be edited, read, written or written new depending on user wishes.

By clicking ***Options → Manage Source Directories*** the window for defining user-specific directories for Source Directories as described below will appear (see Figure 1.1).

Please note that in the following chapters where the respective commands for pulse programs, parameter sets, AU programs, lists and files are described, we will always refer to this chapter and the function ***Options → Manage Source Directories***.

Chapter 2

TOPSPIN parameters

2.1 About TOPSPIN parameters

TOPSPIN parameters are divided in acquisition and processing parameters. In this manual, we will mainly concern ourselves with processing parameters.

The following terms are used:

processing parameters

Parameters which must be set, for example by entering ***edp*** or clicking the ***Procpars*** tab, and are interpreted by processing commands.

acquisition status parameters

Parameters which are set by acquisition commands like ***zg***. They represent the acquisition status of a dataset and can be viewed, for example, by entering ***dpa*** or clicking the ***Acqupars*** tab. Some acquisition status parameters are used as input by processing commands.

processing status parameters

Parameters which are set by processing commands. They represent the processing status of a dataset and can be viewed, for example, by ***dpp*** or by clicking the ***Procpars*** tab. Most processing status parameters get the value of the corresponding processing parameter as it was set by the user (***edp***). Some parameters, however, are explicitly set or modified by the processing command.

input parameters

Parameters which are interpreted by processing commands. These can be:

- processing parameters (set by the user). Most input parameters are processing parameters.
- acquisition status parameters (set by an acquisition command). An example is parameter AQ_mod.
- processing status parameters (set by the previous processing command). An example is the parameter SI set by ***ft*** and then interpreted by ***abs***. This means you cannot change the size between ***ft*** and ***abs***.

output parameters

Parameters which are set or modified by processing commands. These can be:

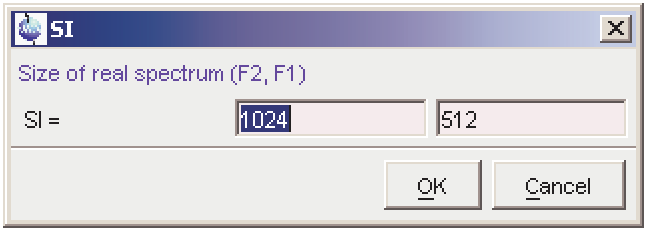
- processing status parameters. Examples are FT_mod and YMAX_p, set by ***ft***. Most output parameters are processing status parameters.
- processing parameters. Examples are PHC0 and PHC1, set by ***apk*** and SR and OFFSET, set by ***sref***.

Processing parameters can be set with the parameter editor ***edp*** and processing status parameters can be viewed with ***dpp***. Alternatively, each parameter can be set or viewed by entering its name in lowercase letters on the command line. For example, the parameter SI:

- ***si*** - set the parameter SI
- ***s si*** - view the status parameter SI

The dimensionality of the dataset is automatically recognized. For example, for a 2D dataset the following dialog box is offered:

Although status parameters are normally not changed by the user, a com-



SI

Size of real spectrum (F2, F1)

SI = 1024 512

mand like ***s si*** allows you to do that. This, however, could make the dataset inconsistent which can be checked with the command ***auditcheck***.

Before any processing has been done, the processing status parameters of a dataset do not contain significant values. After the first processing command, they represent the current processing status of the data. Any further processing command will update the processing status parameters.

After processing, the relevant processing status parameters are usually set to the same values as the corresponding processing parameters. In other words, the command has done what you told it to do. There are, however, some exceptions:

- when a processing command was interrupted, the processing status parameters might not have been updated yet.
- some processing parameters are modified by the processing command, e.g. STSI is rounded to the next higher multiple of 16 by ***xfb***. The rounded value is stored as the processing status parameter.
- the values of some parameters are a result of processing. They cannot be set by the user (they do not appear as processing parameters) but they are stored as processing status parameters. Examples are NC_proc, S_DEV and TILT.

2.2 Parameter values

With respect to the type of values they take, parameters can be divided into three groups:

- parameters taking integer values, e.g. SI, TDeff, ABSG, NSP
- parameters taking float or double values, e.g. LB, PHC0, ABSF1

- parameters using a predefined list of values, e.g. BC_mod, WDW, PSCAL

You can easily see to which group a parameter belongs from the parameter editor opened by entering ***edp*** or clicking ***Procpars***. Note that the values of parameters which use a predefined list are actually stored as integers. The first value of the list is always stored as 0, the second value as 1 etc. Table 2.1 shows the values of the parameter PH_mod as an example:

Parameter value	Integer stored in the proc(s) file
no	0
pk	1
mc	2
ps	3

Table 2.1

2.3 Parameter files

TOPSPIN parameters are stored in various files in the dataset directory tree.

In a 1D dataset:

<dir>/data/<user>/nmr/<name>/<expno>/

`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`proc` - processing parameters
`procs` - processing status parameters

In a 2D dataset:

<dir>/data/<user>/nmr/<name>/<expno>/

`acqu` - F2 acquisition parameters
`acqu2` - F1 acquisition parameters
`acqus` - F2 acquisition status parameters
`acqu2s` - F1 acquisition status parameters

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

`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters

In a 3D dataset:

<dir>/data/<user>/nmr/<name>/<expno>/

`acqu` - F3 acquisition parameters
`acqu2` - F2 acquisition parameters
`acqu3` - F1 acquisition parameters
`acqus` - F3 acquisition status parameters
`acqu2s` - F2 acquisition status parameters
`acqu3s` - F1 acquisition status parameters

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

`proc` - F3 processing parameters
`proc2` - F2 processing parameters
`proc3` - F1 processing parameters
`procs` - F3 processing status parameters
`proc2s` - F2 processing status parameters
`proc3s` - F1 processing status parameters

2.4 List of processing parameters

This paragraph contains a list of all processing parameters with a description of their function and the commands they are interpreted by. Please note that composite processing commands like ***efp*** (which combines ***em***, ***ft*** and ***pk***) are not mentioned here. Nevertheless, they interpret all parameters which are interpreted by the single commands they combine. Processing parameters can be set from the parameter editor, which can be opened by entering ***edp*** or clicking ***Procpars***. Alternatively, you can set parameters by entering their names in lowercase letters on the command line.

ABSF1 - low field limit of the region which is baseline corrected

- used in 1D, 2D and 3D datasets in all directions

- takes a float value (ppm) and must be greater than ABSF2
- interpreted by ***absf***, ***apkf***, ***abs1***, ***abs2***, ***abst****, ***absot****, ***zert****, ***tabs****
- The 1D commands ***abs*** and ***absd*** do not interpret ABSF1 because they work on the entire spectrum. The command ***apkf***, for automatic phase correction, uses ABSF1 as the left limit of the region on which it calculates the phase values.

ABSF2 - high field limit of the region which is baseline corrected

- used in 1D, 2D and 3D datasets in all directions
- takes a float value (ppm), must be smaller than ABSF1
- interpreted by ***absf***, ***apkf***, ***abs2***, ***abs1***, ***abst****, ***absot****, ***zert****, ***tabs****
- The 1D commands ***abs*** and ***absd*** do not interpret ABSF2 because they work on the entire spectrum. The command ***apkf***, for automatic phase correction, uses ABSF2 as the right limit of the region on which it calculates the phase values.

ABSG - degree of the polynomial which is subtracted in baseline correction

- used in 1D, 2D and 3D datasets in all directions
- takes an integer value between 0 and 5 (default is 5)
- interpreted by ***abs***, ***absd***, ***absf***, ***abs2***, ***abs1***, ***abst****, ***absot****, ***tabs****
- A polynomial of degree ABSG is calculated by the baseline correction commands and then subtracted from the spectrum.

ABSL - integral sensitivity factor with reference to the noise

- used in 1D datasets
- takes a float value between 0 and 100 (default is 3)
- interpreted by ***abs***, ***absd***, ***absf***
- Data points greater than ABSL*(standard deviation) are considered spectral information, all other points are considered noise.

ALPHA - correction factor

- used in 2D datasets in F2 and F1

- takes a float value
- interpreted by ***ptilt***, ***ptilt1*** and ***add2d***
- For ***ptilt***, F2 ALPHA is the tilt factor. For ***ptilt1***, F1 ALPHA is the tilt factor. They must have a value between -2.0 and 2.0. For ***add2d***, F2 ALPHA is the multiplication factor for the current dataset (see also parameter GAMMA).

AQORDER - Acquisition order

- used in datasets with dimensionality ≥ 3
- takes one of the values *321*, *312* for 3D data
- takes one of the values *4321*, *4312*, *4231*, etc. for 4D data
- takes ..... etc.
- only interpreted if AQSEQ is not set, by the processing commands ***ftnd*** and ***tf3***
- AQORDER describes the order in which the indirect directions have been acquired. For example, a 3D pulse program usually contains a double nested loop with loop counters `td1` and `td2`. If `td1` is used in the inner loop and `td2` in the outer loop, the acquisition order is 312. Otherwise it is 321.

  Caution: the acquisition order is normally evaluated from the acquisition status parameter AQSEQ. Only if this parameter is not set, AQORDER is used.

ASSFAC - assign the highest or second highest peak as reference for scaling

- used in 1D datasets
- takes a float value (default is 0.0)
- interpreted by ***pp****, ***lipp****
- This parameter is interpreted as follows:

  If ASSFAC > 1, the second highest peak is used as reference for scaling, if the following is true: *h2 < hmax/ASSFAC*, where *h2* is the intensity of the second highest peak and *hmax* the intensity of the highest peak. If this condition is false, the highest peak is used as reference.

  Other values of ASSFAC have no effect on the plot scaling.

ASSWID - region excluded from second highest peak search

- used in 1D datasets
- takes a float value (Hz, default is 0)
- interpreted by ***pp****, ***lipp****
- ASSWID is interpreted as follows:

  If abs(ASSFAC) > 1, a region of width ASSWID around the highest peak is excluded from the search for the second highest peak

AUNMP - processing AU program name

- used in 1D, 2D and 3D datasets in the first direction
- takes a character string value
- interpreted by ***xaup***
- In all Bruker standard parameter sets, the parameter AUNMP is set to a suitable processing AU program.

AZFE - integral extension factor

- used in 1D datasets
- takes a float value (ppm, default 0.1)
- interpreted by ***abs***
- Integral regions are extended at both sides by AZFE ppm. If this extension causes adjacent regions to overlap, the centre of the overlap is used as the limit of the two regions.

AZFW - minimum distance between peaks for independent integration

- used in 1D datasets
- takes a float value (ppm)
- interpreted by ***abs***, ***ldcon***, ***gdcon***, ***mdcon***
- If peaks are more than AZFW apart, they are treated independently. If peaks are less than AZFW ppm apart, they are considered to be overlapping.

BCFW - filter width for FID baseline correction.

- used in 1D datasets
- takes a float value (ppm)

- interpreted by ***bc*** when BC_mod = sfil or qfil
- sfil/qfil is used to suppress signals in the center of the spectrum. BCFW determines the width of the region, around the center of the spectrum, which is affected by ***bc***.

BC_mod - FID baseline correction mode

- used for 1D, 2D, and 3D dataset in all directions
(only useful in the acquisition direction)
- takes one of the values *no*, *single*, *quad*, *spol*, *qpol*, *sfil*, *qfil*
- interpreted by ***bc***, ***em***, ***gm***, ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- The values of BC_mod and the corresponding functions are shown in table 2.2. Most commands evaluate BC_mod for the function to be subtracted but not for the detection mode. The latter is then evaluated from the acquisition status parameter AQ_mod. This means, for example, it does not matter if you set BC_mod to *single* or *quad*. Only ***trf*** and ***xtrf**** evaluate the detection mode from BC_mod and distinguish between BC_mod = single and BC_mod = quad. The same counts for the values *spol/qpol* and *sfil/qfil*.

BC_mod	Function subtracted from the FID	Detection mode
no	no function	
single	average intensity of the last quarter of the FID	single channel
quad	average intensity of the last quarter of the FID	quadrature
spol	polynomial of degree 5 (least square fit)	single channel
qpol	polynomial of degree 5 (least square fit)	quadrature
sfil	Gaussian function of width BCFW [a]	single channel
qfil	Gaussian function of width BCFW [a]	quadrature

Table 2.2

[a] Marion, Ikura, Bax, J. Magn. Res. 84, 425-420 (1989)

COROFFS - correction offset for FID baseline correction

- used in 1D, 2D and 3D datasets in all directions
- takes a double value (Hz, default is 0.0)
- interpreted by ***bc***, ***em***, ***gm***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf3***, ***tf2***, ***tf1***
- COROFFS is only interpreted for BC_mod = qpol or qfil. The center of the
- baseline correction is shifted by COROFFS Hz.

CURPLOT - Default plotter for Plot Editor

- used in 1D and 2D datasets
- interpreted by ***plot*** and ***autoplot***
- The plotter set by CURPLOT overrides the plotter specified in the Plot Editor Layout. It allows you to use the same plotter for all layouts.

DATMOD - data mode: work on ’raw’ or ’proc’essed data

- used in 1D datasets
- takes the value *raw* or *proc*
- interpreted by ***add***, ***addc***, ***and***, ***div***, ***filt***, ***mul***, ***mulc***, ***ls***, ***or***, ***rs***, ***rv***, ***xor***, ***zf***, ***zp***

DC - multiplication factor or addition constant

- used in 1D datasets
- takes a float value
- interpreted by ***add***, ***addc***, ***addfid*** and ***mulc***
- For ***addc***, DC is an addition constant. For ***add***, ***addfid*** and ***mulc***, DC is a multiplication factor.

DFILT - Digital filter filename

- used in 1D datasets
- takes a character string value
- interpreted by ***filt***
- The file specified by DFILT must reside in the directory: `<tshome>/exp/stan/nmr/filt/1d`

and must be set up from a command shell. One standard file called `threepoint` is delivered with TOPSPIN.

FCOR - first (FID) data point multiplication factor

- used in 1D, 2D and 3D datasets in all directions
- takes a float value between 0.0 and 2.0
- interpreted by ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf***, ***xtrfp***, ***tf3***, ***tf2***, ***tf1***
- For 1D digitally filtered Avance data (DIGMOD = digital), FCOR does not play a role because the first raw data point is always zero. FCOR, however, allows you to control the DC offset of the spectrum in the following cases:

  - on A*X data
  - on Avance data measured in analog mode (DIGMOD = analog)
  - on 2D/3D Avance data in the second/second+third direction

FT_mod - Fourier transform mode

- used in 1D, 2D and 3D in all directions
- takes one of the values *no*, *fsr*, *fqr*, *fsc*, *fqc*, *isr*, *iqr*, iqc, *isc*
- interpreted by ***trf***, ***xtrf****, ***xtrfp****
- the Fourier transform commands ***ft*** (1D), ***xfb***, ***xf2***, ***xf1*** (2D) and ***tf**** (3D) do not interpret FT_mod because they evaluate the Fourier transform mode from the acquisition status parameter AQ_mod. They do, however, set the processing status parameter FT_mod.

- The values of FT_mod have the following meaning:

FT_mod	Fourier transform mode
no	no Fourier transform
fsr	forward, single channel, real
fqr	forward, quadrature, real
fsc	forward, single channel, complex
fqc	forward, quadrature, complex
isr	inverse, single channel, real
iqr	inverse, quadrature, real
isc	inverse, single channel, complex
iqc	inverse, quadrature, complex

Table 2.3

GAMMA - multiplication factor

- used in 2D datasets in F2
- takes a float value
- interpreted by ***add2d***
- GAMMA is the multiplication factor for the second dataset (see also parameter ALPHA).

GB - Gaussian broadening factor for Gaussian window multiplication

- used in 1D, 2D and 3D datasets in all directions
- takes a float value between 0.0 and 1.0
- interpreted by ***gm***
- interpreted by ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf**** if WDW = EM or GM

INTBC - automatic baseline correction of integrals created by ***abs***

- used in 1D datasets
- takes the value *yes* or *no*
- interpreted by ***li***, ***lipp***, ***lippf***

- INTBC has no effect on integrals which were created interactively in the ***Integration*** mode.

INTSCL - scale 1D integrals relative to a reference dataset

- used in 1D datasets
- takes an integer value
- interpreted by ***li***, ***lipp***, ***lippf***
- INTSCL is used as follows:

  For INTSCL > 0, the integral values are scaled individually for each spectrum.

  For INTSCL = 0, the integrals on the plot will obtain the same numeric values as defined interactively in the integration mode.

  For INTSCL = -1, scaling is performed relatively to the last spectrum plotted.

ISEN - integral sensitivity factor with reference to the largest integral

- used in 1D datasets
- takes a positive float value (default 128)
- interpreted by ***abs***, ***absd***, ***absf***
- Only the regions of integrals which are larger (area) than the largest integral divided by ISEN are stored.

LB - Lorentzian broadening factor for exponential window multiplication

- used in 1D, 2D and 3D datasets in all directions
- takes a float value
- interpreted by ***em***, ***gm***
- interpreted by ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf**** if WDW = EM or GM
- LB must be positive for an exponential and negative for Gaussian window multiplication.

LPBIN - number of points for linear prediction

- used in 1D, 2D and 3D datasets in all directions
- takes a positive integer value
- interpreted by ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****

- also interpreted by ***em***, ***gm***, ****sin****, ***tm***, ***traf****

For backward prediction, LPBIN represents the number of input points with a maximum of TD - abs(TDoff). The default value of LPBIN is zero, which means all data points are used as input. The status parameter LPBIN (***dpp***) shows how many input points were actually used. For forward prediction, LPBIN can be used to reduce the number of prediction output points as specified in table 2.4. Note LPBIN only has an effect in the last two cases. If LPBIN is smaller than TD or greater than 2*SI this has the same effect as LPBIN = 0.

parameter values	normal points	predicted points	zeroes
LPBIN = 0, 2*SI < TD	2*SI	-	-
LPBIN = 0, TD < 2*SI < 2*TD	TD	2*SI - TD	-
LPBIN = 0, 2*TD < 2*SI	TD	TD	2*SI - 2*TD
TD < LPBIN < 2*SI< 2*TD	TD	LPBIN - TD	2*SI - LPBIN
TD < LPBIN < 2*TD < 2*SI	TD	LPBIN - TD	2*SI - LPBIN

Table 2.4 Linear forward prediction

MAXI - maximum relative intensity for peak picking

- used in 1D datasets
- takes a float value (cm)
- interpreted by ***pp****, ***li***, ***lipp****
- only peaks with an intensity smaller than MAXI will appear in the peak list. MAXI can also be set from the ***pp*** dialog box and, interactively, in peak picking mode.

MC2 - Fourier transform mode of the second (and third) direction

the processing parameter MC2 is only interpreted if the acquisition status parameter FnMODE (***dpa***) does not exist or has the value *undefined*. FnMODE must be set (with ***eda***) according to the experiment type before the acquisition is started. As MC2, FnMODE only exists in the second (and third) direction. On datasets acquired with XWIN-NMR 2.6 or earlier, MC2 is interpreted and must be set before the data are processed. The parameter MC2:

- is used in 2D datasets in the second direction (F1)
- is used in 3D datasets in the second and third direction (F2 and F1)
- takes one of the values *QF*, *QSEQ*, *TPPI*, *States*, *States-TPPI*, *echo-antiecho*
- is interpreted by ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****

ME_mod - FID linear prediction mode

- used in 1D, 2D and 3D datasets in all directions
- takes one of the values *no*, *LPfr*, *LPfc*, *LPbr*, *LPbc*, *LPmifr*, *LPmifc*
- interpreted by ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- also interpreted by ***em***, ***gm***, ****sin****, ***tm***, ***traf****
- The values of ME_mod have the following meaning:

LPfr	forward LP on real data
LPfc	forward LP on complex data
LPbr	backward LP on real data
LPbc	backward LP on complex data
LPmifr	mirror image forward LP on real data
LPmifc	mirror image forward LP on complex data

Table 2.5

Linear prediction is only performed for NCOEF > 0. Furthermore, LPBIN and, for backward prediction, TDoff play a role. The commands ***ft***, ***xfb***, ***xf2*** and ***xf1*** evaluate ME_mod but do not distinguish between LPfr and LPfc nor do they distinguish between LPbr and LPbc. The reason is that the detection mode (real or complex) is evaluated from the acquisition status parameter AQ_mod. However, ***trf***, ***xtrf*** and ***xtrf2*** evaluate the detection mode from ME_mod. In 1D, a combination of forward and backward prediction can be done by running ***trf*** with ME_mod = LPfc and ***trfp*** (or ***ft***) with ME_mod = LPbc. In 2D, this would be the sequence ***xtrf*** - ***xtrfp*** (or ***xfb***). Note that not only Fourier transform but also window multiplication commands perform linear prediction when ME_mod is set. This allows you to easily see the effect of linear prediction on the FID, for example by executing ***em*** with LB = 0.

MI - minimum relative intensity for peak picking

- used in 1D datasets
- takes a float value (cm)
- interpreted by ***pp****, ***li***, ***lipp****
- only peaks with an intensity greater than MI will appear in the peak list. MI can also be set from the ***pp*** dialog box and, interactively, in peak picking mode.

NCOEF - number of linear prediction coefficients

- used in on 1D, 2D and 3D datasets in all directions
- takes a positive integer value (default is 0)
- interpreted by ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- also interpreted by ***em***, ***gm***, ****sin****, ***tm***, ***traf****
- NCOEF is typically set to 2-3 times the number of expected peaks. For NCOEF = 0, no prediction is done. Linear prediction also depends on the parameters ME_mod, LPBIN and TDoff.

NOISF1 - low field (left) limit of the noise region

- used in 1D datasets
- takes a float value (ppm)
- interpreted by ***sino***
- The noise in the region between NOISF1 and NOISF2 is calculated according to the algorithm described for the command ***sino***.

NOISF2 - high field (right) limit of the noise region

- used in 1D datasets
- takes a float value (ppm)
- interpreted by ***sino***
- The noise in the region between NOISF1 and NOISF2 is calculated according to the algorithm described for the command ***sino***.

NSP - number of data points shifted during right shift or left shift

- used in 1D datasets
- takes a positive integer value (default is 1)
- interpreted by ***ls*** and ***rs***
- NSP points are discarded from one end and NSP zeroes are added to the other end of the spectrum.

NZP - number of data points set to zero intensity

- used in 1D datasets
- takes a positive integer value (default is 0)
- interpreted by ***zp***
- ***zp*** sets the intensity of the first NZP points of the dataset to zero.

OFFSET - the ppm value of the first data point of the spectrum

- used in 1D, 2D and 3D datasets in all directions
- takes a float value (ppm)
- set by ***sref*** or interactive calibration
- also set by ***accumulate***
- The value is calculated according to the relation:

  OFFSET = (SFO1/SF-1) * 1.0e6 + 0.5 * SW * SFO1/SF

  where SW and SFO1 are acquisition status parameters. In fact, the relation for OFFSET depends on the acquisition mode. When the acquisition status parameter AQ_mod is *qsim*, *qseq* or *DQD*, which is usually the case, the above relation count. When AQ_mod is *qf*, the equation:

  OFFSET = (SFO1/SF-1) * 1.0e6

  is used.

PC - peak picking sensitivity

- used in 1D datasets
- takes a float value
- interpreted by ***pp****, ***li***, ***lipp****
- a spectral point is only a considered peak if it is a maximum which is greater than the previous minimum plus 4*PC*noise. In addition to

MI, PC provides an extra way of controlling the peak picking sensitivity. It allows you, for instance, to detect a shoulder on a large peak.

PHC0 - zero order phase correction value (frequency independent)

- used in 1D, 2D and 3D datasets in all directions
- takes a float value (degrees)
- set by ***apk***, ***apks***, ***apkf***, ***apk0*** on 1D datasets
- set interactively in Phase correction mode on 1D and 2D datasets
- interpreted by ***pk***, ***xfbp***, ***xf2p***, ***xf1p***, ***tf*p***
- interpreted by ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf3***, ***tf2***, ***tf1*** when PH_mod = pk
- PHC0 is one of the few examples where a processing parameter is set by a processing command. For example, ***apk*** sets both the processing and processing status parameter PHC0. ***pk*** reads the processing parameter and updates the processing status parameter. For multiple phase corrections, the total zero order phase value is stored as the processing status parameter PHC0.

PHC1 - first order phase correction value (frequency dependent)

- used in 1D, 2D and 3D datasets in all directions
- takes a float value (degrees)
- set by ***apk***, ***apks***, ***apkf***, ***apk1*** on 1D datasets
- set interactively in Phase correction mode on 1D and 2D datasets
- interpreted by ***pk***, ***xfbp***, ***xf2p***, ***xf1p***, ***tf*p***
- interpreted by ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf3***, ***tf2***, ***tf1*** when PH_mod = pk
- PHC1 is one of the few examples where a processing parameter is set by a processing command. For example, ***apk*** sets both the processing and processing status parameter PHC1. ***pk*** reads the processing parameter and updates the processing status parameter. For multiple phase corrections the total first order phase value is stored as the processing status parameter PHC1.

PH_mod - phase correction mode

- used in 1D, 2D and 3D datasets in all directions

- takes one of the value *no*, *pk*, *mc*, *ps*
- interpreted by ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- The values of PH_mod are described in table 2.6.

PH_mod	mode
no	no phase correction
pk	phase correction according to PHC0 and PHC1
mc	magnitude calculation
ps	power spectrum

Table 2.6

- The value PH_mod = pk is only useful if the phase values are known and the parameters PHC0 and PHC1 have been set accordingly. In 1D, they can be determined with ***apk*** or ***apks***, or, interactively, from the Phase correction mode. In 2D and 3D, they can only be determined interactively.

PKNL - group delay compensation (Avance) or filter correction (A*X)

- used in 1D, 2D and 3D datasets in the first direction
- takes the value *true* or *false*
- interpreted by ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- On A*X spectrometers, PKNL = true causes a non linear 5th order phase correction of the raw data. This corrects possible errors caused by non linear behaviour of the analog filters. On Avance spectrometers, PKNL must always be set to TRUE. For digitally filtered data, it causes ***ft*** to handle the group delay of the FID. For analog data it has no effect.

PSCAL - determines the region with reference peak for vertical scaling

- used in 1D datasets
- takes one of the values *global*, *preg*, *ireg*, *pireg*, *sreg*, *psreg*, *noise*
- interpreted by ***pp****, ***li***, ***lipp****

- the values of PSCAL have the following meaning:.

PSCAL	Peak used as reference for vertical scaling
global	The highest peak of the entire spectrum.
preg	The highest peak within the plot region.
ireg	The highest peak within the regions specified in the `reg` file. If the `reg` file does not exist, *global* is used.
pireg	as *ireg*, but the peak must also lie within the plot region.
sreg	The highest peak in the regions specified in scaling region file. This file is specified by the parameter SREGLST. If SREGLST is not set or specifies a file which does not exist, *global* is used.
psreg	as *sreg* but the peak must also lie within the plot region.
noise	The intensity of the noise.

Table 2.7

- For PSCAL = ireg or pireg, the `reg` file is interpreted. The `reg` file can be created in interactive ***integration*** mode and can be viewed or edited with the command ***`edmisc reg`***.
- For PSCAL = sreg or psreg, the scaling region file is interpreted. This feature is used to exclude the region in which the solvent peak is expected. The name of a scaling region file is typically of the form NUCLEUS.SOLVENT, e.g. 1H.CDCl3. For all common nucleus/solvent combinations, a scaling region file is delivered with TOPSPIN. These can be viewed or edited with the command ***`edlist scl`***. In several 1D standard parameter sets which are used during automation, PSCAL is set to *sreg* and SREGLIST to NUCLEUS.SOLVENT as defined by the parameters NUCLEUS and SOLVENT.

PSIGN - peak sign for peak picking

- used in 1D datasets
- takes the value *pos*, *neg* or *both* (default is *pos*)
- interpreted by ***`pp*`***, ***`lipp*`***
- in most 1D standard parameter sets PSIGN is set to *pos* which means only positive peaks are picked

REVERSE - flag indicating to reverse the spectrum during Fourier transform

- used in 1D, 2D and 3D datasets in all directions
- takes the value *true* or *false* (default is *false*)
- interpreted by ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- Reversing the spectrum can also be done after Fourier transform with the commands ***rv*** (1D) or ***rev2***, ***rev1*** (2D).

SF - spectral reference frequency

- used in 1D, 2D and 3D datasets in the first direction
- takes a positive float value
- set by ***sref*** or interactive calibration
- ***sref*** calculates SF according to the relation:

  SF=BF1/(1.0+RShift * 1e-6)

  where *RShift* is taken from the ***edlock*** table and BF1 is an acquisition status parameter. SF is interpreted by display and plot routines for generating the axis (scale) calibration.

SI - size of the processed data

- used in 1D, 2D and 3D datasets in all directions
- takes an integer value
- interpreted by processing commands which work on the raw data (commands working on processed interpret the processing status parameter SI)
- The total size of the processed data (real+imaginary) is 2*SI. In Bruker standard parameter sets (see ***rpar***), SI is set to TD/2, where TD is an acquisition status parameter specifying the number of raw data points.

SIGF1 - low field (left) limit of the signal region

- used in 1D and 2D datasets
- takes a float value (ppm), must be greater than SIGF2
- interpreted by ***sino***

- If SIGF1 = SIGF2, the signal region is defined by the entire spectrum minus the first 16th part or, if the scaling region file exists, by the regions in this file. The name of the scaling region file is NUC1.SOLVENT where NUC1 and SOLVENT are acquisition status parameters.
- SIGF1 is also used in 2D datasets as the low field limit for 2D baseline correction by ***abst2***, ***abst1***, ***absot2***, ***absot1***, ***zert1***, and ***zert2***.

SIGF2 - high field (right) limit of the signal region

- used in 1D and 2D datasets
- takes a float value (ppm), must be smaller than SIGF1
- interpreted by ***sino***
- If SIGF1 = SIGF2, the signal region is defined by the entire spectrum minus the first 16th part or, if the scaling region file exists, by the regions in this file. The scaling region file is defined as NUC1.SOLVENT where NUC1 and SOLVENT are acquisition status parameters.
- SIGF2 is also used in 2D datasets as the high field limit for 2D baseline correction by ***abst2***, ***abst1***, ***absot2***, ***absot1***, ***zert1***, and ***zert2***.

SINO - signal to noise ratio

- used in 1D datasets
- takes a float value
- used in AU as an acquisition criterion (not used by processing commands)
- the processing parameter SINO (set with ***edp***) can be used in an AU program to specify a signal/noise ratio which must be reached in an acquisition. The acquisition runs until the value of SINO is reached and then it stops. An example of such an AU program is ***au_zgsino***. SINO can be set with ***edp*** but not from the command line. The reason is that entering ***sino*** on the command line would execute the command ***sino***. Note that the processing parameter SINO (***edp***) has a different purpose than the processing status parameter SINO

(***dpp***). The latter represents the signal to noise ratio calculated by the processing command ***sino***.

SREGLST - name of the scaling region file

- used in 1D datasets
- takes a character string value
- interpreted by ***li***, ***lipp**** if PSCAL = sreg or psreg
- interpreted by ***sino***
- scaling region files contain the regions in which the reference peak is searched. They are used to exclude the region in which the solvent peak is expected. Because this region is nucleus and solvent specific the name of a scaling region file is of the form NUCLEUS.SOLVENT, e.g. 1H.CDCl3. For all common nucleus/solvent combinations, a scaling region file is delivered with TOPSPIN. They can be viewed or edited with ***edlist scl***.

SSB - sine bell shift

- used in 1D, 2D and 3D datasets in all directions
- takes a positive float value
- interpreted by ***sinm***, ***qsin***, ***sinc***, ***qsinc***
- interpreted by ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf**** if WDW = sine, qsine, sinc or qsinc

SR - spectral reference

- used in 1D, 2D and 3D datasets in all directions
- takes a float value (Hz)
- set by ***sref*** or interactive calibration
- The spectral reference is calculated according to the relation:

  SR = SF - BF1

STSI - strip size: number of output points of strip transform

- used in 1D, 2D and 3D datasets in all directions
- takes an integer value between 0 and SI (default 0)
- interpreted ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf***, ***xtrf2***, ***tf3***, ***tf2***, ***tf1***

- During strip transform, only the region determined by STSI and STSR is stored. For STSI = 0, a normal (full) transform is done. STSI is always rounded; in 1D to the next lower multiple of 4, in 2D and 3D to the next higher multiple of 16. Furthermore, when the 2D (3D) data are stored in submatrix (subcube) format, STSI is rounded to the next multiple of the submatrix (subcube) size.

STSR - strip start: first output point of a strip transform

- used in 1D, 2D and 3D datasets in all directions
- takes an integer value between 0 and SI (default 0)
- interpreted ***ft***, ***xfb***, ***xf2***, ***xf1***, ***xtrf***, ***xtrf2***, ***tf3***, ***tf2***, ***tf1***
- During strip transform, only the region determined by STSI and STSR is stored.

TDeff - number of raw data points to be used for processing

- used in 1D, 2D and 3D datasets in all directions
- takes an integer value between 0 and TD (default is 0 which means all)
- interpreted by processing commands which work on the raw data
- The first TDeff raw data points are used for processing. For TDeff = 0, all points are used, with a maximum of 2*SI.

TDoff - number of raw data points ignored or predicted

- used in 1D, 2D and 3D datasets in all directions
- integer value between 0 and TD (default is 0)
- interpreted by 2D and 3D processing commands which work on raw data
  The first raw data point that contributes to processing is shifted by TDoff points. For 0 < TDoff < TD the first TDoff raw data points are cut off at the beginning and TDoff zeroes are appended at the end (corresponds to left shift). For TDoff < 0 -TDoff zeroes are prepended at the beginning and:
  - for SI < (TD-TDoff)/2 raw data are cut off at the end
  - for DIGMOD=digital, the zeroes would be prepended to the group delay which does not make sense. You can avoid that by

converting the raw data with ***convdta*** before you process them.

- also interpreted by 1D, 2D and 3D processing commands which do linear backward prediction, i.e. ***ft***, ***xfb*** of ***tf3*** when ME_mod is *lpbr* or *lpbc*.
  For TDoff > 0, the first TDoff points are replaced by predicted points. For TDoff < 0, abs(TDoff) predicted points are added to the beginning and cut off at the end of the raw data. If zero filling occurs (2*SI > TD), then only zeroes are cut off at the end as long as abs(TDoff) < 2*SI - TD. Note that digitally filtered Avance data start with a group delay. This means that a backward prediction does not make sense unless the data are first converted AMX format with ***convdta***.

TM1 - the end of the rising edge of a trapezoidal window

- used in 1D, 2D and 3D datasets in all directions
- takes a float value between 0.0 and 1.0
- interpreted by ***tm***
- TM1 represents a fraction of the acquisition time and must be smaller than TM2

TM2 - the start of the falling edge of a trapezoidal window

- used in 1D, 2D and 3D datasets in all directions
- takes a float value between 0.0 and 1.0
- interpreted by ***tm***
- TM2 represents a fraction of the acquisition time and must be greater than TM1.

WDW - FID window multiplication mode

- used in 1D, 2D and 3D datasets in all directions
- takes one of the values *no*, *em*, *gm*, *sine*, *qsine*, *trap*, *user*, *sinc*, *qsinc*, *traf*, *trafs*
- interpreted by ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- On 1D data, window multiplication is usually done with commands like ***em***, ***gm***, ***sinm*** etc. which do not interpret WDW. These command

are already specific for one type of window multiplication. The values of WDW have the following meaning:

WDW value	Function	Dependent parameters	Specific 1D command
em	Exponential	LB	***em***
gm	Gaussian	GB, LB	***gm***
sine	Sine	SSB	***sinm***
qsine	Sine squared	SSB	***qsin***
trap	Trapezoidal	TM2, TM1	***tm***
sinc	Sine	SSB, GB	***sinc***
qsinc	Sine squared	SSB, GB	***qsinc***
traf	Traficante (JMR, **71**, 1987, 237)		***traf***
trafs	Traficante (JMR, **71**, 1987, 237)		***trafs***

Table 2.8

2.5 Processing status parameters

After processing, most processing status parameters have been set to the same value as the corresponding processing parameter. For some processing status parameters, however, this is different. The reason can be that:

- the corresponding processing parameter does not exist, e.g. NC_proc
- the corresponding processing parameter is not interpreted, e.g. FT_mod
- the value of the corresponding processing parameter is adjusted, e.g. STSI

These type of processing status parameters are listed below and described as output parameters for each processing command. They can be viewed with ***dpp*** (see also chapter 2.1).

BYTORDP - byte order of the processed data

- used in 1D, 2D and 3D datasets in the first direction
- takes the value *little* or *big*
- set by the first processing command
- interpreted by various processing commands
- Big endian and little endian are terms that describe the order in which a sequence of bytes are stored in a 4-byte integer. Big endian means the most significant byte is stored first, i.e. at the lowest storage address. Little-endian means the least significant byte is stored first. TOPSPIN only runs on computers with byte order little endian. However, TOPSPIN's predecessor XWIN-NMR also runs on SGI workstations which are big endian. The byte order of the raw data is determined by the computer which controls the spectrometer and is stored in the acquisition status parameter BYTORDA (type ***s bytorda***). This allows raw data to be processed on computers of the same or different storage types. The first processing command interprets BYTORDA, stores the processed data in the byte order of the computer on which it runs and sets the processing status parameter BYTORDP accordingly (type ***s bytordp***). All further processing commands interpret this status parameter and store the data accordingly. As such, the byte order of the computer is handled automatically and is user transparent. 2D and 3D processing commands, however, allow you to store the processed data with a byte order different from the computer on which they run. For example, the commands ***xfb big*** and ***tf3 big*** on a Windows or Linux PC store the data in big endian although the computer is little endian. The processing status parameter BYTORDP is set accordingly.

FT_mod - Fourier transform mode

- used in 1D, 2D and 3D datasets in all directions
- takes one of the values *no*, *fsr, fqr*, *fsc*, *fqc*, *isr*, *iqr*, *iqc*, *isc*
- set by all Fourier transform commands, e.g. ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***trf****, ***xtrf****, ***tf3***, ***tf2***, ***tf1***
- interpreted by ***trf*** and ***xtrf****.

- also exists as processing (***edp***) parameter (interpreted by ***trf*** and ***xtrf****)
- The values of FT_mod are described in chapter 2.4.

MC2 - Fourier transform mode of the second (and third) direction

- is used in 2D datasets in the second direction (F1)
- is used in 3D datasets in the second and third direction (F2 and F1)
- takes one of the values *QF*, *QSEQ*, *TPPI*, *States*, *States-TPPI*, *echo-antiecho*
- is set by ***xfb***, ***xf2***, ***xf1***, ***xtrf****, ***tf****
- is interpreted by ***xf1***, ***xtrf1***, ***tf2***, ***tf1***
- The processing status parameter MC2 is set according to the acquisition status parameter FnMODE. If, however, FnMODE = undefined, the processing status parameter MC2 is set according to the processing parameter MC2. Furthermore, status MC2 is interpreted during 2D processing in F1, on processed data, for example by ***xf1*** on data which have already been processed with ***xf2***.

NC_proc - intensity scaling factor

- used in 1D, 2D and 3D datasets in the first direction
- takes an integer value
- set by all processing commands
- only exists as processing status parameter
- Processing in TOPSPIN performs calculations in double precision floating point but stores the result in 32-bit integer values. During double to integer conversion, the data are scaled up or down such that the highest intensity of the spectrum lies between 2^{28} and 2^{29}. This means the 32 bit resolution is not entirely used. This allows for the highest intensity to be increased, for example during phase correction, without causing data overflow. NC_proc shows the amount of scaling that was done, for example:

  NC_proc = -3 : data were scaled up (multiplied by 2) three times
  NC_proc = 4 : the data were scaled down (divided by 2) four times

- Although NC_proc is normally calculated by processing commands, 2D processing also allows you to predefine the scaling factor with the argument ***nc_proc***, for example:

  xfb nc_proc 2

  scales down the data twice. However, you can only scale the data more down (or less up) than the command would have done without the argument ***nc_proc***. The latter is shown by the processing status parameter NC_proc (type ***dpp***). Smaller (more negative) values of ***nc_proc*** are ignored to avoid data overflow. The command:

  xfb nc_proc last

  takes the current value of the processing status parameter NC_proc (type ***dpp***) as input value.

PPARMOD - dimensionality of the processed data

- takes one of the values 1D, 2D,..., 8D
- interpreted by TOPSPIN display, parameter editor ***edp*** and processing commands that access processed data like ***abs*** and ***apk***.
- can be set by changing the dimension from the parameter editor (***edp***) toolbar.
- The status parameter PPARMOD defines the dimensionality of the processed data. Note the following restriction: PPARMOD <= PARMODE.

PHC0 - zero order phase correction value (frequency independent)

- used in 1D, 2D and 3D datasets in all directions
- takes a float value (degrees)
- set by ***apk***, ***apks***, ***apkf***, ***apk0***, ***apk0f*** in 1D datasets
- set interactively in Phase correction mode in 1D and 2D datasets
- also exists as processing parameter (***edp***)
- PHC0 is one of the few examples where a processing parameter is set by a processing command. For example, ***apk*** sets both the processing and processing status parameter PHC0. ***pk*** reads the processing parameter and updates the processing status parameter. After multiple phase corrections, the processing status parameter PHC0 shows the total zero order phase correction.

PHC1 - first order phase correction value (frequency dependent)

- used in 1D, 2D and 3D datasets in all directions
- takes a float value (degrees)
- set by ***apk***, ***apks***, ***apkf***, ***apk1*** in 1D datasets
- set interactively in Phase correction mode in 1D and 2D datasets
- also exists as processing parameter (***edp***)
- PHC1 is one of the few examples where a processing parameter is set by a processing command. For example, ***apk*** sets both the processing and processing status parameter PHC1. ***pk*** reads the processing parameter and updates the processing status parameter. For multiple phase corrections, the processing status parameter PHC1 shows the total first order phase correction.

SINO - signal to noise ratio

- used in 1D datasets
- takes a float value
- set by ***sino***
- also exists as processing parameter
- The signal is determined in the region between SIGF2 and SIGF1. The noise is determined in the region between NOISF2 and NOISF1. Note that SINO also exists as a processing parameter (***edp***) which has a different purpose (see chapter 2.4)

SW_p - spectral width of the processed data

- used in 1D, 2D and 3D datasets in all directions
- takes a double value
- set by all processing commands
- only exists as processing status parameter
- Normally, SW_p will be the same as the acquisition status parameter SW. However, in case of stripped data, the processing spectral width differs from the acquired spectral width.

SYMM - 2D symmetrization type done

- used in 2D datasets in the F2 direction

- takes the value *no*, *sym*, *syma* or *symj*
- set by ***sym***, ***syma*** and ***symj***
- only exists as processing status parameter (***dpp***)
- SYMM shows the (last) kind of symmetrization that was done.

STSI - strip size; the number of output points of a strip transform

- used in 1D, 2D and 3D datasets in all directions
- takes an integer value between 0 and SI (default 0)
- also exists as processing parameter (***edp***)
- rounded by ***ft***, ***trf***, ***xfb***, ***xf2***, ***xf1***, ***xtrf***, ***xtrf2***, ***tf3***, ***tf2***, ***tf1***
- During strip transform, only the region determined by STSI and STSR is stored. Processing commands round the value of the processing parameter STSI; in 1D to the next lower multiple of 4, in 2D and 3D to the next higher multiple of 16. Furthermore, when the 2D (3D) data are stored in submatrix (subcube) format, STSI is rounded to the next multiple of the submatrix (subcube) size. The rounded value is stored as the processing status parameter STSI. If no strip transform is done (STSI = 0), the status STSI is set to the value of SI.

TDeff - number of raw data points that were used for processing

- used in 1D, 2D and 3D datasets in all directions
- set by ***ft***, ***xfb***, ***xf2***, ***xf1***, ***trf****, ***xtrf****
- also exists as processing parameter (***edp***)
- Normally, all raw data points are used as input. However, the number of input points can be decreased with the processing parameter TDeff or increased by doing linear forward or backward prediction with TDoff < 0. The number of raw data points that were actually used is stored in the processing status parameter TDeff.

TILT - flag indicating whether a tilt command has been performed

- used in 2D datasets in the F2 direction
- takes the value TRUE or FALSE
- set by ***ptilt***, ***ptilt1*** or ***tilt***
- only exists as processing status parameter (***dpp***)

XDIM - submatrix or subcube size

- used in 2D and 3D datasets in all directions
- takes an integer value
- set by ***xfb***, ***xf2***, ***xf1***, ***xtrf***, ***xtrf2***, ***tf3***
- also exists as processing parameter
- Although XDIM is normally calculated by processing commands, 2D and 3D processing also allow you to predefine the submatrix sizes. On a 2D dataset, the command:

  xfb xdim

  interprets the processing parameter XDIM in both F2 and F1. Note that the submatrix sizes cannot be set with ***edp*** but only with ***2 xdim*** and ***1 xdim***. On a 3D dataset, the command:

  tf3 c

  prompts you for the XDIM values in F3, F2 and F1. It does not interpret the processing parameter XDIM.

FTSIZE - Fourier transform size

- used in 1D, 2D and 3D datasets in all directions
- takes an integer value
- set by all processing command that perform Fourier transform
- Normally, the status parameter FSIZE has the same value as the status parameter SI. Only in case of strip transform (STSR > 0 and/or STSI > 0), they are different. FTSIZE then represents the size with which the raw data were Fourier transformed whereas SI represents the size with which the processed data are stored.

YMAX_p - maximum intensity of the processed data

- used in 1D, 2D and 3D datasets in the first direction
- takes a float value
- set by all processing commands
- only exists as processing status parameter (***dpp***)

YMIN_p - minimum intensity of the processed data

- used in 1D, 2D and 3D datasets in the first direction

- takes a float value
- set by all processing commands
- only exists as processing status parameter (***dpp***)

2.6 Relaxation parameters

Relaxation parameters can be set with the command ***edt1*** which can be entered from the Relaxation menu.

COMPNO - number of components contributing to the relaxation curve

- used in pseudo 2D relaxation datasets
- takes an integer value (default is 1)
- interpreted by ***simfit***
- Peak positions are determined on a row which is specified by the parameter START (usually the first row). These positions are then used by ***pd*** for each row of the 2D data. However, peak positions sometimes drifts in the course of the experiment, i.e. they might shift one or more points in successive rows. Therefore, ***pd*** searches for the maximum intensity at the predefined peak position plus or minus DRIFT.

DRIFT - drift of the peak positions in the course of the experiment

- used in pseudo 2D relaxation datasets
- takes an integer value (must be 1 or greater, default is 5)
- interpreted by ***pd***
- Relaxation analysis is usually done with a series of relaxation curves, one for each peak in the spectrum. One curve shows the intensity distribution of one peak over a series of experiments, i.e. a series of rows in a pseudo 2D dataset. First the peak positions are determined on one row, for example with ***ppt1***. Then the command ***pd*** determines the intensity at these positions in each row. However, peak positions sometimes drifts in the course of the experiment, i.e. they can be slightly different in different rows. Therefore, ***pd*** searches for the maximum intensity in a range around a each peak position. This range is determined by the parameter DRIFT.

EDGUESS - table of initial values and step rates of the function variables

- used in pseudo 2D relaxation datasets
- interpreted by ***simfit***
- The EDGUESS table shows all variables of the function specified by FCTTYPE. For each variable, the initial guess (G) and step rate (S) can be set for each component (C). Table 2.9 shows the EDGUESS table for an inversion recovery experiment, with 2 components. The initial guess for I[0] must be such that the total value 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 or the initial guess. If the step rate of a variable is set to zero, then this variable is not changed during the iterations. Note that the commands ***ct1***, ***ct2***, ***dat1*** or ***dat2*** do not use the EDGUESS table. They calculate the initial values and step rates of the T1/T2 function variables I[0], P and T1.

GC1I0	0.5	SC1I0	0.05
GC1A	1.0	SC1A	0.1
GC1T1	2.0	SC1T1	0.2
GC2I0	0.5	SC2I0	0.05
GC2A	1.0	SC2A	0.1
GC2T1	2.0	SC2T1	0.2

Table 2.9

FCTTYPE - function type used for fitting the relaxation curve

- used in pseudo 2D relaxation datasets
- takes one of the values listed in Table 2.10
- interpreted by ***simfit***
- Table 2.10 shows the experiment types which ***simfit*** can handle and the corresponding fit functions. Note that ***ct1***, ***ct2***, ***dat1*** and ***dat2*** do not evaluate FCTTYPE because they can only handle T1/T2 experiments. They do, however, set FTCTYPE to the value *t1/t2.*

Exp. type	Comp	Fit function
uxnmrt1t2	1	I[t] = I[0]+P*exp(t/T1)
invrec	1 - 4	I[t] = I[0]*(1-2A*exp(-t/T1))
satrec	1 - 6	I[t] = I[0]*(1-exp(-t/T1))
cpt1rho	1 - 4	I[t] = I[0]/(1-TIS/T1rho)*(exp(-t/T1rho)-exp(t/TIS))
expdec	1 - 6	I[t] = I[0]*exp(-t/T)
gaussdec	1 - 6	I[t] = I[0]*exp(-SQR(t/T))
lorgauss	1 - 3	I[t] = IL*exp(-t/TL)+IG*exp(-SQR(t/TG))
linear	1 - 6	I[t] = A+B*t
varbigdel	1 - 6	I = I[0]*exp(-D*SQR(2*PI*gamma*G*LD)*(BD-LD/3)*1e4)
varlitdel	1 - 6	I = I[0]*exp(-D*SQR(2*PI*gamma*G*LD)*(BD-LD/3)*1e4)
vargrad	1 - 6	I = I[0]*exp(-D*SQR(2*PI*gamma*G*LD)*(BD-LD/3)*1e4)
raddamp	1 - 6	MZ[t]=A0+MZ[0]*tanh((t-T0)/TRD)

Table 2.10

- used in pseudo 2D relaxation datasets
- takes the value *area* or *intensity* (default is *intensity*)
- interpreted by ***pd***, ***ct1***, ***dat1*** and ***simfit***
- Before you run ***pd***, both the integral ranges and peak positions should be determined (see ***rspc*** and ***ppt1***). ***pd*** then picks the points storing both their integrals and intensities but it only displays one curve; the one defined by FITTYP. ***ct1*** or ***simfit*** then calculate the relaxation value for one peak according to FITTYPE. You can change FITTYP and recalculate the relaxation value without running ***pd*** again. The same counts for the commands ***dat1*** and ***simfit all*** which fit all peaks.

INC - point (1D) or row (2D) increment

- used in 1D and pseudo 2D relaxation datasets
- takes an integer value (default is 1)
- interpreted by ***pft2*** (1D data)

- interpreted by ***pd*** (pseudo 2D data)
- Starting with START, every INC point (1D) or row (pseudo 2D) is used for relaxation analysis.

NUMPNTS - number of data points used for relaxation analysis

- used in 1D and pseudo 2D relaxation datasets
- takes an integer value (default is TD)
- interpreted by ***pft2*** (1D)
- interpreted by ***pd*** (pseudo 2D)
- The default value of NUMPNTS is the number of available points, i.e. TD (1D) or F1 TD (pseudo 2D). TD is the acquisition status parameter which can be viewed with ***dpa*** or ***s td***. Note that if you increase INC, you must reduce NUMPNTS such that INC*NUMPNTS does not exceed TD.

START - first point (1D) or row (2D) used for relaxation analysis

- used in 1D and pseudo 2D relaxation datasets
- takes an integer value (default is 1)
- interpreted by ***pft2*** (1D data)
- interpreted by ***pd*** (pseudo 2D data)
- Note that the default value (1) is not the first but the second point of a 1D dataset. It is, however, the first row of a pseudo 2D dataset. The point or row used is START + n*INC.

Chapter 3

1D Processing commands

This chapter describes all TOPSPIN 1D processing commands. Several of them can also be used to process one row of 2D or 3D data. They store their output in processed data files and do not change the raw data.

For each command, the relevant input and output parameters are mentioned. Furthermore, the relevant input and output files and their location are mentioned. Although file handling is completely transparent, it is sometimes useful to know which files are involved and where they reside. For example, if you have permission problems or if you want to process or interpret your data with third party software.

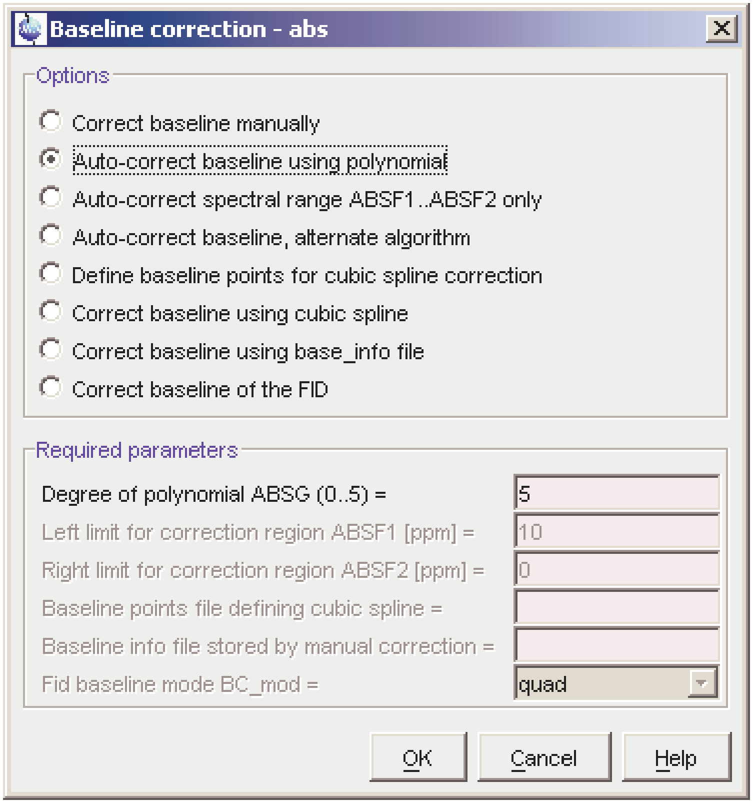
abs, absf, absd, bas

NAME

abs - Automatic baseline correction (1D)
absf - Automatic baseline correction of the plot region (1D)
absd - Automatic baseline correction, special algorithm (1D)
bas - Open baseline correction dialog box (1D)

DESCRIPTION

Baseline correction commands can be started on the command line or from the baseline correction dialog box. The latter is opened with the



Baseline correction - abs

Options

○ Correct baseline manually
● Auto-correct baseline using polynomial
○ Auto-correct spectral range ABSF1..ABSF2 only
○ Auto-correct baseline, alternate algorithm
○ Define baseline points for cubic spline correction
○ Correct baseline using cubic spline
○ Correct baseline using base_info file
○ Correct baseline of the FID

Required parameters

Degree of polynomial ABSG (0..5) = 5
Left limit for correction region ABSF1 [ppm] = 10
Right limit for correction region ABSF2 [ppm] = 0
Baseline points file defining cubic spline =
Baseline info file stored by manual correction =
Fid baseline mode BC_mod = quad

Figure 3.1

command ***bas***.

This dialog box offers several options, each of which selects a certain command for execution.

Auto-correct baseline using polynomial

This option selects the command ***abs*** for execution. It performs an automatic baseline correction of the spectrum by subtracting a polynomial. The degree of the polynomial is determined by the parameter ABSG which has a value between 0 and 5, with a default of 5. ***abs*** first determines which parts of the spectrum contain spectral information and stores the result in the file `intrng` (integral regions). The remaining part of the spectrum is considered baseline and used to fit the polynomial function.

abs also interprets the parameters ABSL, AZFW, AZFE and ISEN. Since these parameters apply to integration rather than baseline correction, they do not appear in the ***bas*** dialog box. They do appear in the integration dialog box (command ***int***). Data points greater than ABSL*(standard deviation) are considered spectral information, all other points are considered noise. If two peaks are more than AZFW apart, they are treated independently. If they are less than AZFW ppm apart, they are considered to be overlapping. Integral regions are extended at both sides by AZFE ppm. If this extension causes adjacent regions to overlap, the centre of the overlap is used as the limit of the two regions. Only regions whose integrals are larger (area) than the largest integral divided by ISEN are considered.

abs n does not store the integral ranges. It is, for example, used in the command sequence ***ef***, ***mc***, ***abs***, ***efp***, ***abs n*** to store the integral regions of both positive and negative peaks. The command ***abs*** only stores the regions of positive peaks.

Auto-correct spectral range ABSF1 .. ABSF2 only

This option selects the command ***absf*** for execution. It works like ***abs***, except that it only corrects the spectral region which is determined by the processing parameters ABSF1 and ABSF2.

Auto-correct baseline, alternate algorithm

This option selects the command ***absd*** for execution. It works like

abs, except that it uses a different algorithm[1]. It is, for example, used when a small peak lies on the foot of a large peak. In that case, ***absd*** allows you to correct the baseline around the small peak which can then be integrated. Usually ***absd*** is followed by ***abs***.

To display the integral regions determined by one of the above commands:

1. Right-click inside the data window and select ***Display Properties***
2. Check the entry ***Integrals*** and click ***OK***

The integral regions are also used by various commands which calculate spectral integrals like ***li***, ***lipp*** and ***plot***.

If you run a command like ***abs*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.

If automatic baseline correction does not give satisfactory results, you can apply an interactively determined polynomial, exponential, sine or spline baseline correction. This can be started with the first entry of the ***bas*** dialog box, by clicking the button in the toolbar or by entering ***.basl*** on the command line.

The ***bas*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***bas*** dialog box, with ***edp*** or by typing ***absg***, ***absf1*** etc.:

ABSG - degree of the polynomial (input of ***abs***, ***absf***, ***absd***)
ABSF1 - low field (left) limit of the region corrected by ***absf***
ABSF2 - high field (right) limit of the region corrected by ***absf***

set from the ***int*** dialog box, with ***edp*** or by typing ***absl***, ***azfw*** etc.:

ABSL - integral sensitivity factor with reference to the noise
AZFW - minimum distance between peaks for independent integration
AZFE - integral extension factor
ISEN - integral sensitivity factor with reference to the largest integral

[1] It uses the same algorithm as the command ***abs*** in DISNMR

INPUT FILES

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

`1r` - real processed 1D data
`proc` - processing parameters

OUTPUT FILES

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

`1r` - real processed 1D data
`procs` - processing status parameters
`intrng` - integral regions (output of ***abs***, ***absf*** , ***absd***)
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

ABS

ABSD

ABSF

SEE ALSO

bcm, sab, bc, .basl

add, duadd, addfid, addc, adsu

NAME

add - Add two datasets point-wise, multiply 2nd with DC (1D)
duadd - Add two datasets ppm/Hz-wise, mult. 2nd with DC (1D)
addfid - Add two FIDs, multiply 2nd with DC (1D)
addc - Add the constant DC to the current dataset
adsu - Open add/subtract/multiply dialog box (1D, 2D)

DESCRIPTION

Addition commands can be entered on the command line or started from the add/subtract/multiply dialog box. The latter is opened with the command ***adsu***.

This dialog box offers several options, each of which selects a certain command for execution.

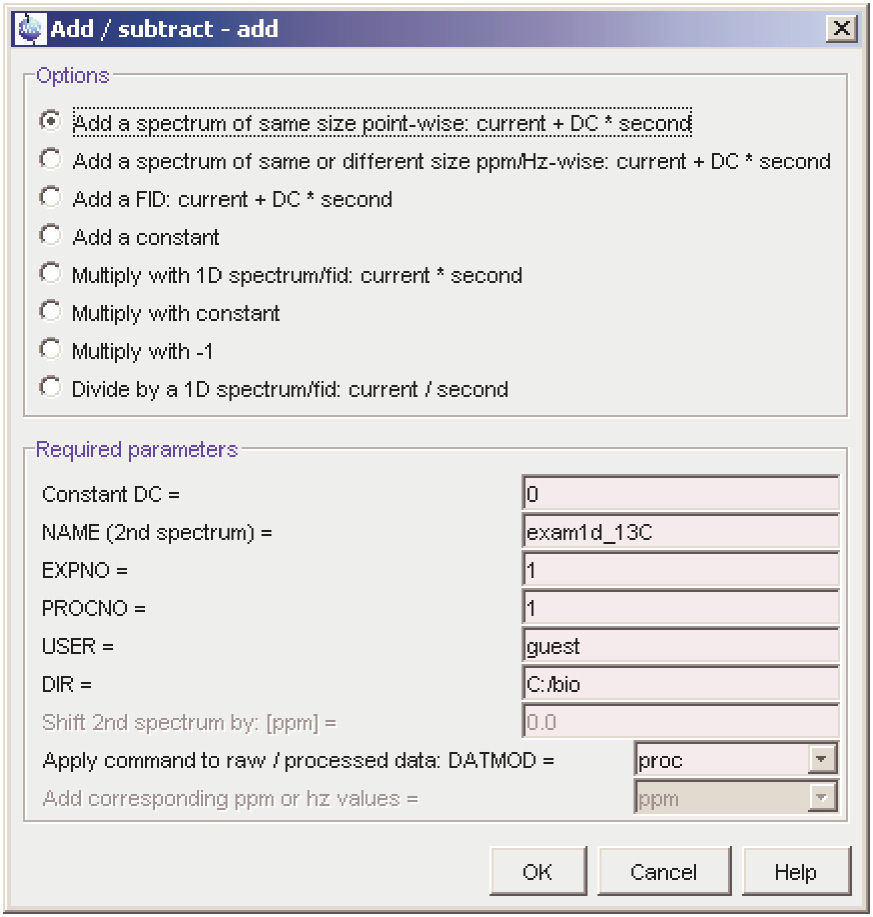
Add a 1D spectrum point-wise

This option selects the command ***add*** for execution. It adds the second dataset, multiplied with the constant DC, to the current dataset. ***add*** performs a point to point addition which is independent of the spectrum calibration.The result is stored in the current dataset. DC can be set by entering ***dc*** on the command line or in the ***Procpars*** pane. If the second dataset has not been defined yet, the add/subtract dialog box is opened. Here you can define the second dataset and start the ***add*** command. ***add*** works on raw or on processed data, depending on the value of DATMOD. For DATMOD = raw, ***add*** adds the raw data of the current and second dataset but stores the result as processed data in the current dataset. As such, the raw data of the current dataset are not overwritten.

Add a 1D spectrum ppm/Hz-wise

This option selects the command ***duadd*** for execution. It works like ***add***, except that it adds two datasets according to their chemical shift values. Each ppm value of one dataset is added to the same ppm value of a second dataset.

duadd is useful when the two input spectra are:



Add / subtract - add

Options

● Add a spectrum of same size point-wise: current + DC * second

○ Add a spectrum of same or different size ppm/Hz-wise: current + DC * second

○ Add a FID: current + DC * second

○ Add a constant

○ Multiply with 1D spectrum/fid: current * second

○ Multiply with constant

○ Multiply with -1

○ Divide by a 1D spectrum/fid: current / second

Required parameters

Constant DC =	0
NAME (2nd spectrum) =	exam1d_13C
EXPNO =	1
PROCNO =	1
USER =	guest
DIR =	C:/bio
Shift 2nd spectrum by: [ppm] =	0.0
Apply command to raw / processed data: DATMOD =	proc
Add corresponding ppm or hz values =	ppm

Figure 3.2

- of different size
- referenced differently
- acquired with different frequencies (i.e. on different spectrometers)

For data with equal size, reference and spectrometer frequency, ***add*** and ***duadd*** give the same result.

Furthermore, ***duadd*** allows you to shift the second spectrum by a user defined number of ppm. The parameter *ppm* or *hz* is only relevant if the input data were acquired with different basic frequencies, i.e. when they come from different spectrometers. ***duadd*** only works on processed data, independent of the value of DATMOD.

Add an FID

This option selects the command ***addfid*** for execution. It adds two 1D raw datasets multiplying one of them with the factor DC. The result is stored in the current dataset. It works like ***add*** with DATMOD = raw, except that it overwrites the raw data.

Add a constant

This option selects the command ***addc*** for execution. It adds the value of DC to the current dataset. It works on raw or processed data, depending on the value of DATMOD. The result is stored as processed data in the current dataset.

If you run a command like ***add*** from the command line, it behaves slightly different. It adds the second and the third dataset, as specified with ***edc2*** and stores the result in the current dataset. dataset you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.

The ***adsu*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***adsu*** dialog box, with ***edp*** or by typing ***dc***, ***datmod*** etc.:

DC - multiplication factor
DATMOD - data mode: work on 'raw' or 'proc'essed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - current raw data (input of ***add***/***addc*** if DATMOD = raw)

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

`1r`, `1i` - current processed data (input of ***add***/***addc*** if DATMOD = proc)

`proc` - processing parameters
curdat2 - definition of the second dataset

<dir2>/data/<user2>/nmr/<name2>/<expno2>/

`fid` - second raw data (input of ***add*** if DATMOD = raw, ***addfid***)

<dir2>/data/<user2>/nmr/<name2>/<expno2>/pdata/<procno2>/

`1r`, `1i` - second processed data (input of ***add*** if DATMOD = proc)

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - current raw data (output of ***addfid***)
`audita.txt` - acquisition audit trail (output of ***addfid***)

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

`1r`, `1i` - current processed data (output of ***add*** and ***addc***)
`procs` - processing status parameters
`auditp.txt` - processing audit trail (output of ***add*** and ***addc***)

USAGE IN AU PROGRAMS

ADD

ADDFID

ADDC

SEE ALSO

mul, mulc, div, add2d

accumulate

NAME

accumulate - Accumulate 1D datasets ppm/Hz-wise (1D)

SYNTAX

accumulate [start] offset scale Hz|ppm procno [expno [name [user [dir]]]]

DESCRIPTION

The command ***accumulate*** accumulates 1D datasets. It adds a specified processed dataset to the current dataset. ***accumulate*** has the following features:

- the specified data can be shifted and scaled with respect to the current data.
- addition can be performed ppm-wise or hz-wise
- the specified data can overwrite the current data or can be added to the current data

All required information must be specified by command line arguments. As such, ***accumulate*** takes 4 to 9 arguments. Here are some examples of its usage:

accumulate <offset> <scale> ppm |hz <procno>

Add the processed data of the specified *procno* to the current *procno* as follows:

- shift the added data by <offset> ppm
- scale added data by the value <scale>
- perform the addition ppm-wise or hz-wise as specified

Example: ***accumulate 0.0 1.0 ppm 3***

accumulate start <offset> <scale> ppm |hz <procno>

Same as above, except that the processed data of the specified *procno* are copied to the current *procno*, overwriting possibly existing data.

Example: ***accumulate start 0.0 1.0 ppm 3***

Note that here, the arguments ***offset*** and ***ppm**|**hz*** do not affect the data but do affect the status parameter OFFSET.

In the examples above, the accumulated dataset has the same datapath as the original data except for the *procno*. To accumulate data with a different datapath, you can specify other parts of the datapath as arguments. Parts that are not specified are taken from the current dataset.

Examples:

accumulate <offset> <scale> ppm|hz <procno> <expno>

accumulate start <offset> <scale> ppm|hz <procno> <expno> <user> <dir>

accumulate works like the command ***duadd***, except that all information is specified on the command line. ***accumulate*** is typically used repeatedly to accumulate a series of 1D processed data. The first instance of ***accumulate*** overwrites the current data with the specified data, defining the accumulation start. All further instances add the specified data to the current data.

OUTPUT PARAMETERS

OFFSET - the ppm value of the first data point of the spectrum

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>/
`1r`, `1i` - current processed data
`proc` - processing parameters

<dir2>/data/<user2>/nmr/<name2>/<expno2>/pdata/<procno2>/
`1r`, `1i` - second processed data

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>/
`1r`, `1i` - current processed data
`procs` - processing status parameters
`auditp.txt` - processing audit trail

SEE ALSO

duadd

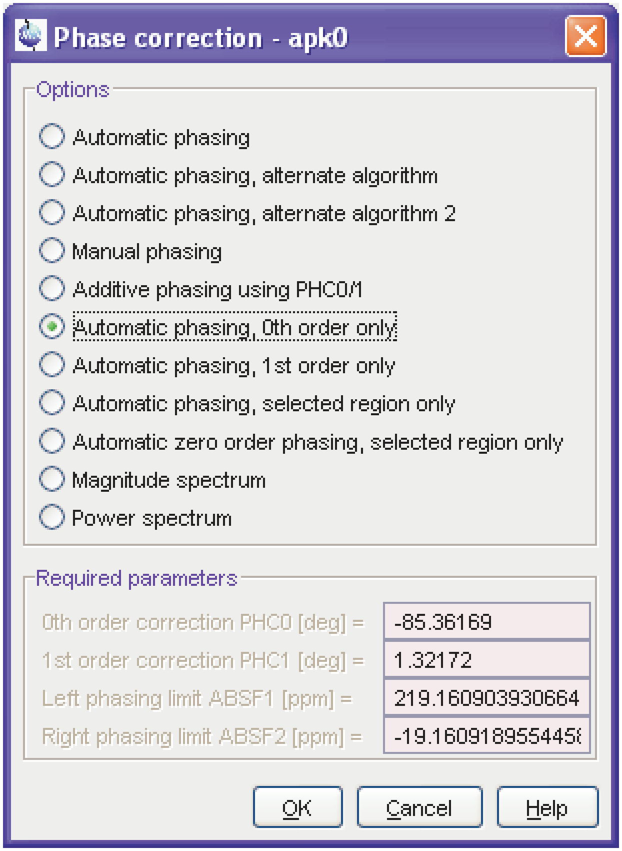
apk0, apk1, apk0f, ph

NAME

apk0 - Zero-order automatic phase correction (1D)
apk1 - First-order automatic phase correction (1D)
apk0f - Customized zero-order automatic phase correction (1D)
ph - Open phase correction dialog box (1D/2D)

DESCRIPTION

Phase correction commands can be can be entered on the command line or started from the phase correction dialog box (see Figure 3.3). This di-



Phase correction - apk0

Options

○ Automatic phasing
○ Automatic phasing, alternate algorithm
○ Automatic phasing, alternate algorithm 2
○ Manual phasing
○ Additive phasing using PHC0/1
● Automatic phasing, 0th order only
○ Automatic phasing, 1st order only
○ Automatic phasing, selected region only
○ Automatic zero order phasing, selected region only
○ Magnitude spectrum
○ Power spectrum

Required parameters

0th order correction PHC0 [deg] = -85.36169
1st order correction PHC1 [deg] = 1.32172
Left phasing limit ABSF1 [ppm] = 219.160903930664
Right phasing limit ABSF2 [ppm] = -19.160918955445

Figure 3.3

alog is opened with the command ***ph***. It offers several options, each of which selects a certain command for execution.

Automatic phasing, 0th order only

This option selects the command ***apk0*** for execution. It works like ***apk***, except that it only performs the zero order phase correction.

Automatic phasing, 1st order only

This option selects the command ***apk1*** for execution. It works like ***apk***, except that it only performs the first order phase correction.

Automatic zero order phasing, selected region order only

This option selects the command ***apk0f*** for execution. It works like ***apkf***, except that it only performs the zero order phase correction.

If you run a command like ***apk0f*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.

If automatic phase correction does not give satisfactory results, you can perform interactive phase correction. This can be started with the entry ***Manual phasing*** in the ***ph*** dialog box, by clicking the button in the toolbar or by entering ***.ph*** on the command line.

The ***ph*** command can be used on 1D, 2D or 3D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***ph*** dialog box, with ***edp*** or by typing ***absf1***, ***absf2*** etc.:

ABSF1 - low field (left) limit of the region used by ***apk0f***
ABSF2 - high field (right) limit of the region used by ***apk0f***

OUTPUT PARAMETERS

can be viewed with ***edp***, ***dpp*** or by typing ***phc0***, ***s phc0*** etc.:

PHC0 - zero order phase correction value (output of ***apk0*** and ***apk0f***)
PHC1 - first order phase correction value (output of ***apk1***)

Note that this is one of the rare cases where the output parameters of a command are stored as processing (***edp***) and as processing status parameters (***dpp***).

INPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`proc` - processing parameters
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

APK0

APK1

APK0F

SEE ALSO

apk, apks, apkf, apkm, pk, mc, ps, .ph

apk, apks, apkm, apkf, ph

NAME

apk - Automatic phase correction (1D)
apks - Automatic phase correction with a different algorithm (1D)
apkm - Automatic phase correction with a different algorithm 2 (1D)
apkf - Customized automatic phase correction (1D)
ph - Open phase correction dialog box (1D/2D)

DESCRIPTION

Phase correction commands can be can be entered on the command line or started from the phase correction dialog box (see Figure 3.4). This dialog is opened with the command ***ph***. It offers several options, each of which selects a certain command for execution.

Automatic phasing

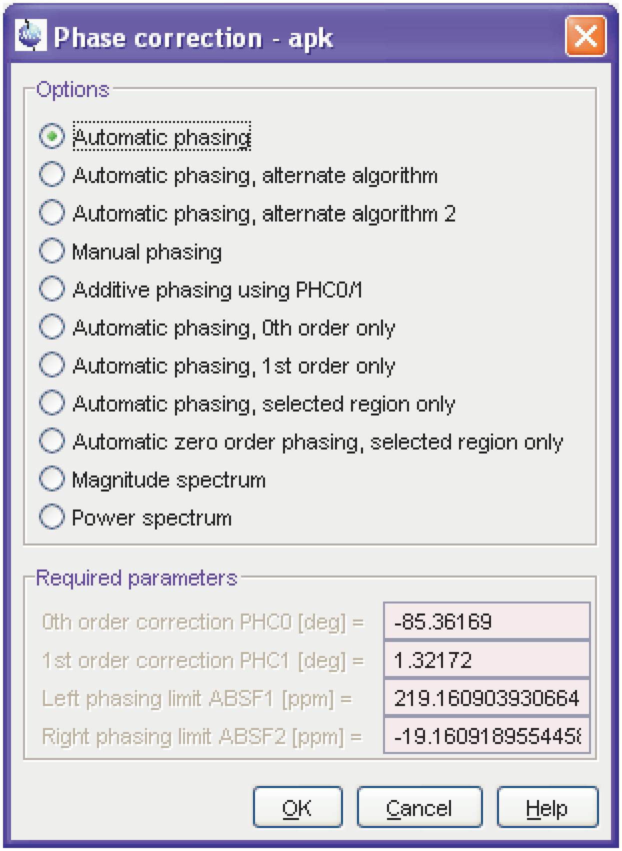
This option selects the command ***apk*** for execution. It calculates the zero and first order phase values and then corrects the spectrum according to these values. The phase values are stored in the parameters PHC0 and PHC1, respectively. Note that ***apk*** stores the calculated phase values both as processing parameters (***edp***) and as processing status parameters (***dpp***).

Automatic phasing, alternate algorithm

This option selects the command ***apks*** for execution. It works like ***apk***, except that it uses a different algorithm which gives better results on certain spectra.

Automatic phasing, alternate algorithm 2

This option selects the command ***apkm*** for execution. It uses symmetric isolated peaks, regions with positive/negative signals and regions of flat baseline for automated phase correction of 1D NMR spectra. The automated phasing is performed by means of minimization of certain penalty function with four terms. The first term is responsible for phases of symmetric isolated peaks, the second accounts for regions with positive/negative signals, the third accounts for baseline regions, and the fourth gives additional penalty for large values of first-order



Phase correction - apk

Options

- ● Automatic phasing
- ○ Automatic phasing, alternate algorithm
- ○ Automatic phasing, alternate algorithm 2
- ○ Manual phasing
- ○ Additive phasing using PHC0/1
- ○ Automatic phasing, 0th order only
- ○ Automatic phasing, 1st order only
- ○ Automatic phasing, selected region only
- ○ Automatic zero order phasing, selected region only
- ○ Magnitude spectrum
- ○ Power spectrum

Required parameters

0th order correction PHC0 [deg] =	-85.36169
1st order correction PHC1 [deg] =	1.32172
Left phasing limit ABSF1 [ppm] =	219.160903930664
Right phasing limit ABSF2 [ppm] =	-19.160918955445(

Figure 3.4

phase correction parameter PHC1. For a full description of ***apkm***, enter the TOPSPIN command ***help apkm***.

Automatic phasing, selected region only

This option selects the command ***apkf*** for execution. It works like ***apk***, except that it uses only a certain region of the spectrum for the calculation of the phase values. This region is determined by the parameters ABSF1 and ABSF2. The calculated phase values are then applied to the entire spectrum. Note that the parameters ABSF1 and ABSF2 are also used by the command ***absf***.

If you run a command like ***apkf*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.

If automatic phase correction does not give satisfactory results, you can perform interactive phase correction. This can be started with the entry ***Manual phasing*** in the ***ph*** dialog box, by clicking the button in the toolbar or by entering ***.ph*** on the command line.

The ***ph*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***ph*** dialog box, with ***edp*** or by typing ***absf1***, ***absf2*** etc.:

ABSF1 - low field (left) limit of the region used by ***apkf***
ABSF2 - high field (right) limit of the region used by ***apkf***

OUTPUT PARAMETERS

can be viewed with ***edp***, ***dpp*** or by typing ***phc0***, ***s phc0*** etc.:

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

Note that this is one of the rare cases where the output parameters of a command are stored as processing (***edp***) and as processing status parameters (***dpp***).

INPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`proc` - processing parameters
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

APK

APKF

APKS

SEE ALSO

apk0, apk1, apk0f

bc

NAME

bc - Baseline correction of the FID (1D)

DESCRIPTION

The command ***bc*** performs a baseline correction of raw 1D data. The type of correction is determined by the processing parameter BC_mod as shown in table 3.1.

BC_mod	Function subtracted from the FID	Detection mode
no	no function	
single	average intensity of the last quarter of the FID	single channel
quad	average intensity of the last quarter of the FID	quadrature
spol	polynomial of degree 5 (least square fit)	single channel
qpol	polynomial of degree 5 (least square fit)	quadrature
sfil	Gaussian function of width BCFW [a]	single channel
qfil	Gaussian function of width BCFW	quadrature

Table 3.1

[a] Marion, Ikura, Bax, J. Magn. Res. 84, 425-420 (1989)

spol/qpol and *sfil/qfil* are especially used to subtract strong signals, e.g. a water signal at the centre of the spectrum. Note that *sfil/qfil* perform a better reduction at the risk of losing valuable signal. For reducing off-centre signal, you can set the parameter COROFFS to the offset frequency.

In this table, *s(ingle)* stands for single detection mode and *q(uad)* for quadrature detection mode. ***bc*** evaluates BC_mod for the function to be subtracted but not for the detection mode. The latter is evaluated from the acquisition status parameter AQ_mod. This means, for example, it does not matter if you set BC_mod to *single* or *quad*. The same counts for the values *spol/qpol* and *sfil/qfil*. Furthermore, for AQ_mod = DQD, no baseline correction is performed for BC_mod = *single* or *quad*. Note that the commands ***trf*** and ***xtrf**** do evaluate the detection mode from BC_mod and perform the baseline correction for BC_mod = *single/quad* when AQ_mod = DQD.

The command ***bc*** is automatically executed as a part of the commands ***em***, ***gm***, ***ft***, or any of the composite Fourier transform commands.

When executed on a 2D or 3D dataset, ***bc*** prompts you for the row and output *procno*. Alternatively, it can be entered with up to four arguments:

bc <row> <procno> n y

process the specified row and store it under the specified *procno*. The last two arguments are optional: ***n*** prevents changing the display to the output 1D data, ***y*** causes a possibly existing data to be overwritten without warning.

When executed on a dataset with 2D or 3D raw data but 1D processed data[1], ***bc*** takes one argument:

bc <row>

process the specified row and store it under the current *procno*.

bc same

process the same row as the previous processing command and store it under the current *procno*. The ***same*** option is automatically used by the AU program macro BC. When used on a regular 1D dataset (i.e. with 1D raw data) it has no effect.

bc can also be started from the baseline dialog box which is opened with the command ***bas***.

INPUT PARAMETERS

set from the ***bas*** dialog box, with ***edp*** or by typing ***bc_mod***, ***bcfw*** etc.:

BC_mod - FID baseline correction mode
BCFW - filter width for BC_mod = sfil or qfil
COROFFS - correction offset in Hz, for BC_mod = spol or qpol and

[1] Usually a result of ***rsr***, ***rsc*** or a 1D processing command on that 2D or 3D dataset.

sfil/qfil

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (time domain)

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

`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed data (time domain)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

BC

SEE ALSO

bas

bcm

NAME

bcm - User defined spectrum baseline correction (1D)

DESCRIPTION

The command ***bcm*** performs a spectrum baseline correction by subtracting a polynomial, sine or exponential function.

This involves the following steps:

1. Click or enter ***.basl*** to change to baseline correction mode.
2. Fit the baseline of the spectrum with a *polynomial*, *exponential* or *sine* function. Click-hold the button **A** and move the mouse to determine the zero order correction. Do the same with the buttons **B**, **C** etc. for higher order corrections until the line matches the baseline of the spectrum.
3. Click to return. The command ***bcm*** is automatically executed.

The interactively determined baseline function is stored in the file `base_info`. This file can be stored for general usage with the command ***wmisc***. After that, you can read it with ***rmisc*** on another dataset and run ***bcm*** to perform the same baseline correction.In this case, ***bcm*** can be started from the command line or from the baseline dialog box which is opened with the command ***bas***.

INPUT FILES

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

`1r` - real processed 1D data
`proc` - processing parameters
`base_info` - baseline correction coefficients

OUTPUT FILES

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

`1r` - real processed 1D data
`procs` - processing status parameters

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

BCM

SEE ALSO

bas, sab, .basl

dt

NAME

dt - Calculate the first derivative of the data (1D)

DESCRIPTION

The command ***`dt`*** calculates the first derivative of the current dataset. Depending on the value of DATMOD, ***`dt`*** works on the raw or on the processed data.

INPUT PARAMETERS

set by the user with ***`edp`*** or by typing ***`datmod`*** :

DATMOD - data mode: work on ’raw’ or ’proc’essed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if DATMOD = raw)

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

`1r`, `1i` - processed 1D data (input if DATMOD = proc)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

DT

ef, efp

NAME

ef - Exponential window multiplication + Fourier transform (1D)
efp - Exponential window multiplication + FT + phase correction (1D)

DESCRIPTION

The composite processing command ***ef*** is a combination of ***em*** and ***ft***, i.e. it performs an exponential window multiplication and a Fourier transform.

efp is a combination of ***em***, ***ft*** and ***pk***, i.e. it does the same as ***ef*** but, in addition, performs a phase correction.

ef and ***efp*** automatically perform an FID baseline correction according to BC_mod.

All composite processing commands can be found under the menu:

Processing → More Transforms → Shortcuts

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if `1r`, `1i` do not exist or are Fourier transformed)
`acqus` - acquisition status parameters

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

`1r`, `1i` - processed data (input if they exist but are not Fourier transformed)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

EF

EFP

SEE ALSO

gf, gfp, fp, fmc

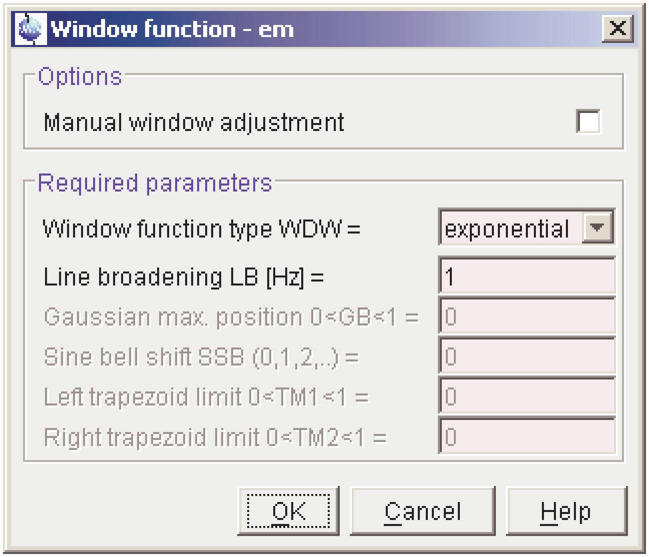
em, gm, wm

NAME

em - Exponential window multiplication of the FID (1D)
gm - Gaussian window multiplication of the FID (1D)
wm - Open window function dialog box (1D, 2D)

DESCRIPTION

Window multiplication commands can be entered on the command line or started from the window function dialog box. The latter is opened with the command ***wm***.



Options

Manual window adjustment □

Required parameters

Window function type WDW = exponential

Line broadening LB [Hz] = 1

Gaussian max. position 0<GB<1 = 0

Sine bell shift SSB (0,1,2,..) = 0

Left trapezoid limit 0<TM1<1 = 0

Right trapezoid limit 0<TM2<1 = 0

Figure 3.5

The parameter section of this dialog box offers several window functions, each of which selects a certain command for execution.

Exponential multiplication

This function selects the command ***em*** for execution. It performs an exponential window multiplication of the FID. It is the most used window function for NMR spectra. ***em*** multiplies each data point *i* with the factor:

$$\exp\left(-\frac{(i-1)\cdot LB\cdot\pi}{2\cdot SWH}\right)$$

where LB (the line broadening factor) is a processing parameter and SWH (the spectral width) an acquisition status parameter.

Gaussian multiplication

This function selects the command ***gm*** for execution. It performs a Gaussian window multiplication of the FID. The result is a Gaussian lineshape after Fourier transform. This lineshape has sharper edges than the lineshape caused by ***em***. ***gm*** multiplies the FID with the function:

$$\exp(((-at)) - (-bt^2))$$

where t is the acquisition time in seconds and a and b are defined by:

$$a = \pi\cdot LB \quad \text{and} \quad b = -\frac{a}{2GB\cdot AQ}$$

In this equation, LB and GB are processing parameters which represent the exponential broadening factor and the Gaussian broadening factor, respectively. AQ is an acquisition status parameter which represents the acquisition time.

gm allows you to separate overlapping peaks. The quality of the separation depends on the choice of the parameters LB and GB. Suitable values can be determined with ***Manual window adjustment***. The value of LB must be negative, typically the half line width of the spectral peaks. Note that for exponential window multiplication (***em***), LB must be positive. The value of GB must lie between 0 and 1. It determines the position of the top of the Gaussian function. For example, for GB = 0.5 the top lies in the middle of the FID. Note that for large values of GB (close to 1), peaks can become negative at the edges which can impair quantitative analysis of the spectrum.

em and ***gm*** implicitly perform a baseline correction of the FID, according to the processing parameter BC_mod. Furthermore, they perform linear prediction according to the parameters ME_mod, NCOEF and LPBIN.

When executed on 2D or 3D data, ***em*** and ***gm*** take up to four arguments, e.g.:

em <row> <procno> n y

process the specified row and store it under the specified *procno*. The last two arguments are optional: ***n*** prevents changing the display to the output 1D data, ***y*** causes a possibly existing data to be overwritten without warning.

When executed on a dataset with 2D or 3D raw data but 1D processed data[1], ***em*** and ***gm*** take one argument, e.g.:

em <row>

process the specified row and store it under the current *procno*.

em same

process the same row as the previous processing command and store it under the current *procno*. The ***same*** option is automatically used by the AU program macros EM and GM. When used on a regular 1D dataset (i.e. with 1D raw data) it has no effect.

If you run a command like ***em*** from the command line, you have to make sure that the required parameters are already set. Click the **Procpars** tab or enter ***edp*** to do that.

The ***wm*** command can be used on 1Dor 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***wm*** dialog box, with ***edp*** or by typing ***lb***, ***bc_mod*** etc.:

LB - Lorentzian broadening factor
GB - Gaussian broadening factor
BC_mod - FID baseline correction mode

set by the acquisition, can be viewed with ***dpa*** or ***s swh***:

SWH - spectral width

[1] Usually a result of ***rsr***, ***rsc*** or a previous 1D processing command on that 2D or 3D data.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if `1r`, `1i` do not exist or are Fourier transformed)
`acqus` - acquisition status parameters

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

`1r`, `1i` - processed data (input if they exist but are not Fourier transformed)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

EM

GM

SEE ALSO

sinm, qsin, sinc, qsinc, tm, traf, trafs

filt

NAME

filt - Digital filtering of the data (1D)

DESCRIPTION

The command ***filt*** smoothes the data by replacing each point with a weighted average of its surrounding points. By default, ***filt*** uses the weighting coefficients 1-2-1 which means that the intensity *p(i)* of data point *i* is replaced by:

$$1 \cdot p(i-1) + 2 \cdot p(i) + 1 \cdot p(i+1).$$

Figure 3.6

Different weighting algorithms can be set up by creating a new file in the directory:

```
<tshome>/exp/stan/nmr/filt/1d
```

Just copy the default file `threepoint` to a different name and modify it with a text editor. The file must look like:

3,1,2,1

or

5,1,2,3,2,1

where the first number represents the number of points used for smoothing and must be odd. The other numbers are the weighting coefficients for the data points. The processing parameter DFILT determines which file is used by ***filt***.

This is one of the few cases where file handling cannot be done from TopSpin and needs to done on operating system level.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***dfilt***, ***datmod*** etc. :

DFILT - digital filter filename
DATMOD - data mode: work on ’raw’ or ’proc’essed data

INPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`proc` - processing parameters

<tshome>/exp/stan/nmr/filt/1d/*

digital filtering file(s)

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

FILT

fp, fmc

NAME

fp - Fourier transform +phase correction (1D)
fmc - Fourier transform + magnitude calculation (1D)

DESCRIPTION

The composite processing command ***fp*** is a combination of ***ft*** and ***pk***, i.e. it performs a 1D Fourier transform and a phase correction.

fmc is a combination of ***ft*** and ***mc***, i.e. it performs a 1D Fourier transform and a magnitude calculation.

fp and ***fmc*** automatically perform an FID baseline correction according to BC_mod.

All composite processing commands can be found under the menu:

Processing → More Transforms → Shortcuts

INPUT AND OUTPUT PARAMETERS

see the commands ***ft***, ***pk*** and ***mc***.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if `1r`, `1i` do not exist or are Fourier transformed)
`acqus` - acquisition status parameters

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

`1r`, `1i` - processed data (input if they exist but are not Fourier transformed)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

FP

FMC

SEE ALSO

ef, efp, gf, gfp

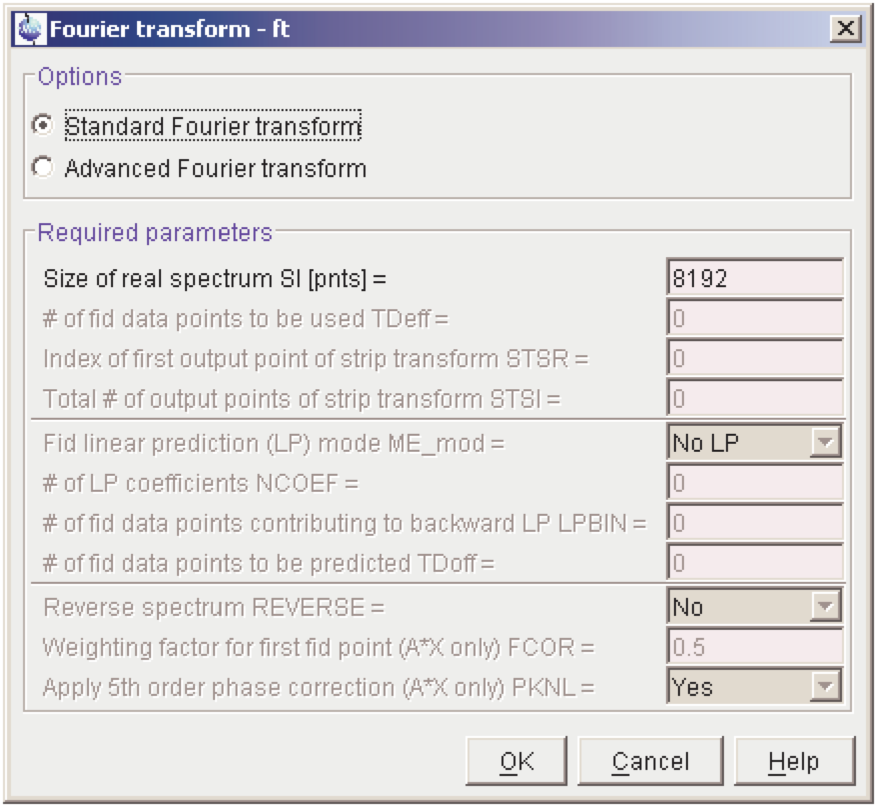
ft, ftf

NAME

ft - Fourier transform (1D)
ftf - Open the Fourier transform dialog box (1D, 2D)

DESCRIPTION

The command ***ft*** Fourier transforms a 1D dataset or a row of a dataset with dimension ≥ 2. It can be started from the command line or from the Fourier transform dialog box. The latter is opened with the command ***ftf***



Fourier transform - ft

Options

● Standard Fourier transform
○ Advanced Fourier transform

Required parameters

Size of real spectrum SI [pnts] = 8192
# of fid data points to be used TDeff = 0
Index of first output point of strip transform STSR = 0
Total # of output points of strip transform STSI = 0
Fid linear prediction (LP) mode ME_mod = No LP
# of LP coefficients NCOEF = 0
# of fid data points contributing to backward LP LPBIN = 0
# of fid data points to be predicted TDoff = 0
Reverse spectrum REVERSE = No
Weighting factor for first fid point (A*X only) FCOR = 0.5
Apply 5th order phase correction (A*X only) PKNL = Yes

Figure 3.7

This dialog box offers two options both of which select the ***ft*** command for execution.

Standard Fourier transform

This option only allows you to set the parameter SI, the size of the real spectrum.

Advanced Fourier transform

This option allows you to set all FT related parameters.

Fourier transform is the main step in processing NMR data. The time domain data (FID) which are created by acquisition are transformed into frequency domain data (spectrum). Usually, Fourier transform is preceded by other processing steps like FID baseline correction (***bc***) and window multiplication (***em***, ***gm***, etc.) and followed by steps like phase correction (***apk***) and spectrum baseline correction (***abs***).

The size of the resulting spectrum is determined by the parameter SI. An FID of TD time domain points is transformed to a spectrum of SI real and SI imaginary data points. A typical value for SI is TD/2. In that case, all points of the FID are used by the Fourier transform and no zero filling is done.

The size of the spectrum and the number of FID points which are used can be determined in the following ways:

- SI > TD/2: the FID is zero filled
- SI < TD/2: only the first 2*SI points of the FID are used
- 0 < TDeff < TD: only the first TDeff points of the FID are used

In the latter two cases, the spectrum will contain less information then the FID. Note that the parameter TDoff only plays a role for linear prediction and in 2D and 3D Fourier transform.

You can also perform a so-called strip transform which means that only a certain region of the spectrum is stored. This can be done by setting the parameters STSR and STSI which represent the strip start and strip size, respectively. They can take values between 0 and SI. The processing status parameters STSI and SI are both set to this value. You can check this by entering ***dpp*** or clicking the ***Procpars*** tab.

The Fourier transform mode depends on the acquisition mode; *single*, *sequential* or *simultaneous*. For this purpose, ***ft*** evaluates the acquisition status parameter AQ_mod as shown in table 3.2 . Note that ***ft*** does not evaluate the processing parameter FT_mod but it does store the Fourier transform mode, as evaluated from the acquisition mode, in the processing status parameter FT_mod. However, the command ***trf*** determines the Fourier transform mode from the processing parameter FT_mod and not from the acquisition mode (see ***trf***).

AQ_mod	FT_mod	Fourier transform mode
qf	fsr	forward, single channel, real
qsim	fqc	forward, quadrature, complex
qseq	fqr	forward, quadrature, real
DQD	fqc	forward, quadrature, complex

Table 3.2

ft evaluates the parameter FCOR. The first point of the FID is multiplied with FCOR which is a value between 0.0 and 2.0. However, on Avance spectrometers, the FID of digitally filtered data starts with a group delay of which the first points are zero so that the value of FCOR is irrelevant. On A*X data, FCOR allows you to control the DC offset of the spectrum.

ft evaluates the parameter PKNL. On A*X spectrometers, PKNL = true causes a non linear 5th order phase correction of the raw data. This corrects possible errors caused by non linear behaviour of the analog filters. On Avance spectrometers, PKNL must always be set to TRUE. For digitally filtered data, it causes ***ft*** to handle the group delay of the FID. For analog data it has no effect.

ft evaluates the parameter REVERSE. If REVERSE = TRUE, the spectrum will be reversed, i.e. the first output data point becomes the last and the last point becomes the first. The same effect is attained by using the command ***rv*** after ***ft***.

ft automatically performs an FID baseline correction according to BC_mod.

ft performs linear prediction according to ME_mod. This parameter can take the following values:

no : no linear prediction

LPfr : forward LP on real data
LPfc : forward LP on complex data
LPbr : backward LP on real data
LPbc : backward LP on complex data
LPmifr : mirror image forward LP on real data
LPmifc : mirror image forward LP on complex data

Forward prediction can, for example, be used to extend truncated FIDs. Backward prediction can be used to improve the initial data points of the FID. ***ft*** determines the detection mode (real or complex) from the acquisition status parameter AQ_mod, not from ME_mod. As such, ***ft*** does not distinguish between ME_mod = LPfr and ME_mod = LPfc. The same counts for backward prediction. Note that the command ***trf*** does determine the detection mode from ME_mod. Linear prediction is only performed for NCOEF > 0. Furthermore, LPBIN and, for backward prediction, TDoff play a role (see these parameters in chapter 2.4). By default, ME_mod is set to *no* which means no linear prediction is done.

When executed on a 2D or 3D dataset, ***ft*** takes up to four arguments, e.g.:

ft <row> <procno> y n

process the specified *row* and store it under the specified *procno*. The last two arguments are optional: ***y*** causes a possibly existing data to be overwritten without warning, n prevents TOPSPIN from changing to the destination dataset.

If you run a command like ***ft*** from the command line, you have to make sure that the required parameters are already set. Click the **Procpars** tab or enter ***edp*** to do that.

The ***ft*** command can be used on multidimensional data. In that case it automatically recognizes the dimensionality of the data and prompt you for the row to be processed and the output *procno*. It only applies to the acquisition direction.

The ***ftf*** command can be used on 1D and 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***ftf*** dialog box, with ***edp*** or by typing ***si***, ***stsr*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
TDeff - number of raw data points to be used for processing
FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
REVERSE - flag indicating to reverse the spectrum
PKNL - group delay compensation (Avance) or filter correction (A*X)
ME_mod - FID linear prediction mode
NCOEF - number of linear prediction coefficients
LPBIN - number of points for linear prediction
TDoff - number of raw data points predicted for ME_mod = LPb*

set by the acquisition, can be viewed with ***dpa*** or by typing ***s aq_mod*** etc.:

AQ_mod - acquisition mode (determines the Fourier transform mode)
TD - time domain; number of raw data points
BYTORDA - byteorder or the raw data
NC - normalization constant

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s ft_mod***, ***s tdeff*** etc.:

FT_mod - Fourier transform mode
TDeff - number of raw data points that were used for processing
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
NC_proc - intensity scaling factor
YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
BYTORDP - data storage order

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if `1r`, `1i` do not exist or are Fourier transformed)
`acqus` - acquisition status parameters

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

`1r`, `1i` - processed data (input if they exist but are not Fourier transformed)
`proc` - processing parameters

OUTPUT FILES

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

FT

SEE ALSO

trf, trfp, ift, ht

gdcon, ldcon, mdcon, ppp, dconpl, dcon

NAME

gdcon - Gaussian deconvolution (1D)
ldcon - Lorentzian deconvolution (1D)
mdcon - Mixed Gaussian/Lorentzian deconvolution (1D)
ppp - Generate peak list for deconvolution (1D)
dconpl - Show result of last deconvolution (1D)
dcon - Open deconvolution dialog box (1D,2D)

DESCRIPTION

Deconvolution commands can be entered on the command line or started from the deconvolution dialog box (see Figure 3.8). The latter is opened with the command ***dcon***.

This offers several options, each of which selects a certain command for execution.

Use Lorentzian shape

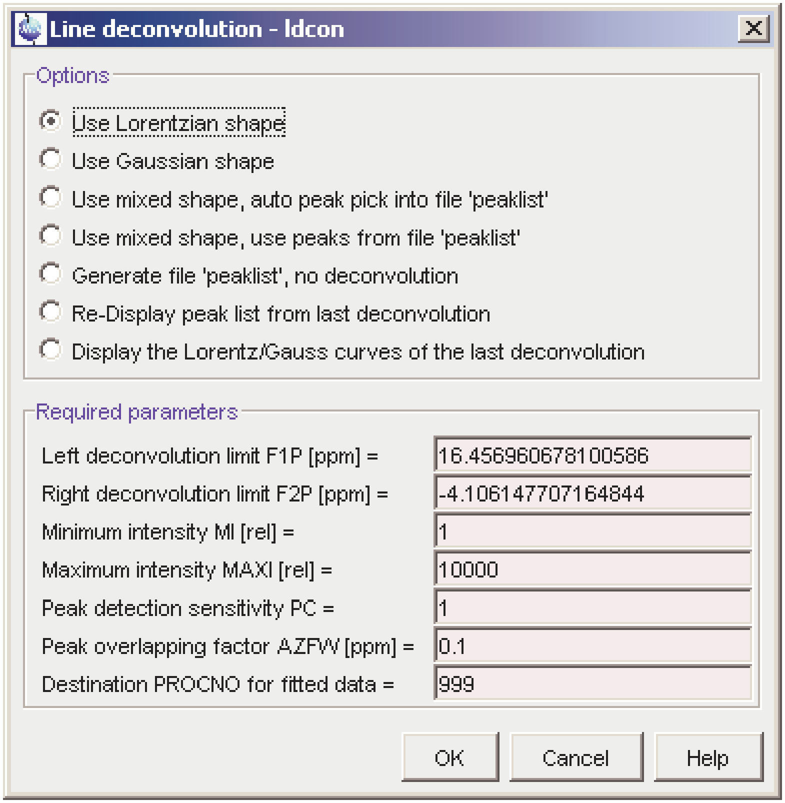
This option selects the command ***ldcon*** for execution. It deconvolves the spectrum fitting a Lorentzian function to the peaks. It is typically used for overlapping peaks with a Lorentzian lineshape to determine the ratio of each individual peak.

Use Gaussian shape

This option selects the command ***gdcon*** for execution. It deconvolves the spectrum by fitting a Gaussian function to the peaks. It is typically used for overlapping peaks with a Gaussian lineshape to determine the ratio of each individual peak.

Use mixed shape, auto peak pick into file ’peaklist’

This option selects the command ***mdcon auto*** for execution. It first picks the peaks for deconvolution and stores them in the `peaklist` file. Then it deconvolves the spectrum by fitting a mixed Lorentzian/Gaussian function to these peaks. This command is typically used to deconvolve spectra which cannot be approximated by a pure Lorentzian or a pure Gaussian lineshape.



Line deconvolution - ldcon

Options

● Use Lorentzian shape

○ Use Gaussian shape

○ Use mixed shape, auto peak pick into file 'peaklist'

○ Use mixed shape, use peaks from file 'peaklist'

○ Generate file 'peaklist', no deconvolution

○ Re-Display peak list from last deconvolution

○ Display the Lorentz/Gauss curves of the last deconvolution

Required parameters

Left deconvolution limit F1P [ppm] =	16.456960678100586
Right deconvolution limit F2P [ppm] =	-4.106147707164844
Minimum intensity MI [rel] =	1
Maximum intensity MAXI [rel] =	10000
Peak detection sensitivity PC =	1
Peak overlapping factor AZFW [ppm] =	0.1
Destination PROCNO for fitted data =	999

Figure 3.8

Use mixed shape, use peaks from file 'peaklist'

This option selects the command ***mdcon*** for execution. It works like ***`mdcon auto`***, except that it uses an existing `peaklist` file. This file must have been created:

by executing ***`mdcon auto`***

by executing ***ppp***

by executing ***pps*** and exporting the peak table (***Peaks*** tab in data window) to the file `peaklist`.

Generate peaklist, no deconvolution

This option selects the command ***ppp*** for execution. It picks the peaks for deconvolution and stores the result in the file `peaklist`. ***ppp*** is implicitly executed by ***mdcon auto***.

Re-Display peaklist from last deconvolution

This option selects the command ***dconpl*** for execution. It shows the peaklist (file `dconpeaks.txt`) which was created with the last deconvolution on the current dataset.

Display the Lorentz/Gauss curves of the last deconvolution

This option selects the command ***dconpl v*** for execution. It shows the individually fitted peaks and their sum.

The deconvolution commands only work on the displayed region, as expressed by the parameters F1P and F2P. Furthermore, they select peaks according to the peak picking parameters MI, MAXI and PC. They also evaluate the parameter AZFW, which determines the minimum distance between two peaks for them to be fitted independently. Peaks which are less than AZFW ppm apart, are considered to be overlapping. As a rule of the thumb, you can set AZFW to ten times the width at half height of the signal.

The result of deconvolution is:

- the quality of the fit expressed by the minimized chi-square value
- a list of peaks within the plot region, and for each peak its frequency, width, intensity and area. This list is displayed on the screen.
- the fitted lineshape which is shown together with the original spectrum in multi-display mode.
- individually fitted peaks and their sum, as shown by ***dconpl v***

All deconvolution commands can be started from the command line. In this case, they use the current values of the required parameters.

Tailor Mixed Shape Deconvolution

Use peak list created by regular peak picking

Mixed deconvolution creates and uses its own peaklist. You can, however, force it use the peaklist created with regular peak picking with the command ***convertpeaklist***. To do that:

1. Perform peak picking, e.g. with ***pps***.
2. Enter ***convertpeaklist peaklist***
3. Enter ***mdcon***.

Select fit parameters for each individual peaks

The deconvolution fit parameters can be enabled/disabled for each individual peak.To do that:

Edit the file `peaklist` in the PROCNO directory of the dataset. At the end of a peak entry, you can specify three flags for the three parameters to be optimized; chemical shift, half width and amplitude:

0 = optimize this parameter

1 = do not optimized this parameter

Here is an example of a peaklist:

H

#frequency half width %gauss/100.

```
3304.390 4.52 0.0 0 0 0
3289.368 2.26 0.0 1 1 1
3262.410 7.91 0.0 0 1 0
3216.022 4.52 0.0 0 0 1
```

Signal 1: All 3 Parameters are optimized (default)
Signal 2: All three Parameters are not optimized
Signal 3:chemical shift and amplitude are optimized, half width is not
Signal 4: chemical shift and half width are optimized, amplitude is not

INPUT PARAMETERS

set from the ***dcon*** dialog box, with ***edp*** or by typing ***azfw***, ***f1p*** etc.:

AZFW - minimum distance in ppm for peaks to be fitted independently
F1P - low field (left) limit of the deconvolution region (= plot region)
F2P - high field (right) limit of the deconvolution region (= plot region)
MI - minimum relative intensity (cm) for peak picking
MAXI - maximum relative intensity (cm) for peak picking
PC - peak picking sensitivity

INPUT FILES

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

`1r` - real processed 1D data
`dconpeaks.txt` - peak list (input of ***dconpl***)
`peaklist` - peak list (input of ***mdcon***)
`proc` - processing parameters

OUTPUT FILES

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

`1r` - real processed 1D data
`dconpeaks.txt` - peak list (output of ***ldcon***, ***gdcon***, ***mdcon***)
`peaklist` - peak list (output of ***ppp*** and ***mdcon auto***)
`procs` - processing status parameters

USAGE IN AU PROGRAMS

LDCON

GDCON

MDCON

PPP

USAGE IN AU PROGRAMS

dcon2d

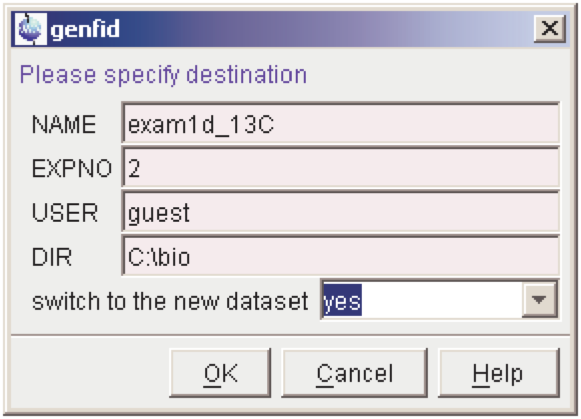
genfid

NAME

genfid - Generate pseudo-raw data (1D)

DESCRIPTION

The command ***genfid*** generates pseudo-raw data from processed data. When entered without arguments, it opens a dialog box where you can specify the destination dataset.



NAME exam1d_13C
EXPNO 2
USER guest
DIR C:\bio
switch to the new dataset yes

Figure 3.9

genfid is normally used in combination with the command ***ift*** which performs an inverse Fourier transform, converting a spectrum into an FID. Actually, ***ift*** transforms processed frequency domain data into processed time domain data. ***genfid*** converts these processed time domain data into pseudo-raw time domain data and stores them under a new name or experiment number (*expno*).

Note that ***genfid*** does not modify the data, but only stores them in a different format. The number of data points of the pseudo-raw data, is twice the size (SI) of the processed data they are created from. The acquisition status parameter TD (types ***s td*** or ***dpa***) is set accordingly; TD = 2*SI.

genfid takes arguments and can be used as follows:

1. ***genfid <expno>***

The FID will be stored under the specified *expno*.

2. ***genfid <expno> <name> y***
   The FID will be stored under the specified *name* and *expno*. The last argument (*y*) causes ***genfid*** to overwrite possibly existing data.

You can use any other combination of arguments as long they are entered in the correct order. The processed data number (*procno*) of the output dataset is always set to 1.

genfid can be used if you want to reprocess a 1D spectrum, for example with different processing parameters, but the raw data do not exist any more. An example of such a procedure is:

ift (if the data are Fourier transformed)

genfid (to create the pseudo-raw data)

edp (to set the processing parameters)

ef (to process the pseudo-raw data)

If the input data are processed but not Fourier transformed, you can skip the first step.

INPUT FILES

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

`1r`, `1i` - processed time domain data (real, imaginary)

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<*expno*>/

`fid` - pseudo-raw data
`audita.txt` - acquisition audit trail

USAGE IN AU PROGRAMS

GENFID(expno)
overwrites possibly existing raw data in the specified *expno*

SEE ALSO

ift, genser

gf, gfp

NAME

gf - Gaussian window multiplication + Fourier transform (1D)
gfp - Gaussian window multiplication + FT + phase correction (1D)

DESCRIPTION

The composite processing command ***gf*** is a combination of ***gm*** and ***ft***, i.e. it performs a Gaussian window multiplication and a Fourier transform.

gfp is a combination of ***gm***, ***ft*** and ***pk***, i.e. it does the same as ***gf*** but, in addition, performs a phase correction.

gf and ***gfp*** automatically perform an FID baseline correction according to BC_mod.

All composite processing commands can be found under the menu:

Processing → More Transforms → Shortcuts

INPUT AND OUTPUT PARAMETERS

see ***gm***, ***ft*** and ***pk***

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if `1r`, `1i` do not exist or are Fourier transformed)
`acqus` - acquisition status parameters

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

`1r`, `1i` - processed data (input if they exist but are not Fourier transformed)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

GF

GFP

SEE ALSO

ef, efp, fp, fmc

ht

NAME

ht - Hilbert transform (1D)

DESCRIPTION

The command ***`ht`*** performs a Hilbert transform which means the imaginary part of a spectrum is calculated from the real part. This is only useful when the real data have been created from zero filled raw data, with SI ≥ TD. Only then, will they contain the entire spectral information.
Imaginary data are required for phase correction. They are normally created together with the real data by Fourier transform. Directly after the Fourier transform, real and imaginary data are consistent and can be used for phase correction. If, however, the real data are manipulated, e.g. by ***`abs`***, they are no longer consistent with the imaginary data. In that case, or when the imaginary data have been deleted, ***`ht`*** can be used to create new imaginary data.
Hilbert transform is based on the so called dispersion relations or Kramers-Kronig relations (see, for example, R. R. Ernst, G. Bodenhausen and A. Wokaun, Principles of nuclear magnetic resonance in one and two dimensions, Clarendon Press, Oxford, 1987).

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>
`1r` - real processed 1D data

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>/
`1i` - imaginary processed data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

HT

SEE ALSO

ft, ift, trf, trfp

ift

NAME

ift - Inverse Fourier transform (1D)

DESCRIPTION

The command ***ift*** performs an inverse Fourier transform of a 1D spectrum, thus creating an artificial FID. Normally, ***ift*** is done when the raw data do not exist any more. If, however, raw data do exist, they are not overwritten. ***ift*** stores the resulting FID as processed data, i.e. it overwrites the current spectrum.

After ***ift***, you can create pseudo-raw data with the command ***genfid*** which creates a new dataset. Note that the number of data points of the pseudo-raw data, is twice the size of the processed data they are created from. The acquisition status parameter TD (***dpa***) is set accordingly; TD = 2*SI.

INPUT FILES

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

`1r`, `1i` - processed 1D data (frequency domain)

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (time domain)
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

IFT

SEE ALSO

genfid, ft, trf, trfp

ls, rs

NAME

ls - Left shift data NSP points (1D)
rs - Right shift data NSP points (1D)

DESCRIPTION

The command ***ls*** shifts 1D data to the left. The number of points shifted is determined by the parameter NSP. The right end of the data is filled with NSP zeroes.

rs shifts 1D data to the right. The number of points shifted is determined by the parameter NSP. The left end of the data is filled with NSP zeroes.

Depending on the parameter DATMOD, ***rs*** and ***ls*** work on raw or processed data.

The value of NSP is the number of the real plus imaginary data points that are shifted. As such, the real data are shifted NSP/2 points and the imaginary data are shifted NSP/2 points. For odd values of NSP the real and imaginary data points are interchanged. As such the displayed spectrum is not only shifted but also changes from real (absorption) to imaginary (dispersion) or vice versa. Note that his only plays a role for DATMOD = proc.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***nsp***, ***datmod*** etc.:

NSP - number of points to be shifted
DATMOD - data mode: work on ’raw’ or ’proc’essed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if DATMOD = raw)

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

`1r`, `1i` - processed 1D data (input if DATMOD = proc*)*
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

LS

RS

SEE ALSO

pk

mc

NAME

mc - Magnitude calculation (1D)

DESCRIPTION

The command ***mc*** calculates the magnitude spectrum of a 1D dataset. The intensity of each point i is replaced by its absolute value according to the formula:

$$ABS(i) = \sqrt{(R(i)^2 + I(i)^2)}$$

Figure 3.10

where R and I are the real and imaginary part of the spectrum, respectively. If no processed input data exist, ***mc*** works on the raw data.

mc can also be started from the phase correction dialog box which is opened with ***ph***.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw 1D data (input if `1r`, `1i` do not exist)

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

`1r`, `1i` - processed 1D data (input if they exist)

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

MC

SEE ALSO

ps, pk, apk, trf, trfp

mul, mulc, nm, div, adsu

NAME

mul - Multiply two datasets (1D)
mulc - Multiply data with a constant (1D)
nm - Negate data (1D)
div - Divide two datasets (1D)
adsu - Open add/subtract/multiply dialog box (1D, 2D)

DESCRIPTION

Multiplication commands can be entered on the command line or started from the add/subtract/multiply dialog box. The latter is opened with ***adsu***.

This dialog box offers several options, each of which selects a certain command for execution.

Multiply with 1D spectrum/fid

This option selects the command ***mul*** for execution. It multiplies the current dataset with the second dataset. The result is stored in the current dataset.

Multiply with constant

This option selects the command ***mulc*** for execution. It multiplies the current data with the value of DC.

Multiply with -1

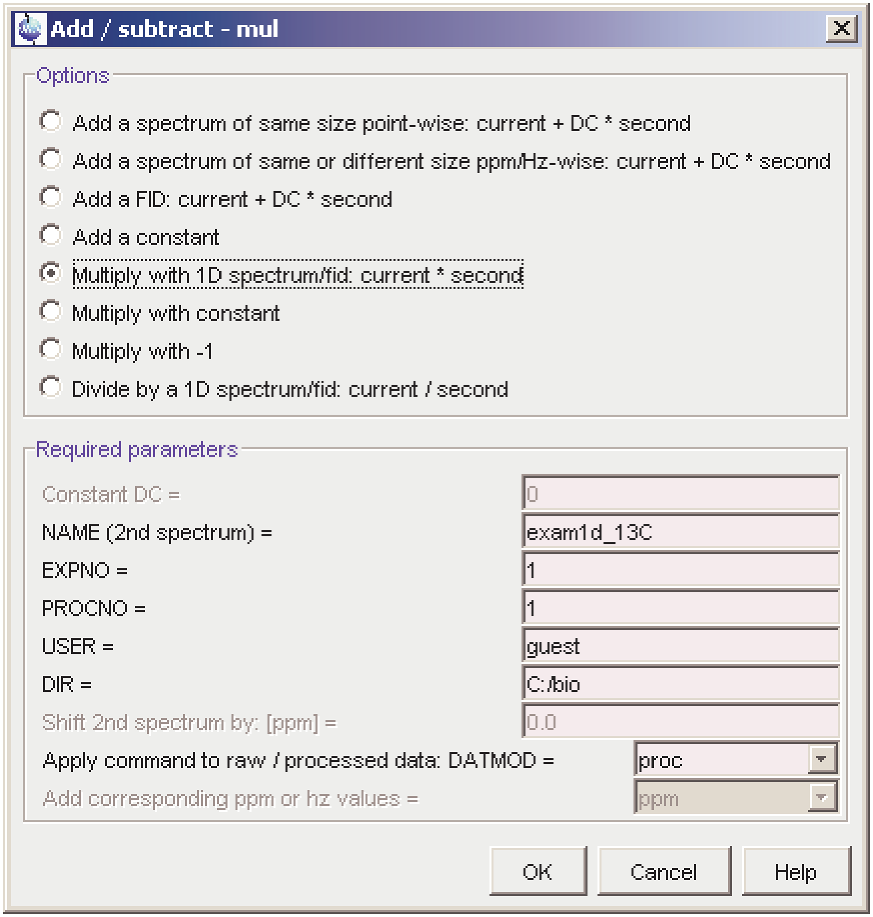
This option selects the command ***nm*** for execution. It negates the current data which means all data points are multiplied by -1.

Divide by 1D spectrum/fid

This option selects the command ***div*** for execution. It divides the current dataset by the second dataset.

mul/***div*** perform a complex multiplication/division on complex spectra. This requires that for both the current and second dataset:

- the status parameter FT_mod = fqc or fsc
- real (file `1r`) and imaginary (file `1i`) data exist



Add / subtract - mul

Options

- ○ Add a spectrum of same size point-wise: current + DC * second
- ○ Add a spectrum of same or different size ppm/Hz-wise: current + DC * second
- ○ Add a FID: current + DC * second
- ○ Add a constant
- ● Multiply with 1D spectrum/fid: current * second
- ○ Multiply with constant
- ○ Multiply with -1
- ○ Divide by a 1D spectrum/fid: current / second

Required parameters

Constant DC =	0
NAME (2nd spectrum) =	exam1d_13C
EXPNO =	1
PROCNO =	1
USER =	guest
DIR =	C:/bio
Shift 2nd spectrum by: [ppm] =	0.0
Apply command to raw / processed data: DATMOD =	proc
Add corresponding ppm or hz values =	ppm

Figure 3.11

This is the case for most data that have been acquired in Avance spectrometers. If the above requirements are not fulfilled, real and imaginary data are multiplied/divided pointwise. When a complex operation has been performed, this is reported in the audit trail output file.

`mul`, ***`div`***, ***`mulc`*** and ***`nm`*** work on raw or on processed data, depending on the value of DATMOD. The result is always stored as processed data in the current dataset. The raw data are not overwritten.

When ***`mul`*** and ***`div`*** are started from the command line, they will run without user interaction if the second dataset is already defined (file `curdat2`). If this is not defined, the ***adsu*** dialog box will be opened. When you run a multiplication or division command from the command line, make sure that the required parameters are set. Click the ***Procpars*** tab or enter ***edp*** to do that.

The ***adsu*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***adsu*** dialog box, with ***edp*** or by typing ***dc***, ***datmod*** etc.:

DC - multiplication factor (input of ***mulc***)
DATMOD - data mode: work on ’raw’ or ’proc’essed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if DATMOD = raw)

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

`1r`, `1i` - processed 1D data (input if DATMOD = proc)
`proc` - processing parameters
curdat2 - definition of the second dataset

<dir2>/data/<user2>/nmr/<name2>/<expno2>/

`fid` - second raw data (input if DATMOD = raw)

<dir2>/data/<user2>/nmr/<name2>/<expno2>/pdata/<procno2>/

`1r`, `1i` - processed 1D data (input if DATMOD = proc*)*

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

MUL

MULC

NM

DIV

SEE ALSO

add, addc, addfid

pk

NAME

pk - Phase correction according to PHC0/PHC1 (1D)

DESCRIPTION

The command ***pk*** performs a zero and first order phase correction according to user defined phase values. These phase values are read from the processing parameters PHC0 and PHC1.

The data, consisting of real points R(i) and imaginary points I(i) are phase corrected according to the formula:

$$\begin{aligned} R0(i) &= R(i)\cos a(i) - I(i)\sin a(i) \\ I0(i) &= I(i)\cos a(i) + R(i)\sin a(i) \end{aligned}$$

Figure 3.12

where:

$$a(i) = PHC0 + (i-1)PHC1$$

Figure 3.13

where i > 0, R0 and I0 represent the corrected values and PHC0 and PHC1 are processing parameters.

pk does not calculate the phase values but uses the preset values. Therefore, ***pk*** is only useful when these values are known. They can be determined, interactively, in Phase correction mode or, automatically, with ***apk*** or ***apks***.

pk is typically used in a series of experiments where the first spectrum is corrected with ***apk*** and each successive spectrum with ***pk***, using the same values (see for example AU program ***proc_noe***).

pk applies but does not change the processing parameters PHC0 and PHC1 (***edp***). It does, however, change the corresponding processing status parameters PHC0 and PHC1 (***dpp***), by adding the applied phase values.

pk is a part of the composite processing commands ***efp***, ***fp*** and ***gfp***.

pk can also be used to perform a phase correction on an FID rather than a spectrum. This is automatically done if you enter ***pk*** on a dataset which does not contain processed data. Phase correction on an FID is used prior to Fourier transform to induce a shift in the resulting spectrum. The spectrum is shifted according to the value of PHC1; one real data point to the left for each 360°. A negative value of PHC1 causes a right shift. The points which are cut off on one side of the spectrum are appended on the other side. Note the difference with performing a left shift (***ls***) or right shift (***rs***) after Fourier transform. This appends zeroes at the opposite side. If processed data do exist and you still want to do a phase correction on the FID, you can do this with the command ***trf***.

The command ***pk*** can also be started from the phase correction dialog box which is opened with ***ph***.

INPUT PARAMETERS

set from the ***ph*** dialog box, with ***edp*** or by typing ***phc0***, ***phc1*** etc.:

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s phc0***, ***s phc1*** etc.:

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if no processed data exist)

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

`1r`, `1i` - processed 1D data (input if they exist)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

PK

SEE ALSO

mc, ps, apk, trf, trfp

prguide

NAME

prguide - Open the Processing Guide (1D,2D,3D)

DESCRIPTION

The command ***prguide*** opens the TOPSPIN Processing Guide (see Figure 3.14). This contains a workflow for processing data, especially suited for new or occasional users. In ***Automatic mode***, the Processing Guide will simply execute a processing command when you click the corresponding button. This requires the processing parameters to be set correctly. In interactive mode (***Automatic mode*** unchecked), the Processing Guide will, at each step, open a dialog box offering you the available options and required parameters. For example, the phase correction button offers various automatic algorithms as well as an option to switch to interactive phasing mode.

Experienced users normally enter the individual processing commands from the command line. This requires that, for each command, the processing parameters are set correctly.

The Processing Guide can be used for 1D and 2D processing.

SEE ALSO

aqguide, t1guide, managuide, solaguide

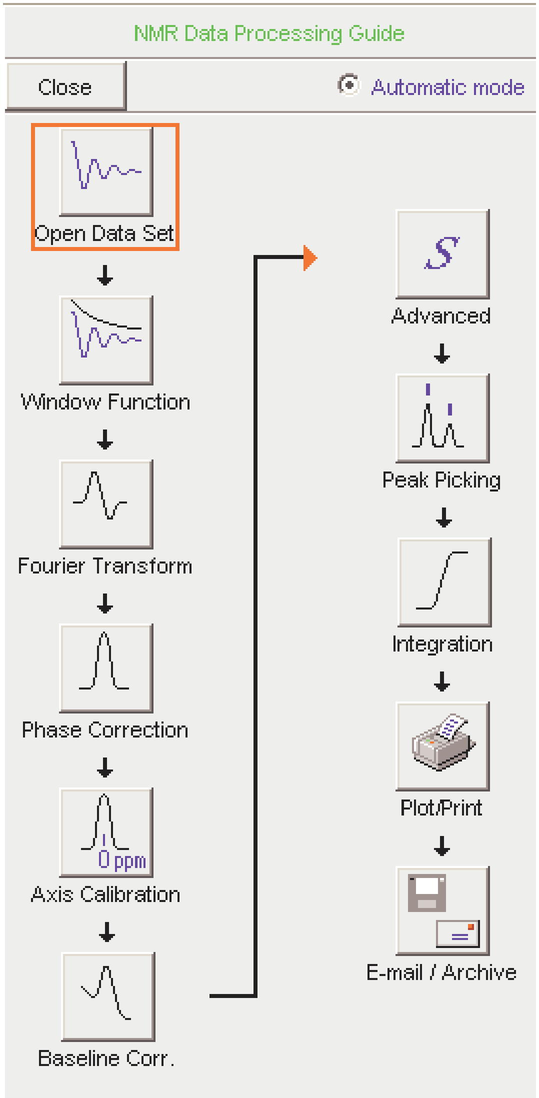

NMR Data Processing Guide
Close
Automatic mode
Open Data Set
Window Function
Fourier Transform
Phase Correction
0 ppm
Axis Calibration
Baseline Corr.
S
Advanced
Peak Picking
Integration
Plot/Print
E-mail / Archive

Figure 3.14

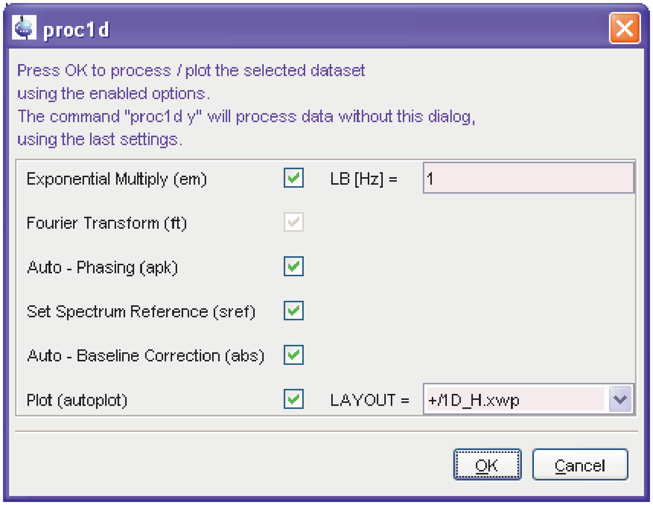
proc1d

NAME

proc1d - Open 1D Processing dialog

DESCRIPTION

The command ***proc1d*** opens a 1D processing dialog (see Figure 3.15).



Press OK to process / plot the selected dataset
using the enabled options.
The command "proc1d y" will process data without this dialog,
using the last settings.

Exponential Multiply (em) ☑ LB [Hz] = 1

Fourier Transform (ft) ☑

Auto - Phasing (apk) ☑

Set Spectrum Reference (sref) ☑

Auto - Baseline Correction (abs) ☑

Plot (autoplot) ☑ LAYOUT = +/1D_H.xwp

Figure 3.15

This dialog can be used for standard 1D processing, including exponential multiplication, Fourier transform, phase correction, referencing, baseline correction and plotting. Processing steps can be switched on or off and two parameters, line broadening and plot layout, can be set. The command takes one argument:

```
proc1d y
```

will process the current dataset without opening the dialog, using the last settings.

SEE ALSO

prguide

ps

NAME

ps - Calculate power spectrum (1D)

DESCRIPTION

The command ***ps*** calculates the power spectrum of the 1D current dataset, replacing the intensity of each data point *i* according to the formula:

$$PS(i) = R(i)^2 + I(i)^2$$

Figure 3.16

where R and I are the real and imaginary part of the spectrum, respectively. If no processed input data exist, ***ps*** works on the raw data. The result is always stored as the real processed data.

ps can also be started from the phase correction dialog box which is opened with ***ph***.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if no processed data exist)

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

`1r`, `1i` - processed 1D data (real, imaginary)

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

PS

SEE ALSO

mc, pk, apk, trf, trfp

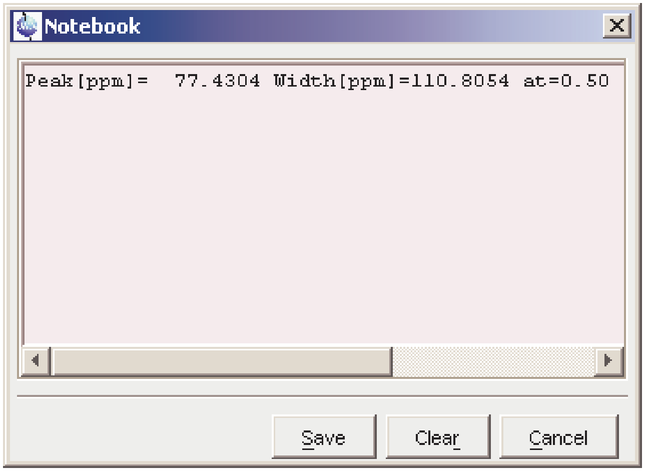
peakw

NAME

peakw - Calculate width of highest peak in displayed region (1D)

DESCRIPTION

The command ***peakw*** calculates the peak width at half height of the highest peak in the displayed region. The result is stored in the notebook and displayed on the screen:



```
Peak[ppm]=   77.4304 Width[ppm]=110.8054 at=0.50
```

Figure 3.17

The command can also be used with one argument, the height at which the width must be calculated:

peakw <height>

For example, ***peakw 0.66*** calculates the width of the highest peak in the displayed region at 66% of the height.

OUTPUT FILES

`<userprop>/notebook.txt` - notebook text file

SEE ALSO

nbook

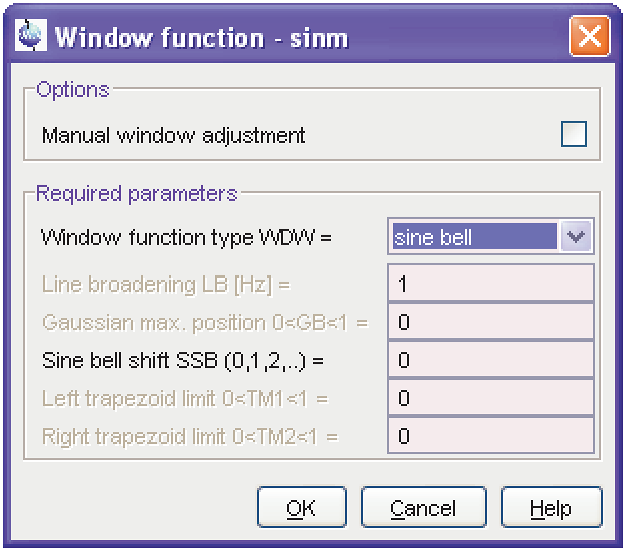
sinm, qsin, sinc, qsinc, wm

NAME

sinm - Sine window multiplication of the FID (1D)
qsin - Sine squared window multiplication of the FID (1D)
sinc - Sinc window multiplication of the FID (1D)
qsinc - Sinc squared window multiplication of the FID (1D)
wm - Open window multiplication dialog box (1D,2D)

DESCRIPTION

Window multiplication commands can be started from the command line or from the window function dialog box. The latter is opened with the command ***wm*** (see Figure 3.18).



Manual window adjustment □

Window function type WDW = sine bell

Line broadening LB [Hz] = 1

Gaussian max. position 0<GB<1 = 0

Sine bell shift SSB (0,1,2,..) = 0

Left trapezoid limit 0<TM1<1 = 0

Right trapezoid limit 0<TM2<1 = 0

Figure 3.18

This dialog box offers several window functions, each of which selects a certain command for execution.

Sine bell

This window function selects the command ***sinm*** for execution. It performs a sine window multiplication, according to the function:

$$SINM(t) = \sin((\pi - PHI) \cdot (t/AQ) + PHI)$$

Figure 3.19

where

$$0 < t < AQ \text{ and } PHI = \pi/SBB$$

Figure 3.20

where AQ is an acquisition status parameter and SSB a processing parameter.

Typical values are SSB = 1 for a pure sine function and SSB = 2 for a pure cosine function. Values greater than 2 give a mixed sine/cosine function. Note that all values smaller than 2, for example 0, have the same effect as SSB = 1, namely a pure sine function.

Squared sine bell

This window function selects the command ***qsin*** for execution. It performs a sine squared window multiplication, according to the function:

$$QSIN(t) = \sin((\pi - PHI) \cdot (t/AQ) + PHI)^2$$

Figure 3.21

where

$$0 < t < AQ \text{ and } PHI = \pi / SBB$$

Figure 3.22

where AQ is an acquisition status parameter and SSB a processing parameter.

Typical values are SSB = 1 for a pure sine function and SSB = 2 for a pure cosine function. Values greater than 2 give mixed sine/cosine functions. Note that all values smaller than 2 have the same effect as SSB = 1, namely a pure sine function.

Sinc

This window function selects the command ***sinc*** for execution. It performs a sinc window multiplication, according to the function:

$$SINC(t) = \frac{\sin t}{t}$$

Figure 3.23

where

$$-2\pi \cdot SBB \cdot GB < t < 2\pi \cdot SSB \cdot (1 - GB)$$

Figure 3.24

and SSB and GB are processing parameters.

Squared sinc

This window function selects the command ***qsinc*** for execution. It performs a sinc squared window multiplication, according to the function:

$$QSINC(t) = \left(\frac{\sin t}{t}\right)^2$$

Figure 3.25

where

$$-2\pi \cdot SBB \cdot GB < t < 2\pi \cdot SSB \cdot (1 - GB)$$

Figure 3.26

and SSB and GB are processing parameters.

The ****sin**** commands implicitly perform a baseline correction of the FID, according to the processing parameter BC_mod. Furthermore, they perform linear prediction according to the parameters ME_mod, NCOEF and LPBIN.

If you run a command like ***sinm*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.

When executed on 2D or 3D data, the ****sin**** commands take up to four arguments, e.g.:

sinm <row> <procno> n y

process the specified row and store it under the specified *procno*. The last two arguments are optional: ***n*** prevents changing the display to the output 1D data, ***y*** causes a possibly existing data to be overwritten without warning.

When executed on a dataset with 2D or 3D raw data but 1D processed data[1], the ***sin**** commands take one argument:

sinm <row>

process the specified row and store it under the current *procno*.

sinm same

process the same row as the previous processing command and store it under the current *procno*. The ***same*** option is automatically used by the AU program macros *SIN*. When used on a regular 1D dataset (i.e. with 1D raw data) it has no effect.

The ***wm*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***wm*** dialog box, with ***edp*** or by typing ***ssb***, ***gb*** etc.:

SSB - sine bell shift
GB - Gaussian broadening factor (input of ***sinc*** and ***qsinc***)

set by the acquisition, can be viewed with ***dpa*** or ***s aq***:

AQ - Acquisition time (input of ***sinm*** and ***qsin***)

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if `1r`, `1i` do not exist or are Fourier transformed)
`acqus` - acquisition status parameters

[1] Usually a result of ***rsr***, ***rsc*** or a previous 1D processing command on that 2D or 3D data.

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

`1r`, `1i` - processed data (input if they exist but are not Fourier transformed)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

SINM

QSIN

SINC

QSINC

SEE ALSO

em, gm, tm, traf, trafs

rv

NAME

rv - Reverse spectrum or FID (1D)

DESCRIPTION

The command ***rv*** reverses the data with respect to the middle data point, i.e. the leftmost data point becomes the rightmost point and vice versa. The real and imaginary parts of the spectrum are thereby interchanged. Depending on the value of DATMOD, ***rv*** works on the raw or on the processed data. The result is always store as processed data.

A spectrum can also be reversed as a part of the Fourier transform by setting the processing parameter REVERSE to TRUE.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***datmod*** :
DATMOD - data mode: work on ’raw’ or ’proc’essed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if DATMOD = raw)

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

`1r`, `1i` - processed 1D data (input if DATMOD = proc)

`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data

`procs` - processing status parameters

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

RV

SEE ALSO

ft, trf

sab

NAME

sab - Spline baseline correction (1D)

DESCRIPTION

The command ***sab*** performs a spline baseline correction. This is based on a predefined set of data points which are considered to be a part of the baseline. The regions between these points are individually fitted. In order to execute ***sab***, the baseline points must have been determined. You can do this as follows:

1. Click or enter ***.basl*** to change to baseline correction mode.
2. Click to switch to *Define baseline points* mode

   (if the baseline points have been defined before, you are first prompted to append to (a) or overwrite (o) the existing list of points)
3. Move the cursor along the spectrum and click the left mouse button at several positions which are part of the baseline.
4. Click to return. The command ***sab*** is automatically executed.

The set of baseline points is saved in the file `baslpnts`. This file can be stored for general usage with the command ***wmisc***. After that, you can read it with ***rmisc*** on another dataset and run ***sab*** to perform the same baseline correction.

sab can be started from the command line or from the baseline dialog box which is opened with the command ***bas***.

INPUT FILES

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

`1r` - real processed 1D data
`baslpnts` - baseline points (points and ppm values)

OUTPUT FILES

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

`1r` - real processed 1D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

SAB

SEE ALSO

bas, bcm, .basl

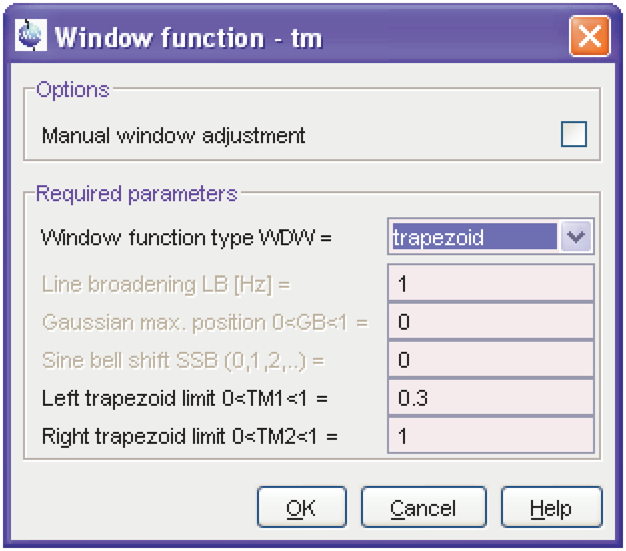
tm, traf, trafs, wm

NAME

tm - Trapezoidal window multiplication of the FID (1D)
traf - Traficante window multiplication of the FID (1D)
trafs - Traficante window multiplication of the FID (1D)
wm - Open window function dialog box (1D,2D)

DESCRIPTION

Window multiplication can be executed from the command line or from the window function dialog box. The latter is opened with the command ***wm*** (see Figure 3.27).



Manual window adjustment □

Window function type WDW =	trapezoid
Line broadening LB [Hz] =	1
Gaussian max. position 0<GB<1 =	0
Sine bell shift SSB (0,1,2,..) =	0
Left trapezoid limit 0<TM1<1 =	0.3
Right trapezoid limit 0<TM2<1 =	1

Figure 3.27

This dialog box offers several window functions, each of which selects a certain command for execution.

Trapezoid

This function selects the command ***tm*** for execution. It performs a trapezoidal window multiplication of the FID. The rising and falling edge of this function are defined by the processing parameters TM1 and TM2. These represent a fraction of the acquisition time as displayed below.

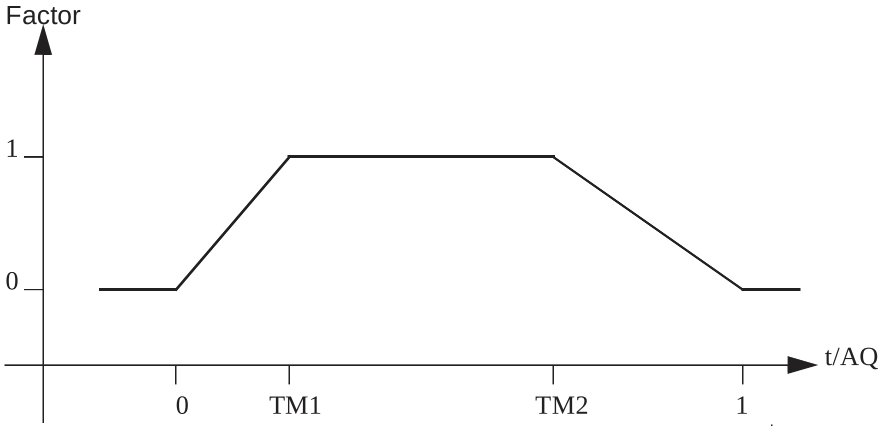


Figure 3.28

Traficante and trafic.s/n

This function selects the commands ***traf*** and ***trafs*** , respectively, for execution. The algorithms used by these commands are described by D. D. Traficante and G. A. Nemeth in J. Magn. Res., 71**,** 237 (1987).

tm, ***traf*** and ***trafs*** implicitly perform a baseline correction of the FID, according to the processing parameter BC_mod. Furthermore, they perform linear prediction according to the parameters ME_mod, NCOEF and LPBIN.

When executed on 2D or 3D data, ***tm*** and ***traf**** take up to four arguments, e.g.:

tm <row> <procno> n y

process the specified row and store it under the specified *procno*. The last two arguments are optional: ***n*** prevents changing the display to the output 1D data, ***y*** causes a possibly existing data to be overwritten without warning.

If you run a command like ***tm*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.

When executed on a dataset with 2D or 3D raw data but 1D processed data[1], ***tm*** and ***traf**** take one argument, e.g.:

tm <row>

process the specified row and store it under the current *procno*.

tm same

process the same row as the previous processing command and store it under the current *procno*. The ***same*** option is automatically used by the AU program macro TM. When used on a regular 1D dataset (i.e. with 1D raw data) it has no effect.

The ***wm*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***wm*** dialog box, with ***edp*** or by typing ***tm1***, ***lb*** etc.:

TM1 - the end of the rising edge of a trapeziodal window (input of ***tm***)
TM2 - the start of the falling edge of a trapezoidal window (input of ***tm***)
LB - Lorentzian broadening factor (input of ***traf****)

set by the acquisition, can be viewed with ***dpa*** or ***s aq***:

AQ - acquisition time (input of ***tm***)

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if `1r`, `1i` do not exist or are Fourier transformed)
`acqus` - acquisition status parameters

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

`1r`, `1i` - processed data (input if they exist but are not Fourier transformed)

[1] Usually a result of ***rsr***, ***rsc*** or a previous 1D processing command on that 2D or 3D data.

`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TM

SEE ALSO

em, gm, sinm, qsin, sinc, qsinc

trf, trfp

NAME

trf - User defined processing of raw data (1D)
trfp - User defined processing of processed data (1D)

DESCRIPTION

The command ***`trf`*** processes the raw data performing the following steps:

- baseline correction according to BC_mod
- linear prediction according to ME_mod
- window multiplication according to WDW
- Fourier transform according to FT_mod
- phase correction according to PH_mod

`trf` offers the following features:

- when all parameters mentioned above are set to *no*, the raw data (file `fid`) are simply stored as processed data (files `1r`, `1i`). The even points are stored as real data (file `1r`) and the odd points as imaginary data (file `1i`). The size of these processed data and the number of input FID points are determined by the parameters SI and TDeff, as described for the command ***`ft`***. For example, if 0 < TDeff < TD, the processed data are truncated. This allows you to create an FID with a smaller size than the original one (see also the command ***`genfid`***).
- ***`trf`*** evaluates BC_mod for the baseline correction mode (e.g. quad, qpol or qfil) and detection mode (e.g. single or quad, spol or qpol, sfil or qfil). Note that the command ***`bc`*** evaluates the acquisition status parameter AQ_mod for the detection mode and ignores the BC_mod detection mode (see parameter BC_mod).
- ***`trf`*** evaluates WDW for the window multiplication mode (*em*, *gm*, *sine*, *qsine*, *trap*, *user*, *sinc*, *qsinc*, *traf* or *trafs*). This allows you to vary the window multiplication by varying the value of WDW rather than the window multiplication command. This can be useful in AU programs.

- the Fourier transform is performed according to FT_mod. Normally, the Fourier transform is done with the command ***ft*** which determines the Fourier transform mode from acquisition status parameter AQ_mod. However, for some datasets, no value of AQ_mod translates to a correct Fourier transform mode. An example of this is when you read a column (with ***rsc***) from a 2D dataset which was measured with FnMODE (or MC2) = States-TPPI and Fourier transformed in the F2 direction only. The resulting FID can only be Fourier transformed correctly with ***trf***. The parameter FT_mod is automatically set to the correct value by the ***rsc*** command. ***trf*** can also be used manipulate the acquisition mode of raw data by Fourier transforming the data with one FT_mod and inverse Fourier transforming them with a different FT_mod. From the resulting data you could create pseudo-raw data (using ***genfid***) with a different acquisition mode than the original raw data. Finally, ***trf*** allows you to process the data without Fourier transform (FT_mod = no). Table 3.3 shows a list of FT_mod values:

FT_mod	Fourier transform mode
no	no Fourier transform
fsr	forward, single channel, real
fqr	forward, quadrature, real
fsc	forward, single channel, complex
fqc	forward, quadrature, complex
isr	inverse, single channel, real
iqr	inverse, quadrature, real
isc	inverse, single channel, complex
iqc	inverse, quadrature, complex

Table 3.3

The command ***trfp*** works like ***trf***, except that it always works on processed data. If no processed data exist, ***trfp*** stops with an error message.

trfp can be used to perform multiple additive baseline corrections, to remove multiple frequency baseline distortions. This cannot be done with ***bc*** or ***trf*** because these commands always work on the raw data, i.e. they are not additive. Note that the window multiplication commands (e.g. ***em***, ***gm***, ***sine*** etc.) are additive. The same counts for linear prediction (part of ***ft***) and phase correction (***pk***).

trf can be used to do a combination of forward and backward prediction. Just run ***trf*** with ME_mod = LPfc and then ***trfp*** (or ***ft***) with ME_mod = LPbc.

When executed on a 2D or 3D dataset, ***trf*** takes up to four arguments:

trf <row> <procno> n y

process the specified row and store it under the specified *procno*. The last two arguments are optional: ***n*** prevents changing the display to the output 1D data, ***y*** causes a possibly existing data to be overwritten without warning.

When executed on a dataset with 2D or 3D raw data but 1D processed data[1], ***trf*** takes one argument:

trf <row>

process the specified row and store it under the current *procno*.

trf same

process the same row as the previous processing command and store it under the current *procno*. The ***same*** option is automatically used by the AU program macro TRF. When used on a regular 1D dataset (i.e. with 1D raw data), it has no effect.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***si***, ***tdeff*** etc.:

SI - size of the processed data
TDeff - number of raw data points to be used for processing
FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
BC_mod - FID baseline correction mode

[1] Usually a result of ***rsr***, ***rsc*** or a previous 1D processing command on that 2D or 3D data.

BCFW - filter width for BC_mod = sfil or qfil
COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil

ME_mod - FID linear prediction mode

NCOEF - number of linear prediction coefficients
LPBIN - number of points for linear prediction
TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode

LB - Lorentzian broadening factor for WDW = em or gm
GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
TM1, TM2 - limits of the trapezoidal window for WDW = trap

FT_mod - Fourier transform mode

REVERSE - flag indicating to reverse the spectrum
PKNL - group delay compensation (Avance) or filter correction (A*X)
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform

PH_mod - phase correction mode

PHC0 - zero order phase correction value for PH_mod = pk
PHC1 - first order phase correction value for PH_mod = pk

set by the acquisition, can be viewed with ***dpa*** or by typing ***s td*** :

TD - time domain; number of raw data points

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s tdeff*** etc.:

TDeff - number of raw data points that were used for processing
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
NC_proc - intensity scaling factor
YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
BYTORDP - data storage order

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input of ***trf***)
`acqus` - F2 acquisition status parameters

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

`1r`, `1i` - processed 1D data (input of ***`trfp`***)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TRF

TRFP

SEE ALSO

ftf, ft, bc, em, pk

zf

NAME

zf - Zero all data points (1D)

DESCRIPTION

The command ***zf*** sets the intensity of all data points to zero. Depending on the value of the parameter DATMOD, ***zf*** works on raw or processed data. The result is always stored as processed data, the raw data are never overwritten.

The output of ***zf*** is usually the same for DATMOD = raw or processed, namely SI processed data points with zero intensity. However, for DATMOD = proc, the existing processed data are set to zero whereas for DATMOD = raw, new processed data are created according to the current processing parameters. The result is different when the data have been Fourier transformed with STSI < SI. ***zf*** with DATMOD = proc creates STSI zeroes whereas ***zf*** with DATMOD = raw creates SI zeroes. The reason is that ***zf*** with DATMOD = raw reprocesses the raw data but does not interpret STSI since no Fourier transform is done.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***datmod***, ***si*** etc.:

DATMOD - data mode: work on ’raw’ or ’proc’essed data
SI - size of the processed data
STSI - strip size (input if DATMOD = proc)

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if DATMOD = raw)

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

`1r`, `1i` - processed 1D data (input if DATMOD = proc)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

ZF

SEE ALSO

zp

zp

NAME

zp - Zero the first NZP data points (1D)

DESCRIPTION

The command ***zp*** sets the intensity of the first NZP points of the dataset to zero. It works on raw or processed data depending on the value of the parameter DATMOD. The parameter NZP can take a value between 0 and the size of the FID or spectrum.

The value of NZP is the number of the real plus imaginary data points that are zeroed. As such, the first (NZP+1)/2 real points and the first NSP/2 imaginary data points are zeroed.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***nzp***, ***datmod*** etc.:

NZP - number of data points set to zero intensity
DATMOD - data mode: work on 'raw' or 'proc'essed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (input if DATMOD = raw)

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

`1r`, `1i` - processed 1D data (input if DATMOD = proc)
`proc` - processing parameters

OUTPUT FILES

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

`1r`, `1i` - processed 1D data (real, imaginary)
`procs` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

ZP

SEE ALSO

zf

Chapter 4

2D processing commands

This chapter describes all TOPSPIN 2D processing commands. Most of them only work on 2D data but some, e.g. ***xfb***, can also be used to process a plane of 3D data. They store their output in processed data files and do not change the raw data.

We will often refer to the two directions of a 2D dataset as the F2 and F1 direction. F2 is the acquisition direction which is displayed horizontally and F1 the orthogonal direction which is displayed vertically. The names of most 2D processing commands express the direction in which they work, e.g. ***xf2*** works in F2, ***xf1*** in F1 and ***xfb*** in both directions. F2 traces are usually referred to as rows, F1 traces as columns. Some commands express this terminology, e.g. ***rsr*** reads and stores rows and ***rsc*** reads and stores columns of a 2D spectrum.

For each command, the relevant input and output parameters are mentioned. Furthermore, the relevant input and output files and their location are mentioned. Although file handling is completely transparent, it is sometimes useful to know which files are involved and where they reside. For example, if you have permission problems or if you want to process or interpret your data with third party software.

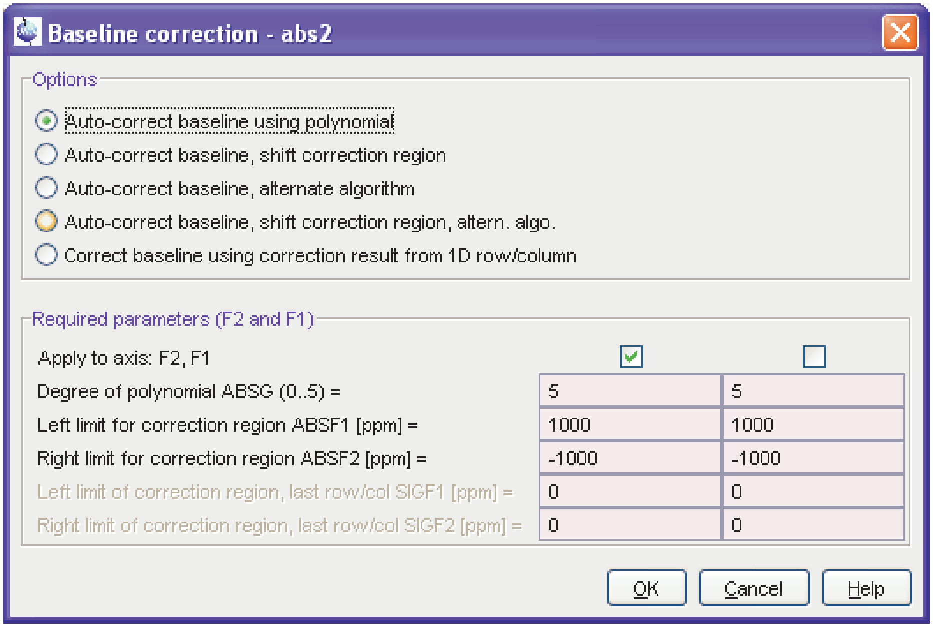
abs2, abst2, absd2, absot2, bas

NAME

abs2 - Automatic baseline correction in F2 (2D)
abst2 - Automatic selective baseline correction in F2 (2D)
absd2 - Automatic baseline correction in F2, diff. algorithm (2D)
absot2 - Automatic selective baseline correction in F2, diff. algorithm (2D)
bas - Open baseline correction dialog box (1D,2D)

DESCRIPTION

Baseline correction commands can be started from the command line, by entering ***abs2***, ***abst2*** etc. or from the baseline dialog box. The latter is opened with the command ***bas***:



Options

● Auto-correct baseline using polynomial
○ Auto-correct baseline, shift correction region
○ Auto-correct baseline, alternate algorithm
○ Auto-correct baseline, shift correction region, altern. algo.
○ Correct baseline using correction result from 1D row/column

Required parameters (F2 and F1)

Apply to axis: F2, F1	☑	□
Degree of polynomial ABSG (0..5) =	5	5
Left limit for correction region ABSF1 [ppm] =	1000	1000
Right limit for correction region ABSF2 [ppm] =	-1000	-1000
Left limit of correction region, last row/col SIGF1 [ppm] =	0	0
Right limit of correction region, last row/col SIGF2 [ppm] =	0	0

Figure 4.1

This dialog box offers several options, each of which selects a certain command for execution. The command further depends on the selected direction. Here we describe the commands for the F2 direction.

F2 Auto-correct baseline using polynomial

This option selects the command ***abs2*** for execution. It performs an automatic baseline correction in the F2 direction. This means it subtracts a polynomial from the rows of the processed 2D data. The degree of the polynomial is determined by the parameter ABSG which has a value between 0 and 5, with a default of 5. It works like ***absf*** in 1D which means it only corrects the spectral region between ABSF1 and ABSF2.

F2 Auto-correct baseline, shift correction region

This option selects the command ***abst2*** for execution. It performs an automatic selective baseline correction in the F2 direction. This means it corrects the rows of the processed 2D data. It works like ***abs2***, except for the following:

- only the rows between F1-ABSF2 and F1-ABSF1 are corrected
- the part (region) of each row which is corrected shifts from row to row. The first row is corrected between F2-ABSF2 and F2-ABSF1. The last row is corrected between F2-SIGF2 and F2-SIGF1. For intermediate rows, the low field limit is an interpolation of F2-ABSF2 and F2-SIGF2 and the high field limit is an interpolation of F2-ABSF1 and F2-SIGF1.

F2 Auto-correct baseline, alternate algorithm

This option selects the command ***absd2*** for execution. It works like ***abs2***, except that it uses a different algorithm[1]. It is, for example, used when a small peak lies on the foot of a large peak. In that case, ***absd2*** allows you to correct the baseline around the small peak which can then be integrated. Usually ***absd2*** is followed by ***abs2***.

F2 Auto-correct baseline, shift correction region, alternate algorithm

This option selects the command ***absot2*** for execution. It works like ***abst2***, except that it has a different algorithm which applies a larger correction.

[1] It uses the same algorithm as the command ***abs*** in DISNMR

If you run a command like ***abs2*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.
The ***bas*** command can be used on 1D, 2D or 3D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***bas*** dialog box, with ***edp*** or by typing ***absg***, ***absf1*** etc.:

ABSG - degree of the polynomial to be subtracted (0 to 5, default is 5)
ABSF1 - low field limit of the region which is baseline corrected
ABSF2 - high field limit of the region which is baseline corrected
SIGF1 - low field limit of the correction region in the last row
SIGF2 - high field limit of the correction region in the last row

INPUT FILES

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

`2rr` - real processed 2D data
`proc` - F2 processing parameters

OUTPUT FILES

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

`2rr` - real processed 2D data
`procs` - F2 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

ABS2

ABST2

ABSD2

ABSOT2

SEE ALSO

abs1, abst1, absd1, absot1

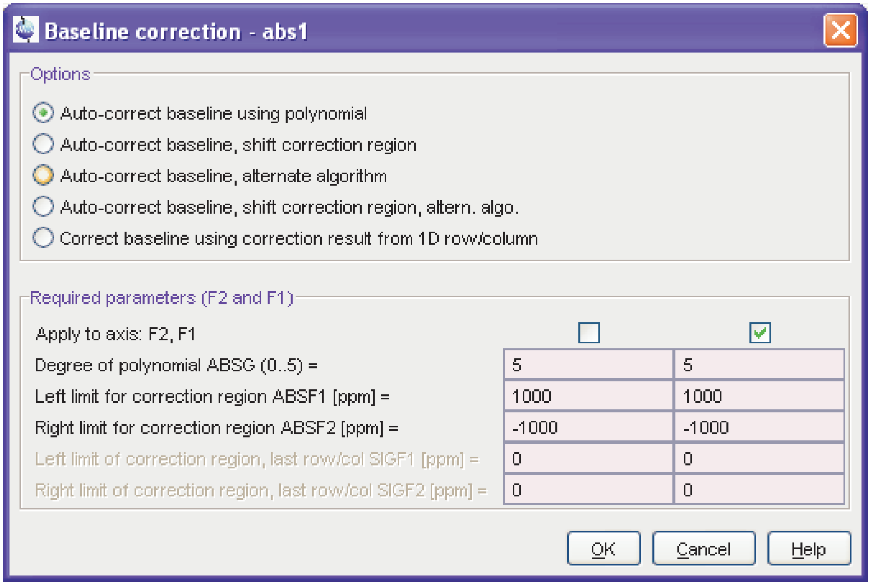
abs1, abst1, absd1, absot1, bas

NAME

abs1 - Automatic baseline correction in the F1 (2D)
abst1 - Automatic selective baseline correction in the F1 (2D)
absd1 - Automatic baseline correction in F1, diff. algorithm (2D)
absot1 - Automatic selective baseline correction in F1, diff. algorithm (2D)
bas - Open baseline correction dialog box (1D,2D)

DESCRIPTION

Baseline correction can be started from the command line, with ***abs1***, ***abst1*** etc., or from the baseline dialog box. The latter is opened with the command ***bas***



Options

● Auto-correct baseline using polynomial
○ Auto-correct baseline, shift correction region
○ Auto-correct baseline, alternate algorithm
○ Auto-correct baseline, shift correction region, altern. algo.
○ Correct baseline using correction result from 1D row/column

Required parameters (F2 and F1)

Apply to axis: F2, F1	□	☑
Degree of polynomial ABSG (0..5) =	5	5
Left limit for correction region ABSF1 [ppm] =	1000	1000
Right limit for correction region ABSF2 [ppm] =	-1000	-1000
Left limit of correction region, last row/col SIGF1 [ppm] =	0	0
Right limit of correction region, last row/col SIGF2 [ppm] =	0	0

Figure 4.2

This dialog box offers several options, each of which selects a certain command for execution.The command further depends on the selected direction. Here we describe the commands for the F1 direction.

F1 Auto-correct baseline using polynomial

This option selects the command ***abs1*** for execution. It performs an automatic baseline correction in the F1 direction. This means it subtracts a polynomial from the columns of the processed 2D data. The degree of the polynomial is determined by the parameter ABSG which has a value between 0 and 5, with a default of 5. It works like ***absf*** in 1D which means it only corrects the spectral region between ABSF1 and ABSF2.

F1 Auto-correct baseline, shift correction region

This option selects the command ***abst1*** for execution. It performs an automatic selective baseline correction in the F1 direction. This means it corrects the columns of the processed 2D data. It works like ***abs1***, except for the following:

- only the columns between F2-ABSF2 and F2-ABSF1 are corrected
- the part (region) of each column which is corrected shifts from column to column. The first column is corrected between F1-ABSF2 and F1-ABSF1. The last column is corrected between F1-SIGF2 and F1-SIGF1. For intermediate columns, the low field limit is an interpolation of F1-ABSF2 and F1-SIGF2 and the high field limit is an interpolation of F1-ABSF1 and F1-SIGF1.

F1 Auto-correct baseline, alternate algorithm

This option selects the command ***absd1*** for execution. It works like ***abs1***, except that it uses a different algorithm[1]. It is, for example, used when a small peak lies on the foot of a large peak. In that case, ***absd1*** allows you to correct the baseline around the small peak which can then be integrated. Usually ***absd1*** is followed by ***abs1***.

F1 Auto-correct baseline, shift correction region, alternate algorithm

This option selects the command ***absot1*** for execution. It works like ***abst1***, except that it has a different algorithm which applies a larger correction.

If you run a command like ***abs1*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that.

The ***bas*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***bas*** dialog box, with ***edp*** or by typing ***absf1***, ***absf2*** etc.:

ABSG - degree of the polynomial to be subtracted (0 to 5, default is 5)
ABSF1 - low field limit of the correction region in the first row
ABSF2 - high field limit of the correction region in the first row
SIGF1 - low field limit of the correction region in the last row
SIGF2 - high field limit of the correction region in the last row

INPUT FILES

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

`2rr` - real processed 2D data
`proc2` - F1 processing parameters

OUTPUT FILES

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

`2rr` - real processed 2D data
`proc2s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

ABS1

ABST1

ABSD1

ABSOT1

SEE ALSO

abs2, abst2, absd2, absot2

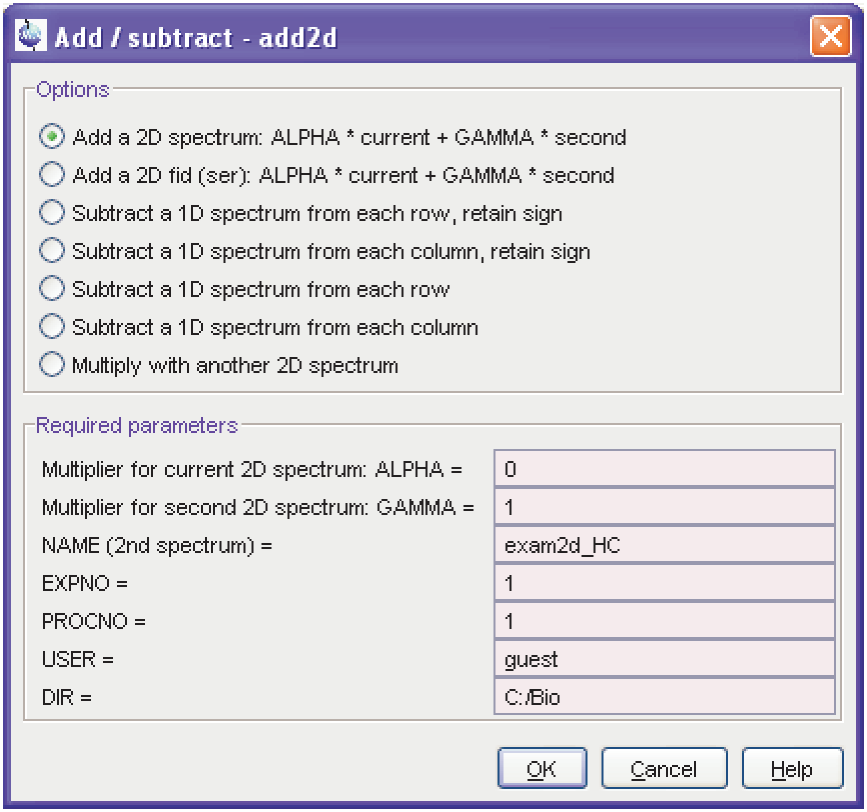
add2d, mul2d, addser, adsu

NAME

add2d - Add or subtract two datasets (2D)
mul2d -Multiply two datasets (2D)
addser - Add two raw datasets (2D)
adsu - Open add/subtract/multiply dialog box (1D, 2D)

DESCRIPTION

Addition commands can be started from the command line or from the add/subtract dialog box. The latter is opened with the command ***adsu***



Options

- ● Add a 2D spectrum: ALPHA * current + GAMMA * second
- ○ Add a 2D fid (ser): ALPHA * current + GAMMA * second
- ○ Subtract a 1D spectrum from each row, retain sign
- ○ Subtract a 1D spectrum from each column, retain sign
- ○ Subtract a 1D spectrum from each row
- ○ Subtract a 1D spectrum from each column
- ○ Multiply with another 2D spectrum

Required parameters

Multiplier for current 2D spectrum: ALPHA =	0
Multiplier for second 2D spectrum: GAMMA =	1
NAME (2nd spectrum) =	exam2d_HC
EXPNO =	1
PROCNO =	1
USER =	guest
DIR =	C:/Bio

Figure 4.3

(see Figure 4.3).

This dialog box offers several options, each of which selects a certain command for execution.

Add a 2D spectrum

This option selects the command ***add2d*** for execution. It adds the processed data of the second dataset to those of the current 2D dataset, according to the following formula:

current = ALPHA*current + GAMMA*second

where ALPHA and GAMMA are processing parameters. Both real and imaginary data are added. The result overwrites the current processed data. For APLHA = 1 and GAMMA = -1, the spectra are subtracted.

Multiply with another 2D spectrum

This option selects the command ***mul2d*** for execution. It multiplies the processed data of the second dataset with those of the current 2D dataset. Both real and imaginary data are multipied.The result overwrites the current processed data.

Add 2D fid (ser)

This option selects the command ***addser*** for execution. It adds the raw data of the second dataset to those of the current 2D dataset. The result overwrites the current raw data.

Caution: the two 2D datasets to be added or multiplied must have equal sizes.

If you run a command like ***add2d*** from the command line, you have to make sure that the required parameters are already set. Click the ***Procpars*** tab or enter ***edp*** to do that. If the second dataset has not been defined yet, ***add2d*** opens the add/subtract (***adsu***) dialog box.

The ***adsu*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***adsu*** dialog box, with ***edp*** or by typing ***alpha***, ***gamma*** etc.:

ALPHA - multiplication factor of the current spectrum
GAMMA - multiplication factor of the second spectrum

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data of the current dataset
`proc` - F2 processing parameters

<dir2>/data/<user2>/nmr/<name2>/<expno2>/pdata/<procno2>/

`2rr`, `2ir`, `2ri`, `2ii` - processed data of the second dataset

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data
`procs` - F2 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

ADD2D

ADDSER

MUL2D

SEE ALSO

add, duadd, mul

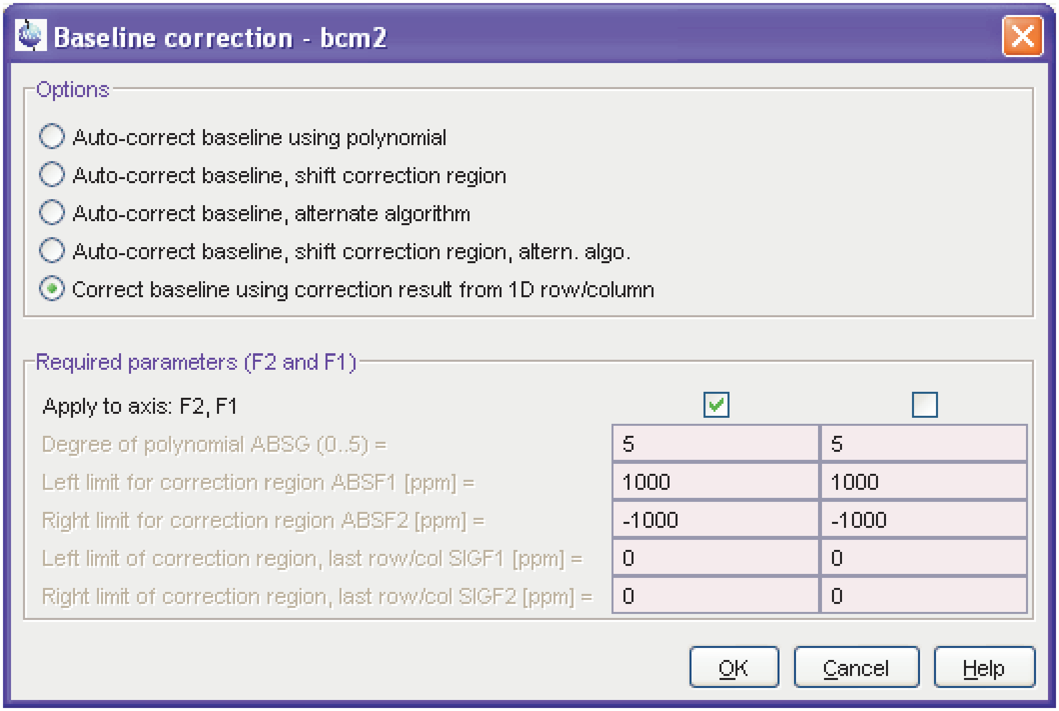
bcm2, bcm1

NAME

bcm2 - User defined baseline correction in F2 (2D)
bcm1 - User defined baseline correction in F1 (2D)

DESCRIPTION

Baseline correction commands can be started from the command line or from the baseline dialog box. The latter is opened with the command ***bas***



Baseline correction - bcm2

Options

○ Auto-correct baseline using polynomial
○ Auto-correct baseline, shift correction region
○ Auto-correct baseline, alternate algorithm
○ Auto-correct baseline, shift correction region, altern. algo.
● Correct baseline using correction result from 1D row/column

Required parameters (F2 and F1)

Apply to axis: F2, F1	☑	□
Degree of polynomial ABSG (0..5) =	5	5
Left limit for correction region ABSF1 [ppm] =	1000	1000
Right limit for correction region ABSF2 [ppm] =	-1000	-1000
Left limit of correction region, last row/col SIGF1 [ppm] =	0	0
Right limit of correction region, last row/col SIGF2 [ppm] =	0	0

Figure 4.4

(see Figure 4.4)

This dialog box offers several options, each of which selects a certain command for execution.

Correct baseline, using correction result from 1D row/column (F2)

This option selects the command ***bcm2*** for execution. It performs a baseline correction in the F2 direction by subtracting a polynomial, sine or exponential function. Before you can use ***bcm2***, you must first do the following:

1. Read a row with ***rsr*** (TOPSPIN will switch to the 1D data window)
2. Click or enter ***.basl*** to switch to baseline mode.
3. Click , or to select the baseline correction function.
4. Fit the baseline of the spectrum with the function you selected in step 2 (initially represented by a straight horizontal line). Click-hold button ***A*** and move the mouse to determine the zero order correction. Do the same with the buttons ***B***, ***C*** for higher order corrections until the line matches the baseline of the spectrum.
5. Click to save the baseline correction to the 2D dataset and leave baseline mode.
6. Select the 2D data window.

Then you can enter ***bcm2*** to perform the baseline correction.

Correct baseline, using correction result from 1D row/column (F1)

This option selects the command ***bcm1*** for execution. It works like ***bcm2***, except that it performs a baseline correction in the F1 direction (columns). Before you can use ***bcm1***, you must read a column with ***rsc*** and define the baseline on it (see above).

bcm* commands only works on the real data. After applying them, the imaginary data no longer match the real data and cannot be used for phase correction.

INPUT FILES

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

`2rr` - real processed 2D data
`base_info` - baseline correction coefficients

OUTPUT FILES

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

`2rr` - real processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

BCM2

BCM1

SEE ALSO

abs2, abs1

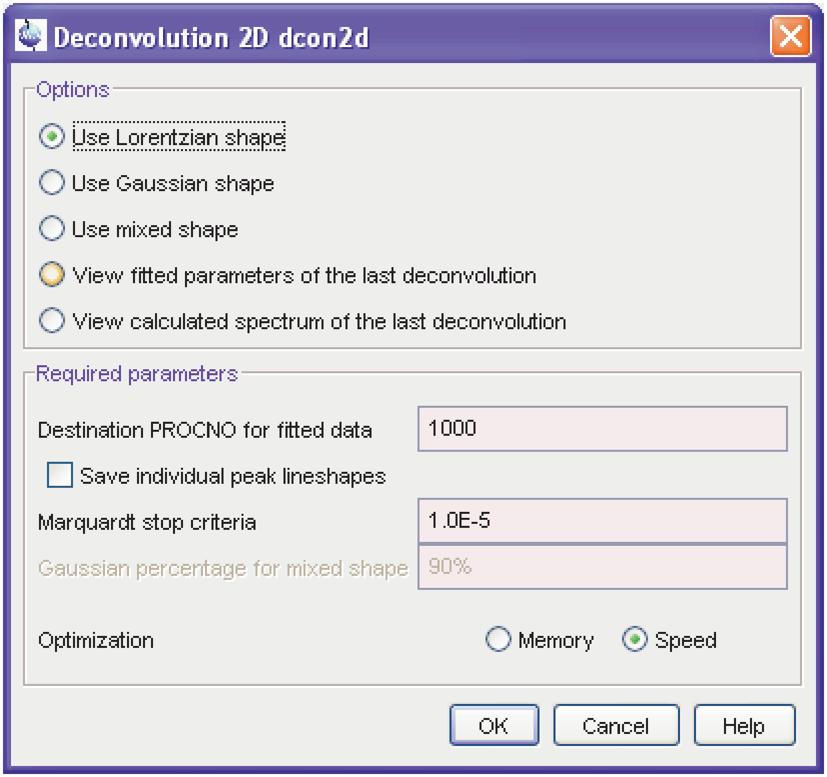
dcon2d, dcon

NAME

dcon2d - Gaussian, Lorentzian or mixed deconvolution (2D)
dcon - Open deconvolution dialog box (1D,2D)

DESCRIPTION

The command ***dcon2d*** performs deconvolution, fitting a Gaussian, Lorentzian or mixed function to the peaks in the displayed region. Before you start this command, you must select the desired region and perform peak picking (command ***pp***). Then enter the command ***dcon*** or ***dcon2d*** to open the dialog box (see Figure 4.5).



Deconvolution 2D dcon2d

Options

● Use Lorentzian shape
○ Use Gaussian shape
○ Use mixed shape
○ View fitted parameters of the last deconvolution
○ View calculated spectrum of the last deconvolution

Required parameters

Destination PROCNO for fitted data: 1000
□ Save individual peak lineshapes
Marquardt stop criteria: 1.0E-5
Gaussian percentage for mixed shape: 90%
Optimization ○ Memory ● Speed

Figure 4.5

This offers several options, each of which selects a certain command for execution.

Use Lorentzian shape

This option deconvolves the spectrum by fitting a Lorentzian function to the peaks. It is typically used for overlapping peaks with a Lorentzian lineshape to determine the ratio of each individual peak.

Use Gaussian shape

This option deconvolves the spectrum by fitting a Gaussian function to the peaks. It is typically used for overlapping peaks with a Gaussian lineshape to determine the ratio of each individual peak.

Use mixed shape

This option deconvolves the spectrum by fitting a mixed Lorentzian/Gaussian function to the peaks. It requires the parameter **Gaussian percentage for mixed shape** to be set. A mixed shape deconvolution is typically used for spectra which cannot be approximated by a pure Lorentzian or a pure Gaussian lineshape.

View fitted parameters of the last deconvolution

This option shows the fitted parameters and peaks of the last performed deconvolution on the current dataset.

View calculated spectrum of the last deconvolution

This option shows the graphical result of the last deconvolution; the original and the deconvolved spectrum in multi-display mode.

The result of deconvolution is:

- The quality of the fit expressed by the minimized chi-square value.
- a list of peaks within the selected region, and for each peak its frequency, width, intensity and integral. This list is displayed on the screen.
- the fitted lineshape, which is shown together with the original spectrum in multi-display mode.

Note that the deconvolution can be optimized for memory usage or speed. Furthermore, you can check the option ***Save individual peak lineshapes*** to store the deconvolution result for each peak in a separate procno. All resulting procnos are shown superimposed in multi-display mode. As such, each deconvolved peak can be separately scaled and shifted.

INPUT FILES

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

`2rr` - real processed 2D data
`peaklist.xml` - peak list
`proc` - processing parameters

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/pdata/1000/

`2rr` - deconvolved processed 2D data (first individual peak)
`dcon2dpeaks.txt` - deconvolution parameters and peaks
`procs` - processing status parameters

<dir>/data/<user>/nmr/<name>/<expno>/pdata/1001/

`2rr` - deconvolved processed 2D data (second individual peak)
`dcon2dpeaks.txt` - deconvolution parameters and peaks
`procs` - processing status parameters

etc.

SEE ALSO

ldcon, gdcon, mdcon

dosy2d

NAME

dosy2d - Process DOSY dataset (2D)

DESCRIPTION

The command ***dosy2d*** processes a 2D DOSY dataset.

DOSY is a special representation of diffusion measurements. Instead of generating just numbers using the T1/T2 fitting package (i.e. diffusion coefficients and error values), the DOSY processing gives pseudo 2D data where the F1 axis displays diffusion constants rather than NMR frequencies.

For more information on ***dosy*** :

click ***Help*** → ***Manuals*** → [**Acquisition Application Manuals**] ***Dosy***

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`difflist` - list of gradient amplitudes in Gauss/cm

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

`2rr` - 2D data processed in F2 only
`dosy` - DOSY processing parameters

OUTPUT FILES

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

`2rr` - 2D processed data
`auditp.txt` - processing audit trail

SEE ALSO

eddosy, dosy3d

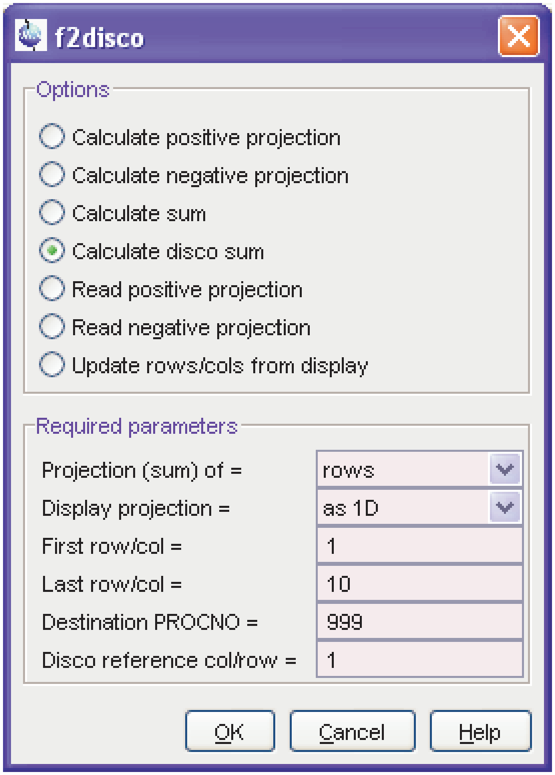
f2disco, f1disco, proj

NAME

f2disco - Calculate disco projection in F2 (2D)
f1disco - Calculate disco projection in F1 (2D)
proj - Open projections dialog box (2D,3D)

DESCRIPTION

The disco projection commands open the projections dialog box (see Figure 4.6) selecting the corresponding command.



Options

○ Calculate positive projection
○ Calculate negative projection
○ Calculate sum
● Calculate disco sum
○ Read positive projection
○ Read negative projection
○ Update rows/cols from display

Required parameters

Projection (sum) of =	rows
Display projection =	as 1D
First row/col =	1
Last row/col =	10
Destination PROCNO =	999
Disco reference col/row =	1

Figure 4.6

This dialog box has several options, each of which selects a certain command for execution.

Calculate disco sum (of rows)

This option selects the command ***f2disco*** for execution. Like ***f2sum***, it calculates the sum of all rows between *firstrow* and *lastrow*. However, for each row, the intensity at the intersection with the reference column is determined. If this intensity is positive, the row is added to the total. If it is negative, the row is subtracted from the total.

Calculate disco sum (of columns)

This option selects the command ***f1disco*** for execution. It works like ***f2disco***, except that it calculates the sum of the specified columns considering the intensities at the intersections with a reference row.

The calculated disco sum is stored under the specified *Destination procno*.

The Required parameter *Display projection* can be set to:

on 2D to display the calculated projection with the 2D dataset. The current 2D dataset remains the active dataset.

as 1D to display the calculated projection as a 1D dataset. The active dataset changes to the destination *procno*.

The required parameters can also be specified as arguments on the command line. As an example we use the command ***f2disco*** here.

f2disco <firstrow>
prompts for *lastrow* and *refrow* and stores the disco projection under data *name* ~TEMP

f2disco <firstrow> <lastrow> <refrow>
stores the specified disco projection under data *name* ~TEMP

f2disco <firstrow> <lastrow> <refrow> <procno>
stores the specified disco projection under the specified *procno* of the current data *name*

f2disco <firstrow> <lastrow> <refcol> <procno> n
stores the specified disco projection under the specified *procno* of the current data *name* but does not change the display to this *procno*

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data

OUTPUT FILES

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

`1r`, `1i`- 1D spectrum containing the F1 disco projection
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

F2DISCO(firstrow, lastrow, refcol, procno)

F1DISCO(firstcol, lastcol, refrow, procno)

for *procno* = -1, the disco projection is written to the dataset ~TEMP

SEE ALSO

f2projn, f2sum, rhpp

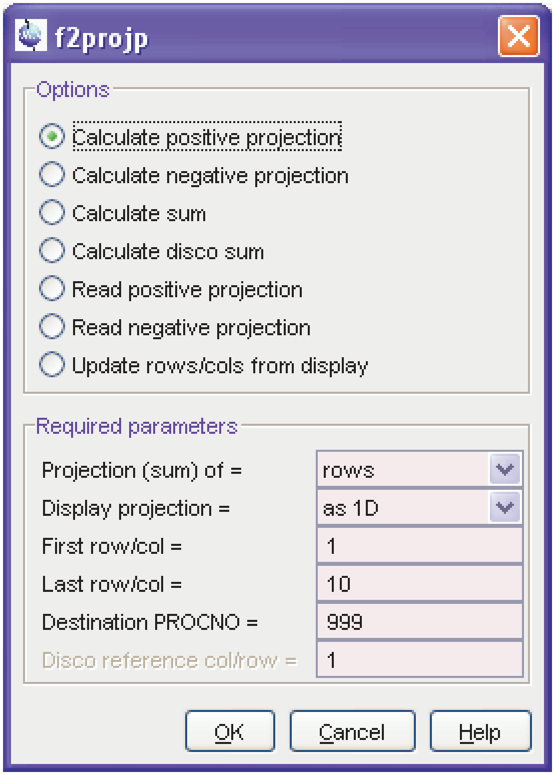
f2projn, f2projp, f1projn, f1projp, proj

NAME

f2projn - Calculate negative partial projection in F2 (2D)
f2projp - Calculate positive partial projection in F2 (2D)
f1projn - Calculate negative partial projection in F1 (2D)
f1projp - Calculate positive partial projection in F1 (2D)
proj - Open projections dialog box

DESCRIPTION

The projection commands open the projections dialog box (see Figure 4.7) selecting the corresponding command.


f2projp

Options

- ● Calculate positive projection
- ○ Calculate negative projection
- ○ Calculate sum
- ○ Calculate disco sum
- ○ Read positive projection
- ○ Read negative projection
- ○ Update rows/cols from display

Required parameters

Projection (sum) of =	rows
Display projection =	as 1D
First row/col =	1
Last row/col =	10
Destination PROCNO =	999
Disco reference col/row =	1

Figure 4.7

This dialog box has several options, each of which selects a certain command for execution.

Calculate positive projection (of rows)

This option selects the command ***f2projp*** for execution. It calculates the positive partial 1D projection of the 2D dataset in the F2 direction

Calculate positive projection (of columns)

This option selects the command ***f1projp*** for execution. It calculates the positive partial 1D projection of the 2D dataset in the F1 direction

Calculate negative projection (of rows)

This option selects the command ***f2projn*** for execution. It calculates the negative partial 1D projection of the 2D dataset in the F2 direction

Calculate negative projection (of columns)

This option selects the command ***f1projn*** for execution. It calculates the negative partial 1D projection of the 2D dataset in the F1 direction

The calculated projection is stored under the specified *Destination procno*.

The Required parameter *Display projection* can be set to:

on 2D to display the calculated projection with the 2D dataset. The current 2D dataset remains the active dataset.

as 1D to display the calculated projection as a 1D dataset. The active dataset changes to the destination PRONCNO.

The required parameters can also be specified as arguments on the command line. As an example we use the command ***f2projn*** here.

f2projn <firstrow>
prompts for *lastrow* and stores the projection under data *name* ~TEMP

f2projn <firstrow> <lastrow>
stores the specified projection under data *name* ~TEMP

f2projn <firstrow> <lastrow> <procno>
stores the specified projection under the specified *procno* of the current data *name*

f2projn <firstrow> <lastrow> <procno> n

stores the specified projection under the specified *procno* of the current data *name* but does not change the display to this *procno*

A projection is a 1D trace where every point has the highest intensity of all points of the corresponding orthogonal trace in the 2D spectrum. Partial means that only a specified range of rows (or columns) is are evaluated, i.e. only a part of the orthogonal trace is scanned for the highest intensity. Negative projections contain only negative intensities, positive projections contain only positive intensities.

A special case is the command ***f1projp*** or ***f1projn*** on a hypercomplex 2D dataset (MC2 ≠ QF) that has been processed in F2 only. Suppose you would perform the following command sequence:

xf2 - to process the data in F2 only

s si - to check the F1 size of the 2D data → click ***Cancel***

s mc2 - to check status MC2 (≠ QF) → click ***Cancel***

f1projp - to store the F1 projection in ~TEMP and change to that dataset

s si - to check the size of the resulting 1D dataset → click ***Cancel***

You will see that the size of the 1D data is only half the F1 size of the 2D data. The reason is that ***f1projp*** unshuffles the input data (file `2rr`). As such, ***f1projp*** behaves like the command ***rsc***. If you want to prevent the unshuffling of the input data (file `2rr`), you can use the following trick. Set the status parameter MC2 to QF before you run ***f1projp*** :

s mc2 → click ***QF***

Then, the size of the 1D data will be the same as the F1 size of the 2D data.

INPUT FILES

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

`2rr` - processed data

OUTPUT FILES

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

`f2projn` - ascii file specifying the range of rows and the 1D data path
`f2projp` - ascii file specifying the range of rows and the 1D data path
`f1projn` - ascii file specifying the range of columns and the 1D data path
`f1projp` - ascii file specifying the range of columns and the 1D data path

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

`1r` - 1D spectrum containing the projection
`auditp.txt` - processing audit trail

If the commands are used with less than three arguments, the files are stored in:

<dir>/data/<user>/nmr/*~TEMP*/1/pdata/1/

USAGE IN AU PROGRAMS

F2PROJN(firstrow, lastrow, procno)

F2PROJP(firstrow, lastrow, procno)

F1PROJN(firstcol, lastcol, procno)

F1PROJP(firstcol, lastcol, procno)

For all these macros counts that if procno = -1, the projection is written to the dataset ~TEMP

SEE ALSO

f2disco, f2sum, rhpp

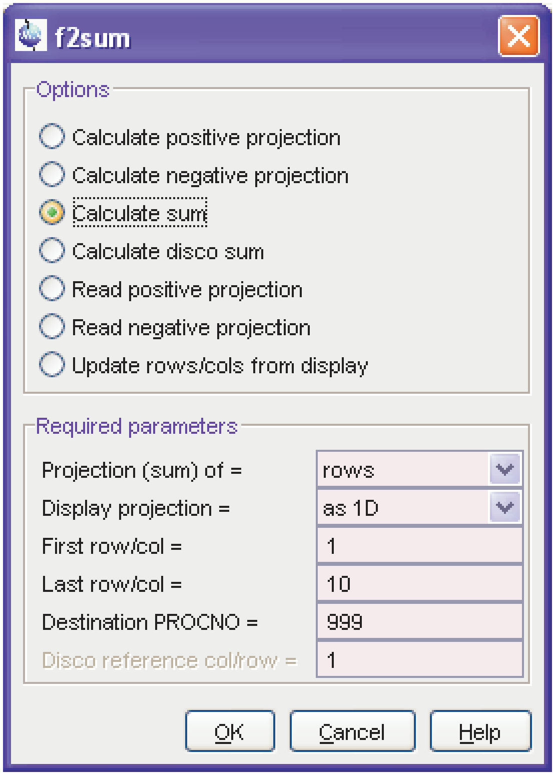
f2sum, f1sum, proj

NAME

f2sum - Calculate partial sum in F2 (2D)
f1sum - Calculate partial sum in F1 (2D)
proj - Open the projections dialog box (2D,3D)

DESCRIPTION

The projection sum commands open the projections dialog box selecting the corresponding command.



○ Calculate positive projection
○ Calculate negative projection
● Calculate sum
○ Calculate disco sum
○ Read positive projection
○ Read negative projection
○ Update rows/cols from display

Projection (sum) of = rows
Display projection = as 1D
First row/col = 1
Last row/col = 10
Destination PROCNO = 999
Disco reference col/row = 1

Figure 4.8

This dialog box has several options, each of which selects a certain command for execution.

Calculate sum (of rows)

This option selects the command ***f2sum*** for execution. It calculates the sum of all rows within a region specified by the parameters.

Calculate sum (of columns)

This option selects the command ***f1sum*** for execution. It calculates the sum of all columns within a region specified by the parameters.

The calculated sum is stored under the specified *Destination procno*.

The Required parameter *Display projection* can be set to:

on 2D to display the calculated projection with the 2D dataset. The current 2D dataset remains the active dataset.

as 1D to display the calculated projection as a 1D dataset. The active dataset changes to the destination *procno*.

The required parameters can also be specified as arguments on the command line. As an example we use the command ***f2sum*** here.

f2sum <firstrow>
prompts for *lastrow* and stores the sum under data *name* ~TEMP

f2sum <firstrow> <lastrow>
stores the specified sum under data *name* ~TEMP

f2sum <firstrow> <lastrow> <procno>
stores the specified sum under the specified *procno* of the current data *name*

f2sum <firstrow> <lastrow> <procno> n
stores the specified sum under the specified *procno* of the current data *name* but does not change the display to this *procno*

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data

OUTPUT FILES

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

`1r`, `1i`- 1D spectrum containing the sum
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

F2SUM(firstrow, lastrow, procno)

F1SUM(firstcol, lastcol, procno)

For both macros counts that if *procno* = -1, the sum is written to the dataset ~TEMP

SEE ALSO

f2projn, f2disco, rhpp

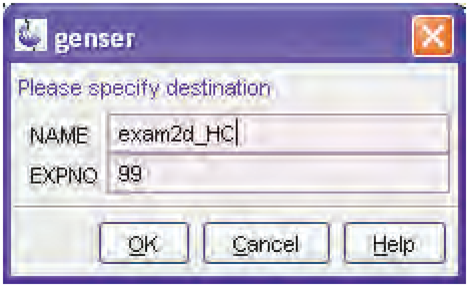
genser

NAME

genser - Generate pseudo-raw data (2D)

DESCRIPTION

The command ***genser*** generates pseudo-raw data from processed 2D data. When entered without arguments, ***genser*** opens the following dialog box:



Please specify destination

NAME exam2d_HC

EXPNO 99

Figure 4.9

Here, you specify the output dataset and click ***OK*** to actually execute the command. ***genser*** is normally used in combination with ***xif2*** and ***xif1***. These commands perform an inverse Fourier transform, converting processed frequency domain data into processed time domain data. ***genser*** converts these processed time domain data into pseudo-raw time domain data and stores them under a new name or experiment number (*expno*).

Note that ***genser*** does not modify the data, but only stores them in a different format. The number of data points of the pseudo-raw data, is twice the size (SI) of the processed data they are created from. The acquisition status parameter TD (type ***dpa***) is set accordingly; TD = 2*SI. This count for both the F2 and F1 direction.

genser takes three arguments and can be used as follows:

- ***genser***
  opens a dialog box where you can specify the output data.

- ***genser <expno>***
  stores the output under the specified *expno* and opens a new data window displaying this expno.
- ***genser <expno> n***
  stores the output under the specified *expno*, but does not open and display this expno.

If the specified expno already exists, you will be prompted to overwrite it or not. You can force the overwrite by specifying the extra argument ***y*** on the command line:

- ***genser <expno> y n***
  stores the output under the specified *expno*, overwriting it if it exists, but does not open and display this expno.

The processed data number (*procno*) of the new dataset is always set to 1.

genser can be useful if you want to reprocess a 2D spectrum, for example with different processing parameters, but the raw data do not exist any more. An example of such a procedure is:

xif2 (if the data are Fourier transformed in F2)

xif1 (if the data are Fourier transformed in F1)

genser (to create the pseudo-raw data)

edp (to set the processing parameters)

xfb (to process the pseudo-raw data)

If the input data are processed but not Fourier transformed, you can skip the first two steps.

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed time domain data

OUTPUT FILES

<*dir*>/data/<*user*>/nmr/<*name*>/<*expno*>/

`ser` - pseudo-raw time domain data

`audita.txt` - acquisition audit trail

USAGE IN AU PROGRAMS

GENSER(expno)

SEE ALSO

xif2, xif1, genfid

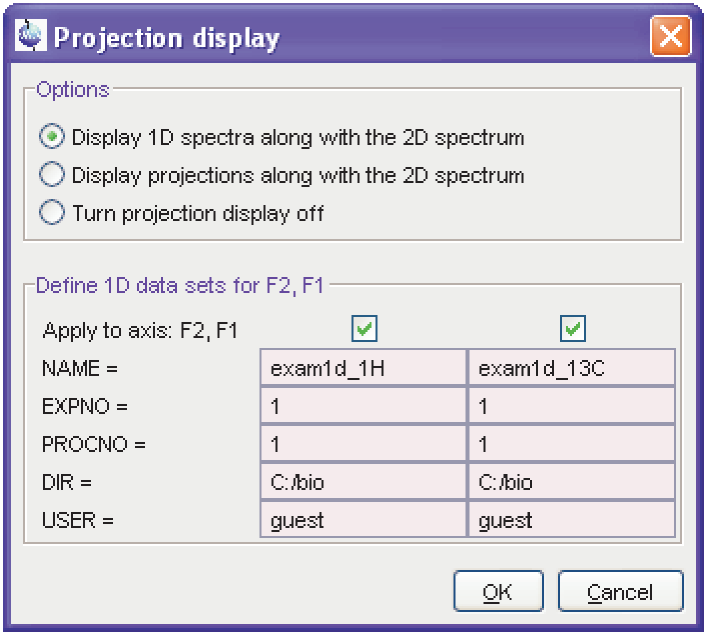
projd

NAME

projd - Display projections along with the 2D spectrum (2D)

DESCRIPTION

The ***projd*** commands opens a dialog box (see Figure 4.10) where you can specify the projections to be displayed along with the 2D spectrum.



Options

● Display 1D spectra along with the 2D spectrum
○ Display projections along with the 2D spectrum
○ Turn projection display off

Define 1D data sets for F2, F1

Apply to axis: F2, F1	☑	☑
NAME =	exam1d_1H	exam1d_13C
EXPNO =	1	1
PROCNO =	1	1
DIR =	C:/bio	C:/bio
USER =	guest	guest

Figure 4.10

This dialog box offers the following tree options:

Display 1D spectra along with the 2D spectrum

Displays the specified 1D dataset(s) as external projections

Display projections along with the 2D spectrum

Displays the internal projections.

Turn projection display off

Turns off the projection display.

In the lower part of the dialog you can specify the 1D datasets to be used for the first option. The checkboxes allow you to display the F2-projection, F1-projection or both. Clicking ***OK*** will show the projections according to the chosen option and close the dialog.

Note that the effect of the second and third option can also be reached by clicking the ▣ button of the toolbar or entering ***`.pr`*** on the command line.

INPUT FILES

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

`1r` - 1D processed data (input for 1st option)

OUTPUT FILES

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

`curdat2` - definition of the second and third dataset

SEE ALSO

f2projn, f2sum, rhpp

rev2, rev1

NAME

rev2 - Reverse spectrum in F2 (2D)
rev1 - Reverse spectrum in F1 (2D)

DESCRIPTION

The command ***rev2*** reverses the spectrum in the F2 direction. This means, each row is mirrored about the central column.

The command ***rev1*** reverses the spectrum in the F1 direction. This means, each column is mirrored about the central row.

Note that the spectrum can also be reversed by during ***xfb*** by setting the F2 and/or F1 processing parameter REVERSE to TRUE.

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

REV2

REV1

SEE ALSO

rv

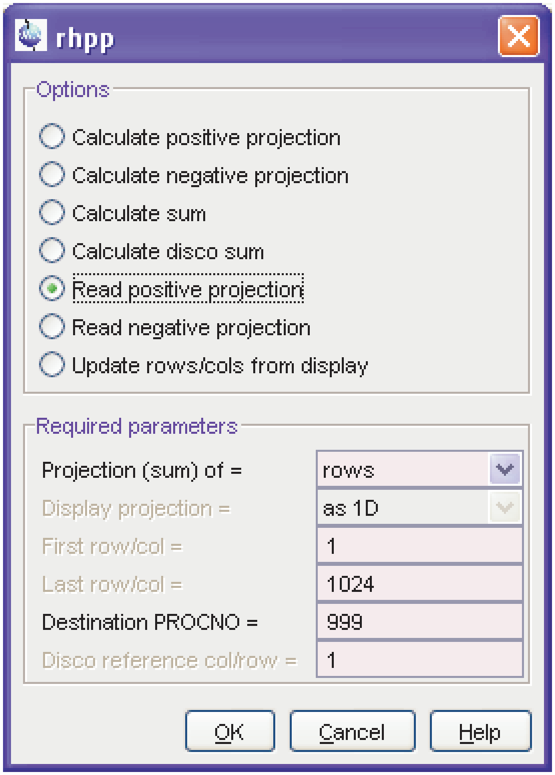
rhpp, rhnp, rvpp, rvnp, proj

NAME

rhpp - Calculate horizontal (F2) positive projection (2D)
rhnp - Calculate horizontal (F2) negative projection (2D)
rvpp - Calculate vertical (F1) positive projection (2D)
rvnp - Calculate vertical (F1) negative projection (2D)
proj - Open the projections dialog box (2D,3D)

DESCRIPTION

The projection commands can be started from the command line or from the projection dialog box selecting the corresponding command.



rhpp

Options

- ○ Calculate positive projection
- ○ Calculate negative projection
- ○ Calculate sum
- ○ Calculate disco sum
- ● Read positive projection
- ○ Read negative projection
- ○ Update rows/cols from display

Required parameters

Projection (sum) of =	rows
Display projection =	as 1D
First row/col =	1
Last row/col =	1024
Destination PROCNO =	999
Disco reference col/row =	1

Figure 4.11

This dialog box has several options, each of which selects a certain command for execution.

Read positive projection (on rows)

This option selects the command ***rhpp*** for execution. It calculates the full positive projection of a 2D spectrum in the F2 direction and stores it as a 1D dataset.

Read positive projection (on columns)

This option selects the command ***rvpp*** for execution. It calculates the full positive projection of a 2D spectrum in the F1 direction and stores it as a 1D dataset.

Read negative projection (on rows)

This option selects the command ***rhnp*** for execution. It calculates the full negative projection of a 2D spectrum in the F2 direction and stores it as a 1D dataset.

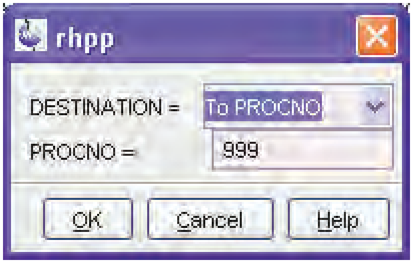
Read negative projection (on columns)

This option selects the command ***rvnp*** for execution. It calculates the full negative projection of a 2D spectrum in the F1 direction and stores it as a 1D dataset.

A projection is a 1D trace where every point has the highest intensity of all points of the corresponding orthogonal trace in the 2D spectrum.

r*p commands only take the projection of the first quadrant data (file `2rr`) and store it as real 1D data (file `1r`)

r*p commands can be started from the command line. When entered without arguments, they open a dialog box as shown in Figure 4.12.


rhpp

DESTINATION = To PROCNO

PROCNO = 999

Figure 4.12

The required arguments can also be specified on the command line.

rhpp <procno>
stores the projection under the specified *procno* of the current data *name*

rhpp <procno> n
stores the projection under the specified *procno* but does not change the display to that *procno*

The three other ***r*p*** command have the same syntax.

A special case is the command ***rvpp*** or ***rvnp*** on a hypercomplex 2D dataset (MC2 ≠ QF) that has been processed in F2 only. Suppose you would perform the following command sequence:

xf2 - to process the data in F2 only

s si - to check the F1 size of the 2D data → click ***Cancel***

s mc2 - to check status MC2 (≠ QF) → click ***Cancel***

rvpp - to store the F1 projection in ~TEMP and change to that dataset

s si - to check the size of the resulting 1D dataset → click ***Cancel***

You will see that the size of the 1D data is only half the F1 size of the 2D data. The reason is that ***rvpp*** unshuffles the input data (file `2rr`). As such, ***rvpp*** behaves like the command ***rsc***. If you want to prevent the unshuffling of the input data (file `2rr`), you can use the following trick. Set the status parameter MC2 to QF before you run ***rvpp*** :

s mc2 → click ***QF***

Then, the size of the 1D data will be the same as the F1 size of the 2D data.

INPUT FILES

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

`2rr` - real processed 2D data

OUTPUT FILES

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

`1r` - 1D spectrum containing the projection
`auditp.txt` - processing audit trail

If the commands are used without arguments, the files are stored in:

<dir>/data/<user>/nmr/~*TEMP*/1/pdata/1/

USAGE IN AU PROGRAMS

RHPP(procno)

RHNP(procno)

RVPP(procno)

RVNP(procno)

For all these macros counts that if *procno* = -1, the projection is written to the dataset ~TEMP

SEE ALSO

f2projn, f2sum, f2disco

rsc

NAME

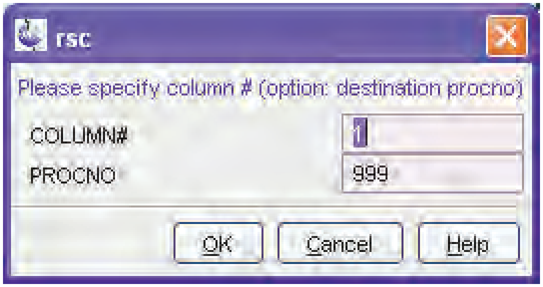
rsc - Read column from 2D data and store as 1D data

SYNTAX

rsc [<column> [<procno>] [n]]

DESCRIPTION

The command ***rsc*** reads a column from a 2D spectrum and stores it as a 1D spectrum. When entered on a 2D dataset without arguments, ***rsc*** opens a dialog box where you can specify the column number and the *procno* of the output data.



rsc

Please specify column # (option: destination procno)

COLUMN# 1

PROCNO 999

Figure 4.13

The column must be specified as a number between 1 and F2-SI. The latter is the F2 processing status parameter SI that can be viewed with ***s si***. The *procno* can be any number other that the current *procno*. If the *procno* field is left empty, the output dataset is stored under data name ~TEMP.

When entered on a 2D dataset, ***rsc*** takes up to three arguments and can be used as follows:

rsc
opens the above dialog box

rsc <column>
stores the specified column under data *name* ~TEMP

rsc <column> <procno>
stores the specified column under the current data *name*, the current *expno* and the specified *procno*. It changes the display to the output 1D data.

rsc <column> <procno> n
stores the specified column under the current data *name*, the current *expno* and the specified *procno*. It does not change the display to the output 1D data.

After ***rsc*** has read a column and the display has changed to the destination 1D dataset, a subsequent ***rsc*** command can be entered on this 1D dataset. This takes two arguments and can be used as follows:

rsc
opens the above dialog box

rsc <column>
reads the specified column from the 2D dataset from which the current 1D dataset was extracted

rsc <column> <procno>
reads the specified column from the 2D dataset that resides under the current data *name* [1], the current *expno* and the specified *procno*. Specifying the *procno* allows you to read a column from a 2D dataset other than the one from which the current 1D dataset was extracted. Furthermore, the AU macro RSC requires two arguments, no matter if it is used on a 1D or on a 2D dataset.

rsr can also be started from the dialog box that is opened with the command ***slice***.

A special case is a 2D dataset that has been Fourier transformed in F2 but not in F1. ***rsc*** then stores 1D processed data that are in the time domain rather than the frequency domain. Below are five different examples of this case.

Example 1

[1] However, if the current data name is ~TEMP, ***rsc <column> <procno>*** reads from the specified *procno* in the dataset from which the current 1D dataset was extracted.

A 2D dataset is Fourier transformed in F2, column 17 (time domain) is extracted and stored under the same name and *expno*, in *procno* 2. The resulting 1D dataset is Fourier transformed.

On the 2D dataset, enter the following commands:

xf2 - to Fourier transform in F2 only

rsc 17 2 - to read column 17 to *procno* 2 and switch to that dataset

ft - to Fourier transform the resulting 1D data according to FnMODE

Explanation: the 1D data shares the *expno*, and the acquisition parameters in it, with the source 2D dataset. 1D processing commands automatically recognize that this 1D dataset is a column from a 2D dataset. The command ***ft*** interprets the F1 acquisition parameter FnMODE to determine the Fourier transform mode.

Example 2

A 2D dataset with F1 acquisition mode *States* is Fourier transformed in F2. Column 17 (time domain) is extracted and stored under data *name* ~TEMP. The resulting 1D dataset is Fourier transformed.

On the 2D dataset, enter the following commands:

s fnmode - check the FnMODE value (*States*) → click ***Cancel***

xf2 - to Fourier transform in F2 only

s mc2 - check the MC2 value (*States*) → click ***Cancel***

rsc 17 - read column 17 to ~TEMP and switch to that dataset

s aq_mod - check the AQ_mod value (*qsim*) → click ***Cancel***

ft - Fourier transform the resulting 1D data according to AQ_mod

Explanation: the source 2D and the destination 1D have a separate a set of acquisition parameters. ***rsc*** reads the F1 status parameter MC2 of the 2D data and translates that to the corresponding AQ_mod of the 1D data. 1D processing commands recognizes this 1D dataset as regular 1D data. This means, for example, that ***ft*** interprets the AQ_mod to determine the Fourier transform mode.

Example 3

A 2D dataset with an F1 acquisition mode States-TPPI is Fourier transformed in F2. Column 17 (time domain) is extracted and stored under data name ~TEMP. The resulting 1D dataset is Fourier transformed.

On the 2D dataset, enter the following commands:

s fnmode - check the FnMODE value (*States-TPPI*) → click ***Cancel***

xf2 - to Fourier transform in F2 only

s mc2 - check the MC2 value (*States-TPPI*) → click ***Cancel***

rsc 17 - to read column 17 to ~TEMP and switch to that dataset

ft_mod - check the FT_mod value (*fsc*) → click ***Cancel***

trfp - to Fourier transform the resulting 1D data according to FT_mod

Explanation: the source 2D and the destination 1D have a separate a set of acquisition parameters. Since there is no value for AQ_mod that corresponds to States-TPPI, ***rsc*** sets the processing parameter FT_mod instead of the acquisition status parameter AQ_mod. As such, the resulting 1D dataset can only be Fourier transformed correctly with ***trfp***.

Example 4

A 2D dataset with an F1 acquisition mode QF is Fourier transformed in F2. Column 17 (time domain) is extracted and stored under data name ~TEMP. From the 2D dataset, enter the following commands:

s fnmode - check the FnMODE value (*QF*) → click ***Cancel***

xf2 - to Fourier transform in F2 only

s mc2 - check the MC2 value (*QF*) → click ***Cancel***

rsc 17 - to read column 17 to ~TEMP and switch to that dataset

s si - check the size of the 1D dataset → click ***Cancel***

Explanation: for FnMODE = QF the 2D storage mode is different than for other values (see the description of ***xfb***). As such, the size of the resulting 1D data is twice as large as for other values of FnMODE. If 2D imaginary data (file `2ii`) exist, 1D imaginary (file `1i`) are created.

Only in that case, the 1D data can be Fourier transformed.

Example 5

From a 3D dataset, a plane is extracted and, from this plane a column is extracted.

On the 3D dataset, enter the following commands:

`xf2 s13 48 2` - to read the F3-F1 plane 48 to *procno* 2

`rsc 19 3` - to read, from plane 48, column 19 to *procno* 3

`ft` : to Fourier transform the resulting 1D data according to FnMODE

Explanation: the 3D, 2D and 1D dataset are stored in three different *procno*'s all under the same *expno*, i.e. they share the same acquisition parameters. 1D processing commands automatically recognize that the 1D dataset is a column from an F3-F1 plane that was extracted from a 3D dataset. As such, ***`ft`*** interprets the F1 parameter FnMODE to determine the Fourier transform mode. Note that F1 is the third direction of the 3D dataset. The parameter handling, however, is transparent to the user.

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - 2D processed data

OUTPUT FILES

If no output *procno* is specified:

<dir>/data/<user>/nmr/*~TEMP*/1/pdata/1/

`1r`, `1i` - 1D spectrum
`used_from` - data path of the source 2D data and the column no.
`auditp.txt` - processing audit trail

If the output *procno* is specified:

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

`1r`, `1i` - 1D spectrum
`used_from` - data path of the source 2D data and the column no.

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

RSC(column, procno)

If *procno* = -1, the column is written to the dataset ~TEMP

SEE ALSO

rtr, rsr, wsr, wsc, rser, rser2d, wser, wserp, slice

rser

NAME

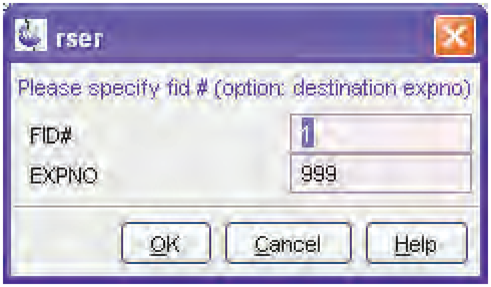
rser - Read row from 2D raw data and store as 1D FID (2D,1D)

SYNTAX

rser [<row> [<expno>] [n]]

DESCRIPTION

The command ***rser*** reads a row from 2D or 3D raw data (a series of FIDs) and stores it as a 1D dataset. It opens a dialog box where you can specify the FID number and the *expno* of the output data.



Please specify fid # (option: destination expno)

FID# 1

EXPNO 999

Figure 4.14

For 2D data, the row must be specified as a number between 1 and F1-TD. The latter is the F1 acquisition status parameter TD that can be viewed with ***s td***.

rser is normally entered on the 2D dataset. It then takes up to three arguments and can be used as follows:

rser
prompts for the row number and stores it under data *name* ~TEMP

rser <row>
stores the specified row under data *name* ~TEMP

rser <row> <expno>
stores the specified row under the current data *name* and the specified *expno* and then changes the display to this *expno*

rser <row> <expno> n
stores the specified row under the current data *name* and the specified *expno* but does not change the display to this *expno*

After ***rser*** has read a row and the display has changed to the destination 1D dataset, a subsequent ***rser*** command can be entered on this 1D dataset. This takes two arguments and can be used as follows:

rser
opens the above dialog box where you can specify the row number and the *procno* of the 2D dataset from which the current 1D dataset was extracted

rser <row>
reads the specified row from the 2D dataset from which the current 1D dataset was extracted

rser <row> <expno>
reads the specified row from the 2D dataset that resides under the current data *name* [1], the specified *expno* and *procno* 1.

Note that on 3D data, ***rser*** does not distinguish between the F2 and F1 direction and treats the 3D dataset as a large 2D dataset. This implies that the row number must lie between 1 and (F2-TD) * (F1-TD).

rser can also be started from the dialog box that is opened with the command ***slice***.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - 2D or 3D raw data

OUTPUT FILES

If the output *expno* is specified:

<dir>/data/<user>/nmr/<name>/<*expno*>/

`fid` - 1D FID
`audita.txt` - acquisition audit trail

[1] However, if the current data name is ~TEMP, the input dataset is the one from which the current 1D dataset was extracted, except for the specified *expno* (*procno*).

<dir>/data/<user>/nmr/<name>/<*expno*>/pdata/1/

`used_from` - data path of the source 2D data and the row no.

If no output *expno* is specified:

<dir>/data/<user>/nmr/*~TEMP*/1/

`fid` - 1D FID

<dir>/data/<user>/nmr/*~TEMP*/1/pdata/1

`used_from` - data path of the source 2D data and the row no.

USAGE IN AU PROGRAMS

RSER(row, expno, procno)

If expno = -1, the row is written to the dataset ~TEMP

SEE ALSO

wser, wserp, rser2d, rsr, rsc, wsr, wsc, slice

rsr

NAME

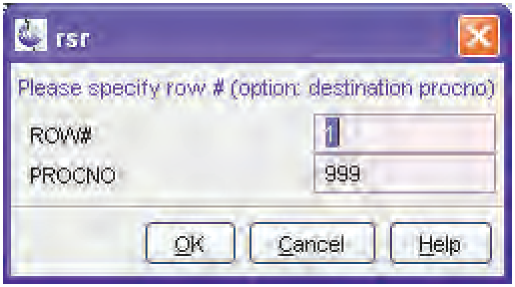
rsr - Read row from 2D data and store as 1D data (2D,1D)

SYNTAX

rsr [<row> [<procno>] [n]]

DESCRIPTION

The command ***rsr*** reads a row from a 2D spectrum and stores it as a 1D spectrum. When entered on a 2D dataset without arguments, ***rsr*** opens a dialog box where you can specify the row number and the *procno* of the output data.



Please specify row # (option: destination procno)

ROW# 1

PROCNO 999

Figure 4.15

The row must be specified as a number between 1 and F1-SI. The latter is the F1 processing status parameter SI that can be viewed with ***s si***. The *procno* can be any number other that the current *procno*. If the *procno* field is left empty, the output dataset is stored under data name ~TEMP.

When entered on a 2D dataset, ***rsr*** takes up to three arguments and can be used as follows:

rsr <row>
stores the specified row under data *name* ~TEMP

rsr <row> <procno>
stores the specified row under the current data *name*, the current *exp-*

no and the specified *procno*. It changes the display to the output 1D data.

rsr <row> <procno> n
stores the specified row under the current data *name*, the current *expno* and the specified *procno*. It does not change the display to the output 1D data.

After ***rsr*** has read a row and the display has changed to the destination 1D dataset, a subsequent ***rsr*** command can be entered on this 1D dataset. This takes two arguments and can be used as follows:

rsr
opens the dialog box where you can specify the row and *procno* of the 2D data

rsr <row>
reads the specified row from the 2D dataset from which the current 1D dataset was extracted

rsr <row> <procno>
reads the specified row from the 2D dataset that resides under the current data *name* [1], the current *expno* and the specified *procno*. Specifying the *procno* allows you to read a row from a 2D dataset other than the one from which the current 1D dataset was extracted. Furthermore, the AU macro RSR requires two arguments, no matter if it is used on a 1D or on a 2D dataset.

rsr can also be started from the dialog box that is opened with the command ***slice***.

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - 2D processed data

[1] However, if the current data name is ~TEMP, ***rsr <row> <procno>*** reads from the specified *procno* in the dataset from which the current 1D dataset was extracted.

OUTPUT FILES

If no *procno* is specified:

<dir>/data/<user>/nmr/*~TEMP*/1/pdata/1/

`1r`, `1i` - 1D spectrum
`used_from` - data path of the source 2D data and the row no.
`auditp.txt` - processing audit trail

If the output *procno* is specified:

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

`1r`, `1i` - 1D spectrum
`used_from` - data path of the source 2D data and the row no.
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

RSR(row, procno)

If *procno* = -1, the row is written to the dataset ~TEMP

SEE ALSO

rtr, rsc, wsr, wsc, rser, rser2d, wser, wserp, slice

sub2, sub1, sub1d12, sub1d1, adsu

NAME

sub2 - Subtract 1D data from 2D data rows, keep sign (2D)
sub1 - Subtract 1D data from 2D data columns, keep sign (2D)
sub1d2 - Subtract 1D data from 2D data rows (2D)
sub1d1 - Subtract 1D data from 2D data columns (2D)
adsu - Open add/subtract/multiply dialog box (1D, 2D)

DESCRIPTION

Subtracting a 1D data from a 2D data can be started from the command line or from the add/subtract dialog box. The latter is opened with the command ***adsu***.

This dialog box offers several options, each of which selects a certain command for execution.

Subtract a 1D spectrum from each row, retain sign

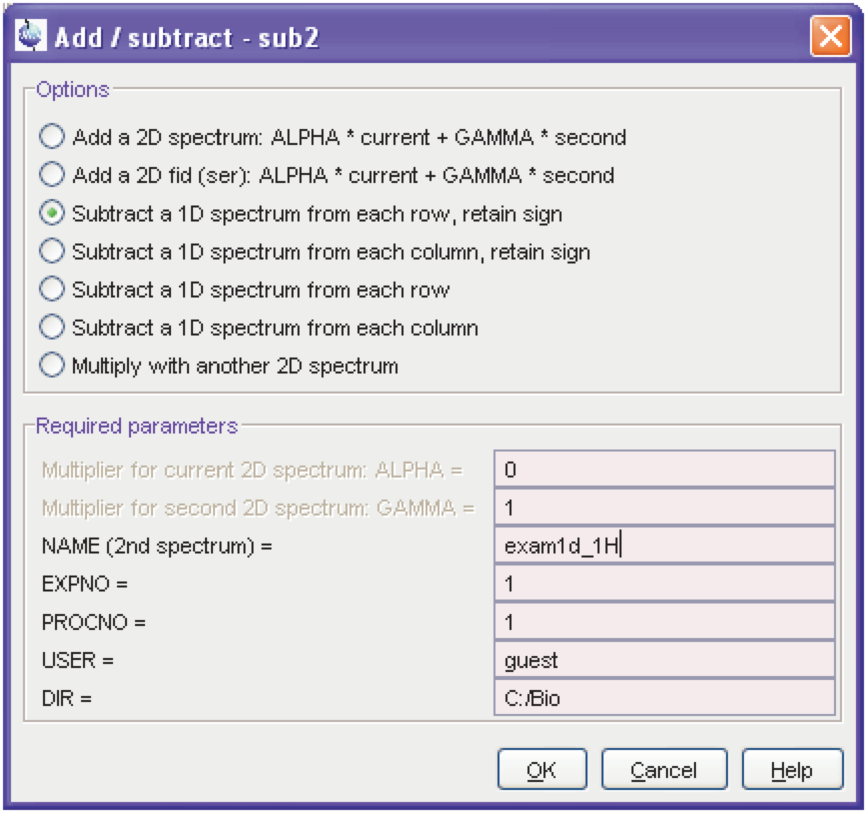
This option selects the command ***sub2*** for execution. It subtracts a 1D dataset from each row of the current 2D spectrum. It first compares the intensity of each data point of the 1D spectrum with the intensity of the corresponding data point in the 2D spectrum. If they have opposite signs, no subtraction is done and the 2D data point remains unchanged. If they have the same sign and the 1D data point is smaller than the 2D data point, the subtraction is done. If the 1D data point is greater than the 2D data point, the latter is set to zero. As such, the sign of the 2D data points always remains the same.

Subtract a 1D spectrum from each column, retain sign

This option selects the command ***sub1*** for execution. It works like ***sub2***, except that it subtracts the 1D second dataset from each column of the current 2D spectrum.

Subtract a 1D spectrum from each row

This option selects the command ***sub1d2*** for execution. It subtracts a 1D dataset from each row of the current 2D spectrum. Unlike ***sub2***, it does not compare intensities.



Options

○ Add a 2D spectrum: ALPHA * current + GAMMA * second
○ Add a 2D fid (ser): ALPHA * current + GAMMA * second
● Subtract a 1D spectrum from each row, retain sign
○ Subtract a 1D spectrum from each column, retain sign
○ Subtract a 1D spectrum from each row
○ Subtract a 1D spectrum from each column
○ Multiply with another 2D spectrum

Required parameters

Multiplier for current 2D spectrum: ALPHA =	0
Multiplier for second 2D spectrum: GAMMA =	1
NAME (2nd spectrum) =	exam1d_1H
EXPNO =	1
PROCNO =	1
USER =	guest
DIR =	C:/Bio

Figure 4.16

Subtract a 1D spectrum from each column

This option selects the command ***sub1d1*** for execution. It subtracts a 1D dataset from each column of the current 2D spectrum. Unlike ***sub1***, it does not compare intensities.

The ***sub**** commands only work on the real data. After using them, the imaginary data no longer match the real data and cannot be used for phase correction.

If the second dataset has not been defined yet, the ***sub**** commands open the add/subtract (***adsu***) dialog box.

The ***adsu*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT FILES

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

`2rr` - real processed 2D data

<dir2>/data/<user2>/nmr/<name2>/<expno2>/pdata/<procno2>/

`1r` - real processed 1D data

OUTPUT FILES

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

`2rr` - real processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

SUB2

SUB1

SUB1D2

SUB1D1

SEE ALSO

add2d

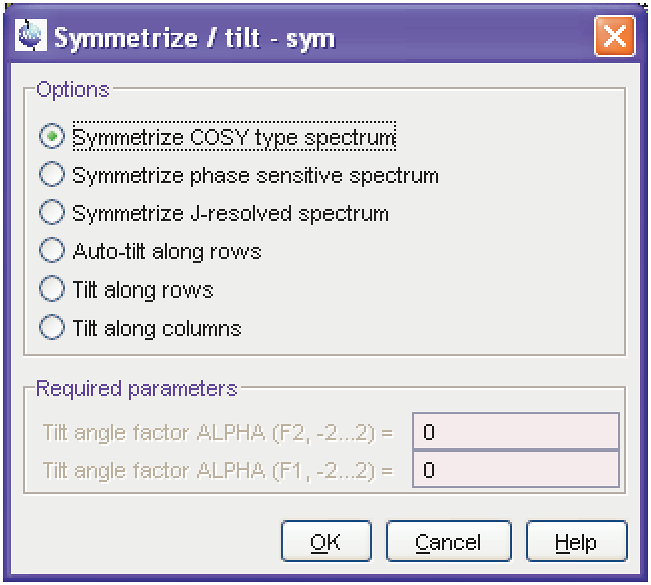
sym, syma, symj, symt

NAME

sym - Symmetrize spectrum about the diagonal (2D)
syma - Symmetrize spectrum about the diagonal, keep sign (2D)
symj - Symmetrize spectrum about central horizontal line (2D)
symt - Open symmetrization and tilt dialog box (2D)

DESCRIPTION

All ***sym**** commands open the symmetrize/tilt dialog box:



Symmetrize / tilt - sym

Options

● Symmetrize COSY type spectrum
○ Symmetrize phase sensitive spectrum
○ Symmetrize J-resolved spectrum
○ Auto-tilt along rows
○ Tilt along rows
○ Tilt along columns

Required parameters

Tilt angle factor ALPHA (F2, -2...2) = 0
Tilt angle factor ALPHA (F1, -2...2) = 0

Figure 4.17

This dialog box offers several options, each of which selects a certain command for execution.

Symmetrize COSY type spectrum

This option selects the command ***sym*** for execution. It symmetrizes a 2D spectrum about a diagonal from the lower left corner (data point 1,1) to the upper right corner (data point F2-SI, F1-SI). It compares each data point with the corresponding data point on the other side of the diagonal and determines which one has the lowest (most negative) intensity. Then both data points are set to that intensity.Table 4.1 shows the intensities of four pairs of data points before and after ***sym***:

before ***sym***	after ***sym***
-370000, 12000	-370000, -370000
1000, -700	-700, -700
18000, 6000	6000, 6000
-13000, -8000	-13000, -13000

Table 4.1

sym is typically used on magnitude cosy spectra.

Symmetrize phase sensitive spectrum

This option selects the command ***syma*** for execution. It works like ***sym***, except that it compares each data point with the corresponding data point on the other side of the diagonal and determines which one has the lowest absolute intensity. Then both data points are set to that intensity while each point keeps its original sign. Table 4.2 shows the intensities of four pairs of data points before and after ***syma***:

before ***syma***	after ***syma***
-370000, 12000	-12000, 12000
1000, -700	700, -700
18000, 6000	6000, 6000
-13000, -8000	-8000, -8000

Table 4.2

syma is typically used on phase sensitive cosy spectra.

Symmetrize J-resolved spectrum

This option selects the command ***symj*** for execution. It symmetrizes a 2D spectrum about a horizontal line through the middle. It is similar to ***sym***, i.e. it compares each data point with the corresponding data point on the other side of the horizontal line and determines which one has the lowest (most negative) intensity. Then both data points are set to that intensity. Table 4.3 shows the intensities of 5 pairs of data points before and after ***symj***:

before ***symj***	after ***symj***
-370000, 12000	-370000, -370000
1000, -700	-700, -700
18000, 6000	6000, 6000
-13000, -8000	-13000, -13000
-8000, -25000	-25000, -25000

Table 4.3

symj is typically used on J-resolved spectra which have been tilted with the command ***tilt***.

sym* commands only work on the real data. After using it, the imaginary data no longer match the real data and cannot be used for phase correction.

When executed from the command line, the command ***sym***, ***syma*** and ***symj*** select the corresponding option in the dialog box. This means, you can just click ***OK*** or hit ***Enter*** to start the command. In contrast, ***symt*** selects the last used symmetrization command.

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s symm*** :

SYMM - type of symmetrization (*no*, *sym*, *syma* or *symj*) done

INPUT FILES

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

`2rr` - real processed 2D data

OUTPUT FILES

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

`2rr` - real processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

SYM

SYMA

SYMJ

SEE ALSO

tilt, ptilt, ptilt1

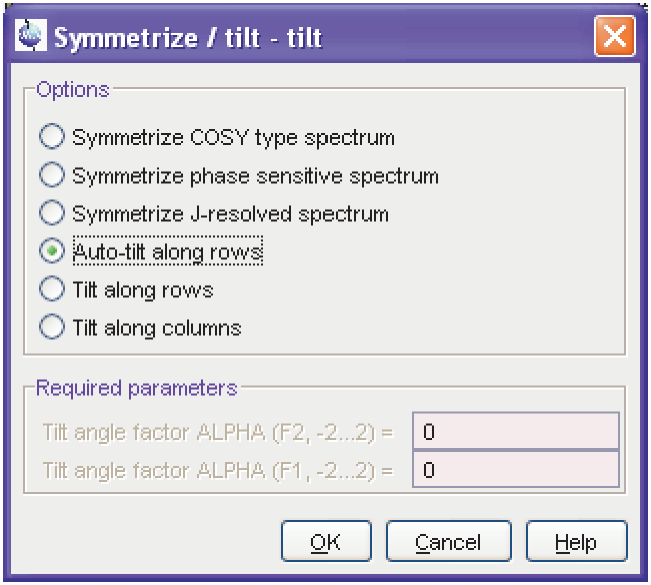
tilt, ptilt, ptilt1, symt

NAME

tilt - Tilt a 2D spectrum
ptilt - Tilt a 2D spectrum by shifting the data in the F2 direction
ptilt1 - Tilt a 2D spectrum by shifting the data in the F1 direction
symt - Open the symmetrize/tilt dialog box

DESCRIPTION

All ***tilt*** commands open the symmetrize/tilt dialog box (see Figure 4.18)



Options

○ Symmetrize COSY type spectrum
○ Symmetrize phase sensitive spectrum
○ Symmetrize J-resolved spectrum
● Auto-tilt along rows
○ Tilt along rows
○ Tilt along columns

Required parameters

Tilt angle factor ALPHA (F2, -2...2) = 0
Tilt angle factor ALPHA (F1, -2...2) = 0

Figure 4.18

This dialog box offers several options, each of which selects a certain command for execution.

Auto-tilt along rows

This option selects the command ***tilt*** for execution. It tilts the 2D spectrum, shifting each row of the 2D spectrum by the value:

n = tiltfactor * (nsrow/2 - row)

The variables in this equation are defined as:

tiltfactor = (SW_p1/SI1) / (SW_p2/SI2)
nsrow = total number of rows
row = the row number

where SW_p1, SI1, SW_p2 and SI2 represent the processing status parameters SW_p and SI in F1 and F2, respectively.

The upper half of the spectrum is shifted to the right, the lower half to the left. Furthermore, this is a circular shift, i.e. the data points which are cut off at the right edge of the spectrum are appended at the left edge and vice versa.

Tilt along rows

This option selects the command ***ptilt*** for execution. It tilts the 2D spectrum about a user defined angle, by shifting the data points in the F2 direction. It is typically used to correct possible magnet field drifts during long term 2D experiments. The tilt factor is determined by the F2 processing parameter ALPHA which can take a value between -2 and 2. Each row of the 2D matrix is shifted by n points where n is defined by:

n = tiltfactor * (nsrow/2 - row)

The variables in this equation are defined by:

tiltfactor = ALPHA*SI2 / SI1
nsrow = total number of rows
row = the row number

where SI2 and SI1 are processing status parameter SI in F2 and F1, respectively.

Tilt along columns

This option selects the command ***ptilt1*** for execution. It tilts the 2D spectrum about a user defined angle, by shifting the data points in the F1 direction. The tilt factor is determined by the F1 processing parameter ALPHA which can take a value between -2 and 2. Each column of the 2D matrix is shifted by n points where n is defined by:

n = tiltfactor * (nscol/2 - col)

The variables in this equation are defined by:

tiltfactor = ALPHA*SI1/ SI2
nscol = total number of columns
col = the column number

where SI2 and SI1 are processing status parameter SI in F2 and F1, respectively.

For F2-ALPHA = 1 and F1-ALPHA = 1:

- the sequence ***ptilt*** - ***ptilt1*** rotates the spectrum by 90°
- the sequence ***ptilt1*** - ***ptilt*** rotates the spectrum by -90°.

The command ***ptilt1*** is used in the AU program shear which can be viewed with the command ***edau shear***.

When executed from the command line, the command ***tilt***, ***ptilt*** and ***ptilt1*** select the corresponding option in the dialog box. This means, you can just click ***OK*** or hit ***Enter*** to start the command. In contrast, ***symt*** selects the last used tilt command.

INPUT PARAMETERS

set from the ***symt*** dialog box, with ***edp*** or by typing ***alpha*** :

ALPHA - tilt factor (used by ***ptilt*** and ***ptilt1***)

set by initial processing command, e.g. ***xfb***, can be viewed with ***dpp***:

SW_p - spectral width of the processed data (used by ***tilt***)
SI - size of the processed data

OUTPUT PARAMETERS

can be viewed with ***dpp***:

TILT - shows whether ***tilt***, ***ptilt*** or ***ptilt1*** was done (true or false)

INPUT FILES

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

`2rr` - real processed 2D data

OUTPUT FILES

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

`2rr` - real processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TILT

PTILT

PTILT1

SEE ALSO

sym, syma, symj

wsc

NAME

wsc - Replace column of 2D spectrum by 1D spectrum

SYNTAX

wsc [<row> [<procno>]]

DESCRIPTION

The command ***wsc*** replaces one column of 2D processed data by 1D processed data. It is normally used in combination with ***rsc*** in the following way:

1. Run ***rsc*** to extract column *x* from a 2D spectrum
2. Manipulate the resulting 1D data with 1D processing commands
3. Run ***wsc*** to replace column *x* of the 2D data with the manipulated 1D data

wsc can be entered on the source 1D dataset or on the destination 2D dataset.

Examples of the usage of ***wsc*** on the source 1D dataset:

wsc
prompts for the column of the destination 2D data which must be replaced by the current 1D data. The 2D dataset is the one from which the 1D dataset was extracted.

wsc <column>
the specified column of the destination 2D data is replaced by the current 1D data. The 2D dataset is the one from which the current 1D dataset was extracted.

wsc <column> <procno>
the specified column of the destination 2D data is replaced by the current 1D data. The 2D dataset must reside under the current data *name* [1], the current *expno* and the specified *procno*.

Examples of usage of ***wsc*** on the destination 2D dataset:

wsc <column>
the specified column of the current 2D processed data is replaced. The source 1D data must reside under the data *name* ~TEMP

wsc <column> <procno>
the specified column of the current 2D processed data is replaced. The source 1D data must reside under the current data *name*, the current *expno* and the specified *procno*.

Although ***wsc*** is normally used as described above, it allows you to specify a full dataset path in the following way:

wsc <column> <procno> <expno> <name> <user> <dir>

When entered on a 1D dataset, the arguments specify the destination 2D dataset. When entered on a 2D dataset, the arguments specify the source 1D dataset. If only certain parts of the destination 2D data path are specified, e.g. the *expno* and *name*, the remaining parts are the same as in the current 1D data path. In AU programs, ***wsc*** must always have 6 arguments (see USAGE IN AU PROGAMS below).

wsc can also be started from the dialog box that is opened with the command ***slice***.

INPUT FILES

<dir>/data/<user>/nmr/~TEMP/1/pdata/1

`1r`, `1i` - 1D processed data
`used_from` - data path of the 2D data (input of ***wsc*** on a 1D dataset)

or

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

`1r`, `1i` - 1D processed data
`used_from` - data path of the 2D data (input of ***wsc*** on a 1D dataset)

OUTPUT FILES

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

[1] However, if the current data name is ~TEMP, ***wsc <column> <procno>*** writes to the specified *procno* in the dataset from which the current 1D dataset was extracted.

`2rr`, `2ri` - processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

WSC(column, procno, expno, name, user, dir)

SEE ALSO

rsc, wsr, rsr, wser, wserp, rser, rser2d, slice

wser

NAME

wser - Replace row of 2D raw data by 1D raw data (2D)

SYNTAX

wser [<row> [<expno>]]

DESCRIPTION

The command ***wser*** replaces one row of 2D raw data by 1D raw data. It can be entered on the source 1D dataset or on the destination 2D dataset. When entered on a 1D dataset, ***wser*** opens the following dialog box:

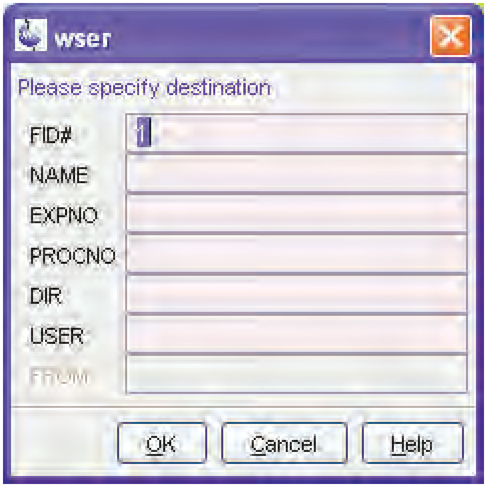


Figure 4.19

Here, you can enter the FID number to be replaced and the destination data path.

Usage of ***wser*** with arguments on the source 1D dataset:

wser <row>
the specified row of the 2D raw data is replaced by the current 1D FID. The destination 2D dataset is the one from which the current 1D dataset was extracted.

wser <row> <expno>

the specified row of the 2D raw data is replaced by the current 1D FID. The 2D dataset must reside under the current data *name*, the specified *expno* and *procno* 1.

Usage of ***wser*** with arguments on the destination 2D dataset:

wser <row> <expno>
the specified row of the current 2D raw data is replaced. The source 1D dataset must reside under the current data *name*, specified *expno* and *procno* 1.

INPUT FILES

<dir>/data/<user>/nmr/~TEMP/1/

`fid` - 1D raw data

<dir>/data/<user>/nmr/~TEMP/1/pdata/1

`used_from` - data path of the 2D data (input of ***wser*** on a 1D dataset)

or

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data

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

`used_from` - data path of the 2D data (input of ***wser*** on a 1D dataset)

wser can also be started from the dialog box that is opened with the command ***slice***.

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<*expno*>/

`ser` - raw 2D data
`audita.txt` - acquisition audit trail

USAGE IN AU PROGRAMS

WSER(row, name, expno, procno, dir, user)

Note that the order of the arguments in AU programs is different from the order on the command line.

SEE ALSO

wserp, rser, rser2d, wsr, wsc, rsr, rsc, slice

wserp

NAME

wserp - Replace row of 2D raw data by 1D processed data

SYNTAX

wserp [<row> [<expno>]]

DESCRIPTION

The command ***wserp*** replaces one row of 2D raw data by processed 1D data. It can be entered on the source 1D dataset or on the destination 2D dataset. When entered on a 1D dataset, ***wserp*** opens the following dialog box:

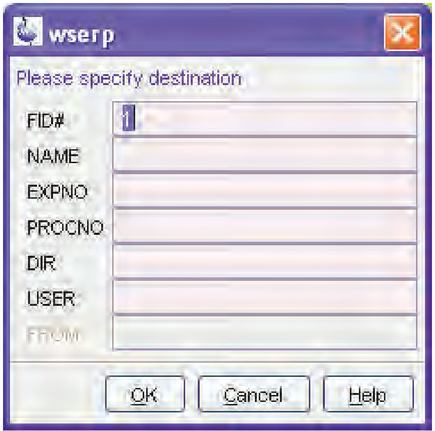


Figure 4.20

Here, you can enter the FID number to be replaced and the destination data path.

Usage of ***wserp*** with arguments on the source 1D dataset:

wserp <row>
the specified row of the 2D raw data is replaced by the current 1D processed data. The 2D dataset is the one from which the current 1D dataset was extracted.

wserp <row> <expno>

the specified row of the 2D raw data under the specified *expno* is replaced by the current 1D processed data. The 2D dataset *name*, *user* and *dir* are the same as in the dataset as the current 1D data were extracted from.

Usage of ***wserp*** with arguments on the destination 2D dataset:

wserp <row> <expno>
the specified row of the current 2D raw data is replaced. The source 1D dataset must reside under the current data *name*, specified *expno* and *procno* 1.

wserp can also be started from the dialog box that is opened with the command ***slice***.

INPUT FILES

<dir>/data/<user>/nmr/~TEMP/1/pdata/1/
`1r`, `1i` - 1D processed data (real, imaginary)
`used_from` - data path of the 2D data (input of ***wserp*** on a 1D dataset)

or

<dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>/
`1r`, `1i` - 1D processed data (real, imaginary)
`used_from` - data path of the 2D data (input of ***wserp*** on a 1D dataset)

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<*expno*>/
`ser` - raw 2D data
`audita.txt` - acquisition audit trail

USAGE IN AU PROGRAMS

WSERP(row, name, expno, procno, dir, user)
Note that the order of the arguments in AU programs is different from the order on the command line.

SEE ALSO

wser, rser, rser2d, wsr, wsc, rsr, rsc, slice

wsr

NAME

wsr - Replace row of a 2D spectrum by 1D spectrum

SYNTAX

wsr [<row> [<procno>]]

DESCRIPTION

The command ***wsr*** replaces one row of 2D processed data by 1D processed data. It is normally used in combination with ***rsr*** in the following way:

- run ***rsr*** to extract row *x* from a 2D spectrum
- manipulate the resulting 1D data with 1D processing commands
- run ***wsr*** to replace row *x* of the 2D data with the manipulated 1D data

wsr can be entered on the source 1D dataset or on the destination 2D dataset.

Examples of the usage of ***wsr*** on the source 1D dataset:

wsr
prompts for the row of the destination 2D data which must be replaced by the current 1D data. The 2D dataset is the one from which the current 1D dataset was extracted.

wsr <row>
the specified row of the destination 2D data is replaced by the current 1D data. The 2D dataset is the one from which the current 1D dataset was extracted.

wsr <row> <procno>
the specified row of the destination 2D data is replaced by the current 1D data. The 2D dataset must reside under the current data *name* [1],

[1] However, if the current data name is ~TEMP, ***wsr <row> <procno>*** writes to the specified *procno* in the dataset from which the current 1D dataset was extracted.

the current *expno* and the specified *procno*.

Examples of usage of ***wsr*** on the destination 2D dataset:

wsr <row>
the specified row of the current 2D processed data is replaced. The source 1D data must reside under the data *name* ~TEMP.

wsr <row> <procno>
the specified row of the current 2D processed data is replaced. The source 1D data must reside under the current data *name*, the current *expno* and the specified *procno*.

wsr can also be started from the dialog box that is opened with the command ***slice***.

INPUT FILES

<dir>/data/<user>/nmr/~TEMP/1/pdata/1

`1r`, `1i` - 1D processed data
`used_from` - data path of the 2D data (input of ***wsr*** on a 1D dataset)

or

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

`1r`, `1i` - 1D processed data
`used_from` - data path of the 2D data (input of ***wsr*** on a 1D dataset)

OUTPUT FILES

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

`2rr`, `2ir` - processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

WSR(row, procno, expno, name, user, dir)

SEE ALSO

wsc, rsr, rsc, wser, wserp, rser, rser2d, slice

xf1

NAME

xf1 - Process data, including FT, in F1 (2D)

DESCRIPTION

The command ***xf1*** processes a 2D dataset in the F1 direction. It can be started from the command line or from the Fourier transform dialog box. The latter is opened with the command ***ftf***.

xf1 Fourier transforms time domain data (FID) into frequency domain data (spectrum). Depending on the F1 processing parameters BC_mod, WDW, ME_mod and PH_mod, ***xf1*** also performs baseline correction, window multiplication, linear prediction and phase correction, respectively. These steps are described in detail for the command ***xfb***.

Normally, 2D data are processed with the command ***xfb*** which performs a Fourier transform in both directions, F2 and F1. In some cases, however, it is useful to process the data in two separate steps using the sequence ***xf2*** - ***xf1***, for example to view the data after processing them in F2 only.

If you run ***xf1*** without running ***xf2*** first, a warning that the F2 transform has not been done will appear. When the command has finished the data are in the time domain in F2 and in the frequency domain in F1. The opposite case, however, is more usual, i.e. data which have only been processed with ***xf2***.

xf1 takes the same options as ***xfb***.

The F1 Fourier transform mode and data storage mode depends on the F1 acquisition mode (see INPUT PARAMETERS below and the description of ***xfb***).

INPUT PARAMETERS

F2 and F1 parameters

set by ***xf2***, can be viewed with ***dpp*** or by typing ***s si***, ***s stsr*** etc.:

SI - size of the processed data

STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)

If ***xf2*** has not been done, ***xf1*** uses the ***edp*** parameters set by the user.

F1 parameters

set from the ***ftf*** dialog box, with ***edp*** or by typing ***bc_mod*** etc.

BC_mod - FID baseline correction mode
- BCFW - filter width for BC_mod = sfil or qfil
- COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil

ME_mod - FID linear prediction mode
- NCOEF - number of linear prediction coefficients
- LPBIN - number of points for linear prediction
- TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode
- LB - Lorentzian broadening factor for WDW = em or gm
- GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
- SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
- TM1, TM2 - limits of the trapezoidal window for WDW = trap

PH_mod - phase correction mode
- PHC0 - zero order phase correction value for PH_mod = pk
- PHC1 - first order phase correction value for PH_mod = pk

FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
REVERSE - flag indicating to reverse the spectrum

set by the ***xf2***, can be viewed with ***dpp*** or by typing ***s mc2*** :

MC2 - Fourier transform mode (input of ***xf1*** on processed data)

set by the acquisition, can be viewed with ***dpa*** or by typing ***s fnmode***:

FnMODE - Acquisition mode (input of ***xf1*** on raw data)

OUTPUT PARAMETERS

F1 parameters

can be viewed with ***dpp*** or by typing ***s ft_mod*** etc.:

FT_mod - Fourier transform mode
FTSIZE - Fourier transform size

F2 parameters

can be viewed with ***dpp*** or by typing ***s ymax_p***, ***s ymin_p*** etc.:

YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - raw data (input if `2rr` does not exist or is Fourier transformed in F1)
`acqu2s` - F1 acquisition status parameters

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

`2rr` - real processed data (input if it exists but is not processed in F1)
`2ir` - second quadrant imaginary processed data (input if FnMODE ≠ QF)
`2ii` - second quadrant imaginary processed data (input if FnMODE = QF)
`proc` - F2 processing parameters
`proc2` - F1 processing parameters

OUTPUT FILES

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

`2rr` - real processed data
`2ir` - third quadrant imaginary processed data (output if FnMODE ≠ QF)
`2ii` - fourth quadrant imaginary processed data (output if FnMODE ≠ QF)
`2ii` - second quadrant imaginary processed data (output if FnMODE = QF)
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XF1

SEE ALSO

xf2, xfb, xtrf, xtrfp1

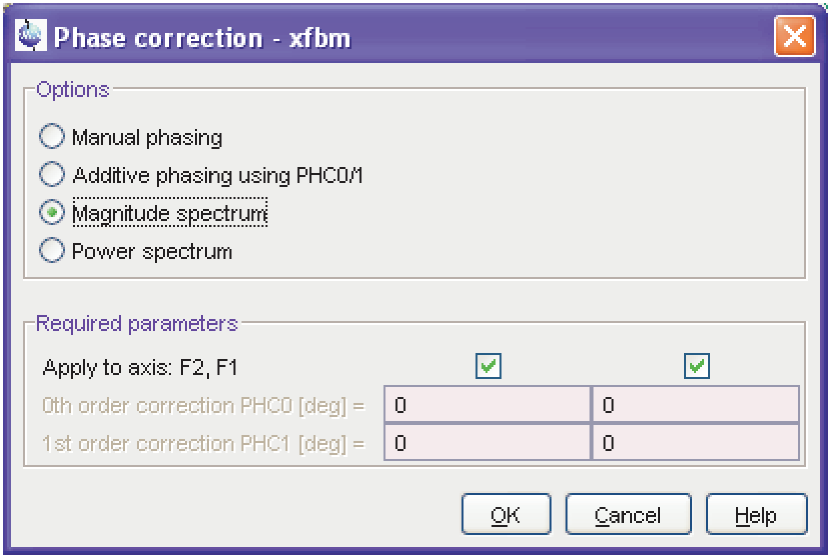
xfbm, xf2m, xf1m, ph

NAME

xfbm - Calculate magnitude spectrum in F2 and F1 (2D)
xf2m - Calculate magnitude spectrum in F2 (2D)
xf1m - Calculate magnitude spectrum in F1 (2D)
ph - Open phase correction dialog box (1D,2D)

DESCRIPTION

The magnitude spectrum commands can be started from the command line or from the phase correction dialog box. The latter is started with the command ***ph***:



Phase correction - xfbm

Options

○ Manual phasing
○ Additive phasing using PHC0/1
● Magnitude spectrum
○ Power spectrum

Required parameters

Apply to axis: F2, F1	☑	☑
0th order correction PHC0 [deg] =	0	0
1st order correction PHC1 [deg] =	0	0

Figure 4.21

This dialog box offers several options, each of which selects a certain command for execution.

Magnitude spectrum (F2)

This option selects the command ***xf2m*** for execution. It calculates the real and F2-imaginary data according to:

$$rr = \sqrt{rr^2 + ir^2}$$

$$ri = \sqrt{ri^2 + ii^2}$$

Figure 4.22

Magnitude spectrum (F1)

This option selects the command ***xf1m*** for execution. It calculates the real and F1-imaginary data according to according to:

$$rr = \sqrt{rr^2 + ri^2}$$

$$ir = \sqrt{ir^2 + ii^2}$$

Figure 4.23

Magnitude spectrum (F12 and F1)

This option selects the command ***xfbm*** for execution. It calculates the real andF1/F2-imaginary data according to according to:

$$rr = \sqrt{rr^2 + ir^2 + ri^2 + ii^2}$$

Figure 4.24

where:

rr = real data (`2rr` file)
ir = F2-imaginary data (`2ir` file)
ri = F1- imaginary data (`2ri` file)
ii = F2/F1-imaginary data (`2ii` file)

The commands ***xf*m*** are, for example, used to convert a phase sensitive spectrum to magnitude spectrum. This is useful for data which cannot be phased properly or data which are not phase sensitive but have been acquired as such.

The ***ph*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XFBM

XF2M

XF1M

SEE ALSO

xf2ps, xf1ps, xfbps

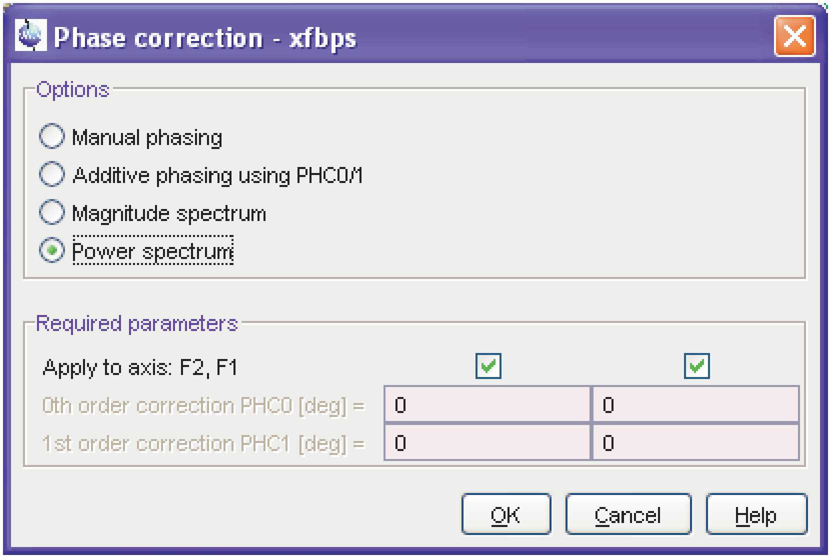
xfbps, xf2ps, xf1ps, ph

NAME

xfbps - Calculate power spectrum in F2 and F1 (2D)
xf2ps - Calculate power spectrum in F2 (2D)
xf1ps - Calculate power spectrum in F1 (2D)
ph - Open phase correction dialog box (1D,2D)

DESCRIPTION

The commands ***xf*ps*** calculate the magnitude spectrum. They can be started from the command line or from the phase correction dialog box. The latter is started with the command ***ph*** (see Figure 4.25).



Phase correction - xfbps

Options

○ Manual phasing
○ Additive phasing using PHC0/1
○ Magnitude spectrum
● Power spectrum

Required parameters

Apply to axis: F2, F1	☑	☑
0th order correction PHC0 [deg] =	0	0
1st order correction PHC1 [deg] =	0	0

Figure 4.25

This dialog box offers several options, each of which selects a certain command for execution.

Power spectrum in F2

This option selects the command ***xf2ps*** for execution. It recalculates the real and F2-imaginary data according to:

$$rr = rr^2 + ir^2$$

$$ri = ri^2 + ii^2$$

Figure 4.26

Power spectrum (F1)

This option selects the command ***`xf1ps`*** for execution. It recalculates the real and F1-imaginary data according to:

$$rr = rr^2 + ri^2$$

$$ir = ir^2 + ii^2$$

Figure 4.27

Power spectrum (F2 and F1)

This option selects the command ***`xfbps`*** for execution. It recalculates the real according to:

$$rr = rr^2 + ir^2 + ri^2 + ii^2$$

Figure 4.28

where:

rr = real data (`2rr` file)
ir = F2-imaginary data (`2ir` file)
ri = F1- imaginary data (`2ri` file)
ii = F2/F1-imaginary data (`2ii` file)

The commands ***`xf*ps`*** is, for example, used in special cases to convert a phase sensitive spectrum to a power spectrum. This is useful for data which cannot be phased properly or data which are not phase sensitive but have been acquired as such.

The ***`ph`*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XFBPS

XF2PS

XF1PS

SEE ALSO

xfbm, xf2m, xf1m

xf2

NAME

xf2 - Process data, including FT, in F2 (2D)

DESCRIPTION

The command ***xf2*** processes a 2D dataset in the F2 direction. It can be started from the command line or from the Fourier transform dialog box. The latter is opened with the command ***ftf***.

xf2 Fourier transforms time domain data (FID) into frequency domain data (spectrum). Depending on the F2 processing parameters BC_mod, WDW, ME_mod and PH_mod, ***xf2*** also performs baseline correction, window multiplication, linear prediction and phase correction, respectively. These steps are described in detail for the command ***xfb***.

Normally, 2D data are processed with the command ***xfb*** which performs a Fourier transform in both directions, F2 and F1. In some cases, however, 2D data must only be processed in the F2 direction. Examples are T1, T2 or Dosy data, or a 2D dataset which has been created from a series on 1D datasets.

Even if a 2D dataset must be processed in both directions, it is sometimes useful to do that in two separate steps using the sequence ***xf2*** - ***xf1***. The result is exactly the same as with ***xfb*** with one exception; ***xfb*** performs a quad spike correction (see ***xfb***) and the sequence ***xf2*** - ***xf1*** does not.

xf2 takes the same options as ***xfb***. Furthermore, ***xf2*** takes the special option ***nd2d*** converting an nD dataset (n>2) to a 2D dataset processing it in the acquisition direction. The size in the orthogonal direction (F1-SI) of the destination 2D dataset, is the product of the TD values of the source nD dataset.

xf2 can also be used to process one 2D plane of a 3D spectrum (see ***xfb***).

INPUT PARAMETERS

F2 and F1 parameters

set from the ***ftf*** dialog box, with ***edp*** or by typing ***si***, ***stsr*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)
XDIM - submatrix size (only used for the command ***xf2 xdim***)

set by the acquisition, can be viewed with ***dpa*** or by typing ***s td***:

TD - time domain; number of raw data points

F2 parameters

set from the ***ftf*** dialog box, with ***edp*** or by typing ***bc_mod*** etc.

BC_mod - FID baseline correction mode
- BCFW - filter width for BC_mod = sfil or qfil
- COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil

ME_mod - FID linear prediction mode
- NCOEF - number of linear prediction coefficients
- LPBIN - number of points for linear prediction
- TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode
- LB - Lorentzian broadening factor for WDW = em or gm
- GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
- SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
- TM1, TM2 - limits of the trapezoidal window for WDW = trap

PH_mod - phase correction mode
- PHC0 - zero order phase correction value for PH_mod = pk
- PHC1 - first order phase correction value for PH_mod = pk

FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
REVERSE - flag indicating to reverse the spectrum

set by the acquisition, can be viewed with ***dpa*** or by typing ***s aq_mod***:

AQ_mod - acquisition mode (determines the Fourier transform mode)
BYTORDA - byteorder or the raw data
NC - normalization constant

F1 parameters

set by the acquisition, can be viewed with ***dpa*** or by typing ***s fnmode*** :

FnMODE - Fourier transform mode

OUTPUT PARAMETERS

F2 and F1 parameters

can be viewed with ***dpp*** or by typing ***s si***, ***s tdeff*** etc.:

SI - size of the processed data
TDeff - number of raw data points that were used for processing
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
FTSIZE - Fourier transform size
XDIM - submatrix size

F2 parameters

can be viewed with ***dpp*** or by typing ***s ft_mod***, ***s ymax_p*** etc.:

FT_mod - Fourier transform mode
YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor
BYTORDP - byte order of the processed data

F1 parameters

set by the acquisition, can be viewed with ***dpp*** or by typing ***s mc2*** :

MC2 - Fourier transform mode

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - raw data (input if `2rr` does not exist or is Fourier transformed in F2)
`acqus` - F2 acquisition status parameters
`acqu2s` - F1 acquisition parameters

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

`2rr` - processed data (input if it exists but is not Fourier transformed in F2)
`proc` - F2 processing parameters

`proc2` - F1 processing parameters

Note that if `2rr` is input, `2ri` is also input if ***xf1*** has been done.

OUTPUT FILES

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

`2rr` - first quadrant real processed data
`2ir` - second quadrant imaginary processed data (output if FnMODE ≠ QF)
`2ii` - second quadrant imaginary processed data (output if FnMODE = QF)
`procs` - F2 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XF2

SEE ALSO

xf1, xfb, xtrf, xtrf2

xfb, ftf

NAME

xfb - Process data, including FT, in F2 and F1 (2D)
ftf - Open Fourier transform dialog box (1D,2D)

DESCRIPTION

The command ***xfb*** processes a 2D dataset or a plane of a dataset with dimension ≥ 3. It can be started from the command line or from the Fourier transform dialog box (see Figure 4.29). The latter is opened with the command ***ftf***.

The ***ftf*** command recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters. For 2D data, two options appear, both of which select the ***xfb*** command for execution, provided the F2 and F1 direction are both enabled.

Standard Fourier transform

This option only allows you to set the parameter SI, the size of the real spectrum.

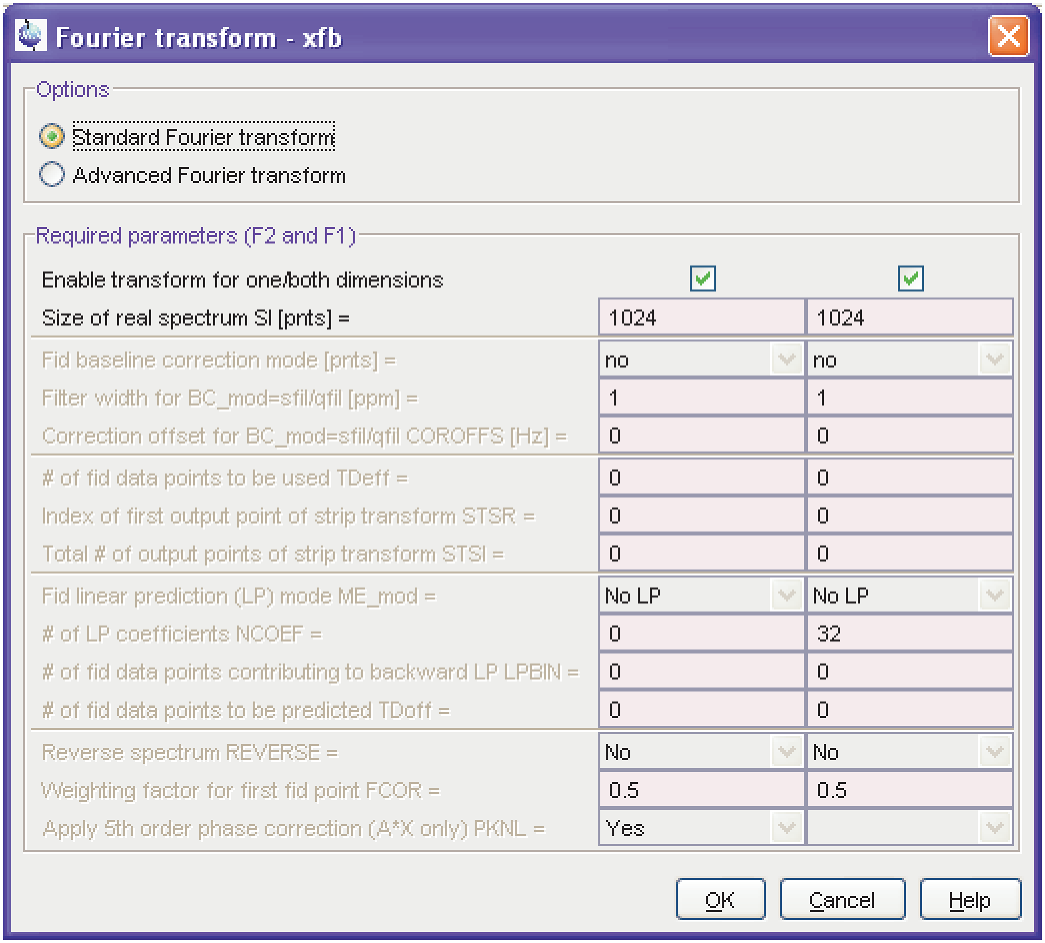
Advanced Fourier transform

This option allows you to set all Fourier transform related parameters.

xfb Fourier transforms time domain data into frequency domain data. Depending on the processing parameters BC_mod, WDW, ME_mod and PH_mod, ***xfb*** also performs baseline correction, window multiplication, linear prediction and spectrum phase correction.

The processing steps done by ***xfb*** can be described as follows:

1. Baseline correction of the 2D time domain data
   Each row and/or column is baseline corrected according to BC_mod. This parameter takes the value *no*, *single*, *quad*, *spol*, *qpol sfil* or *qfil*. More details on BC_mod can be found in chapter 2.4.
2. Linear prediction of the 2D time domain data
   Linear prediction is done according to ME_mod. This parameter takes the value *no*, *LPfr*, *LPfc*, *LPbr*, *LPbc, LPmifr* or *LPmifc*. Usu-



Fourier transform - xfb

Options

● Standard Fourier transform

○ Advanced Fourier transform

Required parameters (F2 and F1)

Enable transform for one/both dimensions	☑	☑
Size of real spectrum SI [pnts] =	1024	1024
Fid baseline correction mode [pnts] =	no	no
Filter width for BC_mod=sfil/qfil [ppm] =	1	1
Correction offset for BC_mod=sfil/qfil COROFFS [Hz] =	0	0
# of fid data points to be used TDeff =	0	0
Index of first output point of strip transform STSR =	0	0
Total # of output points of strip transform STSI =	0	0
Fid linear prediction (LP) mode ME_mod =	No LP	No LP
# of LP coefficients NCOEF =	0	32
# of fid data points contributing to backward LP LPBIN =	0	0
# of fid data points to be predicted TDoff =	0	0
Reverse spectrum REVERSE =	No	No
Weighting factor for first fid point FCOR =	0.5	0.5
Apply 5th order phase correction (A*X only) PKNL =	Yes	

Figure 4.29

ally, ME_mod = no, which means no prediction is done. Forward prediction (*LPfr*, *LPfc*, *LPmifr* or *LPmifc*) can, for example, be used to extend truncated FIDs. Backward prediction (*LPbr* or *LPbc*) can be used to improve the initial data points of the FID. Linear prediction is only performed for NCOEF > 0. Furthermore, LPBIN and, for backward prediction, TDoff play a role (see these parameters in chapter 2.4).

3. Window multiplication of the 2D time domain data

Each row and/or column is multiplied with a window function according to WDW. This parameter takes the value *em*, *gm*, *sine*, *qsine*, *trap*, *user*, *sinc*, *qsinc*, *traf* or *trafs*. More details on WDW can be found in chapter 2.4.

4. Fourier transform of the 2D time domain data
Each row is Fourier transformed according to the acquisition status parameter AQ_mod as shown in table 4.4. Each column (F1) is Fourier transformed according to the acquisition status parameter FnMODE as shown in table 4.5. ***xfb*** does <u>not</u> evaluate the processing parameter FT_mod! However, it stores the Fourier transform mode as it was evaluated from AQ_mod (F2) or FnMODE (F1) in the processing <u>status</u> parameter FT_mod. If, for some reason, you want to Fourier transform a spectrum with a different mode, you can set the processing parameter FT_mod (with ***edp***) and use the command ***xtrf*** (see ***xtrf***). More details on FT_mod can be found in chapter 2.4.

F2 AQ_mod	Fourier transform mode	F2 status FT_mod
qf	forward, single, real	fsr
qsim	forward, quad, complex	fqc
qseq	forward, quad, real	fqr
DQD	forward, quad, complex	fqc

Table 4.4

F1 FnMODE	Fourier transform mode	F1 status FT_mod
QF	forward, quad, complex	fqc
QSEQ	forward, quad, real	fqr
TPPI	forward, single, real	fsr
States	forward, quad, complex	fqc
States-TPPI	forward, single, complex	fsc
Echo-AntiEcho	forward, quad, complex	fqc

Table 4.5

5. Phase correction of the 2D spectrum according to PH_mod. This parameter takes the value *no*, *pk*, *mc* or *ps*. For PH_mod = pk, ***xfb*** applies the values of PHC0 and PHC1. This is only useful if the phase values are known. If they are not, you can do an interactive phase correction in Phase correction mode after ***xfb*** has finished. More details on PH_mod can be found in chapter 2.4.

The size of the processed data is determined by the processing parameter SI; SI real and SI imaginary points are created. A typical value for SI is TD/2 in which case, all raw data points are used and no zero filling is done. In fact, several parameters control the number of input and output data points, for example:

1. SI > TD/2: the raw data are zero filled before the Fourier transform
2. SI < TD/2: only the first 2*SI raw data points are used
3. 0 < TDeff < TD: only the first TDeff raw data points are used
4. 0 < TDoff < TD: the first TDoff raw data points are cut off at the beginning and TDoff zeroes are appended at the end (corresponds to left shift).
5. TDoff < 0: -TDoff zeroes are prepended at the beginning. Note that:
   - for SI < (TD-TDoff)/2 raw data are cut off at the end
   - for DIGMOD=digital, the zeroes would be prepended to the group delay which does not make sense. You can avoid that by converting the raw data with ***convdta*** before you process them.
6. 0 < STSR < SI: only the processed data between STSR and STSR+STSI are stored (if STSI = 0, STSR is ignored and SI points are stored)
7. 0 < STSI < SI: only the processed data between STSR and STSR+STSI are stored.

Note that only in the first case the processed data contain the total information of the raw data. In all other cases, information is lost.

xfb performs a quad spike correction which means that the central data point of the spectrum is replaced by the average of the neighbouring data points in the F1 direction. Note that the quad spike correction is skipped if you process the data with the sequence ***xf2*** - ***xf1***.

xfb evaluates the parameter FCOR. The first point of the FIDs is multiplied with the value of FCOR which lies between 0.0 and 2.0. For digitally filtered Avance data, FCOR is only used in the F1 direction. In F2, it has no effect because the first point is part of the group delay and, as such, is zero. However, A*X data or Avance data measured with DIGMOD = analog, FCOR is used in F1 and F2.

xfb evaluates the F2 parameter PKNL. On A*X spectrometers, PKNL = true causes a non linear 5th order phase correction of the raw data. This corrects possible errors caused by non linear behaviour of the analog filters. On Avance spectrometers, PKNL must always be set to TRUE. For digitally filtered data, it causes ***xfb*** to handle the group delay of the FID. For analog data it has no effect.

xfb evaluates the F2 and F1 parameter REVERSE. If REVERSE = TRUE, the spectrum will be reversed in the corresponding direction, i.e. the first data point becomes the last and the last data point becomes the first. The same effect can be obtained with the commands ***rev2*** and/or ***rev1*** after ***xfb***.

xfb is normally used without options. There are, however, several options available:

n

xfb normally stores real and imaginary processed data. However, the imaginary data are only needed for phase correction. If the parameters PHC0 and PHC1 are set correctly, then you don’t need to store the imaginary data. The option ***n*** allows you to do that. This will save processing time and disk space. If you still want to do a phase correction, you can create imaginary data from the real data with a Hilbert transform (see ***xht2*** and ***xht1***).

nc_proc value

xfb scales the data such that, i.e. the highest intensity of the spectrum lies between 2^{28} and 2^{29}. The intensity scaling factor is stored in the processing status parameter NC_proc and can be viewed with ***dpp***. The option ***nc_proc*** causes ***xfb*** to use a specific scaling factor. However, you can only scale down the data by entering a greater (more positive) value than the one ***xfb*** would use without this option.

If you enter a smaller (more negative) value, the option will be ignored to prevent data overflow. The option ***nc_proc last*** causes ***xfb*** to use the current value of the status processing parameter NC_proc, i.e. the value set by the previous processing step on this dataset.

raw/proc

xfb works on raw data if no processed data exist or if processed data exist and have been Fourier transformed in F2 and/or F1. One of them is usually true, i.e. the data have not been processed yet or they have been processed, for example with ***xfb***. If, however, the data have been processed with ***xtrf*** with FT_mod = no, they are not Fourier transformed and a subsequent ***xfb*** will work on the processed data. The ***raw*** option causes ***xfb*** to work on the raw data, no matter what. The ***proc*** option causes ***xfb*** to work on the processed data. If these do not exist or are Fourier transformed, the command stops and displays an error message. In other words, the option ***proc*** prevents ***xfb*** to work on raw data.

big/little

xfb stores the data in the data byte order (big or little endian) of the computer it runs on e.g. little endian on Windows PCs. Note that TOPSPIN's predecessor XWIN-NMR on SGI UNIX workstations stores data in big endian. The byte order is stored in the processing status parameter BYTORDP which can be viewed with ***s bytordp***. The option ***big*** or ***little*** allows you to predefine the byte order. This, for example, is used to read processed data with third party software which can not interpret BYTORDP. This option is only evaluated when ***xfb*** works on the raw data.

xdim

Large 2D spectra are stored in the so-called submatrix format. The size of the submatrices are calculated by ***xfb*** and depend on the size of the spectrum and the available memory. The option ***xdim*** allows you to use predefined submatrix sizes. It causes ***xfb*** to interpret the F2 and F1 processing parameter XDIM which can be set by entering ***xdim*** on the command line. The actually used submatrix sizes, whether predefined or calculated, are stored as the F2 and F1 processing status parameter XDIM and can be viewed with ***dpp***. Predefining submatrix sizes is, for example, used to read the processed data with third party software which can not interpret the processing status parameter XDIM. This option is only evaluated when ***xfb*** works on the raw data.

Normally, ***xfb*** stores the entire spectral region as determined by the spectral width. You can, however, do a so-called strip transform which means that only a certain region of the spectrum is stored. This can be done by setting the parameters STSR and STSI which represent the strip start and strip size, respectively. They both can take a value between 0 and SI. The values which are actually used can be a little different. STSI is always rounded to the next multiple of 16. Furthermore, when the data are stored in submatrix format (see below), STSI is rounded to the next higher multiple of the submatrix size. Type ***dpp*** to check this; if XDIM is smaller than SI, then the data are stored in submatrix format and STSI is a multiple of XDIM.

Depending on size of the processed data and the available computer memory, ***xfb*** stores the data in sequential or submatrix format. Sequential format is used when the entire dataset fits in memory, otherwise submatrix format is used. ***xfb*** automatically calculates the submatrix sizes such that one row (F2) of submatrices fits in the available memory. The calculated submatrix sizes are stored in the processing status parameter XDIM (type ***dpp***). Table 4.6 and 4.8 show the alignment of the data points for sequential and submatrix format, respectively. This example shows a dataset with the following sizes: F2 SI = 16, F1 SI = 16, F2 XDIM = 8, F1 XDIM = 4. The storage handling is completely transparent to the user and is only of interest when the data are interpreted by third party software.

F2

F1

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
32	33	34	35	36	38	38	39	40	41	42	43	44	45	46	47
48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63
64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79
80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95
96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111
112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127
128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143
144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159
160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175
176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191
192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207
208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223
224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239
240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255

Table 4.6 2D data in sequential storage format

F2

F1

0	1	2	3	4	5	6	7	32	33	34	35	36	37	38	39
8	9	10	11	12	13	14	15	40	41	42	43	44	45	46	47
16	17	18	19	20	21	22	23	48	49	50	51	52	53	54	55
24	25	26	27	28	29	30	31	56	57	58	59	60	61	62	63
64	65	66	67	68	69	70	71	96	97	98	99	100	101	102	103
72	73	74	75	76	77	78	79	104	105	106	107	108	109	110	111
80	81	82	83	84	85	86	87	112	113	114	115	116	117	118	119
88	89	90	91	92	93	94	95	120	121	122	123	124	125	126	127
128	129	130	131	132	133	134	135	160	161	162	163	164	165	166	167
136	137	138	139	140	141	142	143	168	169	170	171	172	173	174	175
144	145	146	147	148	149	150	151	176	177	178	179	180	181	182	183
152	153	154	155	156	157	158	159	184	185	186	187	188	189	190	191
192	193	194	195	196	197	198	199	224	225	226	227	228	229	230	231
200	201	202	203	204	205	206	207	232	233	234	235	236	237	238	239
208	209	210	211	212	213	214	215	240	241	242	243	244	245	246	247
216	217	218	219	220	221	222	223	248	249	250	251	252	253	254	255

Table 4.7 2D data in 8*4 submatrix storage format

As can be seen in table 4.5, the acquisition mode in F1 (FnMODE) determines the Fourier transform mode. Furthermore, FnMODE determines the data storage mode. The description below demonstrates the difference in data storage between a data set with FnMODE = QF and one with FnMODE ≠ QF.

FnMODE = QF

xfb performs complex (two-quadrant) processing. In F2 the data are acquired phase sensitive, in F1 non-phase sensitive. In the example below, the following parameter settings are used:

In F2: TD = 8, SI is 4
In F1: TD = 2, SI = 2

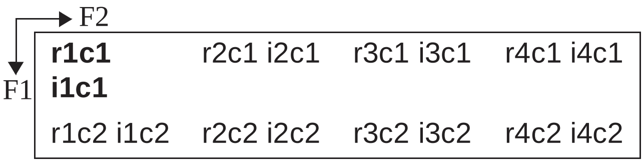
Furthermore, the following notation is used for individual data points:

r*n***c***m* : point *n* of FID *m*. This point is real in F2 and complex in F1
i*n***c***m* : point *n* of FID *m*. This point is imaginary in F2 and complex

in F1

I

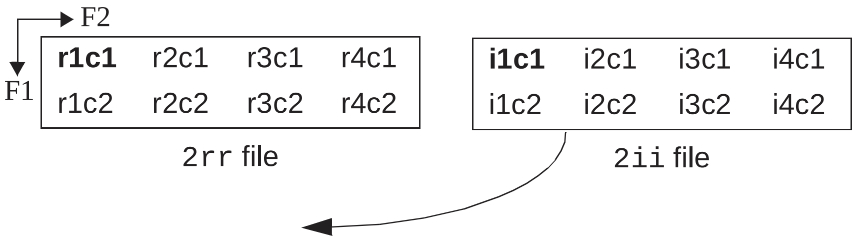
Input F2 processing (raw data)



r1c1 **i1c1**	r2c1 i2c1	r3c1 i3c1	r4c1 i4c1
r1c2 i1c2	r2c2 i2c2	r3c2 i3c2	r4c2 i4c2

For F2 processing, **r1c1 i1c1** is the first complex input point, r2c1 i2c1 the second etc.

Output F2 processing = Input F1 processing



r1c1	r2c1	r3c1	r4c1
r1c2	r2c2	r3c2	r4c2

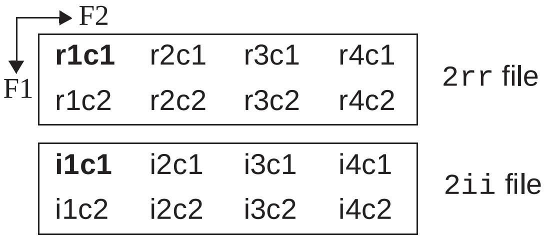
`2rr` file

i1c1	i2c1	i3c1	i4c1
i1c2	i2c2	i3c2	i4c2

`2ii` file

Below, the F1 input data are simply redisplayed in vertical order, with the first complex input point in bold.

Input F1 processing



r1c1	r2c1	r3c1	r4c1
r1c2	r2c2	r3c2	r4c2

`2rr` file

i1c1	i2c1	i3c1	i4c1
i1c2	i2c2	i3c2	i4c2

`2ii` file

Output F1 processing

	F2				
	r1c1	r2c1	r3c1	r4c1	`2rr` file
F1	r1c2	r2c2	r3c2	r4c2	

i1c1	i2c1	i3c1	i4c1	`2ii` file
i1c2	i2c2	i3c2	i4c2	

FnMODE ≠ QF

`xfb` performs hypercomplex (four-quadrant) processing. Both in F2 and F1, the data are acquired phase sensitive. In the example below, the following parameters settings are used:

In F2: TD = 8, SI is 4
In F1: TD = 4, SI = 2

Furthermore, the following notation is used for individual data points:

- **r***n***r***m* : point *n* of FID *m*. This point is real in F2 and F1
- **i***n***r***m* : point *n* of FID *m*. This point is imaginary in F2 and real in F1
- **r***n***i***m*: point *n* of FID *m*. This point is real in F2 and imaginary in F1
- **i***n***i***m* : point *n* of FID *m*. This point is imaginary in F2 and F1

Input F2 processing (raw data)

	F2			
	r1r1 i1r1	r2r1 i2r1	r3r1 i3r1	r4r1 i4r1
F1	r1i1 i1i1	r2i1 i2i1	r3i1 i3i1	r4i1 i4i1
	r1r2 i1r2	r2r2 i2r2	r3r2 i3r2	r4r2 i4r2
	r1i2 i1i2	r2i2 i2i2	r3i2 i3i2	r4i2 i4i2

`ser file`

For F2 processing, **r1r1 i1r1** is the first hypercomplex input data point, r2r1 i2r1 the second etc.

Output F2 processing = Input F1 processing

F2

F1

r1r1	r2r1	r3r1	r4r1
r1i1	r2i1	r3i1	r4i1
r1r2	r2r2	r3r2	r4r2
r1i2	r2i2	r3i2	r4i2

`2rr` file

i1r1	i2r1	i3r1	i4r1
i1i1	i2i1	i3i1	i4i1
i1r2	i2r2	i3r2	i4r2
i1i2	i2i2	i3i2	i4i2

`2ir` file

Below, the F1 input data are simply redisplayed, with the first F1 complex input points in bold.

Input F1 processing

F2

F1

r1r1	r2r1	r3r1	r4r1
r1i1	r2i1	r3i1	r4i1
r1r2	r2r2	r3r2	r4r2
r1i2	r2i2	r3i2	r4i2

`2rr` file

i1r1	i2r1	i3r1	i4r1
i1i1	i2i1	i3i1	i4i1
i1r2	i2r2	i3r2	i4r2
i1i2	i2i2	i3i2	i4i2

`2ir` file

Output F1 processing

F2

F1

r1r1	r2r1	r3r1	r4r1
r1r2	r2r2	r3r2	r4r2

`2rr` file

i1r1	i2r1	i3r1	i4r1
i1r2	i2r2	i3r2	i4r2

`2ir` file

r1i1	r2i1	r3i1	r4i1
r1i2	r2i2	r3i2	r4i2

`2ri` file

i1i1	i2i1	i3i1	i4i1
i1i2	i2i2	i3i2	i4i2

`2ii` file

FnMODE = Echo-Antiecho

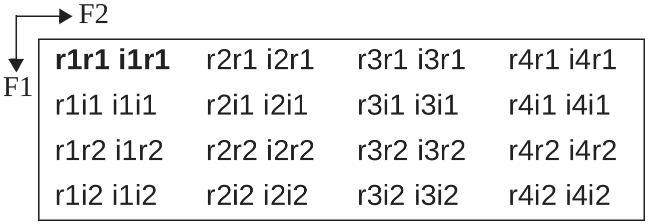
xfb performs hypercomplex (four-quadrant) processing. Both in F2 and F1, the data are acquired phase sensitive. In the example below, the following parameters settings are used:

In F2: TD = 8, SI is 4
In F1: TD = 4, SI = 2

Furthermore, the following notation is used for individual data points:

- **r***n***r***m* : point *n* of FID *m*. This point is real in F2 and F1
- **i***n***r***m* : point *n* of FID *m*. This point is imaginary in F2 and real in F1
- **r***n***i***m*: point *n* of FID *m*. This point is real in F2 and imaginary in F1
- **i***n***i***m* : point *n* of FID *m*. This point is imaginary in F2 and F1

Input F2 processing (raw data)



r1r1 i1r1	r2r1 i2r1	r3r1 i3r1	r4r1 i4r1
r1i1 i1i1	r2i1 i2i1	r3i1 i3i1	r4i1 i4i1
r1r2 i1r2	r2r2 i2r2	r3r2 i3r2	r4r2 i4r2
r1i2 i1i2	r2i2 i2i2	r3i2 i3i2	r4i2 i4i2

`ser file`

For F2 processing, **r1r1 i1r1** is the first hypercomplex input data point, r2r1 i2r1 the second etc.

Output F2 processing = Input F1 processing

F2

F1

-i1r1-i1i1	-i2r1-i2i1	-i3r1-i3i1	-i4r1-i4i1
-r1r1+r1i1	-r2r1+r2i1	-r3r1+r3i1	-r4r1+r4i1
-i1r2-i1i2	-i2r2-i2i2	-i3r2-i3i2	-i4r2-i4i2
-r1r2+r1i2	-r2r2+r2i2	-r3r2+r3i2	-r4r2+r4i2

`2rr` file

r1r1+r1i1	r2r1+r2i1	r3r1+r3i1	r4r1+r4i1
-i1r1+i1i1	-i2r1+i2i1	-i3r1+i3i1	-i4r1+i4i1
r1r2+r1i2	r2r2+r2i2	r3r2+r3i2	r4r2+r4i2
-i1r2+i1i2	-i2r2+i2i2	-i3r2+i3i2	-i4r2+i4i2

`2ir` file

Below, the F1 input data are simply redisplayed, with the first F1 complex input points in bold.

Input F1 processing

F2

F1

-i1r1-i1i1	-i2r1-i2i1	-i3r1-i3i1	-i4r1-i4i1
-r1r1+r1i1	-r2r1+r2i1	-r3r1+r3i1	-r4r1+r4i1
-i1r2-i1i2	-i2r2-i2i2	-i3r2-i3i2	-i4r2-i4i2
-r1r2+r1i2	-r2r2+r2i2	-r3r2+r3i2	-r4r2+r4i2

r1r1+r1i1	r2r1+r2i1	r3r1+r3i1	r4r1+r4i1
-i1r1+i1i1	-i2r1+i2i1	-i3r1+i3i1	-i4r1+i4i1
r1r2+r1i2	r2r2+r2i2	r3r2+r3i2	r4r2+r4i2
-i1r2+i1i2	-i2r2+i2i2	-i3r2+i3i2	-i4r2+i4i2

`2ir` file

Output F1 processing

F2

F1

-i1r1-i1i1	-i2r1-i2i1	-i3r1-i3i1	-i4r1-i4i1
-i1r2-i1i2	-i2r2-i2i2	-i3r2-i3i2	-i4r2-i4i2

`2rr` file

r1r1+r1i1	r2r1+r2i1	r3r1+r3i1	r4r1+r4i1
r1r2+r1i2	r2r2+r2i2	r3r2+r3i2	r4r2+r4i2

`2ir` file

-r1r1+r1i1	-r2r1+r2i1	-r3r1+r3i1	-r4r1+r4i1
-r1r2+r1i2	-r2r2+r2i2	-r3r2+r3i2	-r4r2+r4i2

-i1r1+i1i1	-i2r1+i2i1	-i3r1+i3i1	-i4r1+i4i1
-i1r2+i1i2	-i2r2+i2i2	-i3r2+i3i2	-i4r2+i4i2

`2ii` file

Note that:

- for FnMODE ≠ QF, zero filling once in F1 is done when SI = TD. For FnMODE = QF, zero filling once in F1 is done when SI = 2*TD.
- FnMODE = QF is normally used on magnitude or power data. For this purpose, the F1 processing parameter PH_mod must be set to MC or PS, respectively. Note that in these cases, no imaginary data are stored after F1 processing.
- FnMODE = Echo-Antiecho is equivalent to FnMODE = States, except that two consecutive FIDs (rows of the 2D raw data) are linearly combined according to the following rules:

  re0 = -im1 - im0
  im0 = re1 + re0
  re1 = re1 - re0
  im1 = im1 - im0

- the command ***xfb n*** does not store imaginary data after F1 processing.

2D PROCESSING OF 3D DATA

xfb can also be used to process one 2D plane of a 3D spectrum. This can be a plane in the F3-F2 or in the F3-F1 direction. The output 2D data are stored in a separate *procno*. When the current dataset is a 3D, ***xfb*** will prompt you for the plane axis direction, the plane number, the output *procno* and, if applicable, for the permission to overwrite existing data. Alternatively, you can enter this information as arguments on the command line, for example:

```
xfb s23 17 2 y
```

will read the F3-F2 plane number 17 and store it under procno 2, overwriting possibly existing data. Furthermore, you can use the ***nodisp*** argument to prevent opening/displaying the destination dataset, e.g.:

```
xfb s23 17 2 y nodisp
```

For 2D processing of 3D echo-antiecho (EA) data the option ***eao*** is available. This option ensures EA calculation when:

- the 3D raw data are EA in either F2 or F1 (the acquisition status parameter FnMODE = Echo-Antiecho in F2 or F1, respectively)
- the processed plane does not include the EA direction

For example, to process F2-F3 plane 17 of a 3D dataset which is EA in F1, enter:

```
xfb eao s23 17 2 y
```

If you omit the ***eao*** option, the plane is still processed but no EA calculation is done. Using the ***eao*** option allows you to determine the correct phase values for EA data or compare the processed plane with a plane extracted from a 3D processed data. Note that if the processed plane includes the EA direction, or if the 3D data are not EA in any direction, the option ***eao*** has no effect.

When executed on a dataset with 3D raw data but 2D processed data[1], ***xfb*** takes one argument:

[1] Usually a result of a previous 2D processing command on that 3D dataset.

xfb <plane>

process the specified plane and store it under the current *procno*.

xfb same

process the same plane as the previous processing command and store it under the current *procno*. The ***same*** option is automatically used by the AU program macro XFB. When used on a regular 2D dataset (i.e. with 2D raw data), it has no effect.

INPUT PARAMETERS

F2 and F1 parameters

set from the ***ftf*** dialog box, with ***edp*** or by typing ***bc_mod***, ***bcfw*** etc.

BC_mod - FID baseline correction mode
- BCFW - filter width for BC_mod = sfil or qfil
- COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil

ME_mod - FID linear prediction mode
- NCOEF - number of linear prediction coefficients
- LPBIN - number of points for linear prediction
- TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode
- LB - Lorentzian broadening factor for WDW = em or gm
- GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
- SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
- TM1, TM2 - limits of the trapezoidal window for WDW = trap

PH_mod - phase correction mode
- PHC0 - zero order phase correction value for PH_mod = pk
- PHC1 - first order phase correction value for PH_mod = pk

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)
FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
REVERSE - flag indicating to reverse the spectrum
XDIM - submatrix size (only used for the command ***xfb xdim***)

set by the acquisition, can be viewed with ***dpa*** or by typing ***s td*** :

TD - time domain; number of raw data points

F2 parameters

set from the ***ftf*** dialog box, with ***edp*** or by typing ***pknl*** :

PKNL - group delay compensation (Avance) or filter correction (A*X)

set by the acquisition, can be viewed with ***dpa*** or by typing ***s aq_mod***.:

AQ_mod - acquisition mode (determines the Fourier transform mode)
BYTORDA - byteorder or the raw data
NC - normalization constant

F1 parameters

set by the acquisition, can be viewed with ***dpa*** or by typing ***s fnmode*** :

FnMODE - F1 Acquisition transform mode

set by the user with ***edp*** or by typing ***mc2*** :

MC2 - FT mode in F1 (only used if F1-FnMODE = undefined)

OUTPUT PARAMETERS

F2 and F1 parameters

can be viewed with ***dpp*** or by typing ***s si***, ***s tdeff*** etc.:

SI - size of the processed data
TDeff - number of raw data points that were used for processing
FTSIZE - Fourier transform size
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
XDIM - submatrix size
FT_mod - Fourier transform mode

F2 parameters

can be viewed with ***dpp*** or by typing ***s ymax_p***, ***s ymin_p*** etc.:

YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor
BYTORDP - byte order of the processed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - raw data (input if `2rr` does not exit or is Fourier transformed)

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

`2rr` - real processed 2D data (input if it exists but is not Fourier transformed)
`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`acqus` - F2 acquisition status parameters
`acqu2s` - F1 acquisition status parameters

Note that if `2rr` is input, then `2ir` and `2ri` can also be input, depending on the processing status of the data.

OUTPUT FILES

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

For FnMODE ≠ QF:

`2rr` - real processed 2D data
`2ir` - second quadrant imaginary processed data
`2ri` - third quadrant imaginary processed data
`2ii` - fourth quadrant imaginary processed data

For FnMODE = QF:

`2rr` - real processed 2D data
`2ii` - second quadrant imaginary processed data

For all values of FnMODE:

`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XFB

If you want to use XFB with an option, you can do that with XCMD, e.g. XCMD("xfb raw")

SEE ALSO

xf2, xf1, xfbp, xfbm, xfbps, xtrf

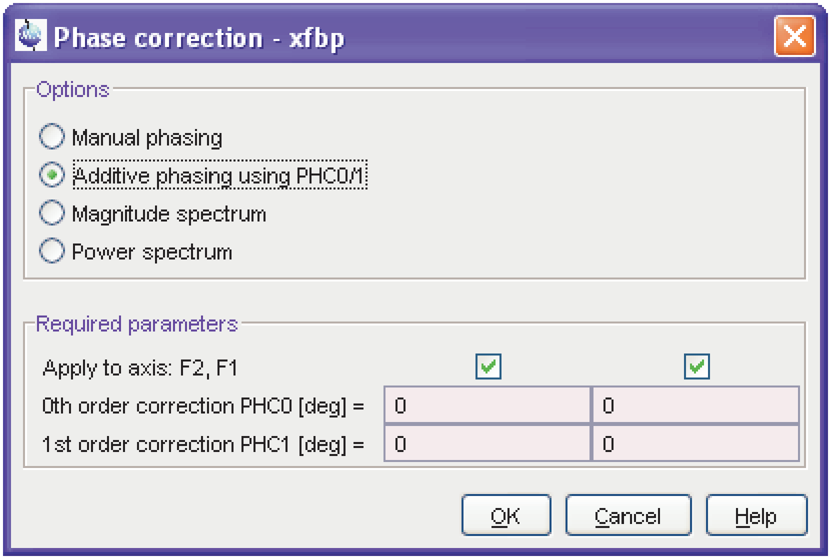
xfbp, xf2p, xf1p, ph

NAME

xfbp - Phase correction in F2 and F1 direction (2D)
xf2p - Phase correction in F2 (2D)
xf1p - Phase correction in F1 (2D)
ph - Open phase correction dialog box (1D,2D)

DESCRIPTION

2D phase correction can be started from the command line or from the phase correction dialog box. The latter is opened with the command ***ph***:



Phase correction - xfbp

Options

○ Manual phasing
● Additive phasing using PHC0/1
○ Magnitude spectrum
○ Power spectrum

Required parameters

Apply to axis: F2, F1	☑	☑
0th order correction PHC0 [deg] =	0	0
1st order correction PHC1 [deg] =	0	0

Figure 4.30

This dialog box offers several options, each of which selects a certain command for execution.

Additive phasing using PHC0/1 (F2 and F1)

This option selects the command ***xfbp*** for execution. It performs a zero and first order 2D phase correction in the F2 and F1 direction. ***xfbp*** works like the 1D command ***pk***. This means it does not calculate the phase values, it simply applies the current values of PHC0 and PHC1.

Additive phasing using PHC0/1 (F2)

This option selects the command ***xf2p*** for execution. It works like ***xfbp***, except that it only corrects the phase in the F2 direction.

Additive phasing using PHC0/1 (F1)

This option selects the command ***xf1p*** for execution. It works like ***xfbp***, except that it only corrects the phase in the F1 direction.

xf*p are only useful when the PHC0 and PHC1 values are known. If they are not, you can perform 2D interactive phase correction. To do that select the option ***Manual Phasing*** in the ***ph*** dialog box or click in the toolbar. The interactive phase correction procedure is described in the TOPSPIN Users Guide.

The phase values can also be determined by the 1D interactive phase correction of a row or column. To do that, read a row (***rsr***) and/or column (***rsc***) and click in the toolbar (see TOPSPIN Users Guide). Alternatively, you can phase correct a row or column with ***apk*** and view the calculated phase values with ***dpp***. Then you can go back to the 2D dataset, set the determined phase values with ***edp*** and run ***xfbp*** to apply them.

xfbp uses but does not change the processing parameters PHC0 and PHC1 (***edp***). It does, however, change the corresponding processing status parameters (***dpp***), by adding the applied phase values.

The ***ph*** command can be used on 1D or 2D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***ph*** dialog box, with ***edp*** or by typing ***phc0***, ***phc1***:

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s phc0***, ***s phc1***:

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

INPUT FILES

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

`2rr`, `ir`, `2ri`, `2ii` - processed 2D data
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters

OUTPUT FILES

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

`2rr`, `ir`, `2ri`, `2ii` - processed 2D data
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XFBP

XF2P

XF1P

SEE ALSO

xfb, xf2, xf1, xtrf, xtrfp, xtrfp2, xtrfp1

xht2, xht1

NAME

xht2 - Hilbert transform in F2 (2D)
xht1 - Hilbert transform in F1 (2D)

DESCRIPTION

The command ***xht2*** performs a Hilbert transform of 2D data in the F2 direction.

The command ***xht1*** performs a Hilbert transform of 2D data in the F1 direction.

Hilbert transform creates imaginary data from the real data. Imaginary data are required for phase correction. They are normally created during Fourier transform with ***xfb***, ***xf2*** or ***xf1***. If, however, if the imaginary data were not stored (***xfb n***) or have been deleted (***deli***), you can (re)create them with ***xht2*** or ***xht1***.

Note that Hilbert Transform is only useful when the real data have been created from zero filled raw data, with SI ≥ TD.

Hilbert transform can also be used if the imaginary data exist but do not match the real data. This is the case when the latter have been manipulated after Fourier transform, for example by ***abs1***, ***abs2***, ***sub****, ***sym*** or third party software.

INPUT FILES

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

`2rr` - real processed 2D data
`2ir` - second quadrant imaginary data (if existing, input of ***xht1***)
`2ri` - third quadrant imaginary data (if existing, input of ***xht2***)

OUTPUT FILES

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

`2rr` - real processed 2D data
`2ir` - second quadrant imaginary data (output of ***xht2***, created from `2rr`)

`2ri` - third quadrant imaginary data (output of ***`xht1`***, created from `2rr`)
`2ii` - fourth quadrant imaginary data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XHT2

XHT1

SEE ALSO

xfb, xf2, xf1

xif2, xif1

NAME

xif2 - Inverse Fourier transform in F2 (2D)
xif1 - Inverse Fourier transform in F1 (2D)

DESCRIPTION

The command ***xif2*** performs an inverse Fourier transform in the F2 direction. This means frequency domain data (spectrum) are transformed into time domain data (FID).

xif1 performs an inverse Fourier transform in the F1 direction.

Note that after ***xif2*** or ***xif1*** (or both), the data are still stored as processed data, i.e. the raw data are not overwritten. You can, however, create pseudo-raw data with the command ***genser*** which creates a new dataset.

Inverse Fourier transform can also be done with the commands ***xtrfp***, ***xtrfp2*** and ***xtrfp1***. To do that:

1. Type ***dpp*** and check the status FT_mod.
2. Type ***edp*** to set the processing parameters; set BC_mod, WDW, ME_mod and PH_mod to *no* and FT_mod to the inverse equivalent of the status FT_mod.
3. Perform ***xtrfp***, ***xtrfp2*** or ***xtrfp1***.

INPUT FILES

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

`2rr`, `ir`, `2ri`, `2ii` - processed 2D data

OUTPUT FILES

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

`2rr`, `ir`, `2ri`, `2ii` - processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XIF2

XIF1

SEE ALSO

genser, xtrfp, xtrfp2, xtrfp1

xtrf, xtrf2

NAME

xtrf - Custom processing of raw data in F2 and F1 (2D)
xtrf2 - Custom processing of raw data in F2 (2D)

DESCRIPTION

The command ***xtrf*** performs customized processing of the raw data in both the F2 and F1 direction. It processes data according to the processing parameters BC_mod, WDW, ME_mod, FT_mod and PH_mod. ***xtrf*** works like ***xfb***, except for the following differences:

- the Fourier transform is performed according to the processing parameter FT_mod, whereas the acquisition status parameter AQ_mod is ignored. This, for example, allows you to process the data without Fourier transform (FT_mod = no). Furthermore, you can choose a Fourier transform mode different from the one that would be evaluated from the acquisition mode. This feature is not used very often because the Fourier transform as evaluated from the acquisition mode is usually the correct one. If, however, you want to manipulate the acquisition mode of the raw data, you can Fourier transform the data with one FT_mod, inverse Fourier transform them with a different FT_mod. Then you can use ***genser*** to create pseudo-raw data with a different acquisition mode than the original raw data. Table 4.8 shows a list of values of FT_mod:

FT_mod	Fourier transform mode
no	no Fourier transform
fsr	forward, single channel, real
fqr	forward, quadrature, real
fsc	forward, single channel, complex
fqc	forward, quadrature, complex
isr	inverse, single channel, real
iqr	inverse, quadrature, real
isc	inverse, single channel, complex
iqc	inverse, quadrature, complex

Table 4.8

- a baseline correction is performed according to BC_mod. This parameter can take the value *no*, *single*, *quad*, *spol*, *qpol*, *sfil* or *qfil*. ***xtrf*** evaluates BC_mod for the baseline correction mode (e.g. quad, qpol or qfil) and for the detection mode (e.g. single or quad, spol or qpol, sfil or qfil). Note that ***xfb*** evaluates the acquisition status parameter AQ_mod for the detection mode. More details on BC_mod can be found in chapter 2.4.
- when all parameters mentioned above are set to *no*, no processing is done but the raw data are still stored as processed data and displayed on the screen. This means the raw data are converted to submatrix format (files `2rr`, `2ir`, `2ri` and `2ii`) and scaled according to the vertical resolution. The intensity scaling factor is stored in the processing status parameter NC_proc and can be viewed with ***dpp***. The size of these processed data and the number of raw data points which are used are determined by the parameters SI, TDeff and TDoff, as described for the command ***xfb***. For example, if 0 < TDeff < TD, the processed data are truncated. This allows you to create pseudo-raw data with a smaller size than the original raw data (see also ***genser***).

The F1 Fourier transform mode and data storage mode depends on the F1 acquisition mode (see INPUT PARAMETERS below and the description of ***xfb***).

xtrf2 works like ***xtrf***, except that it only works in the F2 direction.

xtrf and ***xtrf2*** take the same options as ***xfb***.

xtrf can be used to do a combination of forward and backward prediction. Just run ***xtrf*** with ME_mod = LPfc and ***xtrfp*** (or ***xfb***) with ME_mod = LPbc.

INPUT PARAMETERS

F2 and F1 direction

set by the user with ***edp*** or by typing ***si***, ***bc_mod***, ***bcfw*** etc.:

SI - size of the processed data
TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)
FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
BC_mod - FID baseline correction mode
BCFW - filter width for BC_mod = sfil or qfil
COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil
ME_mod - FID linear prediction mode
NCOEF - number of linear prediction coefficients
LPBIN - number of points for linear prediction
TDoff - number of raw data points predicted for ME_mod = LPb*
WDW - FID window multiplication mode
LB - Lorentzian broadening factor for WDW = em or gm
GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
TM1, TM2 - limits of the trapezoidal window for WDW = trap
FT_mod - Fourier transform mode
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
REVERSE - flag indicating to reverse the spectrum
PKNL - group delay compensation (Avance) or filter correction (A*X)
PH_mod - phase correction mode
PHC0 - zero order phase correction value for PH_mod = pk

PHC1 - first order phase correction value for PH_mod = pk

set by the acquisition, can be viewed with ***dpa*** or by typing ***s td*** :

TD - time domain; number of raw data points

F2 direction

set by the acquisition, can be viewed with ***dpa*** or by typing ***s bytorda***:

BYTORDA - byteorder or the raw data
NC - normalization constant

F1 direction

set by the acquisition, can be viewed with ***dpa*** or by typing ***s fnmode***:

FnMODE - Acquisition mode

OUTPUT PARAMETERS

F2 and F1 parameters

can be viewed with ***dpp*** or by typing ***s si*** etc.:

SI - size of the processed data
TDeff - number of raw data points that were used for processing
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
XDIM - submatrix size

F2 parameters

can be viewed with ***dpp*** or by typing ***s ymax_p***, ***s ymin_p*** etc.:

YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor
BYTORDP - byte order of the processed data

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - raw data
`acqus` - F2 acquisition status parameters

`acqu2s` - F1 acquisition status parameters

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

`proc` - F2 processing parameters
`proc2` - F1 processing parameters

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`procs` - processing status parameters
`proc2s` - processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XTRF

XTRF2

SEE ALSO

xtrfp, xtrfp2, xtrfp1, xfb, xf2, xf1

xtrfp, xtrfp2, xtrfp1

NAME

xtrfp - Custom processing of processed data in F2 and F1 (2D)
xtrfp2 - Custom processing of processed data in F2 (2D)
xtrfp1 - Custom processing of processed data in F1 (2D)

DESCRIPTION

The command ***xtrfp*** performs customized processing of processed data both the F2 and F1 direction. It works like ***xtrf***, except that it only works on processed data. If processed data do not exist, an error message is displayed. If processed data do exist, they are further processed according to the parameters BC_mod, WDW, ME_mod, FT_mod and PH_mod as described for ***xtrf***.

xtrfp2 works like ***xtrfp***, except that it only works in the F2 direction.

xtrfp1 works like ***xtrfp***, except that it only works in the F1 direction.

The ***xtrfp**** commands can, for example, be used to perform multiple additive baseline corrections. This can be necessary if the raw data contain multiple frequency baseline distortions. You cannot do this with ***xfb*** or ***xtrf*** because these commands always work on the raw data, i.e. they are not additive.

xtrfp, ***xtrfp2*** and ***xtrfp1*** can also be used for inverse Fourier transform. To do that:

1. Type ***dpp*** to check the status FT_mod
2. Type ***edp*** to set the processing parameters; set BC_mod, WDW, ME_mod and PH_mod to *no* and FT_mod to the inverse equivalent of the status FT_mod
3. Perform ***xtrfp***, ***xtrfp2*** or ***xtrfp1***

An alternative way to do an inverse Fourier transform is the usages of the commands ***xif2*** and ***xif1***.

INPUT PARAMETERS

F2 and F1 parameters

set by the user with ***edp*** or by typing ***bc_mod***, ***bcfw*** etc.:

BC_mod - FID baseline correction mode

BCFW - filter width for BC_mod = sfil or qfil

COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil

ME_mod - FID linear prediction mode

NCOEF - number of linear prediction coefficients

LPBIN - number of points for linear prediction

TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode

LB - Lorentzian broadening factor for WDW = em or gm

GB - Gaussian broadening factor for WDW = gm, sinc or qsinc

SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc

TM1, TM2 - limits of the trapezoidal window for WDW = trap

FT_mod - Fourier transform mode

PH_mod - phase correction mode

PHC0 - zero order phase correction value for PH_mod = pk

PHC1 - first order phase correction value for PH_mod = pk

FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)

REVERSE - flag indicating to reverse the spectrum

set by a previous processing command, e.g. ***xtrf***, can be viewed with ***dpp*** :

SI - size of the processed data

STSR - strip start: first output point of strip transform

STSI - strip size: number of output points of strip transform

TDeff - number of raw data points to be used for processing

TDoff - first point of the FID used for processing (default 0)

F1 parameters

set by a previous processing command, e.g. ***xtrf***, can be viewed with ***dpp*** :

MC2 - Fourier transform mode

OUTPUT PARAMETERS

F2 parameters

can be viewed with ***dpp*** or by typing ***s ymax_p***, ***s ymin_p*** etc.:

YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor
BYTORDP - byte order of the processed data

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`proc` - F2 processing parameters
`proc2` - F1 processing parameters

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

XTRFP

XTRFP2

XTRFP1

SEE ALSO

xtrf, xtrf2, xfb, xf2, xf1

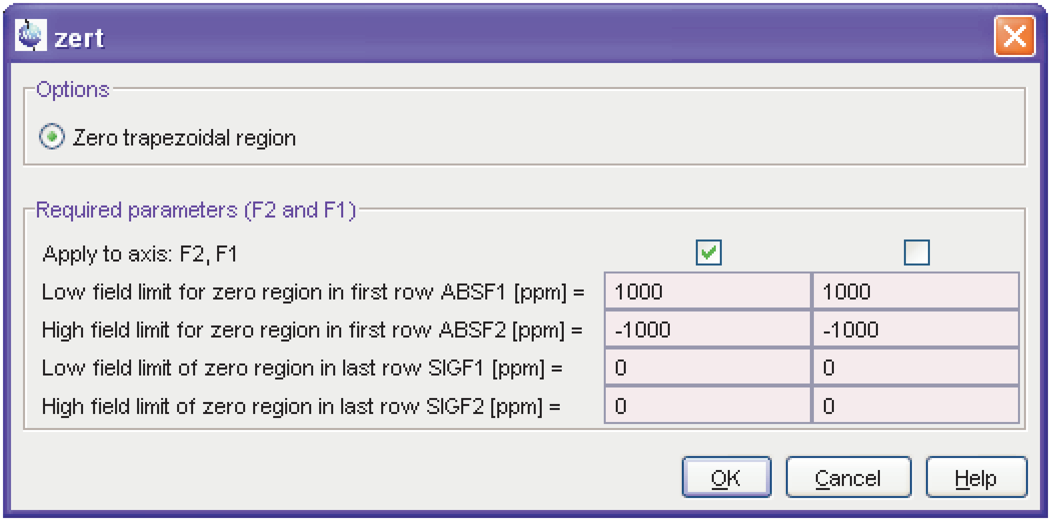
zert2, zert1, zert

NAME

zert2 - Zero a trapezoidal region of each row (2D)
zert1 - Zero a trapezoidal region of each column (2D)
zert - Open zero region dialog box (2D)

DESCRIPTION

The zero region commands can be started from the command line or from the zero region dialog box. The latter is opened with the command ***zert***.



zert

Options

● Zero trapezoidal region

Required parameters (F2 and F1)

Apply to axis: F2, F1	☑	□
Low field limit for zero region in first row ABSF1 [ppm] =	1000	1000
High field limit for zero region in first row ABSF2 [ppm] =	-1000	-1000
Low field limit of zero region in last row SIGF1 [ppm] =	0	0
High field limit of zero region in last row SIGF2 [ppm] =	0	0

Figure 4.31

This dialog box offers only one option which can be used in the F2 or F1 direction.

Zero trapezoidal region in F2

This option selects the command ***zert2*** for execution. The trapezoidal region to be zeroed is defined as follows:

- only the rows between F1-ABSF2 and F1-ABSF1 are zeroed

- the part (region) of each row which is zeroed shifts from row to row. The first row is zeroed between F2-ABSF2 and F2-ABSF1. The last row is zeroed between F2-SIGF2 and F2-SIGF1. For intermediate rows, the low field limit is an interpolation of F2-ABSF2 and F2-SIGF2 and the high field limit is an interpolation of F2-ABSF1 and F2-SIGF1.

zert2 works exactly like ***abst2***, except that the data points are zeroed instead of baseline corrected.

Zero trapezoidal region in F1

This option selects the command ***zert1*** for execution. The trapezoidal region to be zeroed is defined as follows:

- only the columns between F2-ABSF2 and F2-ABSF1 are zeroed
- the part (region) of each column which is zeroed shifts from column to column. The first column is zeroed between F1-ABSF2 and F1-ABSF1. The last column is zeroed between F1-SIGF2 and F1-SIGF1. For intermediate columns, the low field limit is an interpolation of F1-ABSF2 and F1-SIGF2 and the high field limit is an interpolation of F1-ABSF1 and F1-SIGF1.

zert1 works exactly like ***abst1***, except that the data points are zeroed instead of baseline corrected.

INPUT PARAMETERS

set from the ***zert*** dialog box, with ***edp*** or by typing ***absf1***, ***absf2*** etc.:

ABSF1 - low field limit of the zero region in the first row
ABSF2 - high field limit of the zero region in the first row
SIGF1 - low field limit of the zero region in the last row
SIGF2 - high field limit of the zero region in the last row

INPUT FILES

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

`2rr` - real processed 2D data
`proc2` - F1 processing parameters

OUTPUT FILES

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

`2rr` - real processed 2D data
`proc2s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

ZERT2

ZERT1

SEE ALSO

abst2, abst1

Chapter 5

3D processing commands

This chapter describes all TOPSPIN 3D processing commands. They only work on 3D data and store their output in processed data files. 3D raw data are never overwritten.

We will often refer to the three directions of a 3D dataset as the F3, F2 and F1 direction. F3 is always the acquisition direction. For processed data, F2 and F1 are always the second and third direction, respectively. For raw data, this order can be the same or reversed as expressed by the acquisition status parameter AQSEQ. 3D processing commands which work on raw data automatically determine their storage order from AQSEQ.

The name of a 3D processing command expresses the direction in which it works, e.g. ***tf3*** works in F3, ***tf2*** in F2 and ***tf1*** in the F1 direction. The command ***r12*** reads an F1-F2 plane, ***r13*** reads an F1-F3 plane etc.

For each command, the relevant input and output parameters are mentioned.

Furthermore, the relevant input and output files and their location are mentioned. Although file handling is completely transparent, it is sometimes useful to know which files are involved and where they reside. For example, if you have permission problems or if you want to process or interpret your data with third party software.

dosy3d

NAME

dosy3d - Process DOSY dataset (3D)

DESCRIPTION

The command ***dosy3d*** processes a 3D DOSY dataset.

DOSY is a special representation of diffusion measurements. Instead of generating just numbers using the T1/T2 fitting package (i.e. diffusion coefficients and error values), the DOSY processing gives pseudo 3D data where the F2 or F1 axis displays diffusion constants rather than NMR frequencies.

For more information on ***dosy3d*** :

click ***Help*** → ***Manuals*** → [**Acquisition Application Manuals**] ***Dosy***

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`difflist` - list of gradient amplitudes in Gauss/cm

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

`3rrr` - 3D data which are processed in F3 and F2 or in F3 and F1
`dosy` - DOSY processing parameters

OUTPUT FILES

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

`3rrr` - 3D processed data
`auditp.txt` - processing audit trail

SEE ALSO

eddosy, dosy2d

ft3d

NAME

ft3d - Process data, including FT, in the F3, F2 and F1 direction (3D)

DESCRIPTION

The command ***ft3d*** processes a 3D dataset in all three directions F3, F2 and F1. It is equivalent to the command sequence ***tf3***-***tf2***-***tf1*** or ***tf3***-***tf1***-***tf2*** (see below).

ft3d performs a Fourier transform which transforms time domain data (FID) into frequency domain data (spectrum). Depending on the processing parameters BC_mod, WDW, ME_mod and PH_mod, it also performs baseline correction, window multiplication, linear prediction and spectrum phase correction.

ft3d executes the following processing steps:

1. Baseline correction
The time domain data are baseline corrected according to BC_mod. This parameter takes the value *no*, *single*, *quad*, *spol*, *qpol sfil* or *qfil*.
2. Linear prediction
Linear prediction is done according to ME_mod. This parameter takes the value *no*, *LPfr*, *LPfc*, *LPbr*, *LPbc*, *LPmifr* or *LPmifc*. Usually, ME_mod = no, which means no prediction is done. Forward prediction (*LPfr*, *LPfc*, *LPmifr* or *LPmifc*) can, for example, be used to extend truncated FIDs. Backward prediction (*LPbr* or *LPbc*) is usually only done in F3, e.g. improve the initial data points of the FID. Linear prediction is only performed if NCOEF > 0. Furthermore, the parameters LPBIN and, for backward prediction, TDoff are evaluated.
3. Window multiplication
The time domain data are multiplied with a window function according to WDW. This parameter takes the value *em*, *gm*, *sine*, *qsine*, *trap*, *user*, *sinc*, *qsinc*, *traf* or *trafs*.
4. Fourier transform
The time domain data are Fourier transformed in F3 according to

the acquisition status parameter AQ_mod (see table 5.6).

status AQ_mod	Fourier transform mode	status FT_mod
qf	forward, single, real	fsr
qsim	forward, quad, complex	fqc
qseq	forward, quad, real	fqr
DQD	forward, quad, complex	fqc

Table 5.1

In F2 and F1, they are Fourier transformed according to the acquisition status parameter FnMODE [1](see table 5.2).

FnMODE	Fourier transform mode	status FT_mod
undefined	according to MC2	
QF	forward, quad, real	fqc
QSEQ	forward, quad, real	fqr
TPPI	forward, single, real	fsr
States	forward, quad, complex	fqc
States-TPPI	forward, single, complex	fsc
Echo-AntiEcho	forward, quad, complex	fqc

Table 5.2

The Fourier transform mode is stored in the processing status parameter FT_mod. Note that **`ft3d`** does not evaluate the processing parameter FT_mod!

5. Phase correction
The frequency domain data are phase corrected according to PH_mod. This parameter takes the value *no*, *pk*, *mc* or *ps*. For PH_mod = pk, **`ft3d`** applies the values of PHC0 and PHC1. This is only useful if the phase values are known. You can determine them by typing **`xfb`** on the 3D data to process a 23 or 13 plane, do

[1] If FnMODE = undefined, **`ft3d`** evaluates the processing parameter MC2.

a phase correction on the resulting the 2D dataset and store the phase values to 3D.

The size of the processed data is determined by the processing parameter SI; SI real and SI imaginary points are created. A typical value for SI is TD/2 in which case, all raw data points are used and no zero filling is done. In fact, several parameters control the number of input and output data points, for example:

1. SI > TD/2: the raw data are zero filled before the Fourier transform
2. SI < TD/2: only the first 2*SI raw data points are used
3. 0 < TDeff < TD: only the first TDeff raw data points are used
4. 0 < TDoff < TD: the first TDoff raw data points are cut off and TDoff zeroes are appended at the end
5. TDoff < 0: -TDoff zeroes are prepended at the beginning. Note that:
   - for SI < (TD-TDoff)/2 raw data are cut off at the end
   - for DIGMOD=digital, the zeroes would be prepended to the group delay which does not make sense. You can avoid that by converting the raw data with ***convdta*** before you process them.
6. 0 < STSR < SI: only the processed data between STSR and STSR+STSI are stored (if STSI = 0, STSR is ignored and SI points are stored)
7. 0 < STSI < SI: only the processed data between STSR and STSR+STSI are stored.

Note that only in the first case the processed data contain the total information of the raw data. In all other cases, information is lost. Before you run ***ft3d***, you must set the processing parameter SI in all three directions F3, F2 and F1.

ft3d evaluates the acquisition status parameter AQSEQ, which defines the storage order of the raw data. Raw data can be stored in the order 3-2-1 or 3-1-2. Processed data, however, are always stored in the order 3-2-1. For AQSEQ=321, ***ft3d*** is equivalent to the command sequence ***tf3***-***tf2***-***tf1***. For AQSEQ=312, it is equivalent to ***tf3***-***tf1***-***tf2***. Note, however, that for magnitude or power data, the processing order is independent of AQSEQ. ***ft3d*** then behave as follows:

- for F1-PH_mod = mc / ps, ***tf3-tf2-tf1*** is executed
- for F2-PH_mod = mc / ps, ***tf3-tf1-tf2*** is executed

Note that PH_mod = mc/ps is only allowed in either F2 or F1, not in both and also not in F3.

ft3d evaluates the processing parameter FCOR. The first point of the FIDs is multiplied with the value of FCOR which lies between 0.0 and 2.0. For digitally filtered Avance data, FCOR has no effect in F3 because the first point is part of the group delay and, as such, is zero. In that case, it only plays a role in the F2 and F1 direction. However, on A*X data or Avance data measured with DIGMOD = analog, there is no group delay and FCOR also plays a role in F3.

ft3d evaluates the processing parameter PKNL. On A*X spectrometers, PKNL = true causes a non linear 5th order phase correction of the raw data. This corrects possible errors caused by non linear behaviour of the analog filters. On Avance spectrometers, PKNL must always be set to TRUE. For digitally filtered data, it causes ***ft3d*** to handle the group delay of the FID. For analog data it has no effect.

ft3d evaluates the processing parameter REVERSE. If REVERSE = TRUE, the spectrum will be reversed, i.e. the first data point becomes the last and the last data point becomes the first.

ft3d can be used with the following command line arguments:

n

ft3d will not store the imaginary data. Imaginary data are only needed for phase correction in last processed direction. If the phase values are already known and PHC0 and PHC1 have been set accordingly, ***ft3d*** will perform phase correction and there is no need to store the imaginary data. This will save processing time and disk space. If you still need to do a phase correction after ***ft3d***, you can create imaginary data from the real data with a Hilbert transform (see ***tht1***). Note that if the ***n*** option is omitted, imaginary data are only stored in the last processed direction.

21 or ***12***

ft3d 21 is equivalent to the command sequence ***tf3***-***tf2***-***tf1***, whereas ***ft3d 12*** is equivalent to ***tf3***-***tf1***-***tf2***.

xdim

3D spectra are stored in the so-called subcube format. The size of the subcubes is calculated by ***ft3d*** and depends on the size of the spectrum and the available memory. The option ***xdim*** allows you to use predefined subcube sizes. It causes ***ft3d*** to interpret the F3, F2 and F1 processing parameter XDIM which can be set by entering ***xdim***.on the command line. Note that XDIM = 0, is evaluated as XDIM = SI. The actually used subcube sizes, whether predefined or calculated, are stored as the F3, F2 and F1 processing status parameter XDIM and can be viewed with ***dpp***. Predefining subcube sizes is, for example, used to read the processed data with third party software which can not interpret the processing status parameter XDIM.

big/little

ft3d stores the data in the data storage order of the computer it runs on, e.g. little endian on Windows PCs. Note that TOPSPIN's predecessor XWIN-NMR on SGI UNIX workstations stores data in big endian.The storage order is stored in the processing status parameter BYTORDP (type ***s bytordp***). If, however, you want to read the processed data with third party software which can not interpret this parameter, you can use the ***big/little*** option to predefine the storage order.

p<du>

the option ***p*** allows you to store the processed data on a different top level data directory, typically a different disk. The rest of the data directory path is the same as that of the raw data. If the specified top level directory does not exist, it will be created.

Normally, ***ft3d*** stores the entire spectral region as determined by the spectral width. However, you can do a so-called strip transform which means that only a certain region of the spectrum is stored. This can be done by setting the parameters STSR and STSI which represent the strip start and strip size, respectively. They both can take a value between 0 and SI. The values which are actually used can be a little different. STSI is always rounded to the next higher multiple of 16. Furthermore, when the data are stored in subcube format (see below), STSI is rounded to the next multiple of the subcube size. Type ***dpp*** to check this; if XDIM is smaller than SI, then the data are stored in subcube format and STSI is a multiple of XDIM.

ft3d stores the data in subcube format. It automatically calculates the subcube sizes such that one row (F3) of subcubes fits in the available memory. Furthermore, one column (F2) and one tube (F1) of subcubes must fit in the available memory. The calculated subcube sizes are stored in the processing status parameter XDIM (type ***dpp***). The alignment of the data points subcube format is the extension of the alignment in a 2D dataset as it is shown in table 4.7. The storage handling is completely transparent to the user and is only of interest when the data are interpreted by third party software.

INPUT PARAMETERS

F3, F2 and F1 parameters

set by the acquisition, can be viewed with ***dpa*** or ***s td*** :

TD - time domain; number of raw data points

set by the user with ***edp*** or by typing ***si***, ***stsr*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - number of output points of strip transform
TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)
BC_mod - FID baseline correction mode
BCFW - filter width for BC_mod = sfil or qfil
COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil
ME_mod - FID linear prediction mode
NCOEF - number of linear prediction coefficients
LPBIN - number of points for linear prediction
TDoff - number of raw data points predicted for ME_mod = LPb*
WDW - FID window multiplication mode
LB - Lorentzian broadening factor for WDW = em or gm
GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
TM1, TM2 - limits of the trapezoidal window for WDW = trap
PH_mod - phase correction mode

PHC0 - zero order phase correction value for PH_mod = pk
PHC1 - first order phase correction value for PH_mod = pk
FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
REVERSE - flag indicating to reverse the spectrum

F3 parameters

set by the acquisition, can be viewed with ***dpa*** or ***s aq_mod*** etc.:

AQ_mod - acquisition mode (determines the status FT_mod)
AQSEQ - acquisition sequence (3-2-1 or 3-1-2)
BYTORDA - byteorder or the raw data
NC - normalization constant

F2 and F1 parameters

set by the acquisition, can be viewed with ***dpa*** or by typing ***s fnmode***:

FnMODE - Fourier transform mode

OUTPUT PARAMETERS

F3, F2 and F1 parameters

can be viewed with ***dpp*** or by typing ***s si***, ***s stsr*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
FTSIZE - Fourier transform size
TDeff - number of raw data points that were used for processing
TDoff - first point of the FID used for processing (default 0)
XDIM - subcube size
FT_mod - Fourier transform mode

F3 parameters

can be viewed with ***dpp*** or by typing ***s ymax_p*** etc.:

YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor
BYTORDP - byte order of the processed data

F2 and F1 parameters

can be viewed with ***dpp*** or by typing ***s mc2***:

MC2 - Fourier transform mode

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - raw data
`acqus` - F3 acquisition status parameters
`acqu2s` - F2 acquisition status parameters
`acqu3s` - F1 acquisition status parameters

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

`proc` - F3 processing parameters
`proc2` - F2 processing parameters
`proc3` - F1 processing parameters

OUTPUT FILES

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

`3rrr` - real processed 3D data
`3rri` - real/imaginary processed data (for AQSEQ =321, FnMODE ≠ QF)
`3rir` - real/imaginary processed data (for AQSEQ =312, FnMODE ≠ QF)
`3iii` - imaginary processed data (for FnMODE = QF)
`procs` - F3 processing status parameters
`proc2s` - F2 processing status parameters
`proc3s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

FT3D

SEE ALSO

tf3, tf2, tf1

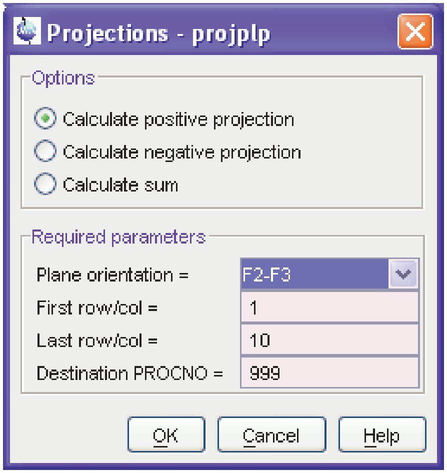
projplp, projpln, sumpl

NAME

projplp - Calculate positive projection (nD)
projpln - Calculate negative projection (nD)
sumpl - Calculate sum projection (nD)

DESCRIPTION

The commands ***projplp***, ***projpln*** and ***sumpl*** calculate the 2D positive, negative and sum projection, respectively. When entered without arguments, they all open the same dialog (see Figure 5.1).


Projections - projplp

Options

● Calculate positive projection
○ Calculate negative projection
○ Calculate sum

Required parameters

Plane orientation = F2-F3
First row/col = 1
Last row/col = 10
Destination PROCNO = 999

Figure 5.1

Here you can select the desired command in the **Options** section and specify the plane orientation, first and last row/column and output PROCNO in the Parameter section.

The parameters can also be specified as arguments. Up to 5 arguments can be used:

<plane orientation>
23, 13, 12 (3D data)
34, 24, 14, 23, 13, 12, 43, ..., 21 (4D data)

<first plane>
the plane included in the calculation

<last plane>
the last plane included in the calculation

<dest. procno>
the *procno* where the 2D output data are stored

n
prevents the destination dataset from being displayed/activated (optional)

Here is an example:

projplp 13 10 128 998 n

calculates the positive F1-F3 projection of the planes 10 to 128 along F2 and stores it under PROCNO 998.

Instead of specifying the first and last plane, you can also use the argument ***all*** for all cubes. For example:

projplp 23 all 10

calculates the positive F2-F3 projection of all planes along F1 and stores it under PROCNO 10.

projplp, ***projpln*** and ***sumpl*** work on data of dimension ≥3D. On 4D and 5D data, the dialog shown in Figure 5.1 does not appear. Instead, the arguments are prompted for one at a time, if they are not specified on the command line.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>/
`3rrr` - real processed 3D data

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/pdata/<*procno*>/
`2rr` - real processed 2D data

SEE ALSO

rpl, wpl, rser2d

r12, r13, r23, slice

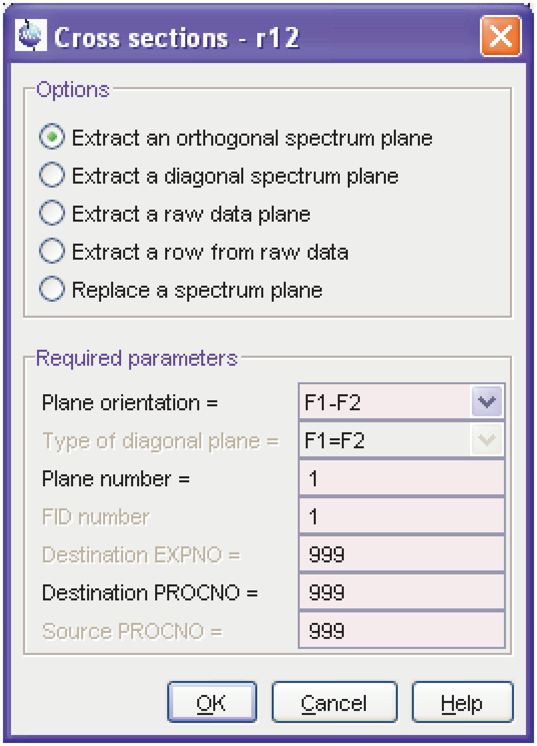
NAME

r12 - Read F1-F2 plane from 3D data and store as 2D data
r13 - Read F1-F3 plane from 3D data and store as 2D data
r23 - Read F2-F3 plane from 3D data and store as 2D data
slice - Open the read plane dialog box (2D,3D)

DESCRIPTION

The commands ***r12***, ***r13*** and ***r23*** read a plane from 3D processed data and store it as a 2D dataset.

When entered without arguments, they open the dialog box shown in Figure 5.2).



Cross sections - r12

Options

● Extract an orthogonal spectrum plane
○ Extract a diagonal spectrum plane
○ Extract a raw data plane
○ Extract a row from raw data
○ Replace a spectrum plane

Required parameters

Plane orientation =	F1-F2
Type of diagonal plane =	F1=F2
Plane number =	1
FID number	1
Destination EXPNO =	999
Destination PROCNO =	999
Source PROCNO =	999

Figure 5.2

This dialog box offers several options, each of which selects a certain command for execution. Furthermore, you must specify three parameters:

Plane orientation: F1-F2, F1-F3 or F2-F3. This parameter determines which of the commands ***r12***, ***r13*** or ***r23*** is executed.

Plane number: the maximum plane number is the SI value in the direction orthogonal to the plane orientation.

Destination procno: the *procno* where the output 2D dataset is stored

For each option described below, a table shows how the processing state of the output 2D data relates to the processing state of the input 3D data. This table can be interpreted as follows:

`FID` - data have not been Fourier transformed (time domain data)
`real` - data have been Fourier transformed but imaginary data do not exist
`real+imag` - data have been Fourier transformed and imaginary data exist

Depending on the processing state, an extracted plane can be further processed with 2D processing commands like ***xf2***, ***xf1***, ***xf2p*** etc.

Extract an orthogonal spectrum plane in F1-F2

This option selects the command ***r12*** for execution. It reads an F1-F2 plane from a 3D dataset and stores it as a 2D dataset (see Table 5.3).

Extract an orthogonal spectrum plane in F1-F3

This option selects the command ***r13*** for execution. It reads an F1-F3 plane from a 3D dataset and stores it as a 2D dataset (see Table 5.4).

Extract an orthogonal spectrum plane in F2-F3

This option selects the command ***r23*** for execution. It reads an F2-F3 plane from a 3D dataset and stores it as a 2D dataset (see Table 5.5).

3D data processed with	3D input data			2D output data	
	F3	F2	F3	F2	F1
tf3	real+imag	FID	FID	FID	FID
tf3, tf2	real	real+imag	FID	real+imag	FID
tf3, tf2, tf1	real	real	real+imag	real	real+imag
tf3, tf1, tf2	real	real+imag	real	real+imag	real

Table 5.3 *r12* input/output data

3D data processed with	3D input data			2D output data	
	F3	F2	F1	F2	F1
tf3	real+imag	FID	FID	real+imag	FID
tf3, tf2	real	real+imag	FID	real	FID
tf3, tf2, tf1	real	real	real+imag	real	real+imag
tf3, tf1, tf2	real	real+imag	real	real	real

Table 5.4 *r13* input/output data

3D data processed with	3D input data			2D output data	
	F3	F2	F1	F2	F1
tf3	real+imag	FID	FID	real+imag	FID
tf3, tf2	real	real+imag	FID	real	real+imag
tf3, tf2, tf1	real	real	real+imag	real	real
tf3, tf1, tf2	real	real+imag	real	real	real+imag

Table 5.5 ***r23*** input/output data

The parameters required by ***r12***, ***r13*** and ***r23*** can also be entered as arguments on the command line. In that case, the command is executed without opening the dialog box. For example:

r12 10 999

reads an F1-F2 plane number 10 and stores it in *procno* 999. Note that the Plane orientation is not specified as an argument but part of the command name.

The commands ***r12***, ***r13*** and ***r23*** are equivalent to the commands ***rpl 12***, ***rpl 13*** and ***rpl 23***, respectively (see the description of ***rpl***).

INPUT FILES

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

`3rrr`, `3irr`, `3rir`, `3rri`, `3iii` - processed 3D data

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

R12(plane, procno)
for example R12(64, 1)

R13(plane, procno)
for example R13(64, 1)

R23(plane, procno)
for example R23(64, 1)

SEE ALSO

r12d, r13d, r23d, rpl, wpl

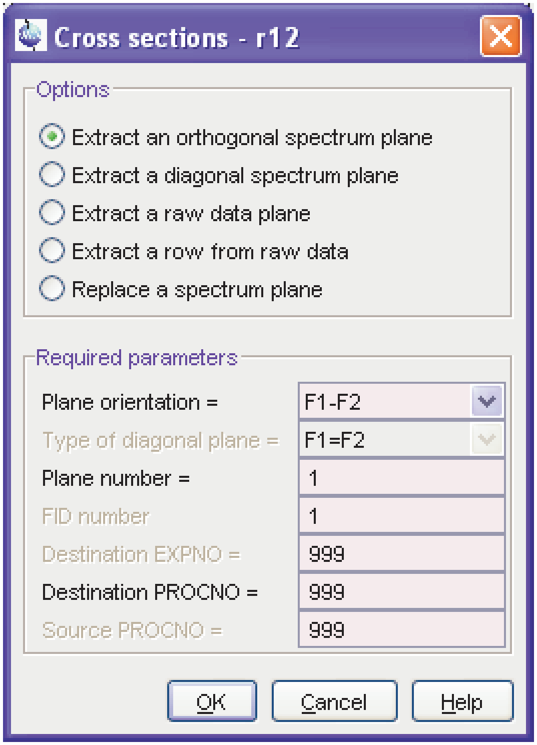
r12d, r13d, r23d

NAME

r12d - Read diagonal F1=F2 plane and store as 2D data (3D)
r13d - Read diagonal F1=F3 plane and store as 2D data (3D)
r23d - Read diagonal F2=F3 plane and store as 2D data (3D)

DESCRIPTION

Read plane commands can be started from the command line or from the read plane dialog box. The latter is opened with the command ***slice***



Cross sections - r12

Options

● Extract an orthogonal spectrum plane
○ Extract a diagonal spectrum plane
○ Extract a raw data plane
○ Extract a row from raw data
○ Replace a spectrum plane

Required parameters

Plane orientation =	F1-F2
Type of diagonal plane =	F1=F2
Plane number =	1
FID number	1
Destination EXPNO =	999
Destination PROCNO =	999
Source PROCNO =	999

Figure 5.3

This dialog box offers several options, each of which selects a certain command for execution.

Extract a diagonal spectrum plane in F1-F2

This option selects the command ***r12d*** for execution. It reads the diagonal F1=F2 plane from a 3D dataset and stores it as a 2D dataset.

Extract a diagonal spectrum plane in F1-F3

This option selects the command ***r13d*** for execution. It reads the diagonal F1=F3 plane from a 3D dataset and stores it as a 2D dataset.

Extract a diagonal spectrum plane in F2-F3

This option selects the command ***r23d*** for execution. It reads the diagonal F2=F3 plane from a 3D dataset and stores it as a 2D dataset.

For each option, you must specify the destination *procno*.

r12d, ***r13d*** and ***r23d*** only store the real data.

INPUT FILES

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

`3rrr` - real processed 3D data

OUTPUT FILES

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

`2rr` - real processed 2D data

SEE ALSO

r12, r13, r23, rpl, wpl

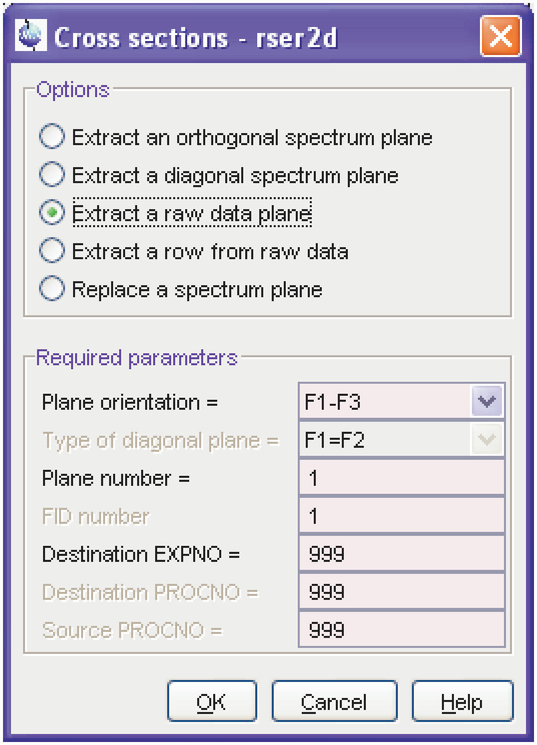
rser2d

NAME

rser2d - Read plane from raw 3D data and store as a 2D (3D)

DESCRIPTION

The command ***rser2d*** reads a plane from 3D raw data (a series of FIDs) and stores it as a pseudo raw 2D dataset. When entered without arguments, it opens the following dialog box:



Cross sections - rser2d

Options

○ Extract an orthogonal spectrum plane
○ Extract a diagonal spectrum plane
● Extract a raw data plane
○ Extract a row from raw data
○ Replace a spectrum plane

Required parameters

Plane orientation =	F1-F3
Type of diagonal plane =	F1=F2
Plane number =	1
FID number	1
Destination EXPNO =	999
Destination PROCNO =	999
Source PROCNO =	999

Figure 5.4

Here you can specify three required parameters:

Plane orientation: F1-F3 or F2-F3 (must contain acquisition (F3) direction)

Plane number: the maximum plane number is the TD value in the direction orthogonal to the plane orientation

Destination EXPNO: the *expno* where the output 2D dataset is stored

The parameters can also be entered as arguments on the command line. In that case, the command is executed without opening the dialog box. For example:

```
rser2d s23 10 999
```

reads an F3-F2 plane number 10 and stores it in *expno* 999

In contrast to **`rser`**, **`rser2d`** can only be entered on the source dataset, not on the destination dataset.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - 3D raw data

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<*expno*>/

`ser` - 2D pseudo raw data
`audita.txt` - acquisition audit trail

<dir>/data/<user>/nmr/<name>/<expno2>/pdata/1/

`used_from` - data path of the source 3D data and the plane number

USAGE IN AU PROGRAMS

RSER2D (direction, plane, expno)

SEE ALSO

rser, wser, wserp, rpl, wpl

tabs3, tabs2, tabs1

NAME

tabs3 - Automatic baseline correction in F3 (3D)
tabs2 - Automatic baseline correction in F2 (3D)
tabs1 - Automatic baseline correction in F1 (3D)

DESCRIPTION

tabs3 performs an automatic baseline correction in the F3 direction, by subtracting a polynomial. The degree of the polynomial is determined by the F3 parameter ABSG which has a value between 0 and 5, with a default of 5. ***tabs3*** works like ***absf*** in 1D and ***abs2*** in 2D. This means that it only corrects a certain spectral region which is determined by the parameters ABSF1 and ABSF2.

tabs2 works like ***tabs3***, except that corrects data in the F2 direction using the F2 parameters ABSG, ABSF2 and ABSF1.

tabs1 works like ***tabs3***, except that corrects data in the F1 direction using the F1 parameters ABSG, ABSF2 and ABSF1.

INPUT PARAMETERS

F3 parameters

set by the user with ***edp*** or by typing ***absg***:

ABSG - degree of the polynomial to be subtracted (0 to 5, default of 5)

F3, F2 and F1 parameters

set by the user with ***edp*** or by typing ***absf1***, ***absf2***:

ABSF1- low field limit of the correction region
ABSF2 - high field limit of the correction region

INPUT FILES

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

`3rrr` - real processed 3D data
`proc` - F3 processing parameters
`proc2` - F2 processing parameters

`proc3` - F1 processing parameters

OUTPUT FILES

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

`3rrr` - real processed 3D data
`procs` - F3 processing status parameters
`proc2s` - F2 processing status parameters
`proc3s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TABS3

TABS2

TABS1

SEE ALSO

abs2, abs1, absf

tf3

NAME

tf3 - Process data, including FT, in F3 (3D)

DESCRIPTION

The command ***tf3*** processes a 3D dataset in the F3 direction. F3 is the first direction of a 3D dataset, i.e. the acquisition direction. ***tf3*** always performs a Fourier transform which transforms time domain data (FID) into frequency domain data (spectrum). Depending on the processing parameters BC_mod, WDW, ME_mod and PH_mod, it also performs baseline correction, window multiplication, linear prediction and spectrum phase correction.

The processing steps done by ***tf3*** can be described as follows:

1. Baseline correction of the F3 time domain data
   Each row is baseline corrected according to BC_mod. This parameter takes the value *no*, *single*, *quad*, *spol*, *qpol sfil* or *qfil*. More details on BC_mod can be found in chapter 2.4.
2. Linear prediction of the F3 time domain data
   Linear prediction is done according to ME_mod. This parameter takes the value *no*, *LPfr*, *LPfc*, *LPbr*, *LPbc, LPmifr* or *LPmifc*. Usually, ME_mod = no, which means no prediction is done. Forward prediction (*LPfr*, *LPfc, LPmifr* or *LPmifc*) can, for example, be used to extend truncated FIDs. Backward prediction (*LPbr* or *LPbc*) can be used to improve the initial data points of the FID. Linear prediction is only performed if NCOEF > 0. Furthermore, the parameters LPBIN and, for backward prediction, TDoff play a role (see these parameters in chapter 2.4).
3. Window multiplication of the F3 time domain data
   Each row is multiplied with a window function according to WDW. This parameter takes the value *em*, *gm*, *sine*, *qsine*, *trap*, *user*, *sinc*, *qsinc*, *traf* or *trafs*. More details on WDW can be found in chapter 2.4.
4. Fourier transform of the F3 time domain data
   Each row is Fourier transformed according to the acquisition sta-

tus parameter AQ_mod as shown in table 5.6. ***tf3*** does not evaluate the processing parameter FT_mod! However, it stores the Fourier transform mode in the processing status parameter FT_mod.

AQ_mod	Fourier transform mode	status FT_mod
qf	forward, single, real	fsr
qsim	forward, quad, complex	fqc
qseq	forward, quad, real	fqr
DQD	forward, quad, complex	fqc

Table 5.6

5. Phase correction of the F3 frequency domain data
Each row is phase corrected according to PH_mod. This parameter takes the value *no*, *pk*, *mc* or *ps*. For PH_mod = pk, ***tf3*** applies the values of PHC0 and PHC1. This is only useful if the phase values are known. You can determine them by typing ***xfb*** on the 3D data to process a 23 or 13 plane, do a phase correction on the resulting the 2D dataset and store the phase values to 3D. More details on PH_mod can be found in chapter 2.4.

The size of the processed data is determined by the processing parameter SI; SI real and SI imaginary points are created. A typical value for SI is TD/2 in which case, all raw data points are used and no zero filling is done. In fact, several parameters control the number of input and output data points, for example:

1. SI > TD/2: the raw data are zero filled before the Fourier transform
2. SI < TD/2: only the first 2*SI raw data points are used
3. 0 < TDeff < TD: only the first TDeff raw data points are used
4. 0 < TDoff < TD: the first TDoff raw data points are cut off and TDoff zeroes are appended at the end
5. TDoff < 0: -TDoff zeroes are prepended at the beginning. Note that:
   - for SI < (TD-TDoff)/2 raw data are cut off at the end

- for DIGMOD=digital, the zeroes would be prepended to the group delay which does not make sense. You can avoid that by converting the raw data with ***convdta*** before you process them.

6. 0 < STSR < SI: only the processed data between STSR and STSR+STSI are stored (if STSI = 0, STSR is ignored and SI points are stored)
7. 0 < STSI < SI: only the processed data between STSR and STSR+STSI are stored.

Note that only in the first case the processed data contain the total information of the raw data. In all other cases, information is lost.

Before you run ***tf3***, you must set the processing parameter SI in all three directions F3, F2 and F1. The command***tf2*** does not evaluate the F2 processing parameter SI, it evaluates the processing status parameter SI as it was set by ***tf3***.

tf3 evaluates the acquisition status parameter AQSEQ. This parameter defines the storage order of the raw data 3-2-1 or 3-1-2. For processed data, F2 and F1 are always the second and third direction, respectively. For raw data, this order can be the same or reversed as expressed by AQSEQ.

tf3 evaluates the processing parameter FCOR. The first point of the FIDs is multiplied with the value of FCOR which lies between 0.0 and 2.0. For digitally filtered Avance data, FCOR has no effect in F3 because the first point is part of the group delay and, as such, is zero. In that case, it only plays a role in the F2 and F1 direction (see ***tf2*** and ***tf1***). However, on A*X data or Avance data measured with DIGMOD = analog, there is no group delay and FCOR also plays a role in F3.

tf3 evaluates the processing parameter PKNL. On A*X spectrometers, PKNL = true causes a non linear 5th order phase correction of the raw data. This corrects possible errors caused by non linear behaviour of the analog filters. On Avance spectrometers, PKNL must always be set to TRUE. For digitally filtered data, it causes ***tf3*** to handle the group delay of the FID. For analog data it has no effect.

tf3 evaluates the processing parameter REVERSE. If REVERSE = TRUE, the spectrum will be reversed in F3, i.e. the first data point becomes the last and the last data point becomes the first.

tf3 can be used with the following command line options:

n

tf3 will not store the imaginary data. Imaginary data are only needed for phase correction. If the phase values are already known and PHC0 and PHC1 have been set accordingly, ***tf3*** will perform phase correction and there is no need to store the imaginary data. This will save processing time and disk space. If you still need to do a phase correction after ***tf3***, you can create imaginary data from the real data with a Hilbert transform (see ***tht3***).

xdim

3D spectra are stored in the so-called subcube format. The size of the subcubes is calculated by ***tf3*** and depends on the size of the spectrum and the available memory. The option ***xdim*** allows you to use predefined subcube sizes. It causes ***tf3*** to interpret the F3, F2 and F1 processing parameter XDIM which can be set with the command ***xdim***. The actually used subcube sizes, whether predefined or calculated, are stored as the F3, F2 and F1 processing status parameter XDIM and can be viewed with ***dpp***. Predefining subcube sizes is, for example, used to read the processed data with third party software which can not interpret the processing status parameter XDIM.

big/little

tf3 stores the data in the data storage order of the computer it runs on, e.g. little endian on Windows PCs. Note that TOPSPIN's predecessor XWIN-NMR on SGI UNIX workstations stores data in big endian.The storage order is stored in the processing status parameter BYTORDP (type ***s bytordp***). If, however, you want to read the processed data with third party software which can not interpret this parameter, you can use the ***big/little*** option to predefine the storage order.

p<du>

the option ***p*** allows you to store the processed data on a different top level data directory, typically a different disk. The rest of the data directory path is the same as that of the raw data. If the specified top level directory does not exist, it will be created.

Normally, ***tf3*** stores the entire spectral region as determined by the spectral width. However, you can do a so-called strip transform which means that only a certain region of the spectrum is stored. This can be done by setting the parameters STSR and STSI which represent the strip start and strip size, respectively. They both can take a value between 0 and SI. The values which are actually used can be a little different. STSI is always rounded to the next higher multiple of 16. Furthermore, when the data are stored in subcube format (see below), STSI is rounded to the next multiple of the subcube size. Type ***dpp*** to check this; if XDIM is smaller than SI, then the data are stored in subcube format and STSI is a multiple of XDIM.

tf3 stores the data in subcube format. It automatically calculates the subcube sizes such that one row (F3) of subcubes fits in the available memory. Furthermore, one column (F2) and one tube (F1) of subcubes must fit in the available memory. The calculated subcube sizes are stored in the processing status parameter XDIM (type ***dpp***). The alignment of the data points for sequential and subcube format is the extension of the alignment in a 2D dataset as it is shown in table 4.6 and 4.7. The storage handling is completely transparent to the user and is only of interest when the data are interpreted by third party software.

INPUT PARAMETERS

F3, F2 and F1 parameters

set by the user with ***edp*** or by typing ***si***, ***stsr*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - number of output points of strip transform
TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)

F3 parameters

set by the user with ***edp*** or by typing ***bc_mod***, ***bcfw*** etc.:

BC_mod - FID baseline correction mode
BCFW - filter width for BC_mod = sfil or qfil
COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil
ME_mod - FID linear prediction mode

NCOEF - number of linear prediction coefficients
LPBIN - number of points for linear prediction
TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode

LB - Lorentzian broadening factor for WDW = em or gm
GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
TM1, TM2 - limits of the trapezoidal window for WDW = trap

PH_mod - phase correction mode

PHC0 - zero order phase correction value for PH_mod = pk
PHC1 - first order phase correction value for PH_mod = pk

FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
REVERSE - flag indicating to reverse the spectrum
PKNL - group delay compensation (Avance) or filter correction (A*X)

set by the acquisition, can be viewed with ***dpa*** or ***s aq_mod*** etc.:

AQ_mod - acquisition mode (determines the status FT_mod)
AQSEQ - acquisition sequence (3-2-1 or 3-1-2)
TD - time domain; number of raw data points
BYTORDA - byteorder or the raw data
NC - normalization constant

F2 and F1 parameters

set by the acquisition, can be viewed with ***dpa*** or by typing ***s fnmode*** etc.:

FnMODE - Fourier transform mode

OUTPUT PARAMETERS

F3, F2 and F1

can be viewed with ***dpp*** or by typing ***s si***, ***s stsi*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
TDeff - number of raw data points that were used for processing
TDoff - first point of the FID used for processing (default 0)
XDIM - subcube size

F3 parameters

can be viewed with ***dpp*** or by typing ***s si***, ***s tdeff*** etc.:

FTSIZE - Fourier transform size
FT_mod - Fourier transform mode
YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor
BYTORDP - byte order of the processed data

F2 and F1 parameters

can be viewed with ***dpp*** or by typing ***s mc2*** etc.:

MC2 - Fourier transform mode

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - raw data
`acqus` - F3 acquisition status parameters
`acqu2s` - F2 acquisition status parameters
`acqu3s` - F1 acquisition status parameters

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

`proc` - F3 processing parameters
`proc2` - F2 processing parameters
`proc3` - F1 processing parameters

OUTPUT FILES

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

`3rrr` - real processed 3D data
`3irr` - real/imaginary processed data (for FnMODE ≠ QF)
`3iii` - real/imaginary processed data (for FnMODE = QF)
`procs` - F3 processing status parameters
`proc2s` - F2 processing status parameters
`proc3s` - F1 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TF3(store_imag, partition)

where *store_image* can be *y* or *n* and *partition* is the top level data directory

SEE ALSO

tf2, tf1, ft3d

tf2

NAME

tf2 - Process data, including FT, in F2 (3D)

DESCRIPTION

The command ***tf2*** processes a 3D dataset in the F2 direction. This involves a Fourier transform which transforms time domain data (FID) into frequency domain data (spectrum). Depending on the processing parameters BC_mod, WDW, ME_mod and PH_mod, ***tf2*** also performs baseline correction, window multiplication, linear prediction and spectrum phase correction.

The processing steps done by ***tf2*** can be described as follows:

tf2 only works on data which have already been processed with ***tf3***. It performs the following processing steps in the F2 direction:

1. Baseline correction of the F2 time domain data
   Each column is baseline corrected according to BC_mod. This parameter takes the value *no*, *single*, *quad*, *spol*, *qpol sfil* or *qfil*. More details on BC_mod can be found in chapter 2.4.
2. Linear prediction of the F2 time domain data
   Linear prediction is done according to ME_mod. This parameter takes the value *no*, *LPfr*, *LPfc*, *LPbr*, *LPbc*, *LPmifr or LPmifc*. Usually, ME_mod = no, which means no prediction is done. Forward prediction in F2 (*LPfr*, *LPfc*, *LPmifr* or *LPmifc*) can, for example, be used to extend truncated FIDs. Backward prediction (*LPbr* or *LPbc*) is not used very often in F2. Linear prediction is only performed for NCOEF > 0. Furthermore, LPBIN and, for backward prediction, TDoff play a role (see these parameters in chapter 2.4).
3. Window multiplication of the F2 time domain data
   Each column is multiplied with a window function according to WDW. This parameter takes the value *em*, *gm*, *sine*, *qsine*, *trap*, *user*, *sinc*, *qsinc*, *traf* or *trafs*. More details on WDW can be found in chapter 2.4.
4. Fourier transform of the F2 time domain data
   tf2 Fourier transforms each column according to the F2 process-

ing status parameter MC2 and stores the corresponding Fourier transform mode in the processing status parameter FT_mod (see table 5.7t). The status MC2 has been set by the ***tf3*** command to

F2 status MC2	Fourier transform mode	status FT_mod
QF	forward, quad, real	fqc
QSEQ	forward, quad, real	fqr
TPPI	forward, single, real	fsr
States	forward, quad, complex	fqc
States-TPPI	forward, single, complex	fsc
Echo-AntiEcho	forward, quad, complex	fqc

Table 5.7

the value of the F2 acquisition status parameter FnMODE [1]. Note that ***tf2*** does not evaluate the processing parameter FT_mod!

5. Phase correction of the F2 frequency domain data.
Each column is phase corrected according to PH_mod. This parameter takes the value *no*, *pk*, *mc* or *ps*. For PH_mod = pk, ***tf2*** applies the values of PHC0 and PHC1. This is only useful if the phase values are known. You can determine them by typing ***xfb*** on the 3D data to process a 23 or 12 plane, do a phase correction on the resulting the 2D dataset and store the phase values to 3D. More details on PH_mod can be found in chapter 2.4.

The F2 processing parameter SI determines the size of the processed data in the F2 direction. This must, however, be set before ***tf3*** is done and cannot be changed after ***tf3***. See ***tf3*** for the role of TD, TDeff and TDoff.

tf2 can do a strip transform according to the F2 parameters STSR and STSI (see ***tf3***).

tf2 evaluates the F2 parameter FCOR. The first point of the FIDs is multiplied with the value of FCOR which is a value between 0.0 and 2.0. As such, FCOR allows you to control the DC offset of the spectrum.

[1] If FnMODE = undefined, ***tf3*** sets processing status MC2 to processing MC2.

tf2 evaluates the F2 parameter REVERSE. If REVERSE = TRUE, the spectrum will be reversed in F2, i.e. the first data point becomes the last and the last data point becomes the first.

tf2 evaluates the F2 status parameter MC2. For MC2 ≠ QF, ***tf2*** uses the file `3rrr` as input and the files `3rrr` and `3rir` as output. For MC2 = QF, ***tf2*** uses the files `3rrr` and `3iii` as input and output. The role of MC2 is described in detail for the 2D processing command ***xfb***.

INPUT PARAMETERS

F2 parameters

set by the user with ***edp*** or by typing ***bc_mod***, ***bcfw*** etc.:

BC_mod - FID baseline correction mode

BCFW - filter width for BC_mod = sfil or qfil

COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil

ME_mod - FID linear prediction mode

NCOEF - number of linear prediction coefficients

LPBIN - number of points for linear prediction

TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode

LB - Lorentzian broadening factor for WDW = em or gm

GB - Gaussian broadening factor for WDW = gm, sinc or qsinc

SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc

TM1, TM2 - limits of the trapezoidal window for WDW = trap

PH_mod - phase correction mode

PHC0 - zero order phase correction value for PH_mod = pk

PHC1 - first order phase correction value for PH_mod = pk

FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)

REVERSE - flag indicating to reverse the spectrum

F3, F2 and F1 parameters

set by ***tf3***, can be viewed with ***dpp*** or by typing ***s si***, ***s stsi*** etc.:

SI - size of the processed data

STSR - strip start: first output point of strip transform

STSI - strip size: number of output points of strip transform

TDeff - number of raw data points to be used for processing

TDoff - first point of the FID used for processing (default 0)

F2 parameters

set by the ***tf3***, can be viewed with ***dpp*** or by typing ***s mc2*** :

MC2 - Fourier transform mode

F1 parameters

set by the acquisition, can be viewed with ***dpa*** or by typing ***s td*** etc.:

TD - time domain; number of raw data points

OUTPUT PARAMETERS

F2 parameters

can be viewed with ***dpp*** or by typing ***s ft_mod*** :

FT_mod - Fourier transform mode
FTSIZE - Fourier transform size

F3 parameters

can be viewed with ***dpp*** or by typing ***s ymax_p***, ***s ymin_p*** etc.:

YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`acqu2s` - F2 acquisition status parameters

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

`3rrr` - processed 3D data (Fourier transformed in F3)
`3iii` - real/imaginary processed data (if MC2 = QF)
`proc2` - F2 processing parameters
`procs`, `proc2s`, `proc3s` - F3, F2, F1 processing status parameters

OUTPUT FILES

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

`3rrr` - real processed 3D data

`3rir` - real/imaginary data (if MC2 ≠ QF)
`3iii` - real/imaginary processed data (if MC2 = QF)
`procs` - F3 processing status parameters
`proc2s` - F2 processing status parameters
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TF2(store_imag)
where *store_image* can be *y* or *n*

SEE ALSO

tf3, tf1, ft3d

tf1

NAME

tf1 - Process data, including FT, in F2 (3D)

DESCRIPTION

The command ***tf1*** processes a 3D dataset in the F1 direction. This involves a Fourier transform which transforms time domain data (FID) into frequency domain data (spectrum). Depending on the processing parameters BC_mod, WDW, ME_mod and PH_mod, ***tf1*** also performs baseline correction, window multiplication, linear prediction and spectrum phase correction.

The processing steps done by ***tf1*** can be described as follows:

tf1 only works on data which have already been processed with ***tf3*** and possibly with ***tf2***. It performs the following processing steps:

1. Baseline correction of the F1 time domain data
   Each tube is baseline corrected according to BC_mod. This parameter takes the value *no*, *single*, *quad*, *spol*, *qpol sfil* or *qfil*. More details on BC_mod can be found in chapter 2.4.
2. Linear prediction of the F1 time domain data
   Linear prediction is done according to ME_mod. This parameter takes the value *no*, *LPfr*, *LPfc*, *LPbr*, *LPbc*, *LPmifr*, *LPmifc*. Usually, ME_mod = no, which means no prediction is done. Forward prediction in F1 (*LPfr*, *LPfc*, *LPmifr* or *LPmifc*) can, for example, be used to extend truncated FIDs. Backward prediction (*LPbr* or *LPbc*) is not used very often in F1. Linear prediction is only performed for NCOEF > 0. Furthermore, LPBIN and, for backward prediction, TDoff play a role (see these parameters in chapter 2.4).
3. Window multiplication of the F1 time domain data
   Each tube is multiplied with a window function according to WDW. This parameter takes the value *em*, *gm*, *sine*, *qsine*, *trap*, *user*, *sinc*, *qsinc*, *traf* or *trafs*. More details on WDW can be found in chapter 2.4.
4. Fourier transform of the F1 time domain data

Each tube is Fourier transformed according to the F1 processing status parameter MC2 as shown in table 5.7. ***tf1*** does not evaluate the processing parameter FT_mod! Instead, it evaluates the F1 processing status parameter MC2, which was set by ***tf3*** to the value of the F1 acquisition status parameter FnMODE [1]. ***tf1*** stores the corresponding Fourier transform mode as the processing status parameter FT_mod (type ***dpp***).

F1 MC2	Fourier transform mode	status FT_mod
QF	forward, quad, real	fqc
QSEQ	forward, quad, real	fqr
TPPI	forward, single, real	fsr
States	forward, quad, complex	fqc
States-TPPI	forward, single, complex	fsc
Echo-AntiEcho	forward, quad, complex	fqc

Table 5.8

5. Phase correction of the F1 frequency domain data.
Each column is phase corrected according to PH_mod. This parameter takes the value *no*, *pk*, *mc* or *ps*. For PH_mod = pk, ***tf1*** applies the values of PHC0 and PHC1. This is only useful if the phase values are known. You can determine them by typing ***xfb*** on the 3D data to process a 13 or 12 plane, do a phase correction on the resulting the 2D dataset and store the phase values to 3D. More details on PH_mod can be found in chapter 2.4.

The F1 processing parameter SI determines the size of the processed data in the F1 direction. This must, however, be set before ***tf3*** is done and cannot be changed after ***tf3***. See ***tf3*** for the role of TD, TDeff and TDoff.

tf1 can do a strip transform according to the F1 parameters STSR and STSI (see ***tf3***).

tf1 evaluates the F1 parameter FCOR. The first point of the FIDs is mul-

[1] If FnMODE = undefined, ***tf3*** sets processing status MC2 to processing MC2.

tiplied with the value of FCOR which is a value between 0.0 and 2.0. As such, FCOR allows you to control the DC offset of the spectrum.

tf1 evaluates the F1 parameter REVERSE. If REVERSE=TRUE, the spectrum will be reversed in F1, i.e. the first data point becomes the last and the last data point becomes the first.

tf1 evaluates the F1 status parameter MC2. For MC2 ≠ QF, ***tf1*** uses the file `3rrr` as input and the files `3rrr` and `3rri` as output. For MC2 = QF, ***tf1*** uses the files `3rrr` and `3iii` as input and output. The role of MC2 is described in detail for the 2D processing command ***xfb***.

INPUT PARAMETERS

F1 parameters

set by the user with ***edp*** or by typing ***bc_mod***, ***bcfw*** etc.:

BC_mod - FID baseline correction mode

BCFW - filter width for BC_mod = sfil or qfil

COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil

ME_mod - FID linear prediction mode

NCOEF - number of linear prediction coefficients

LPBIN - number of points for linear prediction

TDoff - number of raw data points predicted for ME_mod = LPb*

WDW - FID window multiplication mode

LB - Lorentzian broadening factor for WDW = em or gm

GB - Gaussian broadening factor for WDW = gm, sinc or qsinc

SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc

TM1, TM2 - limits of the trapezoidal window for WDW = trap

PH_mod - phase correction mode

PHC0 - zero order phase correction value for PH_mod = pk

PHC1 - first order phase correction value for PH_mod = pk

FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)

REVERSE - flag indicating to reverse the spectrum

F3, F2 and F1 parameters

set by ***tf3***, can be viewed with ***dpp*** or by typing ***s si***, ***s stsi*** etc.:

SI - size of the processed data

STSR - strip start: first output point of strip transform

STSI - strip size: number of output points of strip transform

TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)

F1 parameters

set by the ***tf3***, can be viewed with ***dpp*** or by typing ***s mc2*** :

MC2 - Fourier transform mode

OUTPUT PARAMETERS

F1 parameters

can be viewed with ***dpp*** or by typing ***s ft_mod*** :

FT_mod - Fourier transform mode
FTSIZE - Fourier transform size

F3 parameters

can be viewed with ***dpp*** or by typing ***s ymax_p*** etc.:

YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`acqu3s` - F1 acquisition status parameters

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

`3rrr` - processed 3D data (Fourier transformed in F1)
`3iii` - real/imaginary processed data (if MC2 = QF)
`proc3` - F1 processing parameters

OUTPUT FILES

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

`3rrr` - real processed 3D data
`3rir` - real/imaginary data (if MC2 ≠ QF)
`3iii` - real/imaginary processed data (if MC2 = QF)
`proc3s` - F1 processing status parameters

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TF1(store_imag)
where *store_image* can be *y* or *n*

SEE ALSO

tf3, tf2, ft3d

tf3p, tf2p, tf1p

NAME

tf3p - Phase correction in F3 (3D)
tf2p - Phase correction in F2 (3D)
tf1p - Phase correction in F1 (3D)

DESCRIPTION

tf3p performs a phase correction in the F3 direction applying the values of PHC0 and PHC1. These values must first be determined, for example on a 2D plane. You can do that by typing ***xfb*** on the 3D data to process a 23 or 13 plane, do a phase correction on the resulting the 2D dataset and store the phase values to 3D.

tf2p works like ***tf3p***, except that it works in the F2 direction applying the F2 parameters PHC0 and PHC1. These can be determined on a 2D plane extracted with ***r23*** or ***r12***.

tf1p works like ***tf3p***, except that it works in the F1 direction applying the F1 parameters PHC0 and PHC1. These can be determined on a 2D plane extracted with ***r13*** or ***r12***.

tf3p can only be done:

- directly after ***tf3*** (not after ***tf2*** or ***tf1***)
- if the F3 imaginary data exist

Note that the command ***tf3 n*** does not store the imaginary data. You can, however, create them data from the real data with a Hilbert transform (command ***tht3***).

Phase correction is already done as a part of the commands ***tf3***, ***tf2*** and ***tf1***, if PH_mod = pk and PHC0 and PHC1 are set.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***phc0***, ***phc1*** etc.

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s phc0***, ***s phc1*** etc.:

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

INPUT FILES

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

`3rrr` - real processed 3D data
`3irr` - F3 imaginary processed data (input of ***tf3p***)
`3rir` - F2 imaginary processed data (input of ***tf2p***)
`3rri` - F1-imaginary processed data (input of ***tf1p***)

OUTPUT FILES

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

`3rrr` - real processed 3D data
`3irr` - F3 imaginary processed data (output of ***tf3p***)
`3rir` - F2 imaginary processed data (output of ***tf2p***)
`3rri` - F1-imaginary processed data (output of ***tf1p***)
`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

TF3P(store_imag)
where *store_image* can be *y* or *n*

TF2P(store_imag)
where *store_image* can be *y* or *n*

TF1P(store_imag)
where *store_image* can be *y* or *n*

SEE ALSO

tf3, tf2, tf1, xf2p, xf1p, pk

tht3, tht2, tht1

NAME

tht3 - Hilbert transform in F3 (3D)
tht2 - Hilbert transform in F2 (3D)
tht1 - Hilbert transform in F1 (3D)

DESCRIPTION

`tht3` performs a Hilbert transform in the F3 direction creating imaginary data from the real data. The resulting imaginary data can then be used for phase correction with ***`tf3p`***.

`tht2` performs a Hilbert transform in the F2 direction creating imaginary data from the real data. The resulting imaginary data can then be used for phase correction with ***`tf2p`***.

`tht1` performs a Hilbert transform in the F1 direction creating imaginary data from the real data. The resulting imaginary data can then be used for phase correction with ***`tf1p`***.

Note that Hilbert Transform is only useful when the real data have been created from zero filled raw data, with SI ≥ TD.

Normally, the imaginary data are created during Fourier transform. If, however, the imaginary data are missing or do not match the real data and you want to do a phase correction, you can (re)create them with Hilbert transform. Imaginary data do not match the real data if the latter have been manipulated after the Fourier transform, for example by baseline correction or third party software.

INPUT FILES

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

`3rrr` - real processed 3D data

OUTPUT FILES

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

`3irr` - F3 imaginary processed data (output of ***`tht3`***)
`3rir` - F2 imaginary processed data (output of ***`tht2`***)

`3rri` - F1-imaginary processed data (output of ***`tht1`***)
`auditp.txt` - processing audit trail

SEE ALSO

tf3, tf2, tf1

Chapter 6

nD processing commands

TOPSPIN 2.0 and newer offers nD processing. Datasets up to 5D have been tested by Bruker. nD data can be displayed by reading cubes, planes or traces.

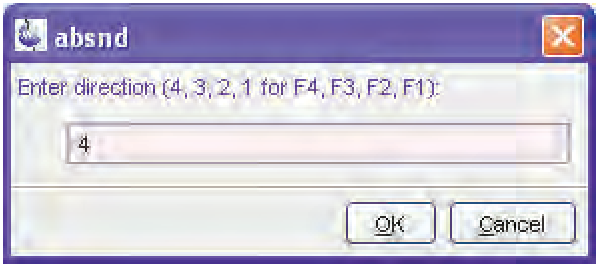
absnd

NAME

absnd - nD automatic baseline correction

DESCRIPTION

The command ***absnd*** performs an automatic baseline correction of data of dimension ≥3D. It takes one argument, the direction to be corrected. If no argument is specified on the command line, it is requested (see Figure 6.1).



absnd

Enter direction (4, 3, 2, 1 for F4, F3, F2, F1):

4

Figure 6.1

absnd subtracts a polynomial, the degree of which is determined by the parameter ABSG, which has a value between 0 and 5, with a default of 5. It only corrects a certain spectral region which is determined by the parameters ABSF1 and ABSF2.

absnd actually processes 2D planes of an nD dataset, performing a series of ***abs2*** or ***abs1*** commands. On 3D data, the commands ***absnd 3***, ***absnd 2*** and ***absnd 1*** are equivalent to **tabs3**, **tabs2** and **tabs1**, respectively.

INPUT PARAMETERS

Acquisition direction:

set by the user with ***edp*** or by typing ***absg***.:

ABSG - degree of the polynomial to be subtracted (0 to 5, default of 5)

All directions:

set by the user with ***edp*** or by typing ***absf1***, ***absf2***:

ABSF1- low field limit of the correction region
ABSF2 - high field limit of the correction region

INPUT FILES

For 4D data:

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

`4rrrr` - processed 4D data
`proc` - F4 processing parameters
`proc2` - F3 processing parameters
`proc3` - F2 processing parameters
`proc4` - F1 processing parameters

For 3D data, the input data file is `3rrr` whereas the `proc4` does not exist. For data of dimension n where n ≥ 5, input data files are named `nr` and `ni`, e.g. `5r`, `5i`, `6r`, `6i` etc.

OUTPUT FILES

For 4D data:

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

`4rrrr` - processed 4D data
`procs` - F4 processing status parameters
`proc2s` - F3 processing status parameters
`proc3s` - F2 processing status parameters
`proc4s` - F1 processing status parameters

For 3D data, the output data file is `3rrr` whereas `proc4s` does not exist. For data of dimension n where n ≥ 5, output data files are named `nr` and `ni`, e.g. `5r`, `5i`, `6r`, `6i` etc.

SEE ALSO

abs2, abs1, tabs3, tabs2, tabs1

ftnd

NAME

ftnd - nD processing including Fourier transform (≥ 3D)

DESCRIPTION

The command ***ftnd*** processes nD data performing fid baseline correction, linear prediction, window multiplication, Fourier transform and phase correction. The command automatically recognizes the data dimensionality and handles data of dimension ≥3D. In TOPSPIN 2.1, ***ftnd*** has been tested by Bruker on 3D, 4D, 5D and 6Ddata. Note that 3D data can also be processed with the conventional commands ***tf3***, ***tf2***, ***tf1*** and ***ft3d***.

As an example, ***ftnd*** is described here for a 4D dataset. It takes the following three arguments:

- ***<direction>***
  the direction(s) to be processed. Allowed values are:

  0 : all directions, in the order defined by AQSEQ
  4321, 4312, 4231, 4213, 4132, 4123 : all directions in specified order
  4, 3, 2, or 1 : F4, F3, F2 or F1, respectively.

- ***<procno>***

  Output procno of the processed data. Optional argument, normally unused. In special cases, however, the data cannot be processed in-place, and must be stored in a different procno. ***ftnd*** will then prompt you for an output procno.

- ***dlp***

  Delayed linear prediction. Optional argument, only applicable when all directions are processed. This argument ensures that when linear prediction is performed in a certain direction, all other directions are already Fourier transformed (see below).

If the arguments are not specified on the command line, ***ftnd*** will normally only prompt you for the direction. The output procno is only prompted for if inplace operation is not possible.

Here are some example of specifying arguments on the command line:

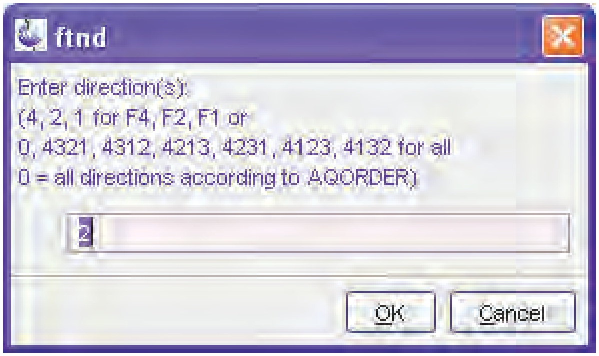
ftnd 0
Process the data in all directions in the order defined by the acquisition status parameter AQSEQ

ftnd 4
Process data in direction F4

ftnd 4312 999
Process the data in all directions, in the order F4-F3-F1-F2 and store the result in procno 999

ftnd 0 dlp
Process the data in all directions, in the order defined by AQSEQ, performing delayed linear prediction according to ME_MOD and NCOEF.

Missing arguments are prompted for, except for the ***dlp*** argument. Note that for the first argument, the direction, only the allowed directions are displayed and the next logical direction is suggested. Figure 6.2 shows the dialog opened by ***ftnd*** on a 4D dataset that has already been processed in F4 and F3.



Enter direction(s):
(4, 2, 1 for F4, F2, F1 or
0, 4321, 4312, 4213, 4231, 4123, 4132 for all
0 = all directions according to AQORDER)

2

Figure 6.2

Extract 1D, 2D or 3D data from 4D, 5D,... processed data.

To view the result of 4D processing, open the dataset (*procno*) where the processed data are stored and read a 3D-cube, 2D-plane or 1D trace. This can be done with the commands ***rcb***, ***rpl*** and ***rtr***, respectively. These commands automatically switch to the destination dataset showing the 3D, 2D or 1D dataset, respectively (see the description of these commands for more information). Furthermore, you can extract positive, negative or sum cube projections with the commands ***projcbp***, ***projcbn*** and ***sumcb***, respectively. Similarly, you can extract plane projections with the commands ***projplp***, ***projpln*** and ***sumpl***, respectively.

Instead of processing the entire 4D dataset and reading a certain plane or trace, you can also process single 2D-planes or 1D fids of the 4D raw data. To process a plane, just enter ***xfb***, ***xf2*** or ***xtrf*** and specify the requested plane axis orientation, plane number and output *procno*. To process a trace, just enter a 1D processing command like ***ft*** or ***trf*** and specify the requested fid number and output *procno*. Obviously, 1D/2D processing commands can also be used to further process or reprocess traces/planes or processed 4D data. For example:

1. Open a 4D dataset
2. ***ftnd 4***
   Perform 4D processing in the F4 direction
3. ***rpl 34 1 999***
   Read F3-F4 plane 1 and store it in *procno* 999. Note that the plane is stored as a F2-processed 2D dataset.
4. ***xf1***
   Perform 2D processing in the F1-direction.

Processing the four directions in separate steps

Normally, ***ftnd*** with the argument ***0*** or one of the arguments 4321, 4312, .. etc. to process all directions. In some cases, you may want to process the different directions in individual steps and perform the sequence ***ftnd 4***, ***ftnd 3***, .. etc. The first direction to be processed must be F4, the other three directions can be processed in any order. Note that every order in which the data are processed in F3, F2 an and F1 gives the same result, unless linear prediction is done (ME_mod and NCOEF ≠ 0)

Delayed linear prediction

Linear prediction is a valuable method for improving the resolution of nD data with small TD values and often truncated FIDs. The effect of linear prediction in one direction can, however, be distorted by modulations introduced by other, untransformed, directions. The ***dlp*** argument allows you to perform linear prediction in a certain direction while all other directions have already been Fourier transformed. Let's take an example to see how this works. Suppose you have a 4D dataset with acquisition order 4321 (parameter AQSEQ), which you want to processed in all 4 directions including Window Multiplication (WM) and Fourier transform (FT). Furthermore, you want to increase the resolution with linear prediction (LP) in the third (F2) and fourth (F1) direction. As such, you have set the parameters WDW, and, in F2 and F1, ME_mod and NCOEF, to appropriate values. If you use the command ***ftnd 0*** the following happens:

1. Processing in F4 (WM - FT)
2. Processing in F3 (WM - FT
3. Processing in F2 (LP - WM - FT
4. Processing in F1 (LP - WM - FT

So when linear prediction is done in F2, data have not been Fourier transformed yet in F1, which can cause distortions.

If, however, you use the command ***ftnd 0 dlp*** for delayed linear prediction, the following happens:

1. Processing in F4 (WM - FT)
2. Processing in F3 (WM - FT)
3. Processing in F2 (FT)
4. Processing in F1 (LP - WM - FT)
5. Processing in F2 (IFT [1])
6. Processing in F2 (LP - WM - FT)

Now when linear prediction is done in F2, the data are Fourier transformed in F1 (and all other directions). For the F1 direction, linear prediction does not have to be delayed because F1 is the last direction being processed. Note that ***ftnd*** also performs fid baseline correction and spectrum phase correction if the parameters BC_mod and PH_mod, respectively, are set.

Delayed linear prediction can also be performed in two steps. The command:

ftnd 0 dlp (with F2-ME_mod ≠ 0 and NCOEF ≠0)

[1] Inverse Fourier transform, including Hilbert Transform to create temporary imaginary data.

is equivalent with the command sequence:

1. ***ftnd 0*** (with F2-ME_mod = 0) and WDW = 0
2. ***lpnd 2*** (with F2-ME_mod ≠ 0, NCOEF ≠ 0 and WDW ≠ 0)

In-place operation

Normally, ***ftnd*** can perform an in-place operation, which means the processed data are stored in the current *procno*. In special cases, however, in-place operation is not possible and the processed data must be stored in a different *procno*. ***ftnd*** will prompt the user for the output *procno*. When processing is finished, the display will automatically change to the destination PROCNO.

Whether or not in-place operation is possible depends on the direction being processed and the zero-filling conditions. In-place operation is done:

- In the first direction: always
- In the second direction: always as long as all directions are processed with one command, e.g. with ***ftnd 0***.
- In the third, fourth etc. directions: if at least single zero filling (SI ≥ TD and (STSI = 0 or STSI ≥ TD)).

Note that if a *procno* is specified on the command line, it is used, i.e. the processed data of the last two directions are stored there.

Restrictions nD processing

The command ***ftnd*** has the following two restrictions:

- Raw and processed data have the same dimensionality, i.e. the values of the status parameters PARMODE and PPARMOD must be the same. Note that 2D processing commands like ***xfb*** also work on datasets with different raw and processed data dimensionality, e.g. 3D raw and 2D processed data.
- If the acquisition mode (acquisition status parameter FnMODE) is QF in one direction, it must be QF in all directions. In other words, you can not process mixed single detection/hypercomplex data.
- For data of dimension ≥ 5D, only the natural acquisition order (AQSEQ = 0) is supported.

- Simultaneous echo-antiecho not supported; the acquisition status parameter FnMODE must not be echo-antiecho in more than 1 direction.

Note that the values of parameters which use a predefined list are stored as integers. The first value of the list is always stored as 0, the second value as 1 etc. Table 6.1 shows the values of the parameter PH_mod as an example:

Parameter value	Integer stored in the proc(s) file
no	0
pk	1
mc	2
ps	3

Table 6.1

INPUT PARAMETERS

F4, F3, F2 and F1 parameters

set by the user with ***edp*** or by typing ***si***, ***stsr*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - number of output points of strip transform
TDeff - number of raw data points to be used for processing
TDoff - first point of the FID used for processing (default 0)
FCOR - first (FID) data point multiplication factor (0.0-2.0, default 0.5)
REVERSE - flag indicating to reverse the spectrum
BC_mod - FID baseline correction mode
BCFW - filter width for BC_mod = sfil or qfil
COROFFS - correction offset for BC_mod = spol/qpol or sfil/qfil
ME_mod - FID linear prediction mode
NCOEF - number of linear prediction coefficients
LPBIN - number of points for linear prediction
TDoff - number of raw data points predicted for ME_mod = LPb*
WDW - FID window multiplication mode
LB - Lorentzian broadening factor for WDW = em or gm

GB - Gaussian broadening factor for WDW = gm, sinc or qsinc
SSB - Sine bell shift for WDW = sine, qsine, sinc or qsinc
TM1, TM2 - limits of the trapezoidal window for WDW = trap

PH_mod - phase correction mode

PHC0 - zero order phase correction value for PH_mod = pk
PHC1 - first order phase correction value for PH_mod = pk

set by the acquisition, can be viewed with ***dpa*** or ***s aq_mod*** etc.:

TD - time domain; number of raw data points

F4 parameters

set by the user with ***edp*** or by typing ***aqorder***, ***pknl*** etc.:

AQORDER - Acquisition order
PKNL - group delay compensation (Avance) or filter correction (A*X)

set by the acquisition, can be viewed with ***dpa*** or ***s aq_mod*** etc.:

AQ_mod - acquisition mode (determines the status FT_mod)
AQSEQ - acquisition sequence (3-2-1 or 3-1-2)
BYTORDA - byteorder or the raw data
NC - normalization constant

F3, F2 and F1 parameters

set by the acquisition, can be viewed with ***dpa*** or by typing ***s fnmode*** etc.:

FnMODE - Fourier transform mode

OUTPUT PARAMETERS

F4, F3, F2 and F1

can be viewed with ***dpp*** or by typing ***s si***, ***s stsi*** etc.:

SI - size of the processed data
STSR - strip start: first output point of strip transform
STSI - strip size: number of output points of strip transform
TDeff - number of raw data points that were used for processing
TDoff - first point of the FID used for processing (default 0)
XDIM - subcube size
FT_mod - Fourier transform mode

FTSIZE - Fourier transform size

F4 parameters

can be viewed with ***dpp*** or by typing ***s si***, ***s tdeff*** etc.:

AQORDER - Acquisition order
YMAX_p - maximum intensity of the processed data
YMIN_p - minimum intensity of the processed data
S_DEV - standard deviation of the processed data
NC_proc - intensity scaling factor
BYTORDP - byte order of the processed data

F3, F2 and F1 parameters

can be viewed with ***dpp*** or by typing ***s mc2*** etc.:

MC2 - Fourier transform mode

INPUT FILES

For 4D data:

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - raw data
`acqus` - F4 acquisition status parameters
`acqu2s` - F3 acquisition status parameters
`acqu3s` - F2 acquisition status parameters
`acqu4s` - F1 acquisition status parameters

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

`proc` - F4 processing parameters
`proc2` - F3 processing parameters
`proc3` - F2 processing parameters
`proc4` - F1 processing parameters

For 3D data `proc4s` does not exist. For data of dimension n where n ≥ 5 the additional files proc5,...,etc. exist.

OUTPUT FILES

For 4D data:

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

`4rrrr` - processed 4D data
`procs` - F4 processing status parameters
`proc2s` - F3 processing status parameters
`proc3s` - F2 processing status parameters
`proc4s` - F1 processing status parameters

For 3D data, the output data file is `3rrr` whereas `proc4s` does not exist. For data of dimension n where n ≥ 5, processed data files are named `nr` and `ni`, e.g. `5r`, `5i`, `6r`, `6i` etc. and the additional files proc5s,..., etc. exist.

SEE ALSO

absnd, pknd, lpnd, projcbp, projcbn, sumcb, projplp, projpln, sumpl

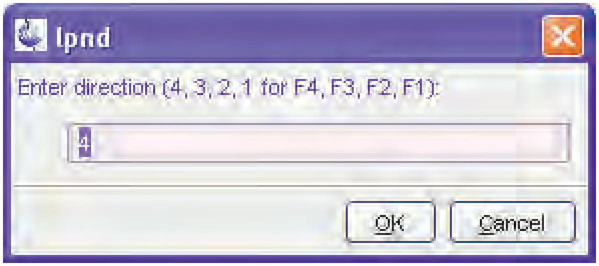
lpnd

NAME

lpnd - nD linear prediction

DESCRIPTION

The command ***lpnd*** performs a linear prediction of data with dimension ≥3D. It takes one argument, the direction to be processed. If no argument is specified on the command line, it is requested (see Figure 6.1).



lpnd

Enter direction (4, 3, 2, 1 for F4, F3, F2, F1):

4

Figure 6.3

lpnd works on data that have already been Fourier transformed in the specified direction, e.g. with ***ftnd***. Since linear prediction is normally performed on a unfiltered FID, the data should first be processed with ***ftnd*** with WDW = no, and then with ***lpnd*** while WDW is set to the desired window function.

lpnd performs the following steps in the specified direction:

1. Inverse Fourier transform[1]
2. Regular processing including:
   - Linear prediction according to ME_mod, NCOEF
   - Window multiplication according to WDW
   - Fourier transform

Linear prediction is a valuable method for improving the resolution of nD data with small TD values and often truncated FIDs. The effect of linear

[1] If imaginary data do not exist, they are automatically created with Hilbert transform.

prediction in one direction can, however, be distorted by modulations introduced by other, untransformed, directions. Therefore, it is a good idea to first process the data in all directions and then perform ***lpnd***. This entire procedure, including the correct window handling, is automatically performed by the command ***ftnd dlp*** (delayed linear prediction). However, if you want both backward and forward prediction, the latter must be done with ***lpnd***. In this case, you have to perform the following steps:

1. Backward prediction with ***ftnd*** while ME_mod=LPbr or LPbc and WDW=no.
2. Forward prediction with ***lpnd*** while ME_mod=LPfr or LPfc and WDW set to the desired window function.

For more information, see the description of ***ftnd***.

INPUT AND OUTPUT PARAMETERS

see ***ftnd***

INPUT FILES

For 4D data:

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

`4rrrr` - processed 4D data
`proc` - F4 processing parameters
`proc2` - F3 processing parameters
`proc3` - F2 processing parameters
`proc4` - F1 processing parameters

For 3D data, the input data file is `3rrr` whereas the `proc4` does not exist. For data of dimension n where n ≥ 5, input data files are named `nr` and `ni`, e.g. `5r`, `5i`, `6r`, `6i` etc.

OUTPUT FILES

For 4D data:

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

`4rrrr` - processed 4D data
`procs` - F4 processing status parameters
`proc2s` - F3 processing status parameters

`proc3s` - F2 processing status parameters
`proc4s` - F1 processing status parameters

For 3D data, the output data file is `3rrr` whereas `proc4s` does not exist. For data of dimension n where n ≥ 5, output data files are named `nr` and `ni`, e.g. `5r`, `5i`, `6r`, `6i` etc.

SEE ALSO

ftnd

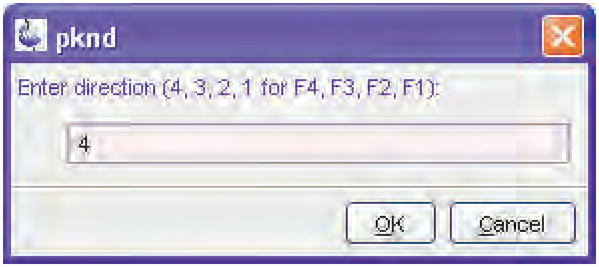
pknd

NAME

pknd - nD phase correction

DESCRIPTION

The command ***pknd*** performs a phase correction of data of dimension ≥3D, applying the values of PHC0 and PHC1. It takes one argument, the direction to be corrected. If no argument is specified on the command line, it is requested (see Figure 6.4).



pknd

Enter direction (4, 3, 2, 1 for F4, F3, F2, F1):

4

Figure 6.4

Before you execute ***pknd***, the phase values must first be determined, for example on a 2D plane. You can do that by typing ***xfb*** on the nD data to process a plane, do a phase correction on the resulting the 2D dataset and store the phase values in the nD dataset.

Note that phase correction normally requires the existence of imaginary data. Usually, however these do not exist for data of dimension ≥ 4. Therefore, ***pknd*** automatically creates temporary imaginary data using Hilbert transform. Actually the command processes 2D planes of an nD dataset, performing a series of ***xht2*** - ***xf2p*** or ***xht1*** - ***xf1*** commands.

On 3D data, the commands ***pknd 3***, ***pknd 2*** and ***pknd 1*** are equivalent to ***tf3p***, ***tf2p*** and ***tf1p***, respectively.

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***phc0***, ***phc1*** etc.

PHC0 - zero order phase correction value (frequency independent)

PHC1 - first order phase correction value (frequency dependent)

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s phc0***, ***s phc1*** etc.:

PHC0 - zero order phase correction value (frequency independent)
PHC1 - first order phase correction value (frequency dependent)

INPUT FILES

For 4D data:

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

`4rrrr` - processed 4D data
`proc` - F4 processing parameters
`proc2` - F3 processing parameters
`proc3` - F2 processing parameters
`proc4` - F1 processing parameters

For 3D data, the input data file is `3rrr` whereas the `proc4` does not exist. For data of dimension n where n ≥ 5, input data files are named `nr` and `ni`, e.g. `5r`, `5i`, `6r`, `6i` etc.

OUTPUT FILES

For 4D data:

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

`4rrrr` - processed 4D data
`procs` - F4 processing status parameters
`proc2s` - F3 processing status parameters
`proc3s` - F2 processing status parameters
`proc4s` - F1 processing status parameters

For 3D data, the output data file is `3rrr` whereas `proc4s` does not exist. For data of dimension n where n ≥ 5, output data files are named `nr` and `ni`, e.g. `5r`, `5i`, `6r`, `6i` etc.

SEE ALSO

ftnd, tf3p, tf2p, tf1p, xf2p, xf1p, xht2, xht1

projcbp, projcbn, sumcb

NAME

projcbp - Calculate positive 3D projection
projcbn - Calculate negative 3D projection
sumcb - Calculate sum 3D projection

DESCRIPTION

The commands ***projcbp***, ***projcbn*** and ***sumcb*** calculate the positive, negative and sum 3D projection, respectively, from a dataset of dimension ≥ 4.
They require take up to 5 arguments:

<cube orientation> *: 234, 134, 124, ..., 432, 321 etc.*

<first cube> : the first cube included in the calculation

<last cube> : the last cube included in the calculation

<dest. procno> : the *procno* where the 3D output data are stored

xdim *:* sets the subcube sizes according to XDIM (optional)

n *:* prevents the destination dataset from being displayed/activated (optional)

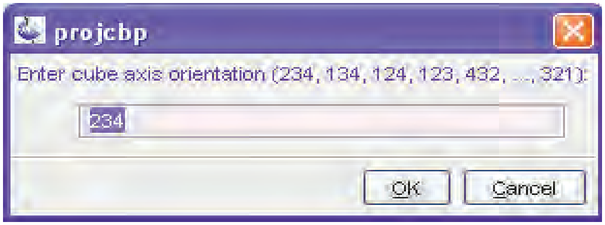
Here is an example of the usage of a 3D projection command:
projcbp 234 1 32 999 n

calculates the positive F2-F3-F4 3D projection of cube 1 to 32 along the F1 direction, stores it under PROCNO 999 but does not change the display to the output data.

Instead of specifying the first and last cube, you can also use the argument ***all*** for all cubes. For example:
projcbp 234 all 10

calculates the positive F2-F3-F4 3D projection of all cubes along F1 and stores it under PROCNO 10.

Missing arguments (except for the optional ones) will be prompted for. For example, if you enter ***projcbp*** without any arguments, it will start with the dialog shown in Figure 6.5:



Enter cube axis orientation (234, 134, 124, 123, 432, ..., 321):

234

Figure 6.5

Note the following aspects:

- the maximum first and last cube is determined by the size of the data in the direction not included cube orientation; i.e. the direction along which the projection is calculated.
- XDIM is a processing parameter which must be set in each direction included cube orientation when with the ***xdim*** argument is used.
- the numerical arguments must be specified in the above order, whereas the arguments ***all***, ***xdim*** and ***n*** can be specified at any position.

INPUT FILES

For a 4D dataset:

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

`4rrrr` - real processed 4D data

OUTPUT FILES

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

`3rrr` - real processed 3D data

`procs` - F3 processing status parameters
`proc2s` - F2 processing status parameters
`proc3s` - F1 processing status parameters
`auditp.txt` - processing audit trail

SEE ALSO

projplp, projpln, sumpl

rcb

NAME

rcb - Read cube from data ≥ 4D and store as 3D data

DESCRIPTION

The command ***rcb*** reads a cube from processed data of dimension ≥ 4. It stores the extracted cube in a different *procno* as a 3D dataset.

rcb takes up to five arguments:

<cube axis orientation> *: 234, 134, 124, ..., 432, 321 etc.*

The digits refer to the F4, F3, F2 and F1 axes of the 4D data. Note that the order of the three digits is relevant:

- the first digit is the 4D axis that corresponds to the 3D-F1 axis
- the second digit is the 4D axis that corresponds to the 3D-F2 axis
- the last digit is the 4D axis that corresponds to the 3D-F3-axis

This means that for values like 234, 134, 124 etc. the axis order or the 3D cube and the 4D dataset are the same. For values like 432, 423, 143 etc., they are different.

<cube number> : 1 - SI

SI is the 4D size in the direction orthogonal to the cube orientation

<***procno***> :

destination 3D *procno* (source 4D *procno* if ***rcb*** is entered on the destination 3D dataset)

xdim *:* optional argument

sets the subcube sizes according to the processing parameter XDIM in the respective directions. This parameter must be set in the source 4D dataset before ***rcb*** is executed.

n *:* optional argument

prevents the destination dataset from being displayed/activated

Arguments which are not specified on the command line will be prompted for, except for ***xdim*** and ***n*** argument.
rcb can be entered on the source 4D dataset or, if this already exists, on the destination 3D dataset. The number of required arguments is different (see below).

rcb entered on a source 4D dataset

In this case, ***rcb*** prompts the user for three arguments. Alternatively, these can be entered on the command line.

Here are some examples:

rcb
Prompt the user for the *cube axis orientation*, the *cube number* and *destination 3D procno* and read the cube accordingly.

rcb 234 10 999

Read F2-F3-F4 cube 10 and store it in *procno* 999.

rcb 324 10 999

Read F2-F3-F4 plane 10 and store it in *procno* 999, exchanging the F2 and F3 axes

rcb 124 64 101 xdim

Read F1-F2-F4 plane 64 with subcube sizes according to the respective XDIM values and store it in *procno* 101.

rcb 124 64

Read F1-F2-F4 plane 64, prompt the user for the destination *procno*

rcb 214 1 10 n

Read an F1-F2-F4 plane number 1 and store it in *procno* 10, exchanging the F2 and F1 axes. Do not display/activate the destination dataset.

rcb entered on a destination 3D dataset

This is typically done on a 3D dataset which is a cube extracted by a previous ***rcb*** command, which was entered on the source 4D dataset. In that case, ***rcb*** requires only one argument; the *cube number*. By default, the same cube *axis orientation* and *source 4D dataset (procno)* are used as with the previous ***rcb*** command (as defined in the `used_from` file of the 3D dataset). You can, however, use two or three arguments to specify a different cube *axis orientation* and/or *4D source procno*. On a regular 3D dataset (not a plane from a 3D), ***rcb*** requires three arguments.

Here are some examples of ***rcb*** executed on a 3D dataset, where the 3D dataset is a cube from a 4D dataset:

rcb

Prompt the user for the *cube number*. Use the *cube axis orientation* and *source 4D procno* as defined in the current 3D dataset.

rcb 11

Read cube 11. Use the *cube axis orientation* and *Source 4D procno* as defined in current 3D dataset.

rcb 123 11

Read F1-F2-F3 plane 11. Use the *source 4D procno* as defined in current 3D dataset.

rcb 123 11 2

Read F1-F2-F3 plane 11 from the 4D dataset under *procno* 2

As described above, the ***rcb*** argument *cube axis orientation* determines whether the axes are exchanged. Axes exchange is sometimes required to match nuclei when you compare a 4D cube with a 3D dataset.

INPUT FILES

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

`4rrrr`, `4iiii` - processed 4D data

OUTPUT FILES

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

`3rrr`, `3iii` - processed 3D data

`auditp.txt` - processing audit trail

`used_from` - data path of the source 4D data and the cube axis orientation

SEE ALSO

rpl, wpl, rtr, wtr

rpl

NAME

rpl - Read plane from data ≥ 3D and store as 2D data

DESCRIPTION

The command ***rpl*** reads a plane from processed data with dimension ≥ 3D and stores it as a 2D dataset in a different *procno*.

rpl takes up to five arguments. As an example we take a plane read from a 3D dataset:

<plane axis orientation> *: 23, 13, 12, 32, 31 or 21*

The digits refer to the F3, F2 and F1 axes of the 3D data. Note that the order of the two digits is relevant:

- the first digit is the 3D axis that corresponds to the 2D-F1 axis
- the last digit is the 3D axis that corresponds to the 2D-F2-axis

This means that for the values 21, 31 and 32, the axes are exchanged, storing rows as columns and vice versa (see below).

<plane number> : 1 - SI

SI is the 3D size in the direction orthogonal to the plane orientation

<***procno***> :

destination 2D *procno* (source 3D *procno* if ***rpl*** is entered on the destination 2D dataset)

<***inmem***> : optional argument for usage in AU programs only

improves performance by data caching. Caution: nD data must not be modified by any command other than ***wpl*** between two consecutive ***rpl inmem*** or ***wpl inmem*** commands.

n *:* optional argument

prevents the destination dataset from being displayed/activated

Obligatory arguments which are not specified on the command line will be prompted for.

rpl can be entered on the source 3D dataset or, if it already exists, on the destination 2D dataset. The number of required arguments is different (see below).

rpl entered on a source 3D dataset

In this case, ***rpl*** prompts the user for three arguments. Alternatively, these can be entered on the command line.

Here are some examples:

rpl
Prompt the user for the *plane axis orientation*, the *plane number* and *source 3D procno* and read the plane accordingly.

rpl 23 10 999
Read F2-F3 plane 10 and store it in *procno* 999.

rpl 32 10 999
Read F2-F3 plane 10 and store it in *procno* 999, exchanging the F2 and F3 axes.

rpl 12 64 101
Read F1-F2 plane 64 and store it in *procno* 101.

rpl 12 64
Read F1-F2 plane 64, prompt the user for the *destination procno*

rpl 31 1 10 n
Read an F1-F3 plane number 1 and store it in *procno* 10, exchanging the F1 and F3 axes. Do not display/activate the destination dataset.

rpl entered on a destination 2D dataset

This is typically done on a 2D dataset which is a plane extracted by a previous ***rpl*** command, which was entered on the source 3D dataset. In that case, ***rpl*** requires only one argument; the *plane number*. By default, the same p*lane axis orientation* and *source 3D dataset (procno)* are used as with the previous ***rpl*** command (as defined in the `used_from` file of the 2D dataset). You can, however, use two or three arguments to specify a different p*lane axis orientation* and/or *3D source procno*. On a regular 2D dataset (not a plane from a 3D), ***rpl*** requires three arguments.

Here are some examples of ***rpl*** executed on a 2D dataset, where the 2D dataset is a plane from a 3D dataset:

rpl

Prompt the user for the plane number, use the *plane axis orientation* and *source 3D procno* as defined in the current 2D dataset and read the plane accordingly.

rpl 11

Read plane 11. Use the *plane axis orientation* and *source 3D procno* as defined in current 2D dataset.

rpl 31 11

Read F1-F3 plane 11, exchanging the F1 and F3 axes. Use the *source 3D procno* as defined in current 2D dataset.

rpl 13 11 2

read F1-F3 plane 11 from the 3D dataset under *procno* 2

As described above, the ***rpl*** argument *plane axis orientation* determines whether the axes are exchanged. This is sometimes required to match nuclei when you compare a 3D plane with a 2D dataset. Example: you have a 3D NOESYHSQC (F3-1H, F2-13C, F1-1H) and want to compare an F2-F1 plane with a 2D HSQC (F2-1H, F1-13C). Now compare the following actions:

rpl 12: The plane is stored as a 2D dataset with F2-13C, F1-1H which cannot be directly compared with the a HSQC.

rpl 21: The plane is stored as a 2D dataset with F2-1H, F1-13C which can be directly compared with the a HSQC.

In special cases, ***rpl*** results in a 2D dataset which is not Fourier transformed in F2. This occurs, for example, if you run ***rpl 12*** on a 3D dataset which has only been transformed in F3. ***rpl*** unshuffles the output data, storing the odd and even points in separate data files (`2rr` and `2ir`). As a result the size in F2 (parameter SI) is only half the size of the corresponding direction in the 3D dataset. If, for some reason, you want keep the same size, you can use ***rpl*** with the option ***keepsize***. The output data are then zero filled once in F2. Here is an example:

```
rpl 12 1 10 keepsize
```

Note that a plane read with ***keepsize*** cannot be written back to the source dataset because the sizes do not match.

Note that the command ***rpl*** replaces the old commands ***r12***, ***r13*** and ***r23*** which do not allow axes exchange. For compatibility reasons, these commands are still available. Note however, their usage in AU programs has changed compared to TOPSPIN 1.1 and XWIN-NMR (see the description of ***r12***).

The behaviour of the command ***rpl*** is similar to the commands ***rsr*** and ***rsc***, in the sense that it can be entered from the source and destination dataset.

On a data with dimension > 3, ***rpl*** works the same as on a 3D dataset, except that there are more plane axis orientations. For example on 4D dataset, possible orientations are *34*, *24*, *14*, *23*, *13*, *12*, *43*, *42*, *41*, *32*, *31* and *21*.

For an example if the ***inmem*** option, see the AU program ***ift3d***.

INPUT FILES

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

`3rrr`, `3irr`, `3rir`, `3rri`, `3iii` - processed data (***rpl*** on 3D data)
`4rrrr`, `4iiii` - processed data (***rpl*** on 4D data)

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`auditp.txt` - processing audit trail
`used_from` - data path of the source 3D data and the plane number

SEE ALSO

wpl, rtr, wtr, rcb, rser, wser, wserp, rser2d

rtr

NAME

rtr - Read trace from data ≥ 2D and store as 1D data

DESCRIPTION

The command ***rtr*** reads a trace from processed data with dimension ≥ 2D and stores it as a 1D dataset.

rtr takes up to four arguments. As an example we take a trace read from a 3D dataset:

<axis orientation> : 1, 2 or 3

The digit refers to the F3, F2 and F1 axis of the 3D data.

<trace number> : 1 - MAX

where MAX is the product of the SI value in the directions orthogonal to the trace orientation.

<***procno***> :

destination 1D *procno* (source 3D *procno* if ***rtr*** is entered on the destination 1D dataset)

n *:* optional argument.

prevents the destination dataset from being displayed/activated

Obligatory arguments that are not specified on the command line will be prompted for.

rtr can be entered on the source 3D dataset or, if this already exists, on the destination 1D dataset. The number of required arguments is different (see below).

rtr entered on a source 3D dataset

In this case, ***rtr*** prompts the user for three arguments. Alternatively, these can be entered on the command line.

rtr

Prompt the user for the *axis orientation*, *trace number* and *destination* *procno* and read the trace accordingly.

rtr 3 10 999

Read F3 trace 10 and store it in *procno* 999.

rtr 1 1 10 n

Read F1 trace 1 and store it in *procno* 10. Do not display/activate the destination dataset.

rtr entered on a destination 1D dataset

This is typically done on a 1D dataset which is a trace extracted by a previous ***rtr*** command, which was entered on the source 3D dataset. In that case, ***rtr*** requires only one argument; the *trace number*. By default, the same *axis orientation* and *source 3D dataset (procno)* are used as with the previous ***rtr*** command (as defined in the `used_from` file of the 1D dataset). You can, however, use two or three arguments to specify a different *axis orientation* and/or *3D source procno*. On a regular 1D dataset (not a trace from a 3D), ***rtr*** requires three arguments.

Here are some examples of ***rtr*** executed on a 1D dataset which is a trace from a 3D dataset:

rtr

Prompt the user for the *trace number*, use the *axis orientation* and *source 3D procno* as defined in the current 1D dataset and read the trace accordingly.

rtr 11

Read trace 11. Use the *axis orientation* and *source 3D procno* as defined in current 1D dataset.

rtr 3 11 2

Read F3 trace 11 from the 3D dataset under *procno* 2

Note that on 2D data the command ***rtr*** works like ***rsr*** and ***rsc***, except that the trace direction can be freely chosen. Furthermore, ***rtr*** always stores the 1D output data in a different *procno* of the same dataset whereas ***rsr*** and ***rsc*** can store data in the dataset ~TEMP.

On 4D or higher dimensional datasets, ***rtr*** works the same as on a 3D dataset, except that there are more axis orientations.

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data (***rtr*** on 2D data)
`3rrr`, `3irr`, `3rir`, `3rri`, `3iii` - processed data (***rtr*** on 3D data)
`4rrrr`, `4iiii` - processed data (***rtr*** on 4D data)

OUTPUT FILES

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

`1r`, `1i` - processed 1D data
`auditp.txt` - processing audit trail
`used_from` - data path of the source data and the trace number

SEE ALSO

wtr, rpl, wpl, rcb, rser, wser, wserp

wpl

NAME

wpl - Write 2D data to a plane of data ≥ 3D

DESCRIPTION

The command ***wpl*** replaces a plane of processed data with dimension ≥ 3D with a 2D processed dataset. It is usually, but not necessarily, used to write back a plane that was extracted with ***rpl***. This plane can be modified and/or written back to a different plane number.

wpl takes up to four arguments. As an example we take a plane written to a 3D dataset:

<plane axis orientation> : 12, 13, 23, 21, 31 or 32

The digits refer to the F3, F2 and F1 axes of the 3D data. Note that the order of the two digits is relevant:

- the first digit is the 3D axis that corresponds to the 2D-F1 axis
- the last digit is the 3D axis that corresponds to the 2D-F2-axis

This means that for the values 21, 31 and 32, the axes are exchanged, i.e. rows are stored as columns and vice versa (see below).

<plane number> : 1 - SI

SI is the 3D size in the direction orthogonal to the plane axis orientation

<***procno***>

destination 3D *procno* (source 3D *procno* if ***wpl*** is entered on the destination 2D dataset)

<***inmem***> : optional argument for usage in AU programs only

improves performance by data caching. Caution: nD data must not be modified by any command other than ***wpl*** between two consecutive ***rpl inmem*** or ***wpl inmem*** commands.

n

do not write imaginary data. Only the real data plane is written to the real destination data. This option prevents ***wpl*** to abort when nD destination data exist, but 2D source data do not. Caution: this options makes the nD imaginary data inconsistent.

wpl can be entered on the 2D source dataset or on the destination 3D dataset. The number of required arguments is different (see below).

wpl entered on the source 2D dataset

In this case, ***wpl*** prompts the user for two arguments only, the *plane number* and the *3D destination procno*. The *plane axis orientation* is taken from the 2D dataset (`used_from` file). The two arguments can also be specified on the command line. If, however, you specify three arguments, the *plane axis orientation* is taken from the first argument rather than from the 2D dataset.

Examples:

wpl

prompt the user for the *plane number* and *destination 3D procno*, take the *plane axis orientation* from the current 2D dataset and write the plane accordingly.

wpl 11 1

write the current 2D data to plane 11 of the 3D dataset in *procno* 1. Take the *plane axis orientation* from the current 2D dataset.

wpl 31 11 2

write the current 2D data to F1-F3 plane number 11 of the 3D data in *procno* 2, exchanging the F1 and F3 axes.

Note that if the source 2D dataset does not contain a `used_from` file, for example because it is not an extracted plane, ***wpl*** will prompt the user for the *plane axis orientation*.

Entering ***wpl*** on the destination 3D dataset

In this case, ***wpl*** prompts the user for three arguments. Alternatively, these can be entered on the command line.

Examples:

wpl 23 10 999

Write the 2D data in *procno* 999 to F2-F3 plane 10 of the current 3D data.

wpl 12 32 101

Write the 2D data in *procno* 101, to the F1-F2 plane 32 of the current 3D data

wpl 12

Prompt the user for the *procno* of the source 2D dataset and the plane number. Write the 2D dataset to the specified F1-F2 plane accordingly.

Entering *wpl* on a 4D dataset

On a data with dimension > 3, ***wpl*** works the same as on a 3D dataset, except that there are more plane axis orientations. For example on 4D dataset, possible orientations are *12, 13, 14, 23, 24, 34, 21, 31, 32, 41, 42* and *43.*

INPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`used_from` - data path of the source 3D data and the plane number

OUTPUT FILES

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

`3rrr`, `3irr`, `3rir`, `3rri`, `3iii` - processed data (***wpl*** on 3D data)
`4rrrr`, `4iiii` - processed data (***wpl*** on 4D data)
`auditp.txt` - processing audit trail

SEE ALSO

rpl, rtr, wtr, rcb, rser, wser, wserp

wtr

NAME

wtr - Write 1D data to a trace of data ≥ 2D

DESCRIPTION

The command ***wtr*** replaces a trace of processed data with dimension ≥ 2D with a 1D processed dataset. It is usually, but not necessarily, used to write back a trace that was extracted with ***rtr***. This trace can be modified and/or written back to a different trace number.

wtr takes up to three arguments. As an example we take a trace written to a 3D dataset:

<axis orientation> : 1, 2 or 3

The digit refer to the F3, F2 and F1 axes of the 3D data.

<trace number> : 1 - MAX

where MAX is the product of the SI value in the directions orthogonal to the trace orientation

<***procno***>

destination 3D *procno* (source 1D *procno* if ***wtr*** is entered on the destination 3D dataset)

wtr can be entered on the 1D source dataset or on the destination 3D dataset. The number of required arguments is different (see below).

wtr entered on the source 1D dataset

In this case, ***wtr*** prompts the user for two arguments only, the *trace number* and the *1D destination procno*. The *axis orientation* is taken from the 3D dataset (`used_from` file). The two arguments can also be specified on the command line. If, however, you specify three arguments, the *axis orientation* is taken from the first argument rather than from the 3D dataset.

Examples:

wtr

prompt the user for the *trace number* and *destination 3D procno*, take the *axis orientation* from the current 1D dataset and write the trace accordingly.

wtr 11 1

write the current 1D data to trace 11 of the 3D dataset in *procno* 1. Take the *axis orientation* from the current 1D dataset.

wtr 3 11 2

write the current 1D data to F3 trace number 11 of the 3D data in *procno* 2.

Note that if the source 1D dataset does not contain a `used_from` file, for example because it is not an extracted trace, ***wtr*** will prompt the user for the *axis orientation*.

Entering *wtr* on the destination 3D dataset

In this case, ***wtr*** prompts the user for three arguments. Alternatively, these can be entered on the command line.

Examples:

wtr 2 10 999

Write the 1D data in *procno* 999 to F2 trace 10 of the current 3D data.

wtr 1 32 101

Write the 1D data in *procno* 101, to the F1 trace 32 of the current 3D data.

wtr 1

Prompt the user for the trace number and the *procno* of the source 1D dataset. Write the 1D dataset to the specified F1 trace accordingly.

Entering *wtr* on a 4D dataset

On a data with dimension > 3, ***wtr*** works the same as on a 3D dataset, except that there are more axis orientations. For example on 4D dataset, possible orientations are *1, 2, 3* and *4*.

INPUT FILES

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

`1r`, `1i` - processed 1D data
`used_from` - data path of the source nD data and the trace number

OUTPUT FILES

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

`2rr`, `2ir`, `2ri`, `2ii` - processed data (***wtr*** on 2D data)
`3rrr`, `3irr`, `3rir`, `3rri`, `3iii` - processed data (***wtr*** on 3D data)
`4rrrr`, `4iiii` - processed data (***wtr*** on 4D data)
`auditp.txt` - processing audit trail

SEE ALSO

rtr, rpl, wpl, rcb, rser, wser, wserp

Chapter 7

Print/Export commands

This chapter describes TOPSPIN print, plot and export commands. Printing can be done directly from the TOPSPIN interface or from the Plot Editor. The data window can be exported into a graphics file. Commands are available for setting the plot title and, for 2D and 3D data, the contour levels.

autoplot

NAME

autoplot - Plot data according to Plot Editor layout (1D,2D)

DESCRIPTION

The command ***autoplot*** plots the current dataset according to a Plot Editor layout. The layout must be specified with the processing parameter LAYOUT. This layout can be a standard Plot Editor layout which is delivered with TOPSPIN or a user defined layout which has been set up from the Plot Editor.

autoplot can take the following arguments:

-s setup.prt
Use printer setup file `setup.prt` instead of the printer setup that was saved with the layout (not available in Windows version).

-l N

Remove N data sets from the portfolio and print again.

-n
Don‘t reset before printing.

-f
Force all 1D and/or 2D objects in the layout to use axis limits as used in TOPSPIN (uses the `F1P/F2P` parameter for each direction).

-e output.ps
Create e.g. a Postscript file instead of printer output. Use the `-?` option to see a complete list of supported file formats.

-v
Show ***autoplot*** version number.

-h
Show help text.

-?
Same as ***-h***.

For a extended description of ***autoplot*** please refer to the Plot Editor online help.

INPUT PARAMETERS

set with ***edp*** or by typing ***layout*** etc.:

LAYOUT - Plot Editor layout
CURPLOT - Default plotter for Plot Editor

INPUT FILES

<tshome>/plot/layouts/*.xwp - Bruker library Plot Editor layouts

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

`1r` - real processed 1D data
`procs` - processing status parameters
`intrng` - integral regions
`parm.txt` - ascii file containing parameters which appear on the plot
`title` - default title file
`outd` - output device parameters
`portfolio.por` - Plot Editor portfolio (input file is it exists)

For a 2D dataset, the files `2rr`, `proc2s` and `clevels` are also input.

USAGE IN AU PROGRAMS

AUTOPLOT

AUTOPLOT_WITH_PORTFOLIO

AUTOPLOT_TO_FILE(outputfile)

AUTOPLOT_WITH_PORTFOLIO_TO_FILE(outputfile)

SEE ALSO

plot, print, prnt

exportfile

NAME

exportfile - Export data window to graphics file (1D,2D,3D)

DESCRIPTION

The command ***exportfile*** saves the contents of a data window in a graphics file of selectable type, e.g. `.png`, `.tif`, `.wmf` etc. It opens an Explorer window.

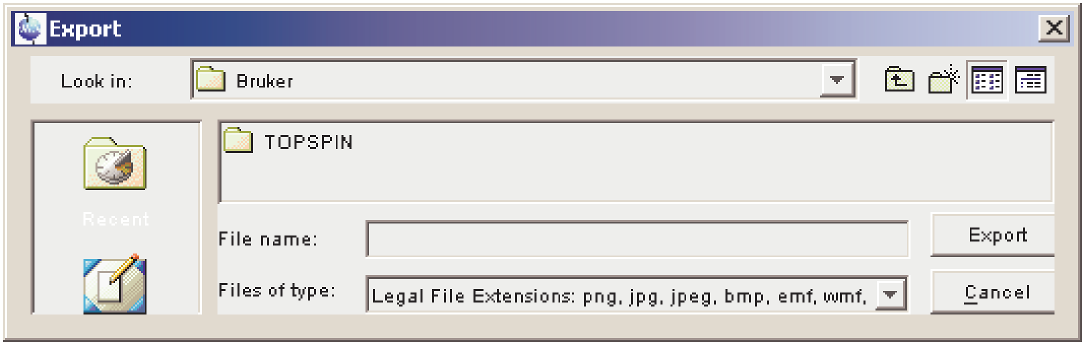


Figure 7.1

Here you can:

- Click or type the output file
- 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.

Entering ***exportfile*** on the command line is equivalent to clicking ***File*** → ***Export***….

In TOPSPIN 2.1 and newer, the pathname of the destination graphics file is available in the Windows clipboard.

OUTPUT FILES

<outputdir>

`outputfile`[`.png`, `.jpg`, `.jpeg`, `.bmp`, `.emf`, `.wmf`] - graphics file

SEE ALSO

plot, autoplot, prnt, print

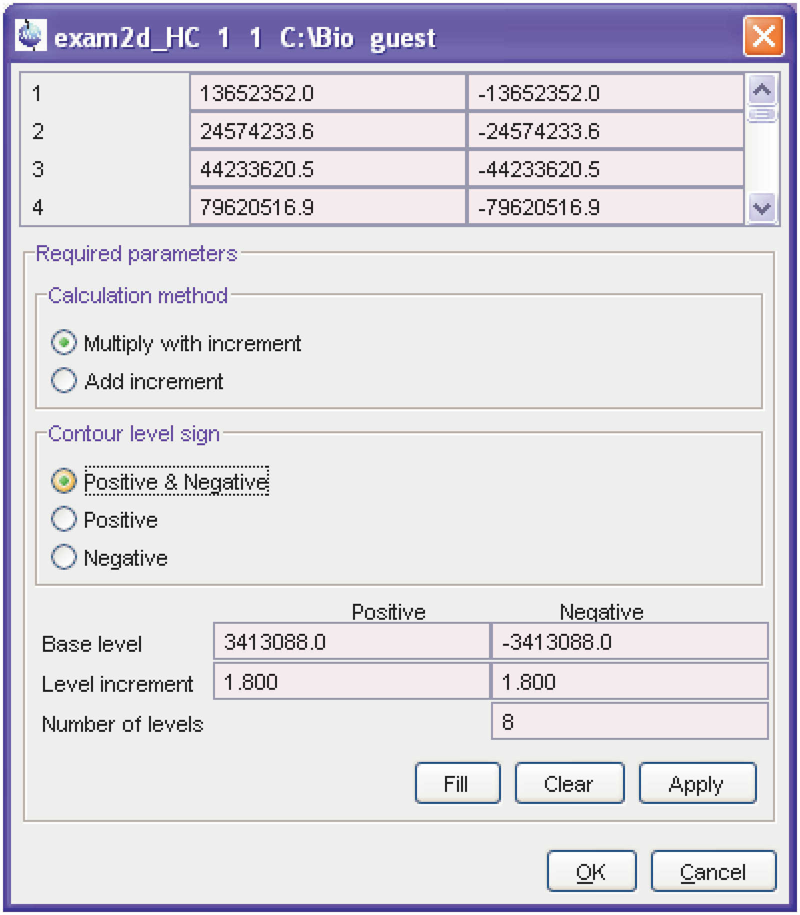
edlev

NAME

edlev - Edit contour levels (2D,3D)

DESCRIPTION

The command ***edlev*** opens a dialog box in which you can set the contour levels of a 2D dataset (see Figure 7.2).



1	13652352.0	-13652352.0
2	24574233.6	-24574233.6
3	44233620.5	-44233620.5
4	79620516.9	-79620516.9

Required parameters

Calculation method

● Multiply with increment
○ Add increment

Contour level sign

● Positive & Negative
○ Positive
○ Negative

	Positive	Negative
Base level	3413088.0	-3413088.0
Level increment	1.800	1.800
Number of levels		8

Figure 7.2

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 or negative levels, or both.

Note that if you change the intensity interactively, for example with the buttons *2 , /2 or ⬍ , the contour levels are automatically adjusted. Entering ***`edlev`*** will show the adjusted levels and clicking 💾 will save them to disk.

INPUT AND OUTPUT FILES

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

`clevels` - Contour levels

SEE ALSO

.ls, .lt

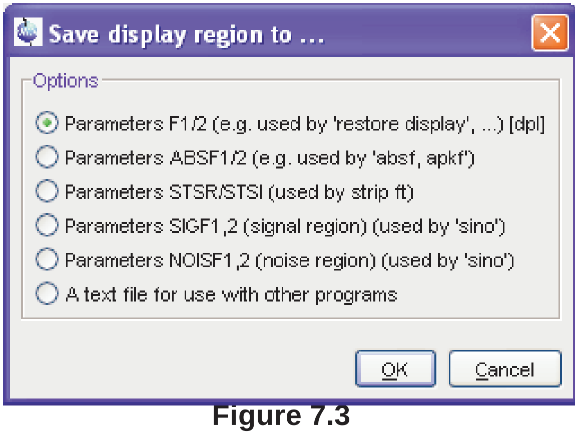
dpl

NAME

dpl - Save the displayed region (1D,2D)

DESCRIPTION

The command ***dpl*** saves the displayed region in the parameters F1P and F2P. The command can also be executed by right-clicking in the data window and selecting ***Save Display Region To...*** This will open the dialog box shown in Figure 7.3. Here select ***Parameters F1/2*** and click ***OK***.



Save display region to ...

Options

● Parameters F1/2 (e.g. used by 'restore display', ...) [dpl]
○ Parameters ABSF1/2 (e.g. used by 'absf, apkf')
○ Parameters STSR/STSI (used by strip ft)
○ Parameters SIGF1,2 (signal region) (used by 'sino')
○ Parameters NOISF1,2 (noise region) (used by 'sino')
○ A text file for use with other programs

Figure 7.3

OUTPUT PARAMETERS

can be viewed with ***edp*** or by typing ***f1p*** or ***f2p*** :
F1P - low field (left) limit of the plot region in ppm
F2P - high field (right) limit of the plot region in ppm

OUTPUT FILES

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

`proc` - plot title

SEE ALSO

plot, prnt, print, autoplot

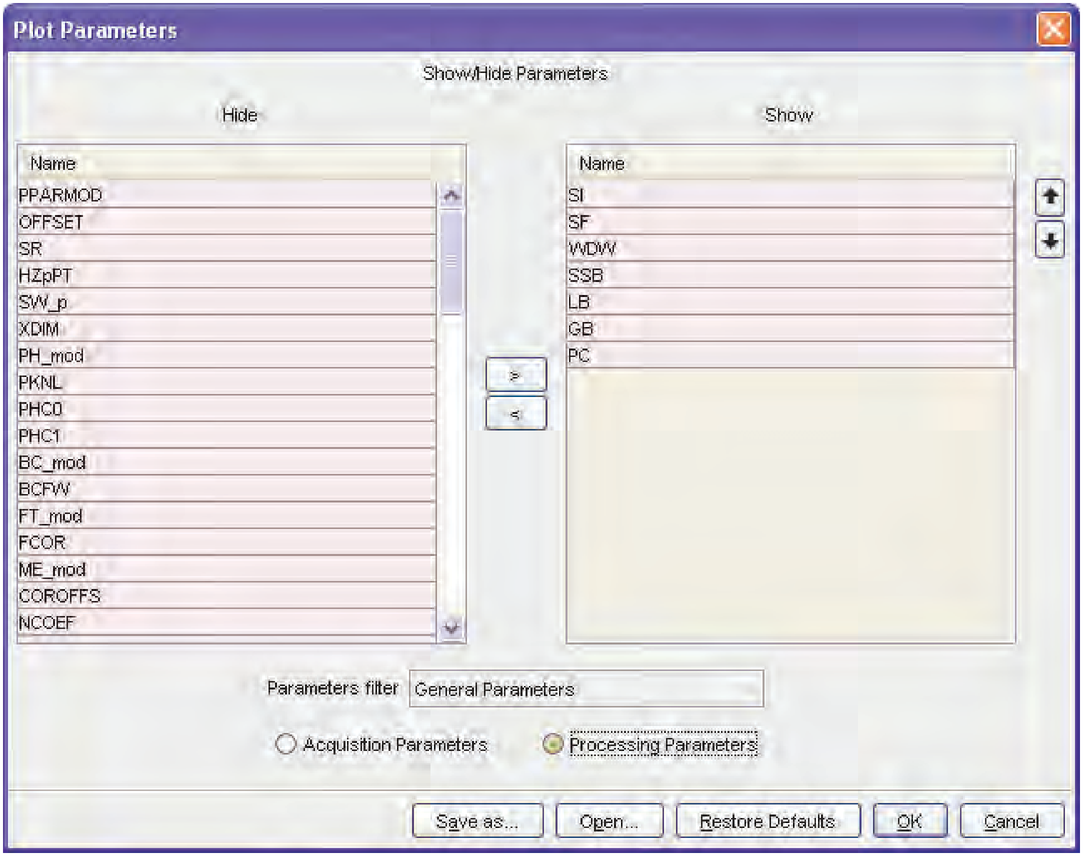
parplot

NAME

parplot - select parameters to appear on the plot (1D,2D)

DESCRIPTION

The command ***`parplot`*** opens a dialog where you can select the acquisition and processing parameters that must appear on the plot (see Figure 7.4).



Name
PPARMOD
OFFSET
SR
HZpPT
SW_p
XDIM
PH_mod
PKNL
PHC0
PHC1
BC_mod
BCFW
FT_mod
FCOR
ME_mod
COROFFS
NCOEF

Name
SI
SF
WDW
SSB
LB
GB
PC

Parameters filter: General Parameters

○ Acquisition Parameters ● Processing Parameters

Figure 7.4

To select the acquisition parameters to be shown on the plot:

1. Enable the radio button ***Acquisition Parameters***

   By default, all acquisition parameters are shown and the *Hide* column is empty.

2. In the *Show* column: select the parameters to be hidden.
3. Click the < button in the center of the dialog.
4. If desired, you can also select experiment specific (***ased***) parameters by selecting the respective ***Parameter filter*** and repeating step 2 and 3.

To select the processing parameters to be shown on the plot:

5. Enable the radio button ***Processing Parameters***

   By default, some processing parameters are shown while most are hidden.

6. In the *Show* column: select the parameters to be hidden.
7. Click the < button in the center of the dialog.
8. In the *Hide* column: select the parameters to be shown.
9. Click the > button in the center of the dialog.

After selecting the acquisition and/or processing parameters:

10. Click ***OK*** to save the selection

The dialog offers the following buttons:

Save as... : save the current selection under a user defined name

Open... : open a user defined selection

Restore Defaults : restore the TOPSPIN default selection

OK : save the current selection

Cancel : Close the dialog

The ***Save as...*** and ***Open*** button allow you to store several selections. Note that these can only be activated from the ***parplot*** dialog by using the ***Open*** and ***OK*** buttons, respectively and then count for all dataset.

Only parameters selected with ***parplot*** will appear on the plot. [1]This counts for both interactive plotting (command ***plot***) and automated plotting (command ***autoplot***).

INPUT AND OUTPUT FILES

<tshome>/exp/stan/nmr/form/acqu.l

`normpl` - acquisition parameters that appear on the plot

<tshome>/exp/stan/nmr/form/proc.l

`normpl` - processing parameters that appear on the plot

<tshome>/exp/stan/nmr/form/

`<name>` - user defined selection of acquisition/processing parameters

INPUT AND OUTPUT FILES

plot, autoplot

[1] On datasets created with TOPSPIN 1.3 or older, first remove the files format.temp in the dataset EXPNO and parm.txt in the dataset PROCNO.

edti

NAME

edti - Set the dataset title (1D,2D,3D)

DESCRIPTION

The command ***edti*** allows you to define the dataset title. Entering this command is equivalent to clicking the ***Title*** tab. Changes in the title will automatically appear in the data window after clicking the ***Spectrum*** or ***Fid*** tab.

The title defined with ***edti*** will also appear on plots created with ***prnt*** or ***autoplot***.

The command ***edti*** replaces the formerly used command ***setti*** which is still available.

INPUT FILES

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

`title` - plot title

OUTPUT FILES

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

`title` - plot title

SEE ALSO

edtix, plot, prnt, print, autoplot

edtix

NAME

edtix - Set the dataset title (1D,2D,3D)

DESCRIPTION

The command ***`edtix`*** allows you to define the dataset title with an external editor. It uses the editor that is defined in the User Preferences. To set this editor:

1. Click ***Options → Preferences*** [**`set`**]
2. Click ***Miscellaneous*** in the left part of the dialog box.
3. Select the *Preferred text editor or* click the respective ***Change*** button to add a new editor.

The title will appear in the data window and on plots created with ***`prnt`*** or ***`autoplot`***.

INPUT FILES

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

`title` - plot title

OUTPUT FILES

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

`title` - plot title

SEE ALSO

edti, plot, prnt, print, autoplot

plot

NAME

plot - Open the Plot Editor (1D,2D)

DESCRIPTION

The command ***plot*** starts the Plot Editor with the current dataset and the layout defined by the processing parameter LAYOUT. The plot limits of all data objects will be the same as in TOPSPIN. The command plot can take various arguments and can be used as follows:

The command ***plot*** can be used with the following arguments:

(no option) Force all data objects to use limits from TOPSPIN

-r Apply *Reset Actions* on all objects after loading the layout

-n Do not change anything after loading the layout

-p `myfile.por` Load the portfolio file `myfile.por`

-i Ignore a `portfolio.por` file found in the data set

The main window of the Plot Editor consists of a drawing area, a menu bar and a toolbar which offers various graphical objects. Here you can display objects like FIDs, one- or two-dimensional NMR spectra, Stacked Plots, parameter lists and titles. You can add integral curves and peak lists to a spectrum, combine several spectra to a stacked plot draw projections around a 2D spectrum.

Furthermore, the Plot Editor offers a set of so-called graphic primitives like lines, text, rectangles and bezier curves. You can place these objects anywhere on the screen and change their appearance . They can be superimposed on NMR-related graphics. All objects can be moved and resized interactively and for each object a range of editing modes is available.

The TOPSPIN command ***autoplot*** allows you to plot a spectrum using a Plot Editor layout.

For a full description, please click:

click ***Help*** → ***Manuals*** → [**Automation and Plotting**] ***TopSpin Plotting***

INPUT PARAMETERS

set with ***edp*** or by typing ***`layout`*** etc.:

LAYOUT - Plot Editor layout
CURPLOT - Default plotter for Plot Editor

INPUT AND OUTPUT FILES

<tshome>/plot/layouts/*.xwp - Bruker library Plot Editor layouts

`portfolio.por` - Plot Editor portfolio (input file is it exists)

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

`layout.xwp` - Plot Editor layout
`last_plot.xwp` - Last stored Plot Editor layout
`portfolio.por` - Plot Editor portfolio

INPUT FILES

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

`1r` - real processed 1D data
`procs` - processing status parameters
`intrng` - integral regions
`parm.txt` - ascii file containing parameters which appear on the plot
`title` - default title file
`outd` - output device parameters

For a 2D dataset, the files `2rr`, `proc2s` and `clevels` are also input.

SEE ALSO

print, prnt, autoplot

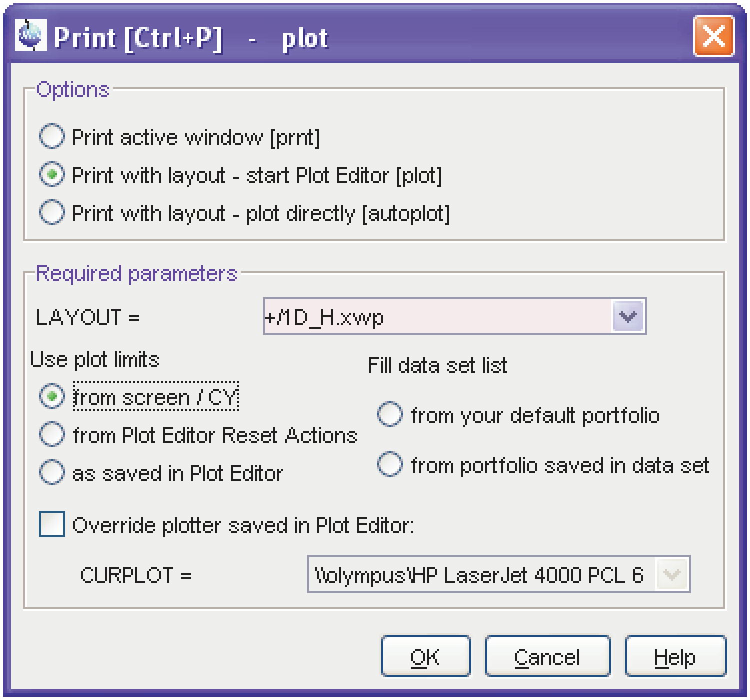
print

NAME

print - Open print dialog box (1D,2D,3D)

DESCRIPTION

The command ***print*** opens the following dialog box



Print [Ctrl+P] - plot

Options

○ Print active window [prnt]

● Print with layout - start Plot Editor [plot]

○ Print with layout - plot directly [autoplot]

Required parameters

LAYOUT = +/1D_H.xwp

Use plot limits

● from screen / CY

○ from Plot Editor Reset Actions

○ as saved in Plot Editor

Fill data set list

○ from your default portfolio

○ from portfolio saved in data set

□ Override plotter saved in Plot Editor:

CURPLOT = \\olympus\HP LaserJet 4000 PCL 6

Figure 7.5

Here, you can choose from three print options:

- *Print active window* [`prnt`]
  The data window is printed as it is displayed on the screen. Before printing starts, the operating system print dialog box will appear where you can, for example, select the printer and printer properties.

- ***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

Override Plotter saved in Plot Editor

If enabled, the plotter defined in the Plot Editor layout will be overridden by the plotter defined by the processing parameter CURPLOT.

For each Option/Required Parameter combination, the corresponding command line command is shown in the title bar of the dialog box. In the example above this is the command ***`plot -f`***.

INPUT FILES

see the description of ***`prnt`***, ***`plot`*** and ***`autoplot`***

SEE ALSO

prnt, plot, autoplot

prnt

NAME

prnt - Print the current dataset (1D,2D,3D)

DESCRIPTION

The command ***`prnt`*** prints the current dataset as it is shown on the screen. Before printing starts, the operating system print dialog box will appear. Here you can, for example, select the printer and printer properties.

SEE ALSO

print, plot, autoplot

savelogs

NAME

savelogs - Save logfiles

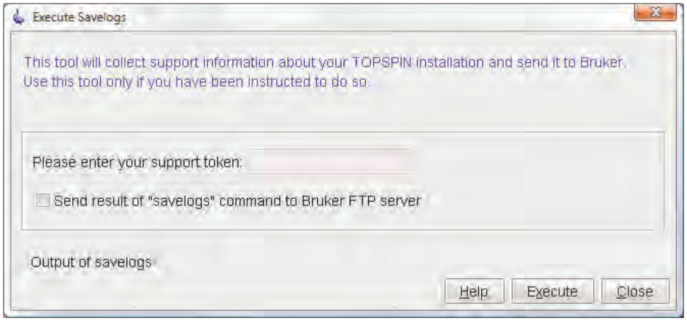
DESCRIPTION

The command ***savelogs*** collects important support information about the userspecific TopSpin installation and saves them on user-pc or on the Bruker FTP-server in a zipped ***tar-file*** (.tar.gz).

Please note only to use the automatic ftp-upload function if you have been instructed by Bruker to do so.If it is insturcted by Bruker NMR Software Support the logfiles can be loaded up automatically to the Bruker FTP-server, but only if the user assertively affirms.

This tool is also available in the menu bar:

- Click ***Options*** → ***Administration*** → ***Execution protocols***
- Click ***Execute savelogs***
- The following window will appear:



This tool will collect support information about your TOPSPIN installation and send it to Bruker.
Use this tool only if you have been instructed to do so.

Please enter your support token:

□ Send result of "savelogs" command to Bruker FTP server

Output of savelogs

Figure 7.6

The recommended token will be told by Bruker support.

If the possibility "Send the result of "savelogs" command to Bruker FTP server is not chosen, the collected logfiles will be saved on user-PC.

- Click ***execute*** to save the output files.
- The output files and information about the ftp-upload (if selected) will be shown in the same window below the line "Output of savelogs". (See Figure 7.6)
- Please note that if ftp-upload doesn’t work the "tar.gz"-file can be send manually to Bruker NMR Software Support under the following address: *nmr-software-support@bruker.de*

If you cannot start TopSpin, but want and are instructed by Bruker NMR Software Support to transfer your log-data to Bruker FTP server, do the following:

Under Windows:

- Click the ***Bruker Utilities****<****topspin version****>* icon on your desktop. An Explorer will be opened.
- Double-click ***Miscellaneous***
- Execute the script ***savelogs***

Under Linux:

- Open a shell.
- Type ***savelogs***

INPUT FILES

User-specific installation files like history files etc. named:

<tshome>/prog/curdir/<user>/*

OUTPUT FILES

- Windows XP:
  <userhome>\AppData\Local Settings\Temp\
  TopSpinSupportFiles_<Support-Token><operating-system-user><year><month><day><hour><minute>.tar.gz
- Windows Vista:
  <userhome>\AppData\Local\Temp\
  TopSpinSupportFiles_<Support-Token><operating-system-user><year><month><day><hour><minute>.tar.gz

- Linux: tmp\TopSpinSupportFiles_<Support-Token>_<operating-system-user><year><month><day><hour><minute>\.tar.gz

SEE ALSO

hist

Chapter 8

Analysis commands

This chapter describes TOPSPIN analysis commands for 1D, 2D and 3D data. Although they do not really process (manipulate) the data, they are part of the processing part of TOPSPIN. Some of them merely interpret the data and display their output, i.e. they do not change the dataset in any way. Others change parameters (like ***sref*** and ***sino***) or create new files (like ***edti*** and ***pps***). None of them, however change the processed data.

autolink

NAME

autolink - Automatic backbone assignment

DESCRIPTION

The command ***`autolink`*** analyses the peak information available on a given set of protein spectra and calculates a backbone assignment. For a step-by-step description of Autolink:

Click ***Help*** → ***Manuals*** → [**Analysis and Simulation**] ***Protein resonance Assignment***

Autolink can be started as follows:

Click ***Analysis*** → ***Proteins*** → ***Automatic Backbone Assignment***

SEE ALSO

ft3d

auremol

NAME

auremol - automated protein structure determination

DESCRIPTION

The command ***auremol*** allows automated spectrum evaluation and protein structure determination.

Auremol can be started as follows:

Click Analysis → Proteins → Structure determination with AUREMOL

For a full description of AUREMOL:

Click ***Help → AUREMOL manual*** from the AUREMOL interface.

daisy

NAME

daisy - 1D simulation program

DESCRIPTION

TOPSPIN 2.1 and newer offers the Daisy package for simulating spectra based on chemical shifts and coupling constants. Daisy supports the following input data:

- TOPSPIN multiplet analysis package
- Windaisy
- HAM
- ACD
- Perch

Daisy can be started as follows:
Click Analysis → Structure Analysis → 1D spectrum Simulation [**`daisy`**]

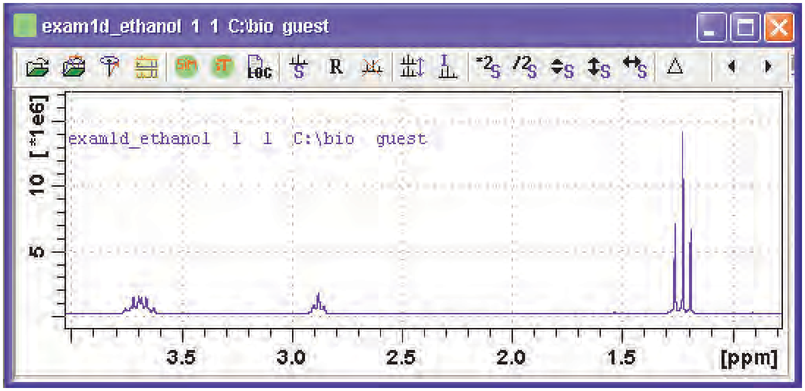


Figure 8.1

For more information on ***`daisy`*** :

click ***Help → Manuals →*** [**Analysis and Simulation**] ***Daisy***

SEE ALSO

daisyguide

daisyguide

NAME

daisyguide - Daisy tutorial

DESCRIPTION

The command ***daisyguide*** opens the Daisy tutorial (see Figure 8.2). This guides you through the Daisy program.

Note that this can also be started with the command daisy.

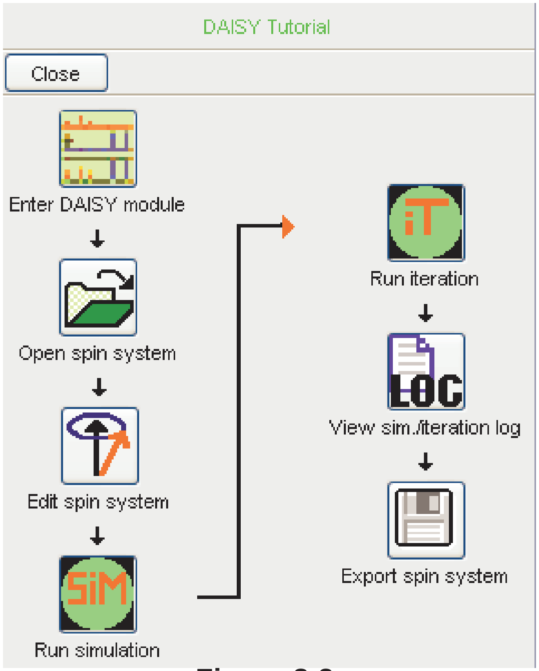


Figure 8.2

For more information on ***daisyguide*** :

click ***Help*** → ***Manuals*** → [**Analysis and Simulation**] ***Daisy***

SEE ALSO

daisy

edstruc

NAME

edstruc - Open the 2D Molecule Structure Editor

DESCRIPTION

The command ***edstruc*** opens the *2D* Molecule Structure Editor. Entering this command is equivalent to clicking the ***Structure*** tab in the 2D data window and the clicking the button ***2D Editor***.

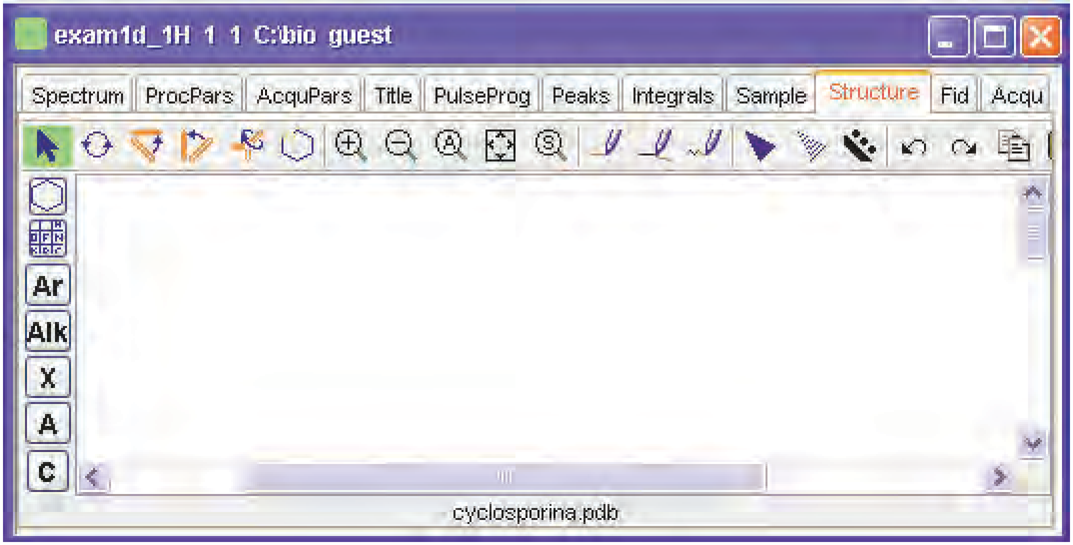


Figure 8.3

A full description of the 2D Structure Editor package can be found under:

Help → ***Manuals*** → [**Analysis and Simulation**] ***Structure Analysis Tools***

SEE ALSO

jmol

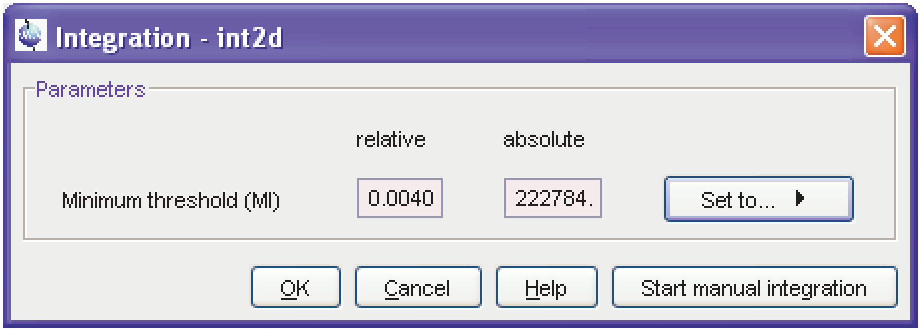
int2d, int3d, int

NAME

int2d - Calculate integrals (2D)
int3d - Calculate integrals (2D)
int - Open integral dialog box (1D,2D,3D)

DESCRIPTION

The command ***int2d*** calculates 2D integrals. It opens the following dialog box:



	relative	absolute
Minimum threshold (MI)	0.0040	222784.

Figure 8.4

Here you can set the minimum threshold for integration. You can enter:

- Enter the relative intensity: value between 0.0 and 1.0
- Enter the absolute intensity: value between 0.0 and YMax_p (processing status parameter).
- Click the ***Set to...*** button and choose from one of the following options:

  lowest contour level - value of the lowest contour level (see ***edlev***)

  value stored in MI - value of the processing parameter MI (see ***edp***)

  most recent MI used - value used by last ***int2d*** command on any dataset

If you enter a relative value, the absolute value is automatically adjusted and vice versa. Setting the ***most recent MI used***, allows you to compare integral value, e.g. of the NOE peak of a series of 2D spectra. Obviously, this only makes sense for spectra that are measured and processing under similar conditions.

The calculated integrals will be marked in the data field and can be listed by clicking the ***Integrals*** tab.

int3d is the same as ***int2d***, except that it works on 3D data.

The ***int*** command can be used on 1D, 2D or 3D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

Figure 8.5 shows a region of peaks after peak picking. Figure 8.6 shows the same region after 2D integration. Here you can see the integral labels and areas. The area color can be set in the user preferences (command ***set***) as *Color of 3rd 1D spectrum*.

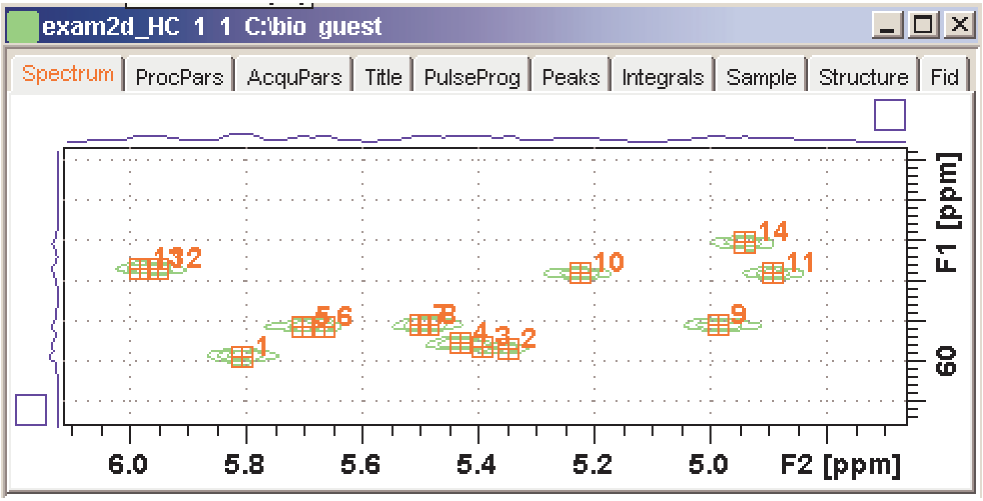


Figure 8.5

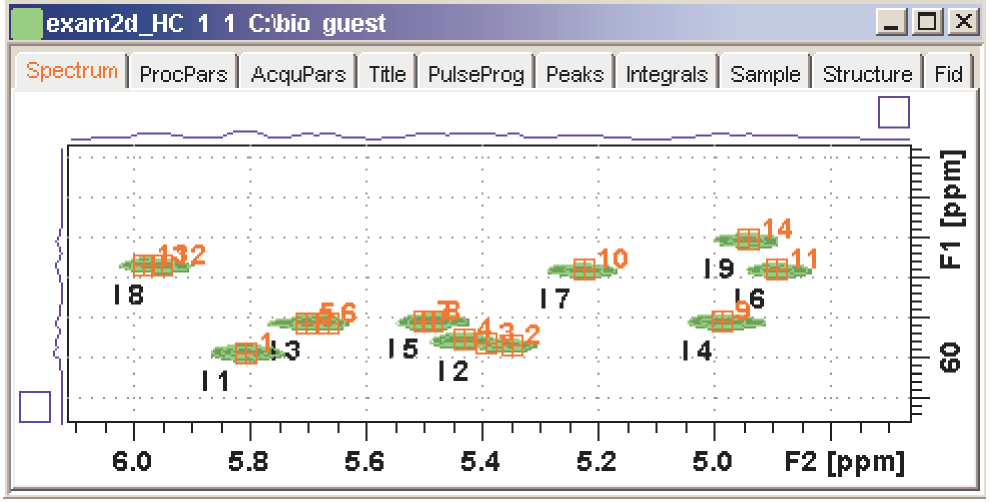


Figure 8.6

INPUT FILES

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

`2rr` - real processed 2D data (input of ***int2d***)
`3rrr` - real processed 3D data (input of ***int3d***)

OUTPUT FILES

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

`integ_points.txt` - data points of integral regions
`integrals.txt` - peaks, integral regions and integral values

SEE ALSO

li

jmol

NAME

jmol - Open the Jmol molecule structure viewer

DESCRIPTION

The command ***jmol*** opens the *Jmol* molecule structure editor. TOPSPIN 1.3 and newer contains Jmol version 10.

A description of the Jmol Molecule Viewer can be found under the Jmol ***Help*** menu, submenu ***User Guide***.

INPUT PARAMETERS

set by the user with ***eda*** or by typing ***chemstr*** :

CHEMSTR - molecule structure filename

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`<name>` - molecule structure file

`acqu` - TOPSPIN acquisition parameters

<tshome>/classes/prop/StructureSamples/* - molecule structure files

SEE ALSO

edstruc

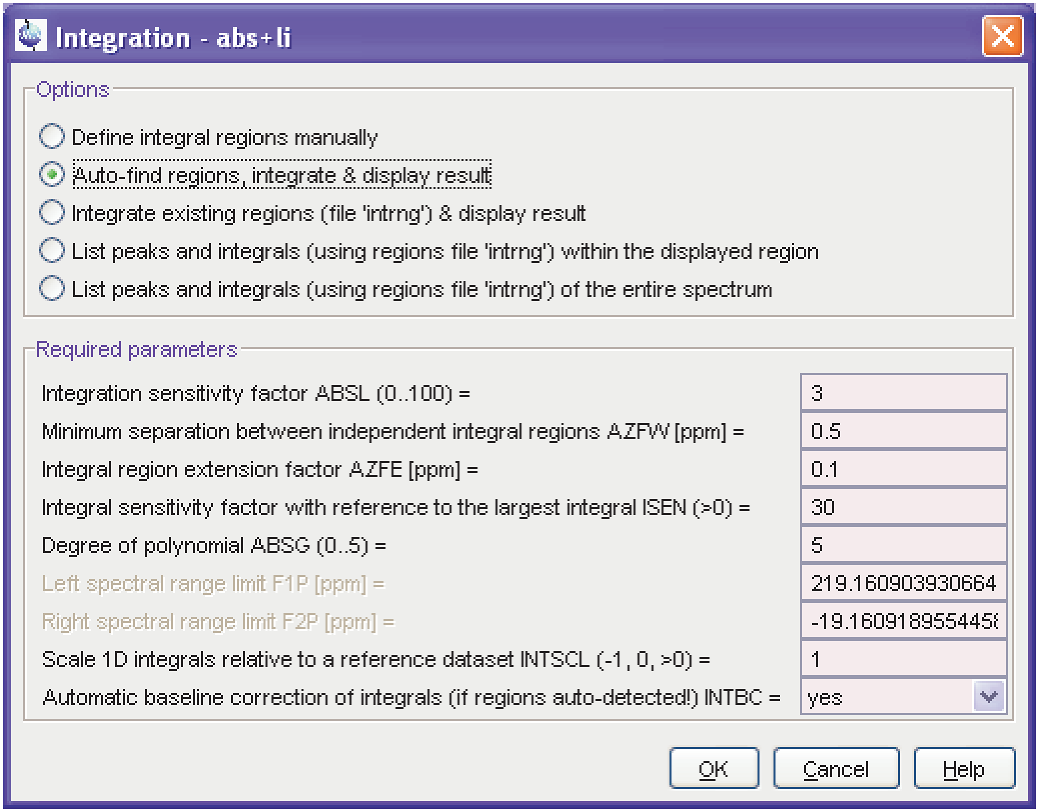
li, lipp, lippf, int

NAME

li - List integrals (1D)
lipp - List integrals and peaks within F1P-F2P (1D)
lippf - List integrals and peaks of the full spectrum (1D)
int - Open integral dialog box (1D,2D,3D)

DESCRIPTION

Integral commands can be started from the command line or from the integration dialog box (see Figure 8.7). The later is opened with the com-



Integration - abs+li

Options

○ Define integral regions manually
● Auto-find regions, integrate & display result
○ Integrate existing regions (file 'intrng') & display result
○ List peaks and integrals (using regions file 'intrng') within the displayed region
○ List peaks and integrals (using regions file 'intrng') of the entire spectrum

Required parameters

Integration sensitivity factor ABSL (0..100) =	3
Minimum separation between independent integral regions AZFW [ppm] =	0.5
Integral region extension factor AZFE [ppm] =	0.1
Integral sensitivity factor with reference to the largest integral ISEN (>0) =	30
Degree of polynomial ABSG (0..5) =	5
Left spectral range limit F1P [ppm] =	219.160903930664
Right spectral range limit F2P [ppm] =	-19.160918955445
Scale 1D integrals relative to a reference dataset INTSCL (-1, 0, >0) =	1
Automatic baseline correction of integrals (if regions auto-detected!) INTBC =	yes

Figure 8.7

mand ***int***

This dialog box has several options, each of which selects a certain command for execution.

Auto-find regions, integrate & display results

> This option executes the command sequence ***abs*** - ***li***. The command ***abs*** determines the integral regions creating the 'intrng' file. The command ***li*** calculates the integral value for each integral region and shows the result in on the screen.

Integrate existing regions and display results

> This option executes the command ***li***. This command calculates the integral value for each integral region and shows the result in on the screen.

List peaks and integrals within the displayed region

> This option executes the command ***lipp***. It works like ***li***, except that it also performs peak picking and shows a list of integral regions and peaks within the region F1P - F2P.

List peaks and integrals of the entire spectrum

> This option executes the command ***lippf***. It works like ***lipp***, except that it only determines the integrals and peaks over the entire spectrum.

The ***li**** commands evaluates the parameter INTSCL if the regions have been determined interactively. For $INTSCL \neq -1$, the current dataset is defined as reference dataset for integral scaling. For $INTSCL = -1$, the integrals of the current dataset are scaled relative to the reference dataset. As such, you can compare the areas of peaks in a series of experiments. Furthermore, the parameter INTBC is evaluated. For INTBC = yes, an automatic baseline correction (slope and bias) of the integrals is performed. This, however, is only done when the integral regions were determined with ***abs***, not if they were determined interactively.

The ***int*** command can be used on 1D, 2D or 3D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set with ***edp***, from the ***int*** dialog box or by typing ***intscl***, ***intbc*** etc.:

INTSCL - scale 1D integrals relative to a reference dataset
INTBC - automatic baseline correction of integrals created by ***abs***
F1P - low field (left) limit of the plot region in ppm (input for ***lipp***)
F2P - high field (right) limit of the plot region in ppm (input for ***lipp***)

INPUT FILES

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

`1r` - real processed 1D data
`intrng` - 1D integral regions (created by ***abs*** or interactive integration)

OUTPUT FILES

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

`integrals.txt` - ascii file containing the output of ***li***
`integrals_lipp.txt` - ascii file containing the output of ***lipp***
`integrals_lippf.txt` - ascii file containing the output of ***lippf***

USAGE IN AU PROGRAMS

LI

LIPP

LIPPF

SEE ALSO

int2d

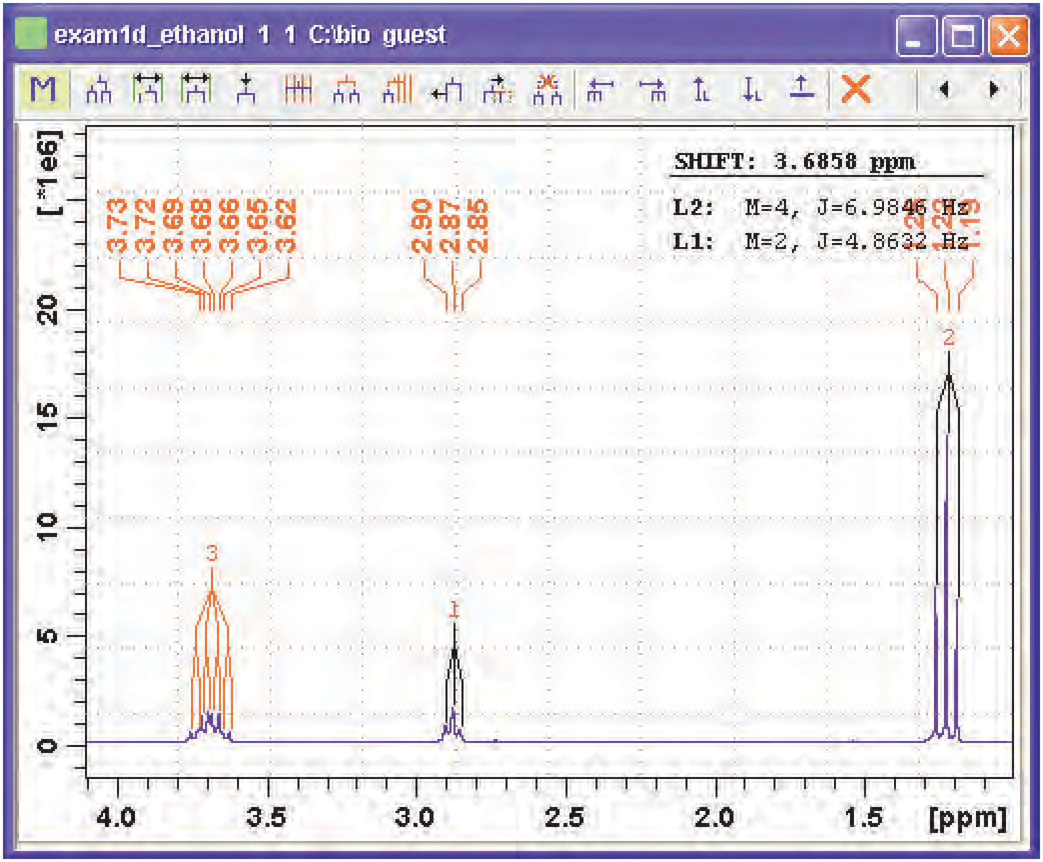
mana

NAME

mana - Switch to multiplet analysis mode (1D)

DESCRIPTION

The command ***mana*** switches to multiple analysis mode (see Figure 8.8).



```
SHIFT: 3.6858 ppm
L2:   M=4, J=6.9846 Hz
L1:   M=2, J=4.8632 Hz
```

Figure 8.8

It can be started as follows:

Click ***Analysis*** → ***Structure Analysis*** → ***Multiplet Definition***.

or from the command line or opened from the Multiplet Analysis Guide (command ***`managuide`***):

A full description of the Multiplet Analysis package can be found under:

Help → ***Manuals*** → [**Analysis and Simulation**] ***Structure Analysis Tools***

SEE ALSO

managuide

managuide

NAME

managuide - Open the Multiplet Analysis Guide (1D)

DESCRIPTION

The command ***managuide*** opens the Multiplet Analysis Guide which guides you through the multiplet analysis procedure (see Figure 8.9).

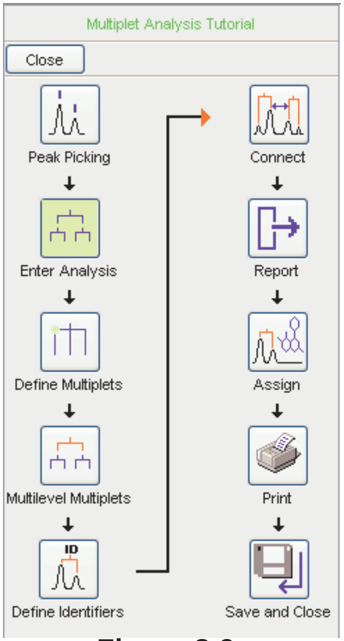


Figure 8.9

A full description of the Multiplet Analysis package can be found under:

Help → ***Manuals*** → [**Analysis and Simulation**] ***Structure Analysis Tools***

SEE ALSO

mana

pps, ppf, ppl, pph, ppj, pp

NAME

pps - Perform peak picking on displayed region
ppf - Perform peak picking on full spectrum
ppl - Perform peak picking in predefined regions
pph - Perform peak picking and also show an intensity histogram
ppj - Perform peak picking and store peaks in JCAMP-DX format
pp - Open the peak picking dialog box

DESCRIPTION

Peak picking commands can be started from the command line or from the peak picking dialog box (see Figure 8.10).

All peak picking commands open the dialog box with the corresponding option selected. The command ***pp***, however, selects the last used option.

Auto-Pick peaks on displayed spectrum region

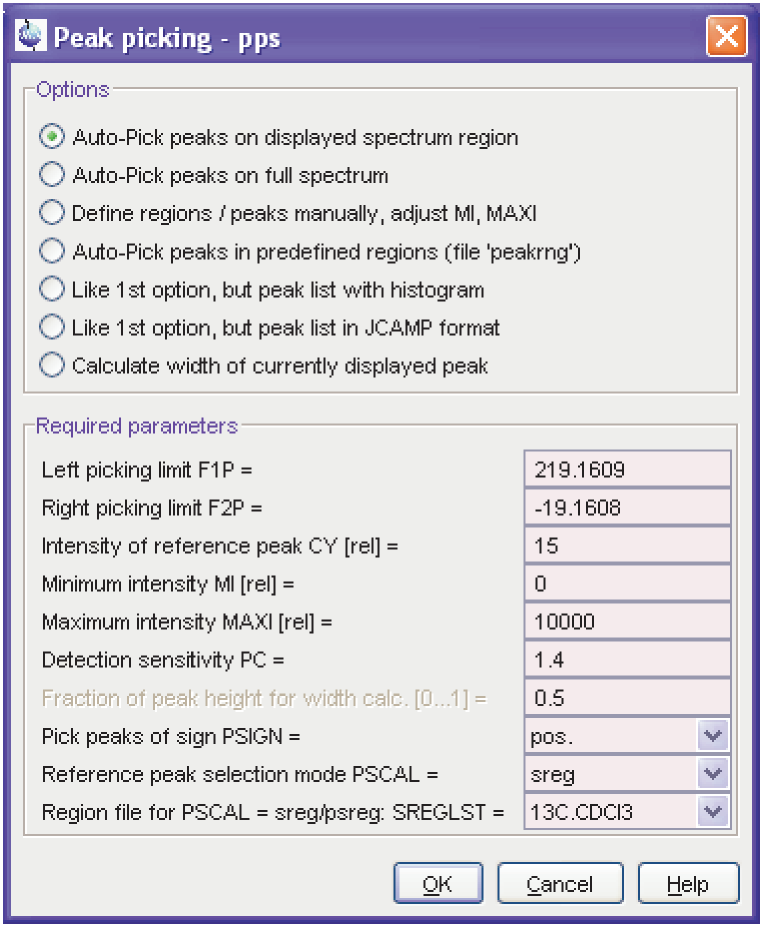
This option selects the command ***pps*** for execution. It determines all peaks within the displayed region. Table 8.1 shows an example of its output.

#	ADDRES S	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	648.7	3698.825	7.3995	0.17
2	658.4	3687.649	7.3771	0.21

Table 8.1

The peak list is created according to several criteria which are determined by various parameters. A data point is added to the peak list if:

- its intensity is higher than its two neighbouring points
- its relative intensity is smaller than MAXI
- its relative intensity is larger than MI



Peak picking - pps

Options

● Auto-Pick peaks on displayed spectrum region

○ Auto-Pick peaks on full spectrum

○ Define regions / peaks manually, adjust MI, MAXI

○ Auto-Pick peaks in predefined regions (file 'peakrng')

○ Like 1st option, but peak list with histogram

○ Like 1st option, but peak list in JCAMP format

○ Calculate width of currently displayed peak

Required parameters

Left picking limit F1P =	219.1609
Right picking limit F2P =	-19.1608
Intensity of reference peak CY [rel] =	15
Minimum intensity MI [rel] =	0
Maximum intensity MAXI [rel] =	10000
Detection sensitivity PC =	1.4
Fraction of peak height for width calc. [0...1] =	0.5
Pick peaks of sign PSIGN =	pos.
Reference peak selection mode PSCAL =	sreg
Region file for PSCAL = sreg/psreg: SREGLST =	13C.CDCl3

Figure 8.10

- its absolute intensity is larger than PC*noise
- it lies within the displayed region as expressed by F2P and F1P

where MAXI, MI and PC are processing parameters and noise is calculated from the first 32th part of the spectrum.

The values of MI and MAXI must be chosen in relation to the plot parameter CY; the intensity (in cm) of the reference peak. The reference peak is the highest peak in the spectrum or in a certain part of it. The spectral region which contains reference peak, is determined by the parameter PSCAL. For PSCAL = global, this is entire spectrum. Table 8.2 shows all possible values of PSCAL and the corresponding regions. For PSCAL = ireg or pireg, the `reg` file is interpreted. To create a `reg` file click ∫ to switch to integration mode, click 💾 and select ***Save regions to 'reg'***. The `reg` file can be viewed or edited with the command ***`edmisc reg`***.

PSCAL	Peak used as reference for vertical scaling
global	The highest peak of the entire spectrum.
preg	The highest peak within the plot region.
ireg	The highest peak within the regions specified in the `reg` file. If it does not exist, *global* is used.
pireg	as *ireg*, but the peak must also lie within the plot region.
sreg	The highest peak in the regions specified in scaling region file. This file is specified by the parameter SREGLST. If SREGLST is not set or it specifies a file which does not exist, *global* is used.
psreg	as *sreg* but the peak must also lie within the plot region.
noise	The intensity height of the noise of the spectrum.

Table 8.2

For PSCAL = sreg or psreg, the scaling region file is interpreted. This is used to make sure the solvent peak is not used as reference. The name of a scaling region file is typically of the form NUCLEUS.SOLVENT, e.g. 1H.CDCl3. For most common nucleus/solvent combinations, a scaling region file is delivered with TOPSPIN. They can be viewed or edited with ***`edlist scl`***. In several 1D standard parameter sets which are used during automation, PSCAL is set to *sreg* and SREGLIST to NUCLEUS.SOLVENT as defined by the parameters NUCLEUS and SOLVENT.

`pps` evaluates the parameter PSIGN which can take three possible value:

- pos - only positive peaks appear in the list
- neg - only negative peaks appear in the list
- both - both positive and negative peaks appear in the list

Auto-Pick peaks on full spectrum

This option selects the command ***ppf*** for execution. It works like ***pps*** except that it picks peaks on the full spectrum.

Auto-Pick peaks in predefined regions (file 'peakrng')

This option selects the command ***ppl*** for execution. It pick the peaks in predefined regions. To define those regions:

- click ***Define regions/peaks manually*** in the peaks dialog box or click the button in the toolbar to switch to peak picking mode
- click the button and drag the cursor inside the data window to defined the regions
- right-click inside the data window and select ***Pick Peaks on ranges*** or enter ***ppl*** on the command line

Like 1st option but peak list with histogram

This option selects the command ***pph*** for execution. It works like ***pps***, except that it also shows an intensity histogram. This allows you to get a quick overview over the intensity distribution.

Like 1st option but peak in JCAMP format

This option selects the command ***ppj*** for execution. It works like ***pps***, except that the peak list is stored in JCAMP-DX format in the file `pp.dx`. This file resides in the processed data directory and can be used for external programs which require JCAMP peak lists. As the file created by ***tojdx*** it contains the acquisition and processing parameters but instead of data points it contains a list of peaks. The

##NPOINTS= 4	
##PEAK TABLE= (XY..XY)	
2.3241	1.58
2.2962	1.18
1.9943	10.00
1.8725	1.36

Table 8.3

last part of the file `pp.dx` looks like:

The ***pp*** command can be used on 1D, 2D or 3D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

For compatibility reasons,

INPUT PARAMETERS

set by the user with ***edp*** or by typing ***mi***, ***maxi*** etc.:

MI - minimum relative intensity (cm)
MAXI - maximum relative intensity (cm)
PC - peak picking sensitivity
PSIGN - peak sign (pos, neg, or both)
PSCAL - determines the region with the reference peak for vertical scaling
SREGLST - name of the scaling region file used for PSCAL = sreg/psreg
ASSFAC - assign the highest or second highest peak as reference for scaling
ASSWID - region excluded from second highest peak search

set by the user with ***edp*** or by typing ***f1p***, ***f2p*** etc.:

F1P - low field (left) limit of the plot region in ppm
F2P - high field (right) limit of the plot region in ppm

INPUT FILES

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

`1r` - real processed 1D data
`proc` - processing parameters
`reg` - region with the reference peak for PSCAL = *ireg* or *pireg*

<tshome>/exp/stan/nmr/lists/scl/

`<SREGLST>` - regions containing the reference peak if PSCAL = *sreg*/*psreg*

OUTPUT FILES

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

`peaks` - peak list containing all peaks in the entire spectrum
`peaklist.xml` - peak list created by ***pp*** and ***pps*** for the Plot Editor (TOPSPIN 2.1 and newer)
`peak.txt` - peak list created by ***pp*** and ***pps*** (TOPSPIN 2.0 and older) or by ***convertpeaklist*** (TOPSPIN 2.1 and newer)
`peakhist.txt` - peak list with histogram, created by ***pph***
`pp.dx` - peak list in JCAMP-DX format created by ***ppj***

USAGE IN AU PROGRAMS

PP

PPL

PPH

PPJ

SEE ALSO

peakw, ppp, lipp, lippf

ppd

NAME

ppd - Perform peak picking with derivative-based algorithm

DESCRIPTION

The command ***ppd*** performs.It can be usefull to pick peak shoulders which are not found by other peak picking commands.

INPUT FILES

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

`1r` - real processed 1D data
`proc` - processing parameters

OUTPUT FILES

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

`peaklist.xml` - peak list created for the Plot Editor

SEE ALSO

pps, ppf, ppl, pph, ppj, pp

pp2d, pp

NAME

pp2d - Perform peak picking (2D)
pp - Open peak picking control dialog (1D,2D,3D)

DESCRIPTION

2D peak picking can be started from the command line or from the peak picking dialog box. The latter can be opened with the command ***pp*** (see Figure 8.11).

In this dialog window, you can set the following options:

- **Append peaks to list**
  When it is checked, the found peaks are appended to a possibly existing list. When it is unchecked, a new list is created [***pp2d append***]
- **Discard new peak(s) if already in list**
  Check this option to avoid duplicate peaks [***pp2d noduplicates***]
- **Export results as XwinNmr peak list**
  In addition to TOPSPIN XML format, the result is also stored in XWIN-NMR format (file `peak.txt`) [***pp2d txt***]. This file is typically used with XWIN-NMR AU programs.

Furthermore, you can set the following peak picking parameters:

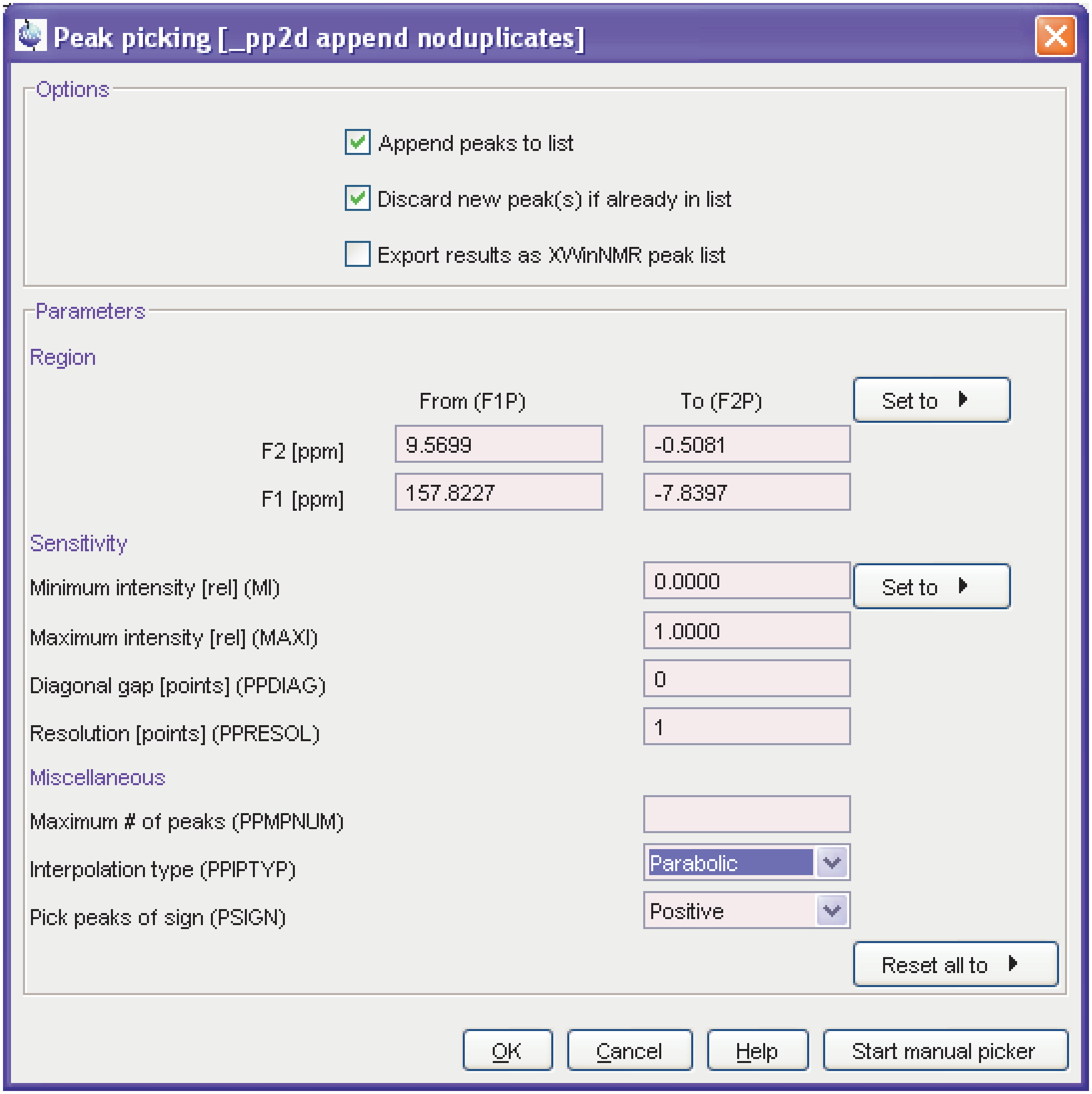
Region parameters

Here you can set the region limits for both the F2 and F1 direction. Only peaks within this region will be picked. Note that the limits can be specified in the text fields or set with the button ***Set to***. The latter allows you to select from:

Full range - full spectrum

Displayed range - range displayed in the data window

Range defined by stored parameters - range stored in parameters F1P/F2P [1]



Peak picking [_pp2d append noduplicates]

Options

☑ Append peaks to list

☑ Discard new peak(s) if already in list

☐ Export results as XWinNMR peak list

Parameters

Region

	From (F1P)	To (F2P)
F2 [ppm]	9.5699	-0.5081
F1 [ppm]	157.8227	-7.8397

Sensitivity

Minimum intensity [rel] (MI)	0.0000
Maximum intensity [rel] (MAXI)	1.0000
Diagonal gap [points] (PPDIAG)	0
Resolution [points] (PPRESOL)	1

Miscellaneous

Maximum # of peaks (PPMPNUM)	
Interpolation type (PPIPTYP)	Parabolic
Pick peaks of sign (PSIGN)	Positive

Figure 8.11

Most recent range stored in peak list - range on which last automatic

[1] To store displayed region: right-click in the data window and select ***Save display region to***

peak picking was done [1].

Sensitivity parameters

Here you can set the peak picking parameters MI and MAXI which are also used for 1D peak picking. Note that MI can also be set interactively with the button ***Set to***, to *the lowest contour level*, *the current value of MI* or *the most recent value stored in the peak list*. Furthermore, you can set the parameters:

PPDIAG - diagonal gap; minimum distance between picked peaks and diagonal signals. Mainly used for homonuclear spectra.

PPRESOL - peak picking resolution

Miscellaneous parameters

Here you can set the following parameters:

PPMPNUM - Maximum number of picked peaks. Note that 0 or no value specified means unlimited.

PPIPTYP - Peak picking interpolation type (parabolic or none).

PSIGN - The sign of the picked peaks (positive, negative or both).

To start peak picking:

Click ***OK***

The peak picking progress will be shown in the TOPSPIN status line. When the peak picking process has finished:

- The number of found peaks is displayed in the status line. Note that if the option ***Append peaks to list*** is checked, only additional peaks are reported as found.
- The peaks and parameters are stored in the processing directory.

To view the peak list, click the ***Peaks*** tab of the data window toolbar.

The peak picking dialog window has two extra buttons:

Reset all to

allows you to reset all parameters to the stored parameters or to the

[1] Only active when peak picking was already done.

most recent values stored in the peak list. Note that the stored parameters and the parameters in the peak list can be different since parameters can also be set with ***edp*** or from the command line. However, right after peak picking they are the same.

Start manual picker

To switch to interactive peak picking mode (equivalent to clicking the button in the TOPSPIN upper toolbar).

The options specified in square brackets in the dialog window and further options can also be specified on the command line. For example:

pp append
open peak picking dialog with the **Append..** option checked.

pp noduplicates
open peak picking dialog with the **Discard new peaks..** option checked.

pp silent
perform peak picking on the displayed region with the last stored options (no dialog). Equivalent to the command ***pps***.

pp nodia
perform peak picking on the last stored region with the last stored options (no dialog).

pp append noduplicates nodia
perform peak picking on the last stored region with the specified options.

The ***pp*** command can be used on 1D, 2D or 3D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***pp*** dialog box, with ***edp*** or by typing ***f1p***, ***mi*** etc.:

F1P - low field (left) limit of the peak picking region in F2 and F1
F2P - high field (left) limit of the deconvolution region F2 and F1
MI - minimum relative intensity (cm)
MAXI - maximum relative intensity (cm)

PC - peak picking sensitivity
PPDIAG - diagonal gap; minimum distance to spectrum diagonal
PPRESOL - peak picking resolution
PPMPNUM - maximum number of picked peaks
PPIPTYP - interpolation type
PSIGN - peak sign (pos, neg, or both)

INPUT FILES

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

`2rr` - real processed 2D data
`proc` - F2 processing parameters, including peak picking parameters

OUTPUT FILES

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

`procs` - F2 processing parameters, including peak picking parameters
`peaklist.xml` - 2D peak list in XML format
`peak.txt` - 2D peak list in TXT format

<userhome>/<.topspin-hostname/prop/

`globals.prop` - peak picking setup

USAGE IN AU PROGRAMS

PP2D

SEE ALSO

pp3d, pps, ppl, pph, ppj

pp3d, pp

NAME

pp3d - Perform peak picking (3D)
pp - Open peak picking control dialog (1D,2D,3D)

DESCRIPTION

3D peak picking can be started from the command line or from the peak picking dialog box. The latter can be opened with the command ***pp*** (see Figure 8.12).

In this dialog window, you can set the following options:

- **Append peaks to list**
  When it is checked, the found peaks are appended to a possibly existing list. When it is unchecked, a new list is created [***pp3d append***]
- **Discard new peak(s) if already in list**
  Check this option to avoid duplicate peaks [***pp3d noduplicates***]
- **Export results as XwinNmr peak list**
  In addition to TOPSPIN XML format, the result is also stored in XWIN-NMR format (file `peak.txt`) [***pp3d txt***]. This file is typically used with XWIN-NMR AU programs.

Furthermore, you can set the following peak picking parameters:

Region parameters

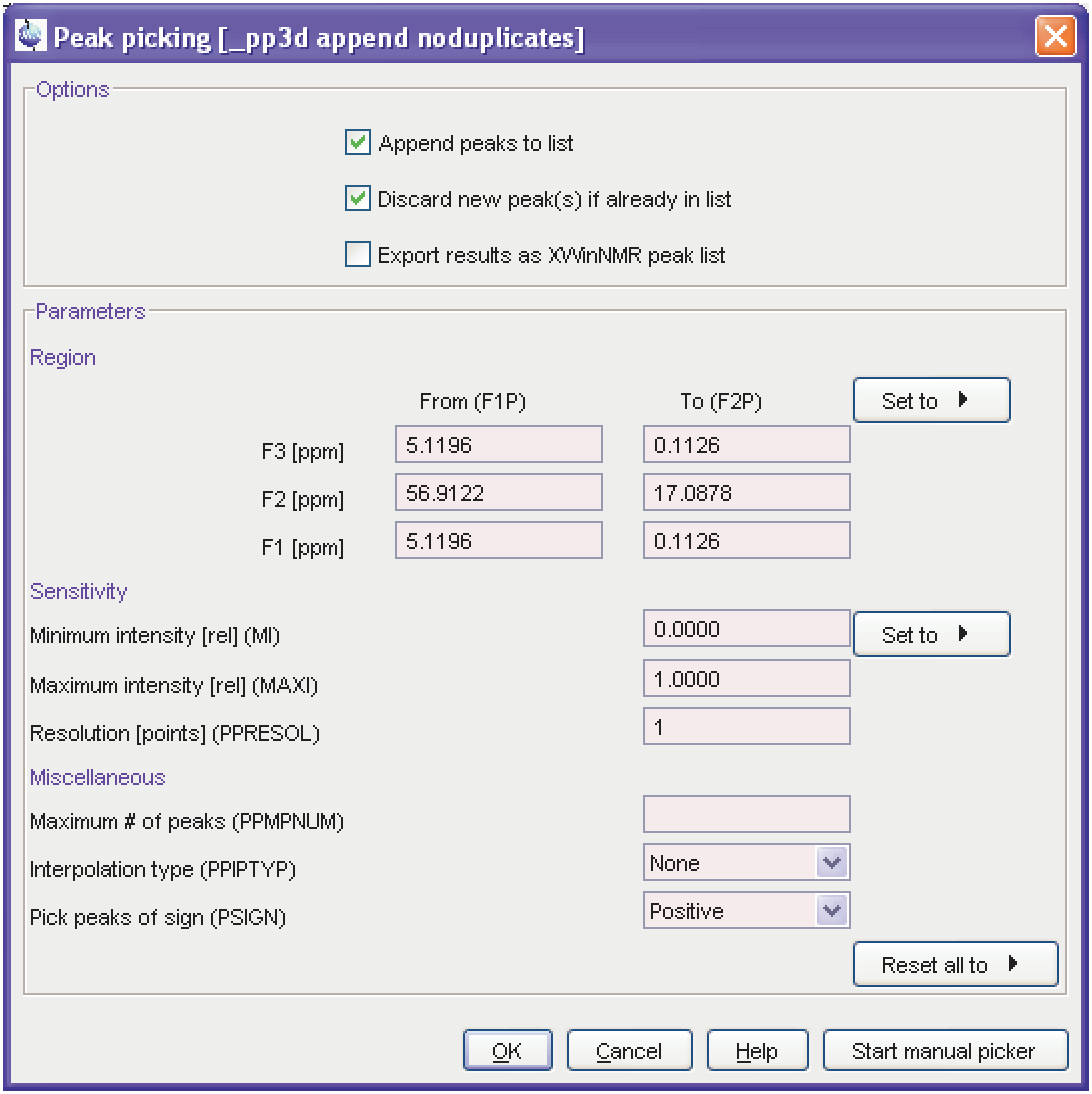
Here you can set the region limits for the F3, F2 and F1 direction. Only peaks within this region will be picked. Note that the limits can be specified in the text fields or set with the button ***Set to*** to:

Full range - full spectrum

Displayed range - range displayed in the data window

Range defined by stored parameters - range stored in parameters F1P/F2P [1]

Most recent range stored in peak list - range on which last automatic



Peak picking [_pp3d append noduplicates]

Options

☑ Append peaks to list

☑ Discard new peak(s) if already in list

☐ Export results as XWinNMR peak list

Parameters

Region

	From (F1P)	To (F2P)
F3 [ppm]	5.1196	0.1126
F2 [ppm]	56.9122	17.0878
F1 [ppm]	5.1196	0.1126

Sensitivity

Minimum intensity [rel] (MI)	0.0000
Maximum intensity [rel] (MAXI)	1.0000
Resolution [points] (PPRESOL)	1

Miscellaneous

Maximum # of peaks (PPMPNUM)	
Interpolation type (PPIPTYP)	None
Pick peaks of sign (PSIGN)	Positive

Figure 8.12

peak picking was done [1].

[1] To store displayed region: right-click in the data window and select ***Save display region to***

[1] Only active when peak picking was already done.

Sensitivity parameters

Here you can set the peak picking parameters MI and MAXI, which are also used for 1D peak picking. Note that MI can also be set interactively with the button ***Set to***, to the current value of MI or the lowest contour level. Furthermore, the parameter PPRESOL for peak picking resolution can be set.

Miscellaneous parameters

Here you can set the following parameters:

PPMPNUM - Maximum number of picked peaks. Note that 0 or no value specified means unlimited.

PPIPTYP - Peak picking interpolation type (parabolic or none).

PSIGN - The sign of the picked peaks (positive, negative or both).

To start peak picking:

Click ***OK***

The peak picking progress will be shown in the TOPSPIN status line. When the peak picking process has finished:

- The number of found peaks is displayed in the status line. Note that if the option ***Append peaks to list*** is checked, only additional peaks are reported as found.
- The peaks and parameters are stored in the processing directory.

To view the peak list, click the ***Peaks*** tab of the data window toolbar.

The peak picking dialog window has two extra buttons:

Reset all to

allows you to reset all parameters to the stored parameters or to the most recent values stored in the peak list. Note that the stored parameters and the parameters in the peak list can be different since parameters can also be set with ***edp*** or from the command line. However, right after peak picking they are the same.

Start manual picker

To switch to interactive peak [picking mode (equivalent to clicking the button in the TOPSPIN upper toolbar).

The options specified in square brackets in the dialog window and further options can also be specified on the command line. For example:

pp append
open peak picking dialog with the **Append..** option checked.

pp noduplicates
open peak picking dialog with the **Discard new peaks..** option checked.

pp silent
perform peak picking on the displayed region with the last stored options (no dialog). Equivalent to the command ***pps***.

pp nodia
perform peak picking on the last stored region with the last stored options (no dialog).

pp append noduplicates nodia
perform peak picking on the last stored region with the specified options.

The ***pp*** command can be used on 1D, 2D or 3D data. It recognizes the data dimensionality and opens a dialog box with the appropriate options and parameters.

INPUT PARAMETERS

set from the ***pp*** dialog box, with ***edp*** or by typing ***f1p***, ***mi*** etc.:

F1P - low field (left) limit of the peak picking region in F3, F2 and F1
F2P - high field (left) limit of the deconvolution region F3, F2 and F1
MI - minimum relative intensity (cm)
MAXI - maximum relative intensity (cm)
PC - peak picking sensitivity
PPRESOL - peak picking resolution
PPMPNUM - maximum number of picked peaks
PPIPTYP - Interpolation type
PSIGN - peak sign (pos, neg, or both)

INPUT FILES

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

`3rrr` - real processed 3D data
`proc` - F3 processing parameters, including peak picking parameters

OUTPUT FILES

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

`procs` - F3 processing parameters, including peak picking parameters
`peaklist.xml` - 3D peak list in XML format
`peak.txt` - 3D peak list in TXT format

<userhome>/<.topspin-hostname/prop/

`globals.prop` - peak picking setup

SEE ALSO

pp2d, pps, ppl, pph, ppj

solaguide

NAME

solaguide - Open the solids analysis guide (1D)

DESCRIPTION

The command ***solaguide*** opens a dialog box with a workflow for Solids Line Shape Analysis. This procedure is completely described in the TOPSPIN Users Guide. To open this:

click ***Help*** → ***Manuals*** → [**Analysis and Simulation**] ***Structure Analysis Tools***

SEE ALSO

sola

sino

NAME

sino - Calculate signal to noise ratio (1D)

SYNTAX

sino [real] [noprint]

DESCRIPTION

The command ***sino*** calculates the signal to noise ratio of a 1D spectrum according to the formula:

$$SINO = \frac{maxval}{2 \cdot noise}$$

where *maxval* is highest intensity in the signal region. The signal region is determined by the processing parameters SIGF1 and SIGF2. If SIGF1 = SIGF2, the signal region is defined by:

- the entire spectrum minus the first 16th part (if the scaling region file is not defined)
- the regions defined in the scaling region file NUC1.SOLVENT where NUC1 and SOLVENT are acquisition status parameters.

Standard scaling region files can be installed with ***expinstall*** and can be edited with ***edlist scl***.

The factor *noise* is calculated according to the algorithm shown in Figure 8.13.

where N is the total number of points in the noise region, n = (N-1)/2, and y(i) is the nth point in the noise region. The limits of the noise region is determined by the processing parameters NOISF1 and NOISF2. If they are equal, the first 1/16th of the spectrum is used as the noise region.

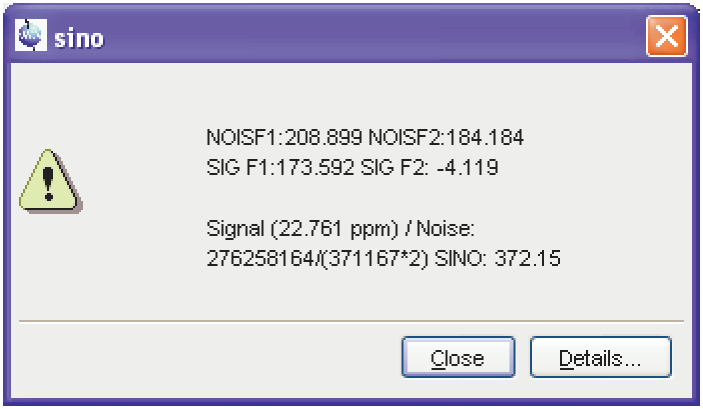
The parameters SIGF1, SIGF2, NOISF1 and NOISF2 can be set from the command line, from the ***Procpars*** tab (command ***edp***) or, interactively, in Signal/Noise display mode. The latter can be entered by clicking ***Analysis* → *Signal/Noise Calculation*** or by entering ***.sino*** on the command line.

$$noise = \sqrt{\frac{\sum_{i=-n}^{n} y(i)^2 - \frac{1}{N}\left(\left(\sum_{i=-n}^{n} y(i)\right)^2 + \frac{3\cdot\left(\sum_{i=1}^{n} i(y(i)-y(-i))\right)^2}{N^2-1}\right)}{N-1}}$$

Figure 8.13

sino internally performs a peak picking to determine the highest peak in the signal region.

The result of ***sino*** appears on the screen, for example:



sino

```
NOISF1:208.899 NOISF2:184.184
SIG F1:173.592 SIG F2: -4.119

Signal (22.761 ppm) / Noise:
276258164/(371167*2) SINO: 372.15
```

Figure 8.14

sino noprint does not show the result on the screen. The *noprint* option is automatically set when ***sino*** is part of an AU program. The result of ***sino*** is also stored in the processing status parameter SINO which can be viewed with ***s sino*** or ***dpp***.

sino real skips the magnitude calculation and works on the real data. Note that ***sino*** without argument first performs a magnitude calculation and then calculates the signal to noise ratio on the magnitude data.

The parameter SINO exists as processing parameter (***edp***) and as processing status parameter (***dpp***) and they have different functions. The latter is used to store the result of the command ***sino*** as discussed above. The former can be used to specify a signal to noise ratio which must be reached in an acquisition (see the parameter SINO in chapter 2.4 and the AU program ***au_zgsino***).

INPUT PARAMETERS

set in ***.sino*** display mode, with ***edp*** or by typing ***noisf1***, ***noisef2*** etc.:

NOISF1 - low field (left) limit of the noise region
NOISF2 - high field (right) limit of the noise region
SIGF1 - low field (left) limit of the signal region
SIGF2 - high field (right) limit of the signal region

set by the acquisition, can be viewed with ***dpa*** or by typing ***s nuc1*** etc.:

NUC1 - observe nucleus
SOLVENT - sample solvent

OUTPUT PARAMETERS

can be viewed with ***dpp*** or by typing ***s sino*** :

SINO - signal to noise ratio

INPUT FILES

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

`1r` - real processed 1D data
`1i` - imaginary processed data (not used for ***sino real***)
`proc` - processing parameters

<tshome>/exp/stan/nmr/lists/scl/

`<NUC1.SOLVENT>` - scaling region file

OUPUT FILES

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

`procs` - processing status parameters

USAGE IN AU PROGRAMS

SINO

SEE ALSO

mc, abs

sola

NAME

sola - Switch to solids lineshape analysis mode

DESCRIPTION

The command ***sola*** switches to solids lineshape analysis mode. This procedure is completely described in the TOPSPIN Users Guide. To open this:

click ***Help*** → ***Manuals*** → [**Analysis and Simulation**] ***Structure Analysis Tools***

SEE ALSO

solaguide

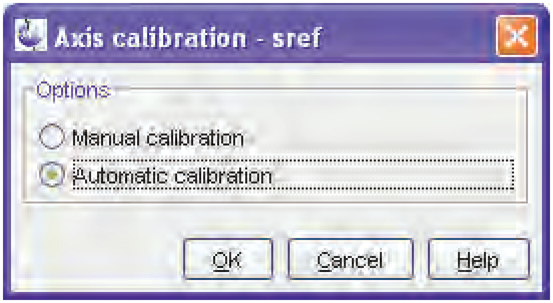
sref, cal

NAME

sref - Calibrate the spectrum; set the TMS signal to 0 ppm (1D,2D)
cal - Open calibration dialog box (1D,2D)

DESCRIPTION

Spectrum calibration can be started from the command line with ***sref*** or from the calibration dialog box which is opened with the ***cal*** command.



Axis calibration - sref

Options

○ Manual calibration

● Automatic calibration

Figure 8.15

This dialog box offers two options, one for manual and one for automatic calibration.

Manual calibration

This option selects the ***.cal*** command for execution. This is equivalent to clicking the button in the toolbar and switches to interactive calibration mode. Click inside the data window at the reference peak, enter the frequency value in the appearing dialog box and click ***OK***.

Automatic calibration

This option selects the ***sref*** command for execution. It calibrates the spectrum by setting the TMS signal of a spectrum to exactly 0 ppm. It works on 1D and 2D spectra.

sref makes use of the lock table. This must be set up once after installing TOPSPIN with the command ***edlock***.

On 1D spectra, ***sref*** involves three steps which are discussed below.

During the first step ***sref*** sets the value of the processing parameter SF according to the formula:

SF=BF1/(1.0+RShift * 1e-6)

where *RShift* is taken from the ***edlock*** table and BF1 is an acquisition status parameter. Changing SF automatically changes the processing parameters SR, the spectral reference, and OFFSET, the ppm value of the first data point, according to the following relations:

SR = SF - BF1

where BF1 is an acquisition status parameter

OFFSET = (SFO1/SF-1) * 1.0e6 + 0.5 * SW * SFO1/SF

where SW and SFO1 are acquisition status parameters

Actually, the relation for OFFSET depends on the acquisition mode. When the acquisition status parameter AQ_mod is *qsim*, *qseq* or *DQD*, which is usually the case, the above relation count. When AQ_mod is *qf*, the relation OFFSET = (SFO1/SF-1) * 1.0e6 is used.

sref then calculates which data point (between 0 and SI) in your spectrum corresponds to the ppm value *Ref*. from the ***edlock*** table. This data point will be used in the second step. The first step is independent of a reference substance.

During the second step, ***sref*** scans a region around the data point found in the first step for a peak. It will normally find the signal of the reference substance. The width of the scanned region is defined by the parameter *Width* in ***edlock*** table, so this region is *Ref. +/- 0.5*Width* ppm. This step is necessary because the lock substance (solvent) will not always resonate at exactly the same position relative to the reference shift. The absolute chemical shift of the lock substance (solvent) differs because of differences in susceptibility, temperature, concentration or pH, for instance.

The third step depends on whether or not a peak was found in the second step. If a peak was found, ***sref*** determines the interpolated peak top and shifts its ppm value to the *ref*. value from the ***edlock*** table. The processing parameters OFFSET, SF and SR are changed accordingly. As such, the result of the default (step 1) is slightly corrected in order to set the peak of the reference substance exactly to 0. You can check this by putting the cursor on this peak. If no peak was found, you will get the message: 'sref: no peak found default calibration done'. The result of the default calibration (step 1) is stored without any further correction.

The three cases below show the calibration of a 1H, 13C and 31P spectrum with C6D6 as a solvent. Table 8.4 shows the corresponding entry in the ***edlock*** table:

Solvent	Field	Lock power	Nucleus	Distance [ppm]	Ref. [ppm]	Width [ppm]	RShift [ppm]
C6D6	-150	-15.0					
			1H	7.28	0.0	0.5	0.000
			2H	7.28	0.0	0.5	0.000
			13C	128.0	0.0	5.0	0.220
			31P	0.00	10.5	5.0	13.356

Table 8.4

case #1 - calibration of a 1H spectrum: A spectrum was acquired while being locked on C6D6. ***sref*** will do a default calibration and look for a signal at 0.0 ppm (*Ref.*) in a window of +/- 0.25 ppm. If a peak is found, its chemical shift will be set to 0 ppm.

case #2 - calibration of a 13C spectrum: A spectrum was acquired while being locked on C6D6. ***sref*** will do a default calibration and look for a signal at 0.0 ppm (*Ref.*) in a window of +/- 2.5 ppm. If a peak is found, its chemical shift will be set to 0 ppm.

case #3 - calibration of a 31P spectrum: A spectrum was acquired while being locked on C6D6. ***sref*** will do a default calibration and look for a signal at 10.5 ppm (*Ref.*) in a window of +/- 2.5 ppm. If a peak is found, its chemical shift will be set to exactly 10.5 ppm.

On 2D spectra, ***sref*** calibrates the F2 and F1 direction and this involves the same steps as described above for 1D spectra.

INPUT PARAMETERS

set by the acquisition, can be viewed with ***dpa*** or by typing ***s solvent*** etc.:

SOLVENT - the solvent of the sample
INSTRUM - configuration name (entered during ***cf***) of the spectrometer
LOCNUC - lock nucleus
SFO1 - spectral frequency
NUC1 - measured nucleus
SW - sweep width

OUTPUT PARAMETERS

processing parameters which can be viewed with ***edp***:
processing status parameters which can be viewed with ***dpp*** :

SF - spectral reference frequency
OFFSET - the ppm value of the first data point of the spectrum
SR - spectral reference

INPUT FILES

<tshome>/conf/instr/<instrum>/

`2Hlock` - edlock table for 2H locked samples
`19Flock` - edlock table for 19F locked samples

OUTPUT FILES

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

`proc` - processing parameters
`procs` - processing status parameters

USAGE IN AU PROGRAMS

SREF

t1guide

NAME

t1guide - Open the relaxation analysis guide (2D)

DESCRIPTION

The command ***`t1guide`*** opens a dialog box with a workflow for relaxation analysis including T1/T2. This procedure is completely described in the TOPSPIN Users Guide. To open this:

click ***Help*** → ***Manuals*** → [**General**] ***User Manual***

Chapter 9

Dataset handling

This chapter describes all TOPSPIN commands which can be used to read or write or delete datasets.

copy

NAME

copy - Copy the contents of the current data window to the Clipboard (nD)

DESCRIPTION

Under Windows, the command ***copy*** copies the contents of the current data window to the clipboard. The data are copied as a bitmap [1]. To copy the data as a windows metafile, use the command ***copy wmf***.

On Linux is the screen dump (***png*** format) copied to a temporary file, the pathname of this file is copied to clipboard.

Entering ***copy*** on the command line is equivalent to clicking ***File → Copy*** in the menu.

SEE ALSO

paste

[1] In Topspin 2.0 and older, data were copied in WMF format.

dalias

NAME

dalias - Create an alias name for a dataset (nD)

DESCRIPTION

The command ***dalias*** creates or interprets alias names for TOPSPIN data. The command requires various arguments and can be used as follows:

Create alias names

dalias add <alias> <name> <eno> <pno> <dir> <usr>
create the alias name <alias> for the specified dataset, e.g.:

dalias add e1h exam1d_1H 1 1 C:/bio joe

dalias add <alias> <pathname>
create the alias name <alias> for the specified dataset, e.g.:

dalias add e1h C:/bio/data/guest/nmr/exam1d_1H/1/pdata/1

Show full names on the screen

dalias pr <alias>
print the name, *expno*, *procno*, *dir* and *user* of the specified alias name

dalias prgen <alias>
print the full pathname of the specified alias name

dalias prall
print the *name*, *expno*, *procno*, *dir* and *user* of all alias names

dalias prallgen
print the full datapath of all alias names

Remove alias names

dalias rm <alias>
remove the specified alias name

dalias rmall
remove all alias names

Note that removing alias names does not remove the corresponding data.

Entering the command ***dalias*** without arguments shows a help message with a summary of the above information.

SEE ALSO

re

del, dela, delp, deldat, delete

NAME

del - Delete data (nD)
dela - Delete raw data (nD)
delp - Delete processed data (nD)
deldat - Delete data acquired at certain dates (nD)
delete - Open the delete dialog box (nD)

SYNTAX

del* [<name>]

DESCRIPTION

Delete commands can be started from the command line or from the delete dialog box. The latter is opened with the command ***`delete`*** (see Figure 9.1).

This dialog box has several options, each of which selects a certain command for execution.

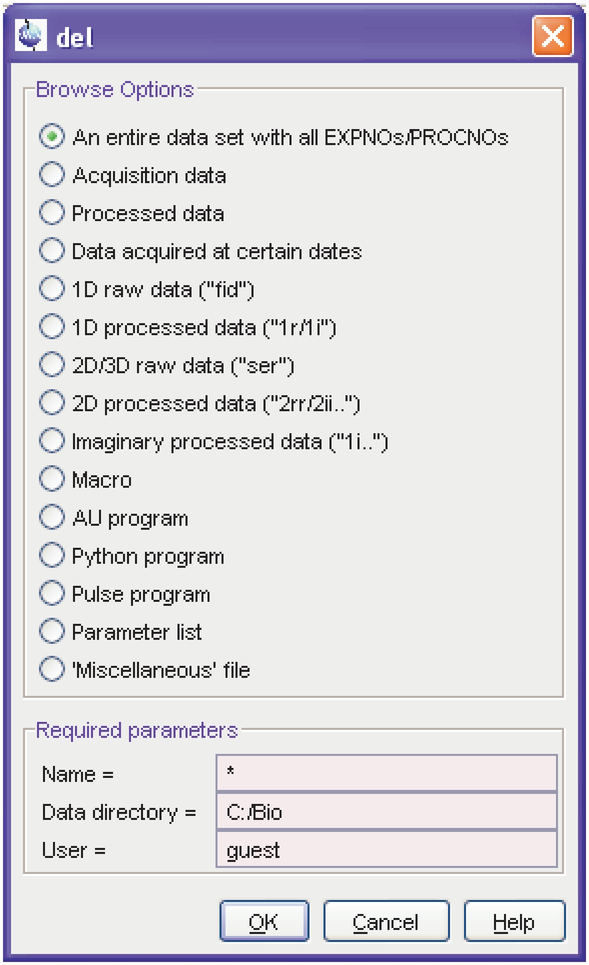
The commands ***`del`***, ***`dela`***, ***`delp`*** and ***`deldat`*** allow you to display a list of datasets. Such a list includes datasets containing raw and/or processed data as well as empty datasets which only contain parameter files. You can click one or more datasets in the list to mark them for deletion and then click ***Delete...*** to actually delete them.

An entire dataset with all expnos/procnos

This option selects the command ***`del`*** for execution. It lists datasets, only showing the dataset name. To delete data, mark one or more datasets and click ***Delete***. The marked datasets are entirely deleted, including data files, parameter files and the data name directory.

Acquisition data

This option selects the command ***`dela`*** for execution. It. It lists datasets showing a separate entry for each experiment number (*expno*). Each entry shows the dataset NAME, EXPNO, ACQU.DATA and SIZE. Datasets which do not contain raw data are displayed with ACQU.DATA *none*. To delete data, mark one or more datasets and click



Browse Options

● An entire data set with all EXPNOs/PROCNOs
○ Acquisition data
○ Processed data
○ Data acquired at certain dates
○ 1D raw data ("fid")
○ 1D processed data ("1r/1i")
○ 2D/3D raw data ("ser")
○ 2D processed data ("2rr/2ii..")
○ Imaginary processed data ("1i..")
○ Macro
○ AU program
○ Python program
○ Pulse program
○ Parameter list
○ 'Miscellaneous' file

Required parameters

Name = *
Data directory = C:/Bio
User = guest

Figure 9.1

one of the following buttons:

- ***Delete selected EXPNOs*** to delete the *expno* directory
- ***Delete raw data files of the selected EXPNOs***

Processed data

This option selects the command ***delp*** for execution. It lists datasets showing a separate entry for each processed data number (*procno*). Each entry shows the dataset NAME, EXPNO, PROCNO, PROC.DA-

TA and SIZE. Datasets which do not contain processed data are displayed with PROC.DATA *none*. To delete data, mark one or more datasets and click one of the following buttons:

- ***Delete selected PROCNOs*** to delete the *procno* directories
- ***Delete processed data files of the selected PROCNOs***

Data acquired at certain dates

This option selects the command ***deldat*** for execution. It prompts the user for a time range as specified in table 9.1. Depending on the time range you select, you are further prompted for one or two specific dates. A list of datasets that were measured within the specified time range is displayed with a separate entry for each experiment number (*expno*).

all	all data acquired by the current user
between	data acquired between two specified dates
day	data acquired on the specified date
earlier	data acquired before the specified date
later	data acquired later than the specified date

Table 9.1

When started from the command line, ***del**** commands can take one argument which may contain wild cards. Examples:

dela exam1d*
list all datasets whose name starts with *exam1d*

dela exam1d???
list all datasets whose name is *exam1d* plus three extra characters

del* commands only list and delete the datasets of current user. The current user here refers to the *user* part of the data path of the currently selected dataset.

Please distinguish:

- the user part of the data path
- the owner of the dataset

- the user who runs TOPSPIN

Usually these three things are the same, i.e. a user works on his own data. However, the user part of the data path can be any character string and does not have to correspond to a user account on the computer. Furthermore, the user who runs TOPSPIN might work on someone else's data. In this case, he/she may or may not have the permission to delete this dataset. In the latter case, the ***del**** commands will not delete the dataset but show an error message instead.

OUTPUT FILES

For *dela* → *Delete raw data files of the selected EXPNOs*:

<dir>/data/<user>/nmr/<name>/<expno>/

`audita.txt` - acquisition audit trail

For *delp* → *Delete processed data files of the selected PROCNOs*:

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

`auditp.txt` - processing audit trail

SEE ALSO

delf, dels, delser, del2d, deli

delf, dels, delser, del2d, deli, delete

NAME

delf - Delete raw data (1D)
dels - Delete processed data (1D)
delser - Delete raw data (2D,3D)
del2d - Delete processed data (2D,3D)
deli - Delete imaginary processed (nD)
delete - Open delete dialog box (nD)

SYNTAX

del* [<name>]

DESCRIPTION

Delete commands can be started from the command line or from the delete dialog box. The latter is opened with the command ***delete*** (see Figure 9.2).

This dialog box has several options, each of which selects a certain command for execution.

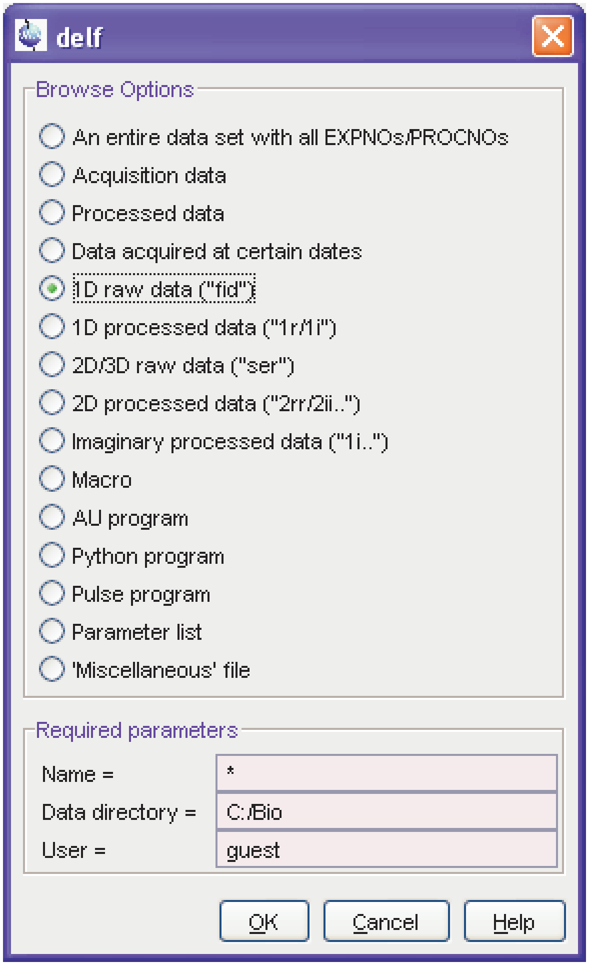
The commands ***delf***, ***dels***, ***delser***, ***del2d*** and ***deli*** display a list of datasets. Such a list only includes datasets which contain data files. As opposed to commands like ***del*** and ***dela***, they do not show empty datasets. You can click one or more datasets to mark them for deletion and then click ***Delete..*** to actually delete them.

1D raw data

This option selects the command ***delf*** for execution. It lists 1D datasets which contain raw data showing a separate entry for each experiment number (*expno*). Each entry shows the dataset NAME, EXPNO, ACQU.DATA and SIZE. To delete data, mark one or more datasets and click one of the following buttons:

- ***Delete selected EXPNOs*** to delete the *expno* directory
- ***Delete raw data files of the selected EXPNOs***

1D processed data



delf

Browse Options

○ An entire data set with all EXPNOs/PROCNOs
○ Acquisition data
○ Processed data
○ Data acquired at certain dates
● 1D raw data ("fid")
○ 1D processed data ("1r/1i")
○ 2D/3D raw data ("ser")
○ 2D processed data ("2rr/2ii..")
○ Imaginary processed data ("1i..")
○ Macro
○ AU program
○ Python program
○ Pulse program
○ Parameter list
○ 'Miscellaneous' file

Required parameters

Name = *
Data directory = C:/Bio
User = guest

Figure 9.2

This option selects the command ***`dels`*** for execution. It lists 1D datasets which contain processed data showing a separate entry for each processed data number (*procno*). Each entry contains the dataset NAME, EXPNO, PROCNO, PROC.DATA and SIZE. To delete data, mark one or more datasets and click one of the following buttons:

- ***Delete selected PROCNOs*** to delete the *procno* directories
- ***Delete processed data files of the selected PROCNOs***

2D/3D raw data

This option selects the command ***delser*** for execution. It lists 2D and 3D datasets which contain raw data showing a separate entry for each experiment number (*expno*). Each entry shows the dataset NAME, EXPNO, ACQU.DATA and SIZE.To delete data, mark one or more datasets and click one of the following buttons:

- ***Delete selected EXPNOs*** to delete the *expno* directory
- ***Delete raw data files of the selected EXPNOs***

2D processed data

This option selects the command ***del2d*** for execution. It lists 2D datasets which contain processed data showing a separate entry for each processed data number (*procno*). Each entry shows the dataset NAME, EXPNO, PROCNO, PROC.DATA and SIZE. To delete data, mark one or more datasets and click one of the following buttons:

- ***Delete selected PROCNOs*** to delete the *procno* directories
- ***Delete processed data files of the selected PROCNOs***

Imaginary processed data

This option selects the command ***deli*** for execution. It lists datasets which contain 1D, 2D or 3D imaginary data showing a separate entry for each processed data number (*procno*). Each entry shows the dataset NAME, EXPNO, PROCNO, PROC.DATA and SIZE. Only the imaginary processed data files are deleted. Raw data, processed data and parameter files are kept. To delete data, mark one or more datasets and click the button:

- ***Delete imaginary processed data of the selected PROCNOs***

When started from the command line, ***del**** commands can take one argument which may contain wild cards. Examples:

delf exam1d*
list all datasets whose name starts with *exam1d*

delf exam1d???
list all datasets whose name is *exam1d* plus three extra characters

del* commands only list and delete the datasets of current user. The current user here refers to the *user* part of the data path of the currently selected dataset. Please distinguish:

- the user part of the data path
- the owner of the dataset
- the user who runs TOPSPIN

Usually these three things are the same, i.e. a user works on his own data. However, the user part of the data path can be any character string and does not have to correspond to a user account on the computer. Furthermore, the user who runs TOPSPIN might work on someone else's data. In this case, he/she may or may not have the permission to delete this dataset. In the latter case, the ***del**** commands will not delete the dataset but show an error message instead.

OUTPUT FILES

For *delf/delser* → *Delete raw data files of the selected EXPNOs*:

<dir>/data/<user>/nmr/<name>/<expno>/

`audita.txt` - acquisition audit trail

For *dels/del2d/deli* → *Delete processed data files of the selected PROCNOs*:

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

`auditp.txt` - processing audit trail

SEE ALSO

del, dela, delp, deldat

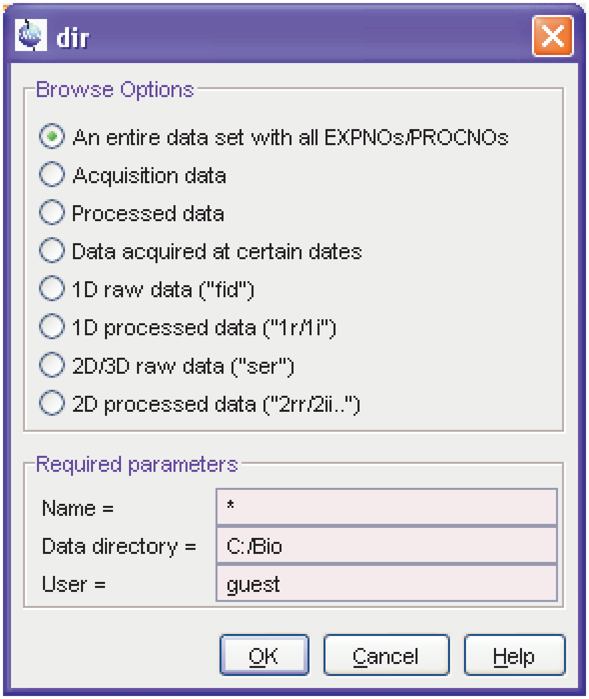
dir, dira, dirp, dirdat, browse

NAME

dir - List datasets (nD)
dira - List raw data (nD)
dirp - List processed data (nD)
dirdat - List data acquired at certain dates (nD)
browse - Open data list dialog box (nD)

DESCRIPTION

Commands to list data directories can be started from the command line or from the directory dialog box. The latter is opened with the command ***browse*** (see Figure 9.3).



Browse Options

● An entire data set with all EXPNOs/PROCNOs
○ Acquisition data
○ Processed data
○ Data acquired at certain dates
○ 1D raw data ("fid")
○ 1D processed data ("1r/1i")
○ 2D/3D raw data ("ser")
○ 2D processed data ("2rr/2ii..")

Required parameters

Name = *
Data directory = C:/Bio
User = guest

Figure 9.3

This dialog box has several options, each of which selects a certain command for execution.

The commands ***dir***, ***dira***, ***dirp*** and ***dirdat*** display all datasets containing raw and/or processed data as well as empty datasets which only contain parameter files. You can mark one or more entries in the list and click:

- ***Display***
  to display the data in the current data window

or

- ***Display in new window***
  to display the data in a new data window

When multiple entries were marked, they will be shown in one data window in multi-display mode.

An entire dataset with all EXPNOs/PROCNOs

This option selects the command ***dir*** for execution. It lists datasets, showing the data names only.

Acquisition data

This option selects the command ***dira*** for execution. It lists datasets showing a separate entry for each *expno*. Each entry shows the dataset NAME, EXPNO, ACQU.DATA and SIZE. The entry *file* refers to the data files and can be *fid* (1D raw data), *ser* (2D or 3D raw data) or *no raw data*.

Processed data

This option selects the command ***dirp*** for execution. It lists datasets showing a separate entry for each processed data number (*procno*). Each entry shows the dataset NAME, EXPNO, PROCNO, PROC.DATA and SIZE. The type refers to the name of the data files and can be *1r 1i* (processed 1D data), *2rr 2ir 2ri 2ii* (2D raw data), *3rrr, 3rri, ..*(processed 3D data) or *no processed data*.

Data acquired at certain dates

This option selects the command ***dirdat*** for execution. It prompts the user for a time range as specified in table 9.2. Depending on the time

all	all data acquired by the current user
between	data acquired between two specified dates
day	data acquired on the specified date
earlier	data acquired before the specified date
later	data acquired later than the specified date

Table 9.2

range you select, you are further prompted for one or two specific dates. A list of datasets which were measured within the specified time range is displayed with a separate entry for each *expno*.

When started from the command line, ***dir**** commands can take one argument which may contain wild cards. Examples:

dir exam1d*
list all datasets whose name starts with *exam1d*

dir exam1d???
list all datasets whose name is *exam1d* plus three extra characters

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data
`ser` - 2D or 3D raw data

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

`1r`, `1i` - processed 1D data
`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`3rrr`, `3irr`, `3rir`, `3iir` - processed 3D data

SEE ALSO

dirf, dirs, dirser, dir2d, open, find, re, rep, rew, repw, reb

dirf, dirs, dirser, dir2d, browse

NAME

dirf - List raw data (1D)
dirs - List processed data (1D)
dirser - List raw data (2D,3D)
dir2d - List processed data (2D,3D)
browse - Open the list data dialog box (nD)

SYNTAX

dir* [<name>]

DESCRIPTION

The ***dir**** commands display a list of datasets according to certain criteria. They can be started from the command line or from the ***browse*** dialog box (see Figure 9.4).

The commands ***dirf***, ***dirs***, ***dirser*** and ***dir2d*** display a list of datasets. This list only includes datasets which contain certain data files. As opposed to commands like ***dir*** and ***dira***, they do not show empty datasets. You can mark one or more datasets in the list and click:

- ***Display***
  to display the data in the current data window

or

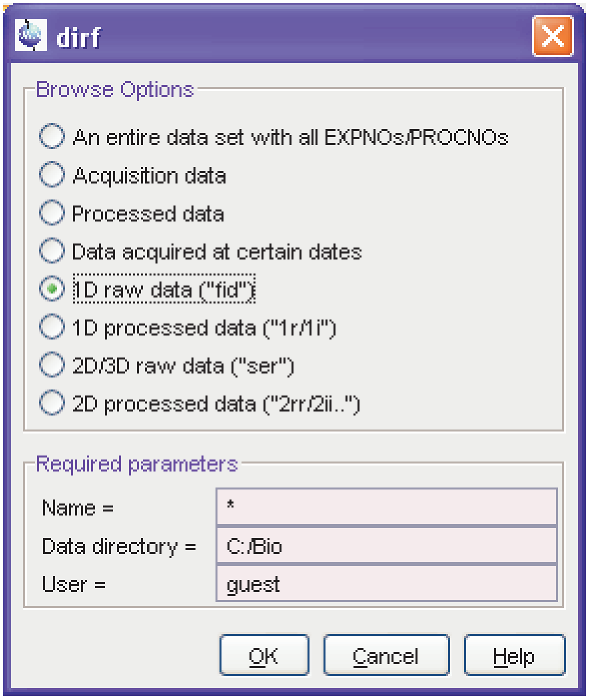
- ***Display in new window***
  to display the data in a new data window

When multiple entries were marked, the will be shown in one data window in multi-display mode.

1D raw data

This option selects the command ***dirf*** for execution. It lists 1D datasets which contain raw data showing a separate entry for each experiment number (*expno*). Each entry shows the dataset NAME, EXPNO, ACQU.DATA and SIZE.

1D processed data



Browse Options

○ An entire data set with all EXPNOs/PROCNOs
○ Acquisition data
○ Processed data
○ Data acquired at certain dates
● 1D raw data ("fid")
○ 1D processed data ("1r/1i")
○ 2D/3D raw data ("ser")
○ 2D processed data ("2rr/2ii..")

Required parameters

Name = *
Data directory = C:/Bio
User = guest

Figure 9.4

This option selects the command ***dirs*** for execution. It lists 1D datasets which contain processed data showing a separate entry for each processed data number (*procno*). Each entry shows the dataset NAME, EXPNO, PROCNO, PROC.DATA and SIZE.

2D/3D raw data

This option selects the command ***dirser*** for execution. It lists 2D and 3D datasets which contain raw data showing a separate entry for each experiment number (*expno*). Each entry shows the dataset NAME, EXPNO, ACQU.DATA and SIZE.

2D processed data

This option selects the command ***dir2d*** for execution. It lists 2D datasets which contain processed data showing a separate entry for each processed data number (*procno*). Each entry shows the dataset NAME, EXPNO, PROCNO, PROC.DATA and SIZE.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data
`ser` - 2D or 3D raw data

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

`1r`, `1i` - processed 1D data
`2rr`, `2ir`, `2ri`, `2ii` - processed 2D data
`3rrr`, `3irr`, `3rir`, `3iir` - processed 3D data

SEE ALSO

dir, dira, dirp, dirdat, browse, find, re, rep, rew, repw, reb

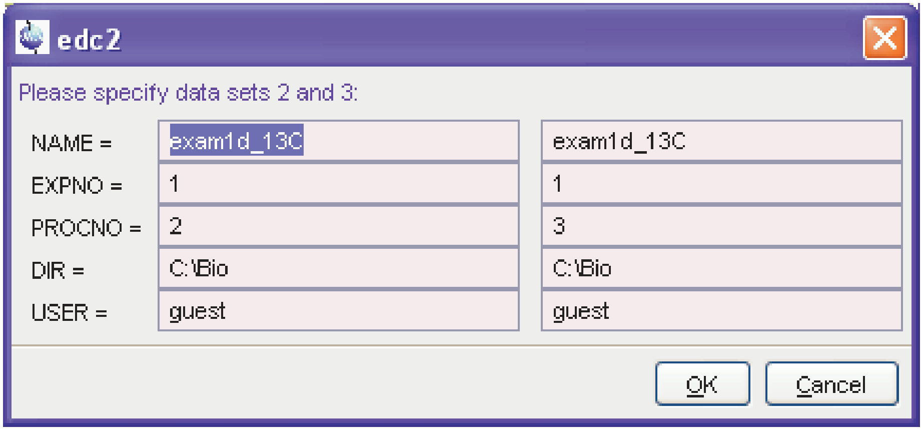
edc2

NAME

edc2 - Define second and third dataset

DESCRIPTION

The command ***edc2*** opens a dialog box in which you can define the second and third dataset (see Figure 9.5).



Please specify data sets 2 and 3:

NAME =	exam1d_13C	exam1d_13C
EXPNO =	1	1
PROCNO =	2	3
DIR =	C:\Bio	C:\Bio
USER =	guest	guest

Figure 9.5

You can define the NAME, EXPNO, PROCNO, DIR (disk unit) and USER. Note that these are all parts of the data pathname:

<dir>\data\nmr\<**user>**\<**name>**\<**expno**>\pdata\<**procno>**

The second dataset is used by 1D commands like ***add***, ***duadd***, ***mul***, ***div*** and ***addfid*** and by 2D commands like ***add2d***, ***mul2d*** and ***addser***. The second dataset is, however, usually set from the add/multiply dialog box (command ***adsu***).

The third dataset is used by the 1D command ***add*** when entered from the command line and in various AU programs (macro DATASET3).

INPUT AND OUTPUT FILES

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

`curdat2` - definition of the second dataset

SEE ALSO

add, duadd, mul, div, addfid, add2d, mul2d, addser

find, search

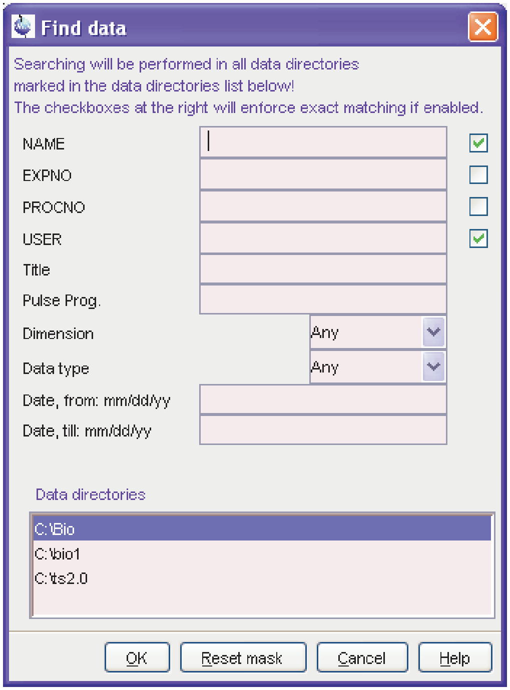
NAME

find - Find data according to specified criteria (nD)

DESCRIPTION

The command ***find*** allows you to 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 Figure 9.6).
2. Enter the search items in the upper part of the dialog. Note that:
   - There will be searched for items containing the specified string
   - Exact matching is performed for dataset variables, NAME, EXPNO, PROCNO and USER, if the checkboxes at the right are enabled.
   - The search is restricted to data created between the specified dates. Note that this refers to the acquisition date.
   - The ***Reset mask*** button allows you to reset the default criteria.
3. Select the **Data directories** to be searched in the lower part of the dialog. If no directories are selected, all will be searched.
4. Click ***OK***
   to start the search. A list of data that fulfil the defined criteria will appear (see Figure 9.7).



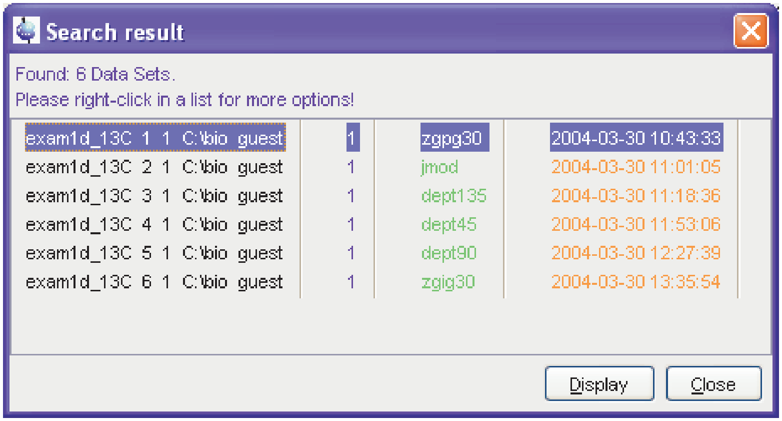
Searching will be performed in all data directories marked in the data directories list below!
The checkboxes at the right will enforce exact matching if enabled.

NAME		☑
EXPNO		□
PROCNO		□
USER		☑
Title		
Pulse Prog.		
Dimension	Any	
Data type	Any	
Date, from: mm/dd/yy		
Date, till: mm/dd/yy		

Data directories

C:\Bio
C:\bio1
C:\ts2.0

Figure 9.6



Found: 6 Data Sets.
Please right-click in a list for more options!

```
exam1d_13C 1 1 C:\bio guest    1    zgpg30    2004-03-30 10:43:33
exam1d_13C 2 1 C:\bio guest    1    jmod      2004-03-30 11:01:05
exam1d_13C 3 1 C:\bio guest    1    dept135   2004-03-30 11:18:36
exam1d_13C 4 1 C:\bio guest    1    dept45    2004-03-30 11:53:06
exam1d_13C 5 1 C:\bio guest    1    dept90    2004-03-30 12:27:39
exam1d_13C 6 1 C:\bio guest    1    zgig30    2004-03-30 13:35:54
```

Figure 9.7

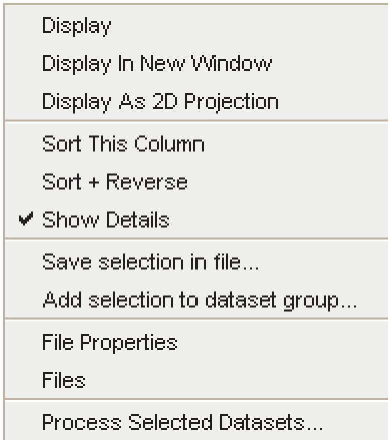
Note that on exiting TOPSPIN, the search criteria will be rest to default.

How to Display one of the Found Datasets

In the search result window (see Figure 9.7):

1. Click one or more datasets to select them.
2. Click ***Display***
   to display the selected dataset(s) in the current data window. If multiple datasets are selected they are displayed in the new data window in multiple display mode.

The search result window offers a right-click context menu with various options (see Figure 9.8).



Display
Display In New Window
Display As 2D Projection
Sort This Column
Sort + Reverse
✓ Show Details
Save selection in file...
Add selection to dataset group...
File Properties
Files
Process Selected Datasets...

Figure 9.8

Display

Display the selected dataset(s) in the current data window. If multiple datasets are selected they are displayed in the same data window in multiple display mode. Equivalent to clicking the ***Display*** button or pressing ***`Enter`***.

Display In New Window

Display the selected dataset(s) in a new window. If multiple datasets are selected they are displayed in the one new data window in multiple display mode.

Display As 2D Projection

Display the selected dataset as a projection of the current 2D dataset. A dialog will appear allowing you to choose F1-projection, F2-projection or both. If multiple datasets are selected, only the first one is considered. If the current dataset is not a 2D dataset, nothing happens.

Sort This Column

Sort the selected column in ascending order.

Sort + Reverse

Sort the selected column in descending order.

Show Details

Show/hide the dataset details Dimension, Pulse program and Acquisition date.

Save Selection to File..

Save the list of selected datasets in a text file. First opens a file dialog where you can select or specify a filename. The saved dataset list can, for example, be used for serial processing (command ***`serial`***, see also ***`Process Selected Datasets`*** below).

Add Selection to dataset group..

Add the list of selected datasets to a dataset group. You will be prompted to enter the group name. The created or modified group can be accessed from the browser.

File properties

Show main dataset parameters like *Dimension*, *Pulse program*, *Acquisition Date*, *Nuclei*, *Spectrometer frequency* and *Solvent*.

Files

Show the files in the processed data directory of the selected dataset.

Process Selected Datasets

Perform serial processing on the selected datasets. Opens a dialog where you can change or edit the dataset list and specify the command, macro or Python program to be executed (starts the command ***`serial`***).

The ***Close*** button allows you to close the search result dialog.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data
`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`1r`, `1i` - processed 1D data
`proc` - processing parameters
`procs` - processing status parameters

Note that these are only the main 1D data files.

SEE ALSO

open, new, re, rep, rew, repw, reb, dir*

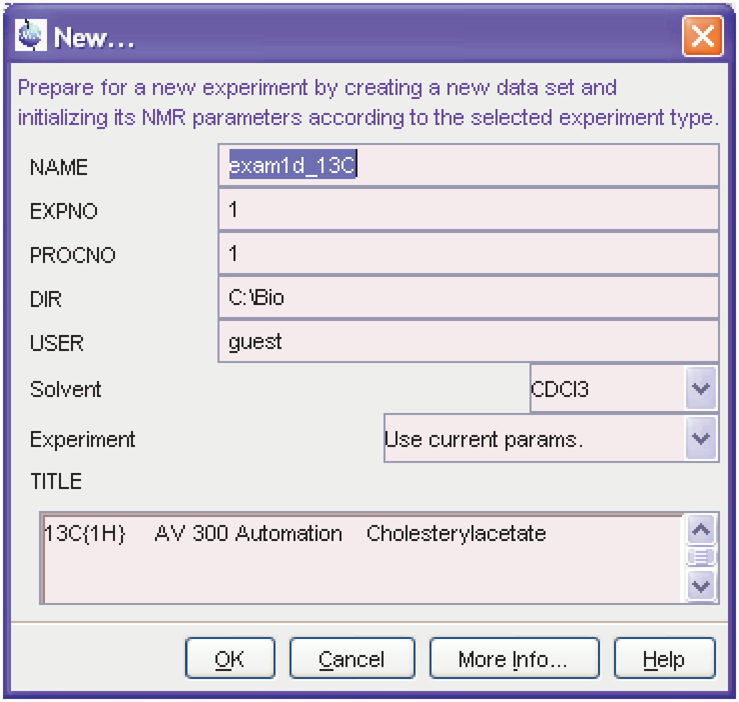
new

NAME

new - Define a new dataset (nD)

DESCRIPTION

The command ***new*** [***Ctrl-n***] opens a dialog box in which you can define a new dataset.



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type.

NAME exam1d_13C

EXPNO 1

PROCNO 1

DIR C:\Bio

USER guest

Solvent CDCl3

Experiment Use current params.

TITLE

13C{1H} AV 300 Automation Cholesterylacetate

Figure 9.9

Here, you can specify the dataset NAME, EXPNO, PROCNO, DIR (disk unit) and USER. Note that these are all parts of the data pathname:

<dir>\data\nmr\<**user>**\<**name>**\<**expno**>\pdata\<**procno>**

Furthermore, you can select:

- ***Solvent***
  sets the acquisition parameter SOLVENT. Default is the solvent of the current dataset.
- ***Experiment*** (=parameter set)
  copies the acquisition and processing parameters. Default is "Use current parameters".

When you click ***OK***, the dataset is created and made the current data window. If the specified dataset already exists, you will be prompted to overwrite this or not. Note that this will only overwrite the parameters, not the data files.

`new` is equivalent to the command ***`edc`***.

INPUT FILES

<tshome>/prog/curdir/<user>/

`curdat` - current dataset definition

If ***Experiment*** = ***Use current params***:

<dir>/data/<user>/nmr/<name>/<expno>/

`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`proc` - processing parameters
`procs` - processing status parameters

If ***Experiment*** ≠ ***Use current params.***:

<tshome>/exp/stan/nmr/par/<experiment>/

`acqu` - acquisition parameters
`proc` - processing parameters

OUTPUT FILES

<tshome>/prog/curdir/<user>/

`curdat` - current dataset definition

If the dataset specified with ***`new`*** does not exist yet, the current dataset is copied:

<*dir*>/data/<*user*>/nmr/<*name*>/<*expno*>/

`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`proc` - processing parameters
`procs` - processing status parameters

For 2D and 3D data the files `acqu2`, `acqu2s` etc. are also output.

SEE ALSO

open, find, re, rep, rew, repw, reb, dir*

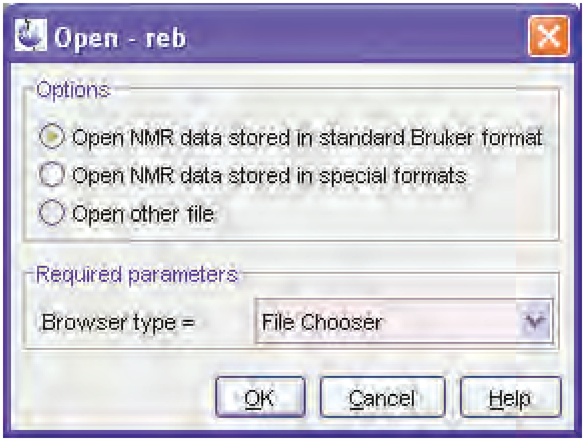
open

NAME

open - Open a dataset, pulse program, AU program etc. (nD)

DESCRIPTION

Opening data, parameters, lists and various other files can be started from the command line or from the open dialog box. The latter is opened with the command ***open*** [***Ctrl-o***] (see Figure 9.10).



● Open NMR data stored in standard Bruker format
○ Open NMR data stored in special formats
○ Open other file

Browser type = File Chooser

Figure 9.10

This dialog box has three options each with several file types. Each file type selects a certain command for execution.

Open NMR data stored in standard Bruker format

This option allows you to open Bruker format data in the following ways:

- File chooser [***reb***]
- RE dialog [***re***]
- PROCNO dialog [***rep***]

Open NMR data stored in special formats

This option allows you to open the following NMR data types (formats):

- JCAMP-DX [***fromjdx***]
- Zipped TOPSPIN [***fromzip***]
- WIN-NMR [***winconv***]
- A3000 [***conv***]
- VNMR [***vconv***]
- JNMR [***jconv***]
- Felix [***fconv***]

Open other file:

This option allows you to open the following lists and programs:

- Pulse programs [***edpul***]
- Au programs [***edau***]
- Gradient programs [***edgp***]
- CPD programs [***edcpd***]
- Miscellaneous files [***edmisc***]
- Parameter lists [***edlist***]
- Python program [***edpy***]

The corresponding command line commands are specified in square brackets.

After clicking ***OK***, a new dialog box will appear according to the selected option and file type.

SEE ALSO

re, rep, rew, repw, reb, fromjdx, fromzip, winconv, conv, vconv, jconv, fconv, edpul, edau, edgp, edcpd, edmisc, edlist, edmac

paste

NAME

paste - Open the dataset that was last copied (nD)

DESCRIPTION

The command ***`paste`*** opens the dataset which was previously copied from the a TOPSPIN data window or from the File Explorer. This involves two steps:

1. **Copy**

   In the File Explorer:

   - Go to a dataset
   - Right-click a dataset folder or file, e.g. the data *name*, *expno* or *procno* folder or any file in it and click **Copy**

2. **Paste**

   In TOPSPIN:

   - Click ***File*** → ***Paste*** or type ***`paste`***

Note that if you select and copy a the dataset in the File Explorer, its data path is copied to the Clipboard. The command ***Paste*** reads this path from the Clipboard. If you run ***Paste*** without first copying a dataset from the Explorer, TOPSPIN tries to read whatever is currently stored in the Clipboard. If that is a data path, TOPSPIN will read it, otherwise you will get an error message.

OUTPUT FILES

<tshome>/prog/curdir/<user>/

`curdat` - current data definition

SEE ALSO

copy

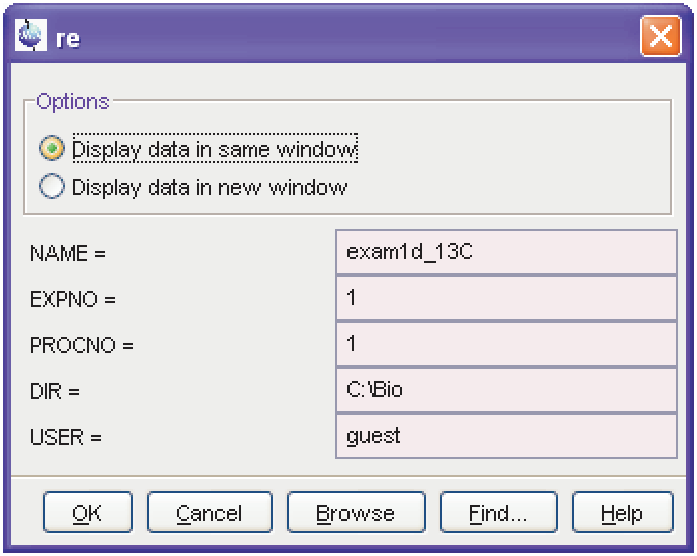
re, rep, rew, repw

NAME

re - Read data of specified *name* or *expno* (nD)
rep - Read data of specified *procno* (nD)
rew - Read data of specified *name*/*expno* in new window (nD)
repw - Read data of specified *procno* in new window (nD)

DESCRIPTION

The commands ***re*** and ***rew*** allow you to read and display a new dataset. They open a dialog box with the corresponding option selected (see Figure 9.11). These options are:



● Display data in same window
○ Display data in new window

NAME = exam1d_13C
EXPNO = 1
PROCNO = 1
DIR = C:\Bio
USER = guest

Figure 9.11

Display data in same window

Selects the command ***re*** for execution. It reads the specified dataset in the current data window.

Display data in new window

Selects the command ***rew*** for execution. It reads the specified dataset in a new data window.

specify the data path variables. A full data path is:

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

re replaces the dataset in the current data window (if it exists).

The data path variables can also be specified on the command line. In this case, the dialog box is not opened and the missing data path variables are taken from the current dataset. Examples:

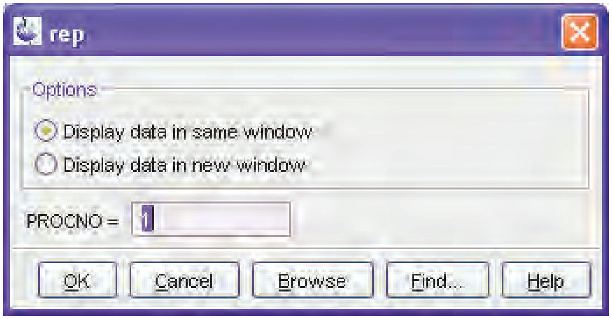
```
re <name>
re <expno>
re <name> <expno>
re <expno> <procno>
re <name> <expno> <procno>
re <name> <expno> <procno> <dir> <user>
```

Alternatively, ***re*** and ***rew*** can be entered with an alias name as argument, i.e.:

```
re <aliasname>
```

Note that the first alphanumeric argument is always interpreted as the name (or alias name) and the first numeric argument as experiment number.

The commands ***rep*** and ***repw*** allow you to read and display a new processed data number (*procno*) of the current dataset. They open a dialog box with the corresponding option selected (see Figure 9.12).



rep

Options

● Display data in same window

○ Display data in new window

PROCNO = 1

Figure 9.12

These options are:

Display data in same window

Selects the command ***rep*** for execution. It reads the specified PROCNO in the current data window.

Display data in new window

Selects the command ***repw*** for execution. It reads the specified PROCNO in a new data window.

The destination *procno* can also be specified on the command line, e.g.:

```
rep 77
```

INPUT FILES

For re and rew:

<dir>/data/<user>/nmr/<name1D>/<expno>/

`fid` - 1D raw data
`acqu` - acquisition parameters
`acqus` - acquisition status parameters

For re, rew, rep and repw:

<dir>/data/<user>/nmr/<name1D>/<expno>/pdata/<procno>/

`1r`, `1i` - processed 1D data
`proc` - processing parameters
`procs` - processing status parameters

Note that these are only the main files of a 1D dataset.

OUTPUT FILES

<tshome>/prog/curdir/<user>/

`curdat` - current data definition

USAGE IN AU PROGRAMS

RE(name)

SEE ALSO

reb, open, new, find, dir*

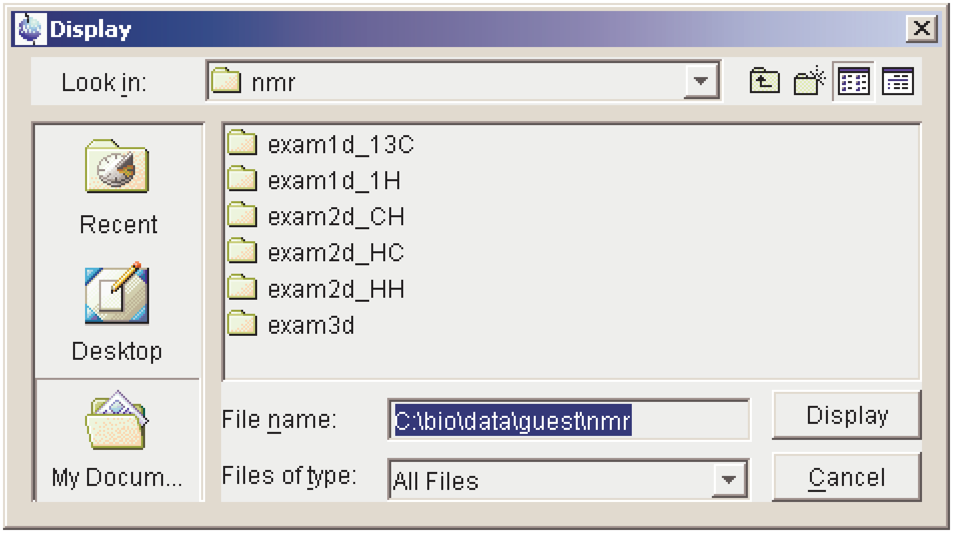
reb

NAME

reb - Open a data browser at the level of data names (nD)

DESCRIPTION

The command ***reb*** opens a file browser (see Figure 9.13).



exam1d_13C
exam1d_1H
exam2d_CH
exam2d_HC
exam2d_HH
exam3d

File name: C:\bio\data\guest\nmr

Files of type: All Files

Figure 9.13

Here you see a list of dataset names under the same <dir> and <user> as the currently selected dataset. Note that TOPSPIN data are stored in a directory:

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

From the browser, you can:

- select the data name to be displayed in the current data window
- move up in the data directory tree to select a different *user* and/or *dir*
- double-click a data *name* to move down the directory tree and select a desired *expno*/*procno*.

Once you have selected the desired *name*, *expno* or *procno*, click ***Display*** or hit ***`Enter`*** to display the dataset in the current data window.

In Topspin 2.0 and newer, ***`reb`*** allows opening datasets stored in the following directories structures:

<mydata>/<dataname>/<expno>/pdata/<procno>

Note that this will create a copy the dataset in the standard Topspin datapath:

<tshome>/data/<user>/nmr/<dataname>/<expno>/pdata/<procno>

where <user> is the current internal Topspin user. This copy can be processed, delete or overwritten, even if the original dataset is write protected. The original data set is left unchanged.

SEE ALSO

open, re, rep, rew, repw, new, find

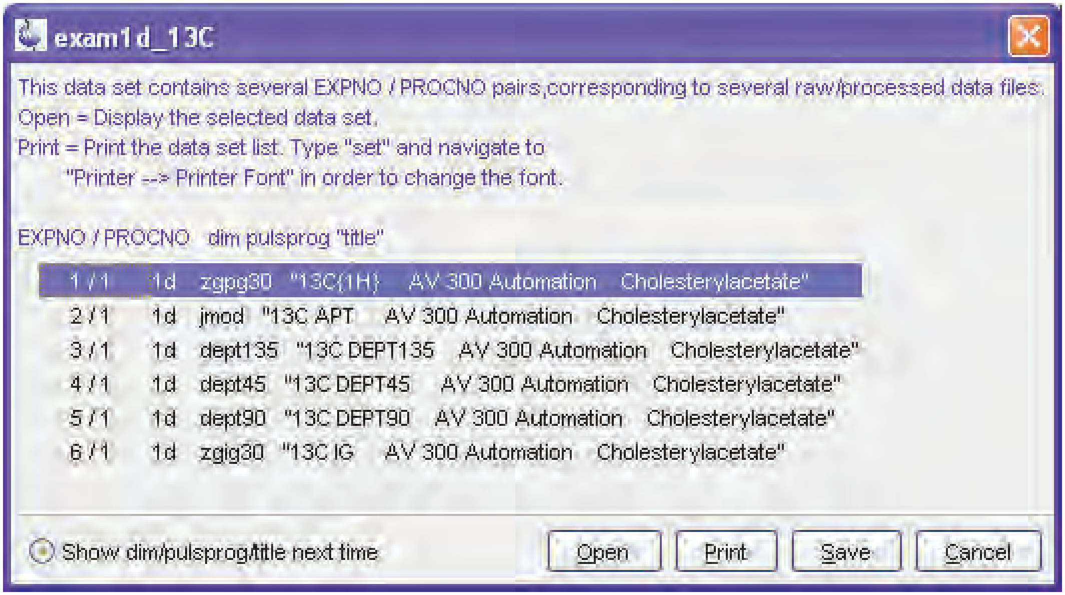
rel, repl

NAME

rel - Open a list of expnos/procnos in current dataset
repl - Open a list of procnos in the current expno

DESCRIPTION

The command ***rel*** lists the available expnos/procnos under the current dataset and allows you to select and open one (see Figure 9.14).



exam1d_13C

This data set contains several EXPNO / PROCNO pairs,corresponding to several raw/processed data files.
Open = Display the selected data set.
Print = Print the data set list. Type "set" and navigate to
"Printer --> Printer Font" in order to change the font.

```
EXPNO / PROCNO   dim pulsprog "title"

   1 / 1    1d   zgpg30  "13C{1H}   AV 300 Automation   Cholesterylacetate"
   2 / 1    1d   jmod  "13C APT   AV 300 Automation   Cholesterylacetate"
   3 / 1    1d   dept135  "13C DEPT135   AV 300 Automation   Cholesterylacetate"
   4 / 1    1d   dept45  "13C DEPT45   AV 300 Automation   Cholesterylacetate"
   5 / 1    1d   dept90  "13C DEPT90   AV 300 Automation   Cholesterylacetate"
   6 / 1    1d   zgig30  "13C IG   AV 300 Automation   Cholesterylacetate"
```

○ Show dim/pulsprog/title next time

Figure 9.14

If the current dataset contains only one expno/procno combination, it is automatically opened.

The dialog offers the following buttons:

Open : open the highlighted dataset (equivalent to pressing the ***Enter*** key)

Print : print the dialog contents

Save : print the dialog contents to a text file

Cancel : Close the dialog

The command ***`repl`*** works like ***`rel`***, except that it lists the available procnos under the current expno.

If no dataset is open, ***`rel`*** refers to the last active dataset. If no dataset has been open yet during the current TOPSPIN session, it shows an error message.

SEE ALSO

repl, re, rep, rew, repw, new

reopen

NAME

reopen - Reopen current dataset in new data window (nD)

DESCRIPTION

The command ***reopen*** reopens the current dataset in a new data window. This is, for example, convenient to view various regions or various objects (spectrum, fid, parameters etc.) of the same dataset. Multiple data windows are indicated with a number in square brackets, e.g. [1], in the title bar.

Entering ***reopen*** on the command line is equivalent to clicking ***File*** → ***Reopen*** in the menu.

SEE ALSO

open

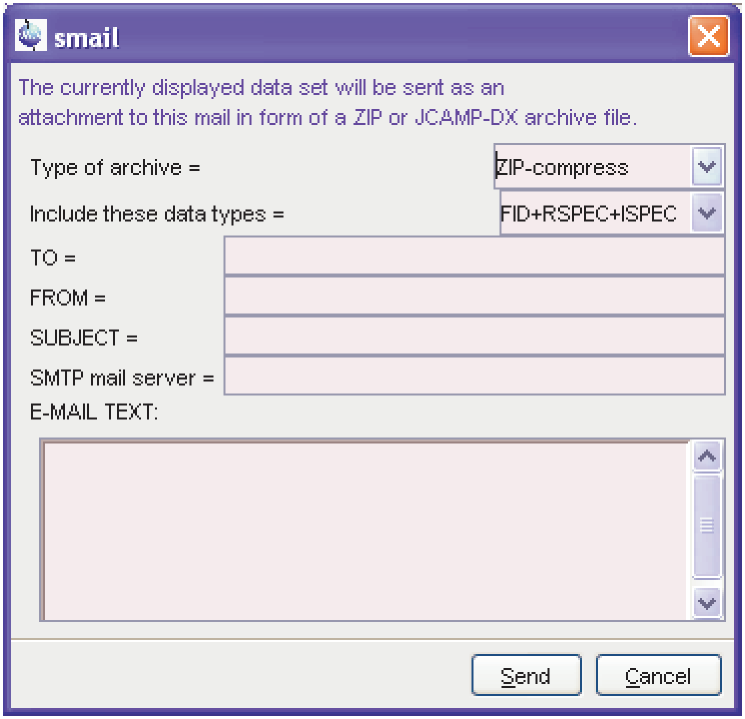
smail

NAME

smail - Send the current dataset by Email (1D,2D,3D)

DESCRIPTION

The command ***smail*** sends the current dataset by Email. It opens a dialog box where you can specify the required information or accept the default values.



The currently displayed data set will be sent as an attachment to this mail in form of a ZIP or JCAMP-DX archive file.

Type of archive = ZIP-compress

Include these data types = FID+RSPEC+ISPEC

TO =

FROM =

SUBJECT =

SMTP mail server =

E-MAIL TEXT:

Figure 9.15

In the dialog box, you can select the:

- Archive type: ZIP or JCAMP
- Data type(s) included: FID, Spectrum and/or Parameters

For ZIP format data you can choose between compression and no compression.

For JCAMP format, you can choose between the following compression modes:

- *FIX* (=0) : table format
- *PACKED* (=1) : no spaces between the intensity values
- *SQUEEZED* (=2) : the sign of the intensity values is encoded in the first digit
- *DIFF/DUP* (=3) : the difference between successive values is encoded, suppressing repetition of successive equal values (default = *DIFF/DUP*)

For the included data types, you have the following choices:

- FID+RSPEC+ISPEC: raw + real and imaginary processed data
- FID+RSPEC: raw + real processed data
- FID: raw data
- RSPEC+ISPEC: real and imaginary processed data
- RSPEC: real processed data
- PARAMS: parameter files

Before you can send the data you must fill in the fields:

- ***To***: the email address of the recipient
- ***From***: your own email address
- ***SMTP mail server***:
- ***Subject***:
- ***Text***:

INPUT FILES

<tshome>/prog/curdir/<user>/

`curdat` - current data definition

If data type includes FID :

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data
`ser` - 2D raw data

If data type includes RSPEC :

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

`1r` - real processed 1D data
`2rr` - real processed 2D data

If data type includes ISPEC :

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

`1i` - imaginary processed 1D data
`2ir` - F2-imaginary processed 2D data
`2ri` - F1-imaginary processed 2D data
`2ii` - F2/F1-imaginary processed 2D data

All other files which are part of a dataset like parameter files, audit trails files etc. are sent for all data types.

OUTPUT FILES

<userhome>/<mydata.dx> - TOPSPIN data in JCAMP-DX format

<userhome>/<mydata.bnmr.zip> - TOPSPIN data in ZIP format

SEE ALSO

tojdx, tozip

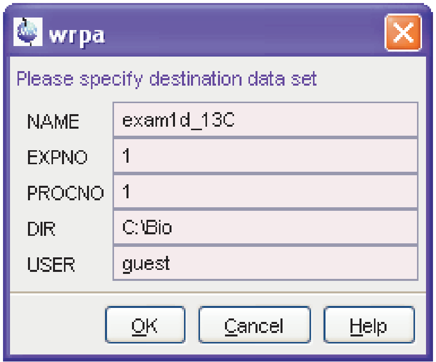
wrpa, wra, wrp, wraparam, wrpparam

NAME

wrpa - Copy a dataset, raw and processed data (nD)
wra - Copy raw data (nD)
wrp - Copy processed data (nD)
wraparam - Copy acquisition dataset (parameters only)
wrpparam - Copy processing dataset (parameters only)

DESCRIPTION

The command ***wrpa*** writes (copies) a dataset. It opens a dialog box where you can specify the destination dataset:



wrpa

Please specify destination data set

NAME exam1d_13C
EXPNO 1
PROCNO 1
DIR C:\Bio
USER guest

Figure 9.16

When you click ***OK***, the entire *expno* directory is copied including raw data, acquisition parameters, processed data and processing parameters. ***wrpa*** takes six arguments:

<name> - the dataset name
<expno> - the experiment number
<procno> - the processed data number
<dir> - the disk unit (data directory)
<user> - the user
y - overwrite the destination dataset if it already exists

All arguments are parts of the destination data path[1], except for the last one which is a flag. You can, but do not have to, specify all of these arguments. If the first argument is a character string, it is interpreted as the destination data name. If the first argument is an integer value, it is interpreted as the destination experiment number. Examples of using ***wrpa*** are:

```
wrpa <name>
wrpa <expno>
wrpa <name> <expno>
wrpa <name> <expno> <procno>
wrpa <name> <expno> <procno> <dir> <user> y
```

wra makes a copy of the current *expno* directory, including raw data, acquisition parameters, and processing parameters. The command takes two arguments and can be used as follows:

wra - prompts you for the destination experiment number
wra <expno> - copies the raw data to <expno>
wra <expno> y - overwrites existing raw data in <expno>

wrp makes a copy of the current *procno* directory, including the processed data and processing parameters. The command takes two arguments and can be used as follows:

wrp - prompts you for the destination processed data number
wrp <procno> - copies processed data to <procno>
wrp <procno> y - overwrites existing processed data in <procno>

wrpparam works like ***wrp***, except that it does not copy the processed data files and `auditp.txt` file.

wraparam works like ***wra***, except that it does not copy the raw data files and `audita.txt` file.
Note that the ***wr**** commands only work if user who started TOPSPIN has the permission to create the destination dataset.

INPUT AND OUTPUT FILES

For ***wrpa***, ***wra*** and ***wraparam***:

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data

[1] The data path of the foreground dataset is displayed above the TOPSPIN data field

`ser` - 2D or 3D raw data
`acqu` - acquisition parameters
`acqus` - acquisition status parameters

For ***wrpa*** and ***wra*** :

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - raw data (1D)
`ser` - raw data (nD)
`audita.txt` - acquisition audit trail

For ***wrpa***, ***wra***, ***wrp*** and ***wrpparam***:

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

`proc` - processing parameters
`procs` - processing status parameters

For ***wrpa***, ***wra*** and ***wrp***:

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

`1r`, `1i` - processed data (1D)
`2rr`, `2ir`, `2ri`, `2ii` - processed data (2D)
`3rrr`, `3irr`, `3rir`, `3rri`, `3iii` - processed data (3D)
`4rrrr`, `4iiii` - processed 4D data
`auditp.txt` - processing audit trail

For 2D data, the additional parameter files `acqu2`, `acqu2s`, `proc2` and `proc2s` will be created. For 3D, 4D etc. data, the respective additional parameter files will be created.
Note that apart from data and parameters several other files are copied.

USAGE IN AU PROGRAMS

WRPA(name, expno, procno, diskunit, user)

WRA(expno)

WRP(procno)

Note that these macros overwrite possibly existing data.

SEE ALSO

new, open, re, rep, rew, repw, reb, dir*

Chapter 10

Parameters, lists, AU programs

This chapter describes all TOPSPIN commands which handle parameters and parameter sets. Furthermore, you will find commands that are used to read or edit lists like pulse programs, gradient programs, frequency lists etc. Note that several commands in this chapter are acquisition related rather than processing related. Nevertheless they play a role in the processing part of TOPSPIN.

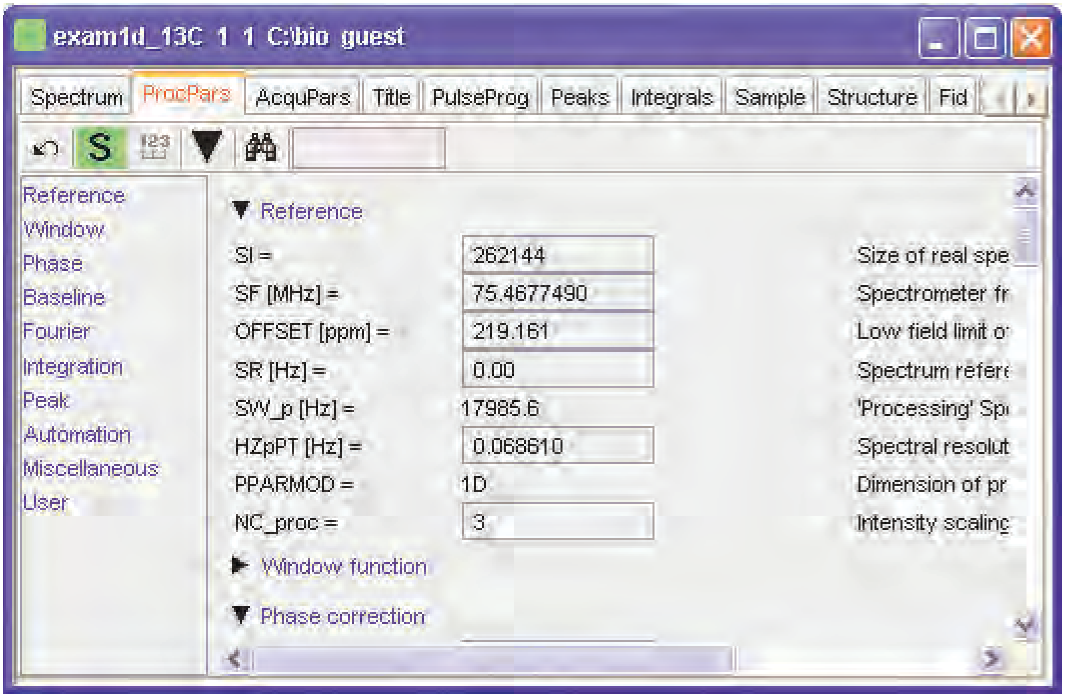
dpp

NAME

dpp - Display processing status parameters (1D,2D,3D)

DESCRIPTION

The command ***dpp*** displays the processing status parameters. Entering ***dpp*** is equivalent to clicking the ***ProcPars*** tab in the data window and clicking the S button.



SI = 262144 Size of real spe
SF [MHz] = 75.4677490 Spectrometer fr
OFFSET [ppm] = 219.161 Low field limit o
SR [Hz] = 0.00 Spectrum refere
SW_p [Hz] = 17985.6 'Processing' Sp
HZpPT [Hz] = 0.068610 Spectral resolut
PPARMOD = 1D Dimension of pr
NC_proc = 3 Intensity scaling

Figure 10.1

The processing status parameters are set by processing commands and represent the status of the processed data. As such, they can only be viewed in the ***dpp*** window.

The following buttons are available:

↶ Undo the last modification (unused for status parameters)

S Switch between processing and processing status parameters

🔍 Search for the parameter specified in the search field

Processing status parameters can also be viewed by entering their names on the command line. For example:

s ft_mod
display the processing status parameter FT_mod

s nc_proc
display the processing status parameter NC_proc

INPUT FILES

<tshome>/classes/prop/

`pared.prop` - parameter properties file

<tshome>/exp/stan/nmr/form/

`proc.e` - processing parameter format file

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

`procs` - processing status parameters

On 2D and 3D data the files `proc2s` and `proc3s` are used for the second and third direction, respectively (see also chapter 2.3).

SEE ALSO

edp, dpa

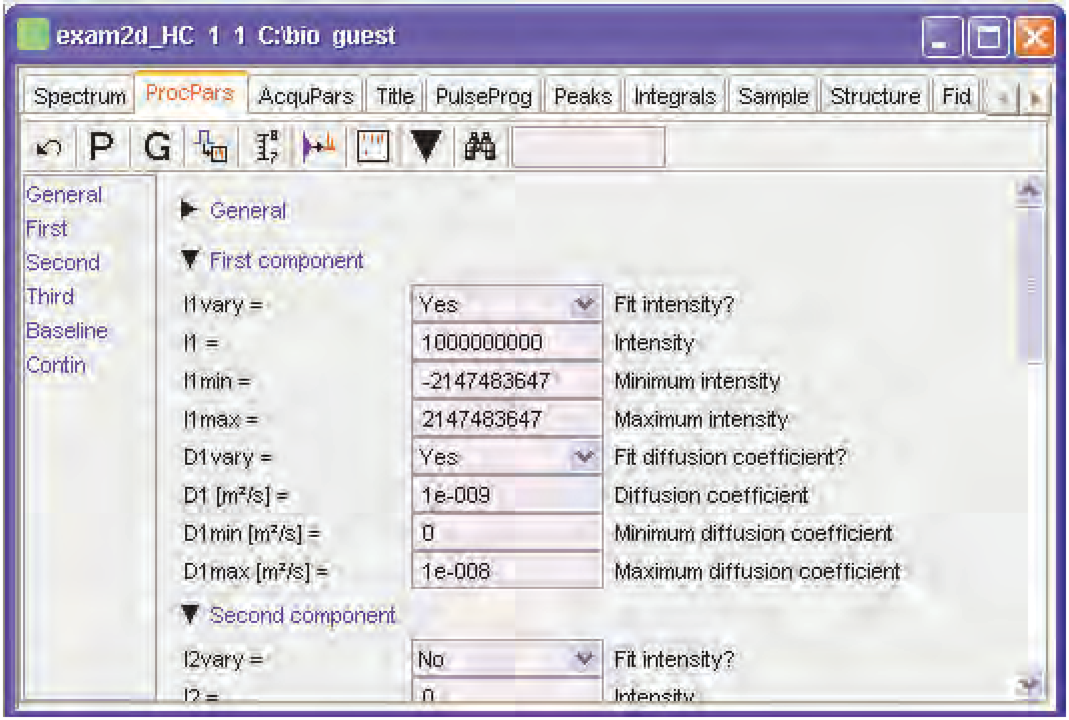
eddosy

NAME

eddosy - Edit DOSY processing parameters (2D,3D)

DESCRIPTION

The command ***eddosy*** opens a dialog box in which you can set DOSY processing parameters.



▶ General

▼ First component

I1vary =	Yes	Fit intensity?
I1 =	1000000000	Intensity
I1min =	-2147483647	Minimum intensity
I1max =	2147483647	Maximum intensity
D1vary =	Yes	Fit diffusion coefficient?
D1 [m²/s] =	1e-009	Diffusion coefficient
D1min [m²/s] =	0	Minimum diffusion coefficient
D1max [m²/s] =	1e-008	Maximum diffusion coefficient

▼ Second component

I2vary =	No	Fit intensity?
I2 =	0	Intensity

Figure 10.2

These parameters are used by the command ***dosy2d*** and ***dosy3d*** on 2D and 3D data, respectively.

The following buttons are available:

↶ Undo the last modification. Can be used repeatedly.

P Switch to processing parameters

G Switch to Gifa parameters

Copy parameters from experiment (AU program ***`setdiffparm`***)

Get display limits from dataset

Execute Fourier Transform (command ***`xf2`***)

Start fitting

Search for the parameter specified in the search field

For more information on ***`eddosy`***:

click ***Help*** → ***Manuals*** → [**Acquisition Application Manuals**] ***Dosy***

INPUT FILES

<tshome>/exp/stan/nmr/form/

`dosy.e` - format file for ***`eddosy`***

INPUT AND OUTPUT FILES

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

`dosy` - DOSY processing parameters

SEE ALSO

dosy2d, dosy3d

edlist

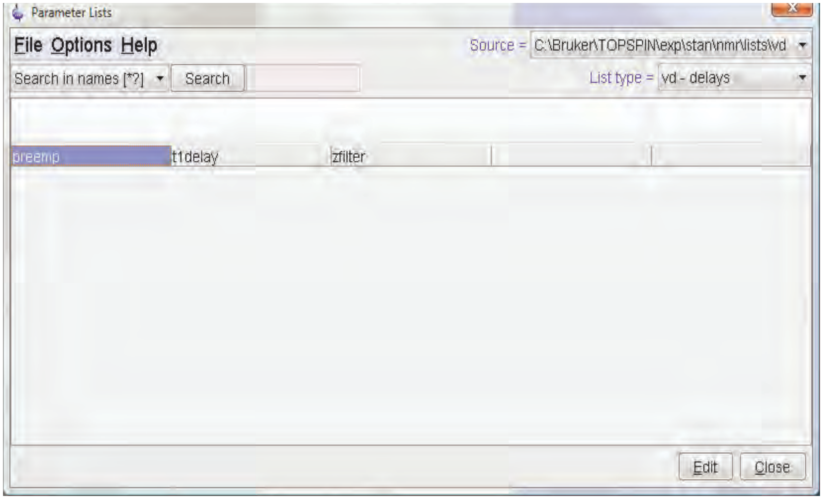
NAME

edlist - Edit Parameter lists

DESCRIPTION

The command ***edlist*** allows you to edit parameter lists like VD Delay lists, VP Pulse lists, VC Loop Counts lists, VA Amplitude lists, VT Temperature lists, F1 Frequency lists, SP Shape lists, DS Data Set lists, SCL Solvent Region lists and PHASE Phases lists.

The command edlist opens the following window (see Figure 10.3).



Source = C:\Bruker\TOPSPIN\exp\stan\nmr\lists\vd

List type = vd - delays

preemp t1delay zfilter

Figure 10.3

On the topright you can change the Source and specifiy the List type with the pull-down menus that should be shown in the table (see figure 10.4). All items shown in the table can be edited in the upcoming text editor.

For detailed information about user-specific definition of ***Source Directories*** and the functionalities of ***Manage Source Directories*** please refer to the information given in Chapter 1.9.

The dialog (Figure 10.3) offers the following buttons:

Edit

After selecting a list by mouseclick the button "edit" opens a text window in which you can edit the chosen list. Same functionality is available by double-click. Saving the modifications will overwrite the existing list.

Close

Closes the dialog.

INPUT/OUTPUT DIRECTORIES

In TopSpin 2.1 and newer the default directory for user-defined lists is:

<tshome>/exp/stan/nmr/lists/<listname>

SEE ALSO

edmisc

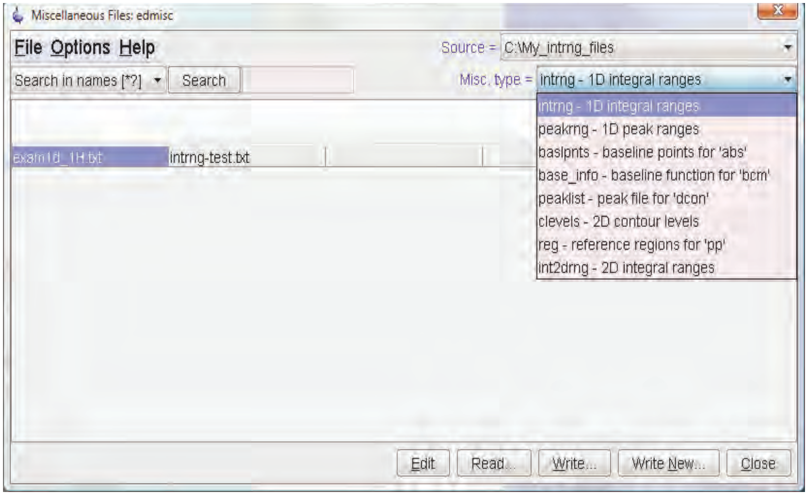
edmisc, rmisc, wmisc, delmisc

NAME

edmisc - Edit miscellaneous lists
rmisc - Read miscellaneous lists
wmisc - Write miscellaneous lists
delmisc - Delete miscellaneous lists

DESCRIPTION

The commands ***misc*** allow you to read, edit, write or delete miscellaneous lists. When entered without arguments, they all open an akin window for Miscellaneous Files. The difference is that ***wmisc*** only offers writing possibilities for Miscellaneous Files, ***rmisc*** only offers reading possibility, whereas with ***edmisc*** and ***delmisc*** you can read, write and edit the correesponding/selected Miscellaneous File, as shown in Figure 10.4.



Miscellaneous Files: edmisc

Source = C:\My_intrng_files
Misc. type = intrng - 1D integral ranges

exam1d_1H.txt
intrng-test.txt

File
Options
Help
Search in names [*?]
Search
intrng - 1D integral ranges
peakrng - 1D peak ranges
baslpnts - baseline points for 'abs'
base_info - baseline function for 'bcm'
peaklist - peak file for 'dcon'
clevels - 2D contour levels
reg - reference regions for 'pp'
int2drng - 2D integral ranges
Edit
Read...
Write...
Write New...
Close

Figure 10.4

On the topright you can change the Source and specifiy the Miscellaneous type that should be shown in the table (see figure 10.4).
All items shown in the table can be edited, read, written or new written. This also corresponds to the commands ***edmisc***, ***rmisc*** and ***wmisc***.

For detailed information about user-specific definition of Source Directories and the functionalities of ***Manage Source Directories*** please refer to the information given in chapter 1.9.

Types of Miscellaneous Files

The lists which can be edited are shown in Table 10.1

list type	contains
`intrng`	integral regions, created by interactive integration or automatic baseline correction (***abs***). Used for spectrum display, print and integral listing.
`base_info`	*polynomial*, *sine* or *exponential* baseline function, created from the baseline mode (***.basl***). Used by the baseline correction command ***bcm***..
`baslpnts`	baseline points created by ***def-pts*** from the baseline mode (***.basl***). Used by the spline baseline correction command ***sab***.
`peaklist`	peak information, created by the command ***ppp*** and ***mdcon auto***. Used by the mixed deconvolution command ***mdcon***.
`reg`	plot regions, created in interactive integration mode (command ***.int***). Used by ***pp***, ***lipp*** when PSCAL=ireg or pireg.

Table 10.1 Miscellaneous list types

When entered on the command line, ***rmisc*** takes two arguments and can be used as follows:

rmisc <type>
Shows all entries of the type <type>. If you select an entry, the corresponding list will be read.

rmisc <type> <name>
Reads the list <name> of the type <type> .

INPUT/OUTPUT DIRECTORIES

In TopSpin 2.1 and newer the default directory of user-defined lists is:

<tshome>/exp/stan/nmr/lists

intrng - integral range files
baslpnts - spline baseline points file
base_info - pol. exp. or sine baseline function files
peaklist - peak information files
reg - plot region files

USGAE IN AU PROGRAMS

RMISC(type, file)

WMISC(type, file)

SEE ALSO

edlist

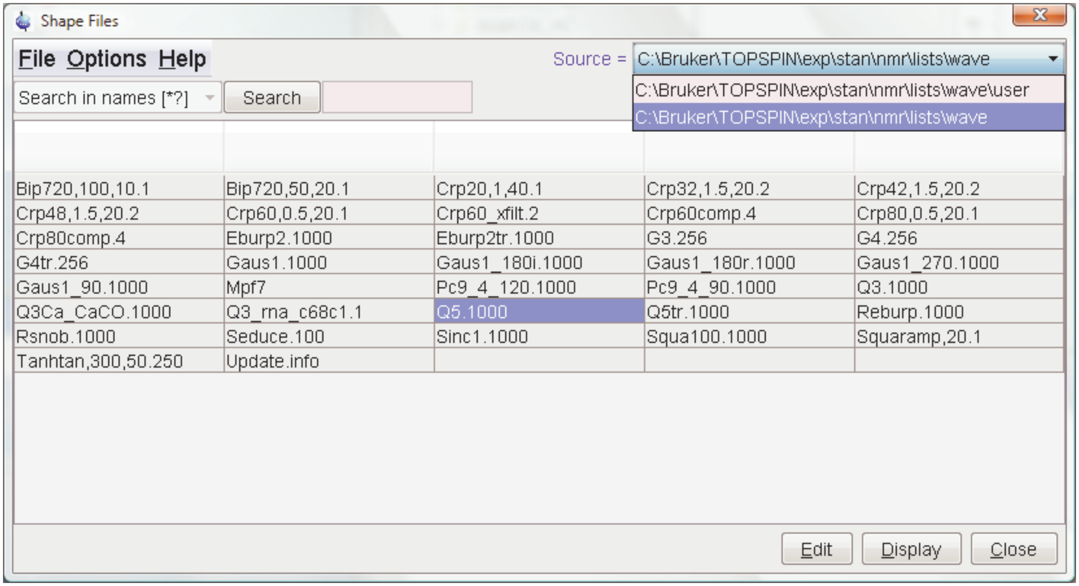
edshape

NAME

edshape - Edit Shape Files
delshape - Delete Shape Files

DESCRIPTION

When entered without arguments, the Shape File commands ***edshape and delshape*** all open the AU program dialog box (see Figure 10.5).



Source = C:\Bruker\TOPSPIN\exp\stan\nmr\lists\wave

C:\Bruker\TOPSPIN\exp\stan\nmr\lists\wave\user
C:\Bruker\TOPSPIN\exp\stan\nmr\lists\wave

Bip720,100,10.1	Bip720,50,20.1	Crp20,1,40.1	Crp32,1.5,20.2	Crp42,1.5,20.2
Crp48,1.5,20.2	Crp60,0.5,20.1	Crp60_xfilt.2	Crp60comp.4	Crp80,0.5,20.1
Crp80comp.4	Eburp2.1000	Eburp2tr.1000	G3.256	G4.256
G4tr.256	Gaus1.1000	Gaus1_180i.1000	Gaus1_180r.1000	Gaus1_270.1000
Gaus1_90.1000	Mpf7	Pc9_4_120.1000	Pc9_4_90.1000	Q3.1000
Q3Ca_CaCO.1000	Q3_rna_c68c1.1	Q5.1000	Q5tr.1000	Reburp.1000
Rsnob.1000	Seduce.100	Sinc1.1000	Squa100.1000	Squaramp,20.1
Tanhtan,300,50.250	Update.info			

Figure 10.5

On the topright of the upcoming window you can find the Sources where the listed Shape Files are stored. With pull-down menu and click on the respective Source you can change the Shape File Source to let them be listed in this dialog.

The AU programs are selected from the **Source** directory as selected at the upper right of the dialog. Note that:

```
<tshome>\exp\stan\nmr\lists\wave
```

contains all Bruker Shape Files.

```
<tshome>\exp\stan\nmr\lists\wave\user
```

contains all user defined Shape Files.

The dialog offers the following buttons:

Edit

Edit the selected Shape File. Equivalent to double-clicking the Shape File name or entering ***`edshape <name>`*** on the command line.

Display

Display the selected Shape File. The Shape Tool will be opened for display the current Shape File (The result can be seen in 10.6).

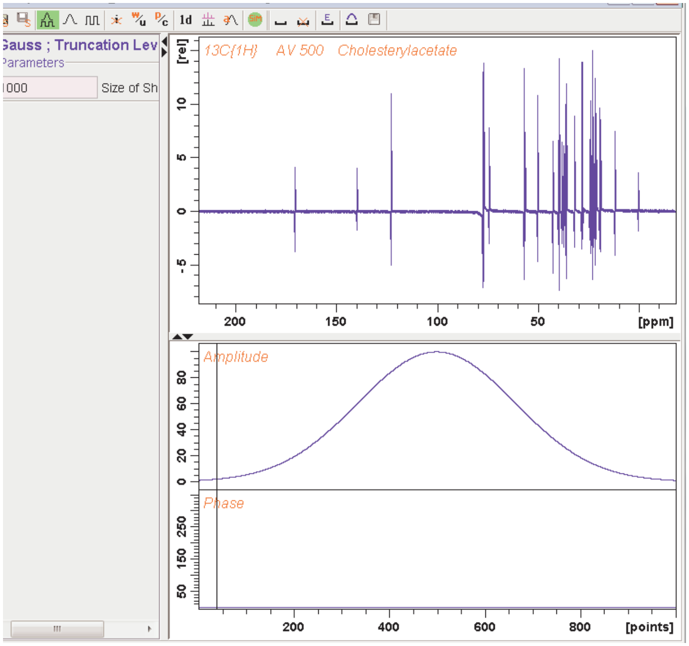


Figure 10.6

Close

Close the dialog.

The File menu

The ***File*** menu offers the following functions:

New...

Create a new Shape File. Note that new Shape Files can only be stored in user defined directories.

Save as...

Save the selected Shape Files under a new name. A dialog will appear where you can specify the Shape File name and destination directory.

Delete...

Delete the selected Shape File.

Rename...

Rename the selected Shape file. Note that only user defined Shape Files can be renamed.

Export...

Export the selected Shape File to an arbitrary directory. A file dialog will appear where you can select/specify the destination directory.

Import...

Import a Shape File from an arbitrary directory. A file dialog will appear where you can select/specify the Shape File.

Close

Close the Shape File lists.

The Options menu

The ***Options*** menu offers the following functions:

Show Comment

Toggles between displaying Shape File with/without comments (see Figure 10.7)

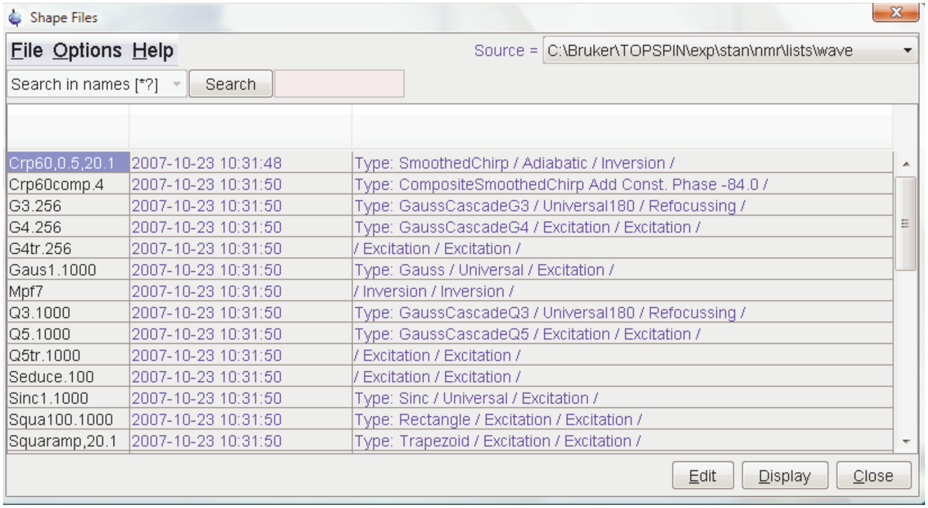
Show Date

Toggles between displaying Shape File with/without date (see Figure

10.7).

Sort by Date

Sort Shape Files by date when selected (see Figure 10.7).



Source = C:\Bruker\TOPSPIN\exp\stan\nmr\lists\wave

Crp60,0.5,20.1	2007-10-23 10:31:48	Type: SmoothedChirp / Adiabatic / Inversion /
Crp60comp.4	2007-10-23 10:31:50	Type: CompositeSmoothedChirp Add Const. Phase -84.0 /
G3.256	2007-10-23 10:31:50	Type: GaussCascadeG3 / Universal180 / Refocussing /
G4.256	2007-10-23 10:31:50	Type: GaussCascadeG4 / Excitation / Excitation /
G4tr.256	2007-10-23 10:31:50	/ Excitation / Excitation /
Gaus1.1000	2007-10-23 10:31:50	Type: Gauss / Universal / Excitation /
Mpf7	2007-10-23 10:31:50	/ Inversion / Inversion /
Q3.1000	2007-10-23 10:31:50	Type: GaussCascadeQ3 / Universal180 / Refocussing /
Q5.1000	2007-10-23 10:31:50	Type: GaussCascadeQ5 / Excitation / Excitation /
Q5tr.1000	2007-10-23 10:31:50	/ Excitation / Excitation /
Seduce.100	2007-10-23 10:31:50	/ Excitation / Excitation /
Sinc1.1000	2007-10-23 10:31:50	Type: Sinc / Universal / Excitation /
Squa100.1000	2007-10-23 10:31:50	Type: Rectangle / Excitation / Excitation /
Squaramp,20.1	2007-10-23 10:31:50	Type: Trapezoid / Excitation / Excitation /

Figure 10.7

Manage Source Directories

Add/modify Shape Files source directories. Shape Files will be searched for in the order of the directories specified.

Detailed information about ***Manage Source Directories*** are described in Chapter 1.9.

INPUT/OUTPUT FILES

In TopSpin 2.1 and newer the default directory for user-defined files is:

```
<tshome>/exp/stan/nmr/lists/files/*
```

SEE ALSO

edlist

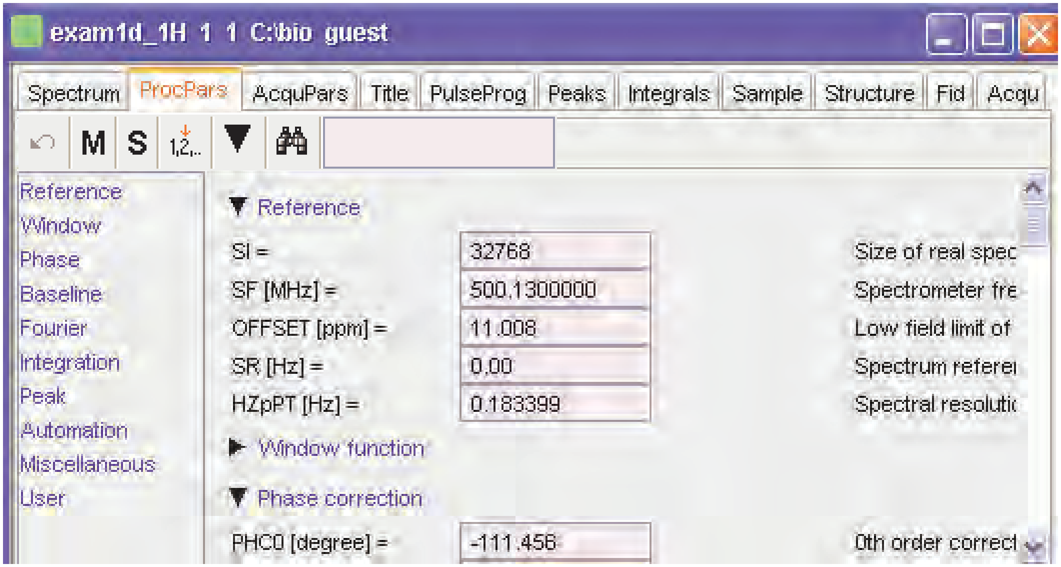
edp

NAME

edp - Edit processing parameters (1D,2D,3D)

DESCRIPTION

The command ***edp*** opens a dialog box in which you can set all processing parameters.



SI = 32768 Size of real spec

SF [MHz] = 500.1300000 Spectrometer fre

OFFSET [ppm] = 11.008 Low field limit of

SR [Hz] = 0.00 Spectrum referei

HZpPT [Hz] = 0.183399 Spectral resolutic

PHC0 [degree] = -111.456 0th order correct

Figure 10.8

Entering ***edp*** on the command line is equivalent to clicking ***ProcPars*** in the tab bar of the data window.

The following buttons are available:

↶ Undo the last modification. Can be used repeatedly.

M Switch to Maxent parameters

S Switch to processing status parameters

Change raw dataset dimensionality (parameter PPARMOD)

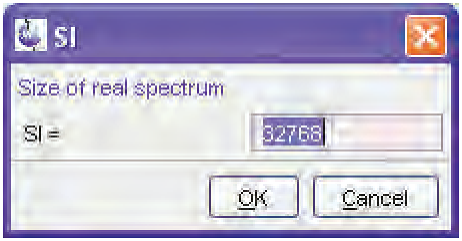
Search for the parameter specified in the search field

Inside the parameter editor, you can do the following actions:

- click a processing step, e.g. Window at the left of the dialog box. The step becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.
- click in a parameter field, e.g. SI to set the parameter value. It is automatically stored.
- 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.

Note that you can also set parameters by entering there names on the command line. A dialog window will appear where you can enter the parameter value(s). For example:

si
on a 1D dataset.



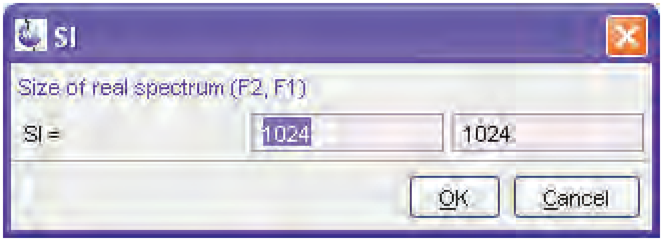
SI = 32768

Figure 10.9

or on a 2D dataset:

Alternatively, you can specify the parameter value as an argument on the command line, For example;

si 4k
The size will be set to 4k



Size of real spectrum (F2, F1)

SI = 1024 1024

Figure 10.10

INPUT AND OUTPUT PARAMETERS

All processing parameters.

INPUT FILES

<tshome>/classes/prop/

`pared.prop` - parameter properties file

<tshome>/exp/stan/nmr/form/

`proc.e` - format file for ***edp***

INPUT AND OUTPUT FILES

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

`proc` - processing parameters
`proc2` - processing parameters for the second direction (2D or 3D)
`proc3` - processing parameters for the third direction (3D)

SEE ALSO

dpp, eda

edpul, edcpd, edpy, edmac

NAME

edpul - Edit pulse programs
edcpd - Edit composite pulse decoupling (CPD) programs
edpy - Edit Python programs
edmac - Edit macros

DESCRIPTION

The commands ***edpul***, ***edcpd***, ***edpy*** and ***edmac*** open a dialog that lists pulse programs, CPD programs, Python programs and macros, respectively. The dialog offers various functions like edit, create, search, delete, import and export. In TOPSPIN 2.1 and newer, these programs are stored in a database.

The dialog for the command ***edpul*** is shown in Figure 10.11. The dialogs for ***edcpd***, ***edpy*** and ***edmac*** have the same menu but can offer different buttons.

Search List Box

Database items can be searched in two possible ways, as can be chosen from the list box at the upper left of the dialog:

- *Search in names*
  to search for a string in the item names.
- *Search in text*
  to search for a string in item text contents.

Search Text Field

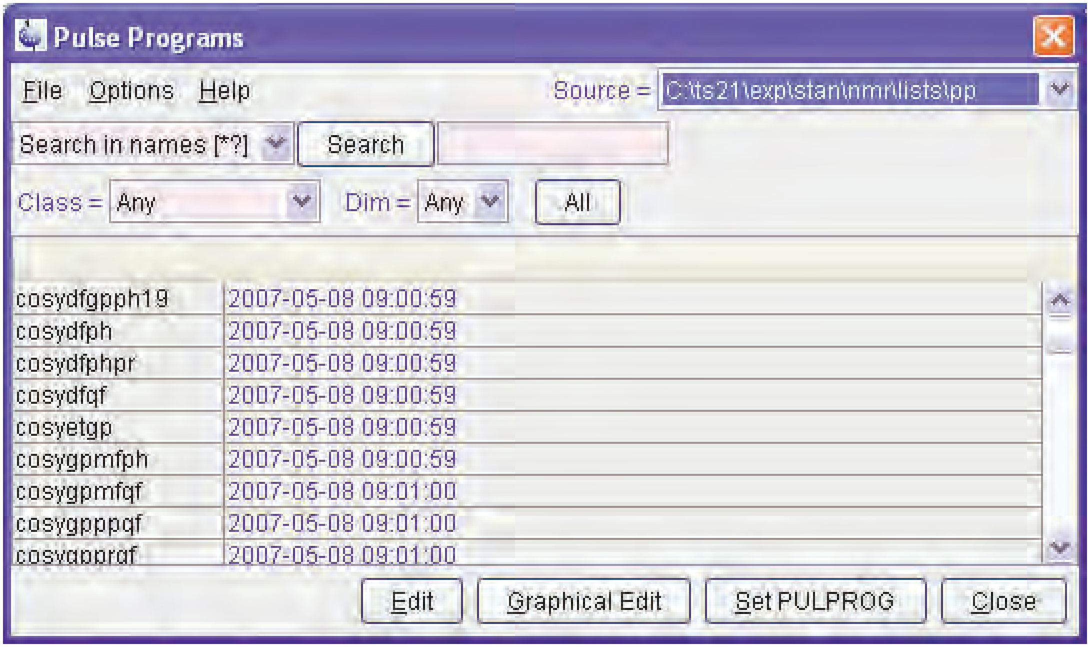
Here you can enter one or more characters of the item name or contents. The following wildcards can be used=:

* : for zero or more occurrences of any character

? : for a single occurrence of any character

Here are some examples:

- *xxx* finds all occurrences of xxx.



Source = C:\ts21\exp\stan\nmr\lists\pp

Search in names [*?]

Class = Any   Dim = Any

```
cosydfgpph19   2007-05-08 09:00:59
cosydfph       2007-05-08 09:00:59
cosydfphpr     2007-05-08 09:00:59
cosydfqf       2007-05-08 09:00:59
cosyetgp       2007-05-08 09:00:59
cosygpmfph     2007-05-08 09:00:59
cosygpmfqf     2007-05-08 09:01:00
cosygpppqf     2007-05-08 09:01:00
cosygpprqf     2007-05-08 09:01:00
```

Figure 10.11

- ??xxx* finds all occurrences of xxx preceded by two arbitrary characters.

A search mask for item names can also be specified on the command line, e.g. ***edpul ??cos****

Conditional List boxes

These list boxes are only offered if the selected item has the corresponding item defined. For example, most high resolution pulse programs have a Class and Dim definition but not Type or SubType definition.

Class

Allows you to show a particular class of items or all items (any).

Dim

Allows you to show items of a particular dataset dimension or all items (any).

Type

Allows you to show a particular type of items or all items (any).

SubType

Allows you to show items of a particular subtype of items or all items (any).

Available Buttons

All

Show items of all classes, dimensions, types and subtypes.

Edit

Opens the selected item (pulse program, CPD program, ...) in the TOPSPIN text editor or viewer, depending on whether the selected item is writable for the current user or not (see below). Writable items can be modified in the editor. They can be saved from the editor as follows:

Click ***File* → *Save*** [**`Ctrl-s`**]

Write-protected items can be saved under a different name as follows:

Click ***File* → *Save as..***

The new item is owned by and writable for the current TOPSPIN user.

Items can also be created /modified with an external (non-TOPSPIN) editor. They can then be imported in the database as described below.

Graphical Edit (for pulse programs only)

Opens a symbolic graphical display of the selected pulse program, with the possibility of graphical editing.

Set PULPROG (for pulse programs only)

Sets the acquisition parameter PULPPROG to the name of the selected pulse program.

The Options menu

The ***Options*** menu offers the following functions:

Show Comment

Toggles between displaying items with/without comments.

Show Date

Toggles between displaying items with/without date.

Sort by Date

Sort items by date when selected.

Manage Source Directories

Add/modify item source directories. Items will be searched for in the order of the directories specified.

For detailed information about Source Directory Handling and ***Manage Source Directories*** please refer to Chapter 1.9.

Export Sources...

Opens a dialog to export an entire item library to a user defined directory. Note the difference to the ***Export*** function under the ***File*** menu (see below).

The File menu

The ***File*** menu offers the following functions:

New

Opens an empty editor for creating a new item, e.g. a pulse program. Saving the text will prompt you for the item name, and will store it in the database. The owner of the item will be the current TOPSPIN user.

Save As...

Saves the selected item under a new name. Opens a dialog where you can selected a source directory and specify a filename.

Delete...

Deletes all selected items from the database (if not write protected). You will be prompted to confirm deletion.

Rename...

Allows you to rename the selected item in the database (if not write protected).

Export...

Exports one or more items to text files. To do that:

1. Mark one or more items in the dialog.
2. Click ***File*** → ***Export...***
3. Select or enter the storage directory and click ***Export...***

The selected item(s) will be stored under their original names, provided there is write permission.

Import...

Imports external item (e.g. pulse program) files into the database and lists it in the dialog. First, it opens a file browser where you can navigate to a directory containing your text files (which may have been created outside of TOPSPIN). Select or enter the desired files in the browser and click the ***Import*** button. The dialog will be updated showing the imported item. Please note that:

- The owner of imported items is the current TOPSPIN user.
- Write-protected items in the database cannot be overwritten by importing items with the same name.
- Writable items with the same name are only overwritten by import, after user confirmation.

Close

Close the dialog

Current TopSpin User

The current TOPSPIN user can be one of the following users:

- the system login user, i.e. the user who started TOPSPIN. This is the case if '*TOPSPIN internal login/logoff*'is disabled.
- the current internal TOPSPIN user. This is the case if '*TOPSPIN internal login/logoff*' is enabled.

To enable/disable '*TOPSPIN internal login/logoff* ', enter **`set`** and click the ***Change*** button to the right of the item *Setup users for internal*....

Write Protection

An item (e.g. pulse program) in the database is write-protected (cannot be modified or deleted), if its owner is *Bruker* or if its owner is not the current TOPSPIN user.

Owner

Each item (e.g. pulse program) in the database has an assigned owner. Please note the following aspects:

- For all items (e.g. pulse programs) delivered by Bruker, the owner is *Bruker*
- The description of the ***Edit**, **New** and **Import*** functions above shows how an owner is assigned to an item.
- Bruker-owned items are write protected (cannot be changed/deleted). They may, however, be copied to a new name (see ***Edit*** above).
- Pulse programs names MUST be unique across all owners! The database cannot contain two pulse programs with same name, even if their assigned owners are different.

Using Pulse/CPD Programs from a User-defined Directory

When you run an acquisition, using commands like ***zg**, **gs**, ..*, the required pulse or CPD program is normally taken from the database. You might, however, want to use pulse programs from an arbitrary, user-defined directory, e.g. for development purposes. You can do this by setting the operating system environment variables *PULPPROG_DIR* and *CPDPROG_DIR*. They can be set in two different ways, with or without a minus sign, determining the item search order.

Examples:

- `PULPPROG_DIR=c:\mydir`
  will cause ***zg***, ***gs***... to search for the pulse program in the database and then, if it did not find it there, in `c:\mydir`. So the database is searched first, then the defined directory.
- `PULPPROG_DIR=-c:\mydir`
  will cause ***zg***, ***gs***... to search for the pulse program in `c:\mydir`, and then, if it did not find it there, in the database. So the directory is searched first, then the database.

Each time a pulse or CPD program is taken from a directory (rather than from the database), a message is written into the history file (to be viewed with command ***hist***).

Please note:

- the commands ***edpul*** and ***edcpd*** do not evaluate the above environment variables.
- When TOPSPIN is running as a client that controls a remote spectrometer, the remote environment variables are evaluated.

About Macros

Macros are text files which contain a sequence of TOPSPIN commands and/or Python commands. A simple macro for processing and plotting the current dataset is:

```
# 1D processing macro

em
ft
apk
sref
autoplot # plot according to Plot Editor layout
```

TOPSPIN commands can be inserted in lower or uppercase letters. Python commands must be entered as follows:

```
xpy <name>
```

All text behind a # character is treated as comment.

About Python programs

Python programming is extensively described in a separate document available under:

click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***Python programming***

INPUT AND OUTPUT FILES

In TopSpin 2.1 and newer the default directories for pulse programs, CPD programs, Macros and Python programs are listed below, just like Bruker default directories:

<tshome>/exp/stan/nmr/lists/pp/* - Bruker pulse programs

<tshome>/exp/stan/nmr/lists/pp/user/* - User defined pulse programs

<tshome>/exp/stan/nmr/lists/cpd/* - Bruker/CPD programs

<tshome>/exp/stan/nmr/lists/cpd/user/* - User CPD programs

<tshome>/exp/stan/nmr/lists/mac/* - Bruker TOPSPIN macros

<tshome>/exp/stan/nmr/lists/mac/user/* - User TOPSPIN macros

<tshome>/exp/stan/nmr/py/* - Bruker Python programs

<tshome>/exp/stan/nmr/py/user/* - User Python programs

SEE ALSO

edlist, delpul, delcpd, delpy, delmac, xmac, xpy

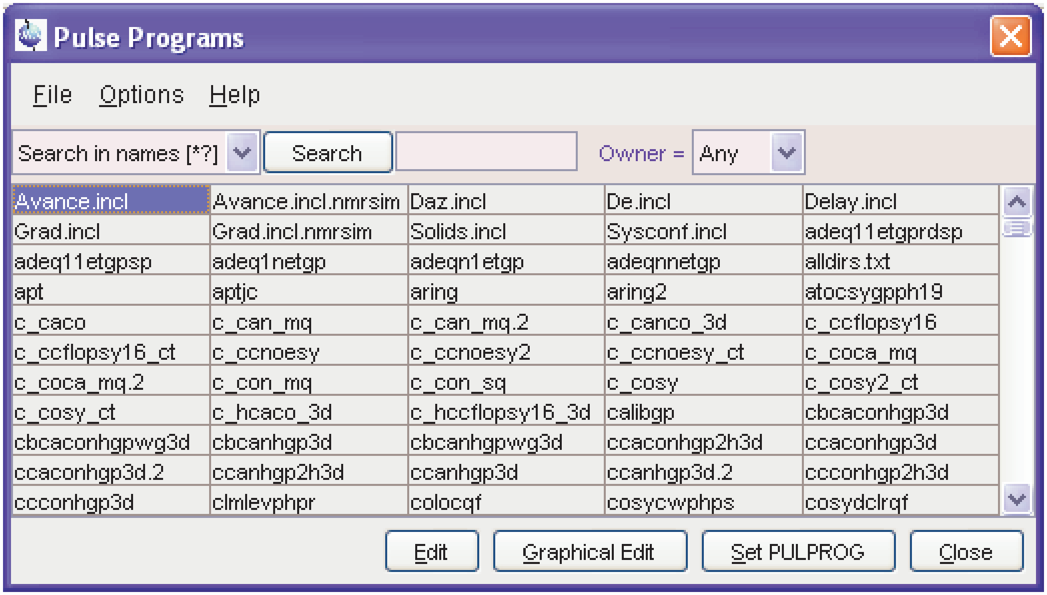
delpul, delcpd, delpy, delmac

NAME

delpul - Delete pulse programs
delcpd - Delete composite pulse decoupling (CPD) programs
delmac - Delete macros
delpy - Delete Python programs

DESCRIPTION

The commands ***delpul***, ***delcpd***, ***delpy*** and ***delmac*** open a dialog from which you can delete pulse programs, CPD programs, Python programs and macros, respectively. In TOPSPIN 2.0 and newer, these programs are stored in a database. The commands open the same dialog as the corresponding commands ***edpul***, ***edcpd***, etc. (see the description of these commands and Figure 10.12).



Avance.incl	Avance.incl.nmrsim	Daz.incl	De.incl	Delay.incl
Grad.incl	Grad.incl.nmrsim	Solids.incl	Sysconf.incl	adeq11etgprdsp
adeq11etgpsp	adeq1netgp	adeqn1etgp	adeqnnetgp	alldirs.txt
apt	aptjc	aring	aring2	atocsygpph19
c_caco	c_can_mq	c_can_mq.2	c_canco_3d	c_ccflopsy16
c_ccflopsy16_ct	c_ccnoesy	c_ccnoesy2	c_ccnoesy_ct	c_coca_mq
c_coca_mq.2	c_con_mq	c_con_sq	c_cosy	c_cosy2_ct
c_cosy_ct	c_hcaco_3d	c_hccflopsy16_3d	calibgp	cbcaconhgp3d
cbcaconhgpwg3d	cbcanhgp3d	cbcanhgpwg3d	ccaconhgp2h3d	ccaconhgp3d
ccaconhgp3d.2	ccanhgp2h3d	ccanhgp3d	ccanhgp3d.2	ccconhgp2h3d
ccconhgp3d	clmlevphpr	colocqf	cosycwphps	cosydclrqf

Figure 10.12

You can delete items as follows:

1. Select the items to be deleted

2. Click ***More ...* → *Delete...***
3. Confirm the appearing warning by clicking ***OK***.

INPUT FILES

<tshome>/exp/stan/nmr/lists/pp/* - pulse programs

<tshome>/exp/stan/nmr/lists/cpd/* - CPD programs

<tshome>/exp/stan/nmr/lists/mac/* - TOPSPIN macros

<tshome>/exp/stan/nmr/py/* - Python programs

SEE ALSO

edpul, edcpd, edpy, xpy, edmac, xmac

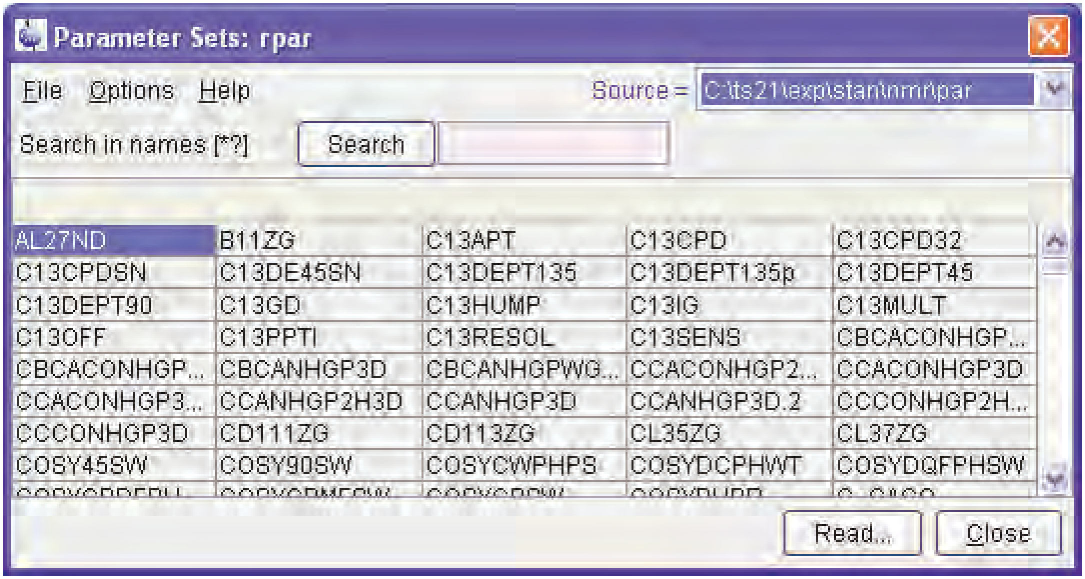
rpar

NAME

rpar - Read a parameter set (1D,2D,3D)

DESCRIPTION

The command ***rpar*** reads a parameter set (experiment) to the current dataset. When it is entered without arguments, ***rpar*** opens a dialog box with a list of available parameter sets.



Source = C:\ts21\exp\stan\nmr\par

AL27ND	B11ZG	C13APT	C13CPD	C13CPD32
C13CPDSN	C13DE45SN	C13DEPT135	C13DEPT135p	C13DEPT45
C13DEPT90	C13GD	C13HUMP	C13IG	C13MULT
C13OFF	C13PPTI	C13RESOL	C13SENS	CBCACONHGP...
CBCACONHGP...	CBCANHGP3D	CBCANHGPWG...	CCACONHGP2...	CCACONHGP3D
CCACONHGP3...	CCANHGP2H3D	CCANHGP3D	CCANHGP3D.2	CCCONHGP2H...
CCCONHGP3D	CD111ZG	CD113ZG	CL35ZG	CL37ZG
COSY45SW	COSY90SW	COSYCWPHPS	COSYDCPHWT	COSYDQFPHSW

Figure 10.13

Here you can select a **Source** directory at the upper right of the dialog, then select a parameter set and click ***Read..*** to read it to the current dataset (for detailed information please refer to paragraphe 1.9). This will open the dialog shown in Figure 10.14. In this dialog, you can select the file types to be read, or just click ***OK*** to read all types.

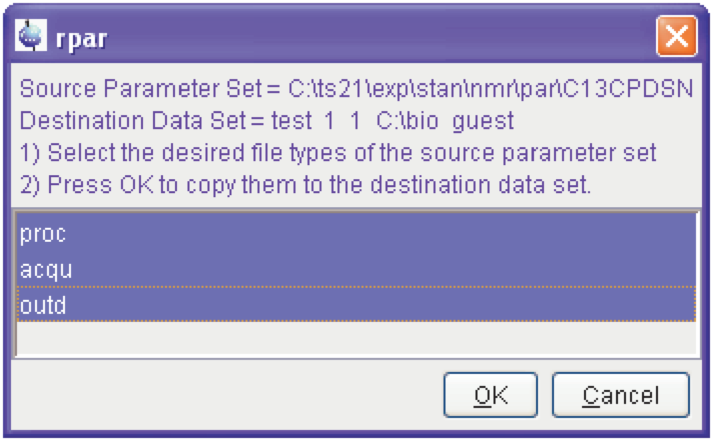
The following buttons are available:

Read...

Read the parameters of the selected parameter set to the current dataset.

Close

Close the ***rpar*** dialog.



Source Parameter Set = C:\ts21\exp\stan\nmr\par\C13CPDSN
Destination Data Set = test 1 1 C:\bio guest
1) Select the desired file types of the source parameter set
2) Press OK to copy them to the destination data set.

Figure 10.14

rpar can be used with arguments

- ***rpar <name>***
  opens a dialog box where you can select individual parameter files of the parameter set <name>. Upon clicking ***OK***, this file is copied to the current dataset.
- ***rpar <name> acqu***
  reads the acquisition parameters (file acqu) of the parameter set <name> to the current dataset.
- ***rpar <name> proc***
  reads the processing parameters (file `proc`) of the parameter set <name> to the current dataset.
- ***rpar <name> acqu proc***
  reads the acquisition and processing parameters (files `acqu` and `proc`) of the parameter set <name> to the current dataset.

- ***rpar <name> all***
  reads all parameter files of the parameter set <name> to the current dataset.
- ***rpar <name> all remove=yes***
  reads all parameter files of the parameter set <name> to the current dataset, deleting all data files and all status parameters

The first argument may contain wildcards, e.g.:

rpar C* shows all parameter sets beginning with the letter C

The ***remove=yes*** argument can be used together with any other argument.

After reading a parameter set with ***rpar***, you can modify parameters of the various types with the commands:

- ***eda*** - acqu parameters
- ***edp*** - processing parameters

Note that Bruker parameter sets contain all parameter types, but user defined parameter sets contain only those parameter types that were stored when the parameter set was created (see ***wpar***). Usually, however, user defined parameter sets are also stored with all parameter types.

Bruker parameter sets are delivered with TOPSPIN and installed with the command ***expinstall***.

User defined parameter sets are created with ***wpar***, which stores the parameters of the current dataset under a new or existing parameter set name.

rpar allows you to read parameters sets of various dimensionalities, 1D, 2D, etc. If the dimensionality of the current dataset and the parameter set you want to read are the same, e.g. both 1D, the current parameter files are overwritten. If the current dataset contains data (raw and/or processed data), these are kept. Furthermore, the status parameters are kept so you still have a consistent dataset. However, as soon as you process the data, the new processing parameters are used, the processed data files are overwritten and the processing status parameters are updated. When you start an acquisition, the new acquisition parameters are used, the raw data are overwritten and the acquisition status parameters are updated.

If the dimensionality of the current dataset and the parameter set you want to read are different, the current parameter files are overwritten, all data files are deleted and status parameters are kept. If the dimensionality is reduced, the superfluous parameter files are deleted.

INPUT FILES

<tshome>/exp/stan/nmr/par/<1D parameter set>/

`acqu` - acquisition parameters
`proc` - processing parameters
`outd` - output device parameters

<tshome>/exp/stan/nmr/par/<2D parameter set>/

`acqu` - F2 acquisition parameters
`acqu2`- F1 acquisition parameters
`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`outd` - output device parameters
`clevels` - 2D contour levels

3D parameter sets also contain the files `acqu3` and `proc3` for the third direction.

OUTPUT FILES

<dir>/data/<user>/nmr/<1D data name>/<expno>/

`acqu` - acquisition parameters

<dir>/data/<user>/nmr/<1D data name>/<expno>/pdata/<procno>/

`proc` - processing parameters
`outd` - output device parameters

<dir>/data/<user>/nmr/<2D data name>/<expno>/

`acqu` - F2 acquisition parameters
`acqu2` - F1 acquisition parameters

<dir>/data/<user>/nmr/<2D data name>/<expno>/pdata/<procno>/

`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`outd` - output device parameters

`clevels` - 2D contour levels

In TOPSPIN 2.1 and newer, the default directory for user defined parameter sets is:

<tshome>/exp/stan/nmr/par/user

USAGE IN AU PROGRAMS

RPAR(name, type)

SEE ALSO

wpar, delpar, expinstall

wpar, edpar

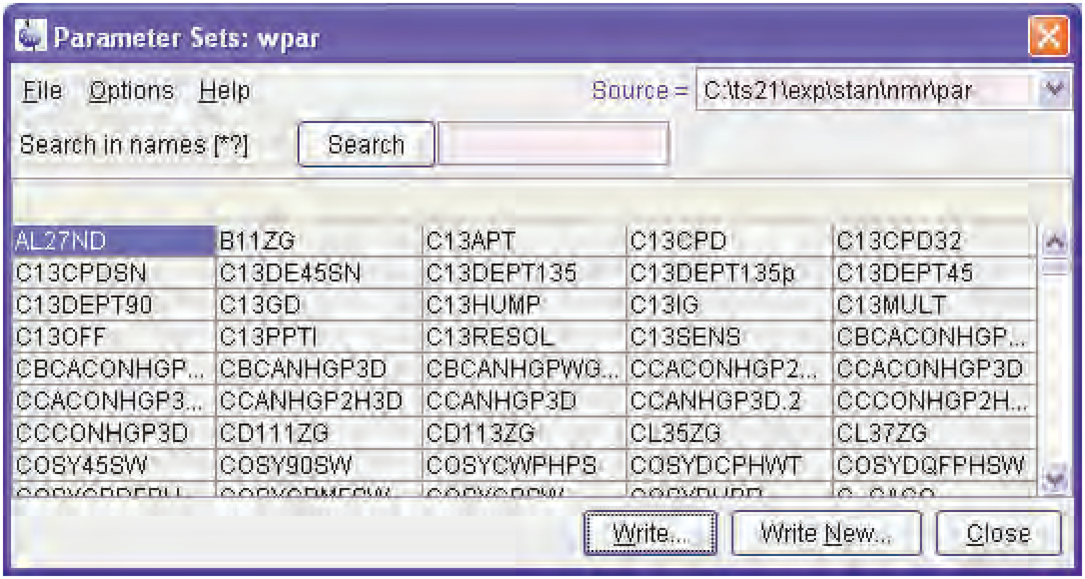
NAME

wpar - Write a parameter set
edpar - Edit a parameter set

DESCRIPTION

The command ***wpar*** stores the parameters of the current dataset in a parameter set. It opens a dialog box where you can select an experiment name and then click ***Write..*** to store it or click ***Write New...*** to store the them under a new name. (see Figure 10.15).

The command ***edpar*** opens an ankin dialog as ***rpar*** and ***wpar*** command. The difference to ***wpar*** and ***rpar*** is that with ***edpar*** parameter sets can be read, written, written new and edited, whereas ***rpar*** only offer reading possibilities for parameter sets and ***wpar*** gives the possibility to write and create (button "Write New ...") parameter sets. Same possibilities as ***edpar*** offers the command ***delpar***.



Source = C:\ts21\exp\stan\nmr\par

Search in names [*?]

AL27ND	B11ZG	C13APT	C13CPD	C13CPD32
C13CPDSN	C13DE45SN	C13DEPT135	C13DEPT135p	C13DEPT45
C13DEPT90	C13GD	C13HUMP	C13IG	C13MULT
C13OFF	C13PPTI	C13RESOL	C13SENS	CBCACONHGP...
CBCACONHGP...	CBCANHGP3D	CBCANHGPWG...	CCACONHGP2...	CCACONHGP3D
CCACONHGP3...	CCANHGP2H3D	CCANHGP3D	CCANHGP3D.2	CCCONHGP2H...
CCCONHGP3D	CD111ZG	CD113ZG	CL35ZG	CL37ZG
COSY45SW	COSY90SW	COSYCWPHPS	COSYDCPHWT	COSYDQFPHSW

Figure 10.15

The following buttons are available:

Write...

Write the parameters of the current dataset to the selected parameter set.

Write New...

Write the parameters of the current dataset to a new experiment name. You will be prompted to enter this name.

Close

Close the ***wpar*** dialog.

The parameters are written to the **Source** directory as selected at the upper right of the dialog.

wpar can be used with arguments

- ***wpar <name>***
  opens a dialog box where you can select individual parameter files of the parameter set <name>. Upon clicking ***OK***, this file is copied to the current dataset.
- ***wpar <name> acqu***
  reads the acquisition parameters (file acqu) of the parameter set <name> to the current dataset.
- ***wpar <name> proc***
  reads the processing parameters (file `proc`) of the parameter set <name> to the current dataset.
- ***wpar <name> acqu proc***
  reads the acquisition and processing parameters (files `acqu` and `proc`) of the parameter set <name> to the current dataset.
- ***wpar <name> all***
  reads all parameter files of the parameter set <name> to the current dataset.

The first argument may contain wildcards, e.g.:

wpar C* shows all parameter sets beginning with the letter C

Bruker standard experiment names should not be used when storing your own experiments with ***wpar***. The reason is that they are overwritten when a new version of TOPSPIN is installed.

wpar is often used in the following way:

1. Define a new dataset with the command ***new***.
2. Enter ***rpar*** to read a Bruker parameter set which defines the experiment you want to do.
3. Modify the acquisition parameters (with ***eda***) to your preference and run the acquisition.
4. Modify processing parameters (with ***edp***) to your preference and process the data.
5. Store the parameters with ***wpar*** under a new experiment name for general usage.

son is that is that ***rpar*** with two arguments is used in automation.

INPUT FILES

<dir>/data/<user>/nmr/<1D data name>/<expno>/

`acqu` - acquisition parameters

<dir>/data/<user>/nmr/<1D data name>/<expno>/pdata/<procno>/

`proc` - processing parameters
`outd` - output device parameters

<dir>/data/<user>/nmr/<2D data name>/<expno>/

`acqu` - F2 acquisition parameters
`acqu2` - F1 acquisition parameters

<dir>/data/<user>/nmr/<2D data name>/<expno>/pdata/<procno>/

`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`outd` - output device parameters
`clevels` - 2D contour levels

OUTPUT FILES

<tshome>/exp/stan/nmr/par/user/<1D parameter set>

`acqu` - acquisition parameters

`proc` - processing parameters
`outd` - output device parameters

<tshome>/exp/stan/nmr/par/user/<2D parameter set>

`acqu` - F2 acquisition parameters
`acqu2`- F1 acquisition parameters
`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`outd` - output device parameters
`clevels` - 2D contour levels

3D parameter sets also contain the files `acqu3` and `proc3` for the third direction.

Note that in TOPSPIN 2.0 and older, the user subdirectory does not exist and user defined parameter sets are stored in:

<tshome>/exp/stan/nmr/par

the same location as Bruker parameter sets.

USAGE IN AU PROGRAMS

WPAR(name, type)

SEE ALSO

rpar, expinstall

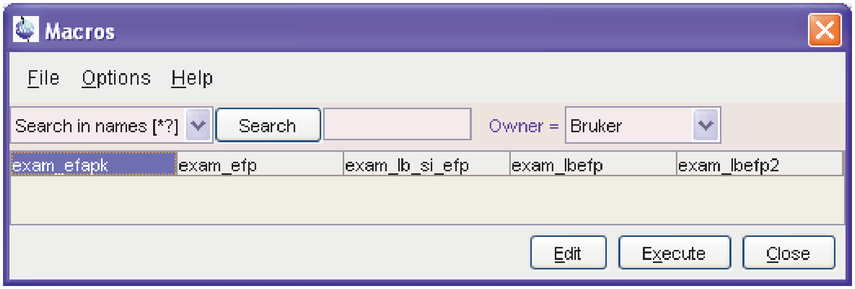
xmac

NAME

xmac - Execute macro

DESCRIPTION

The command ***xmac*** opens a dialog showing all available macros (see Figure 10.16). Just select the desired macro and click the ***Execute*** button to execute it.



Owner = Bruker

Figure 10.16

Macros can also be executed from the command line by entering the macro name, e.g.:

exam_efp

or

xmac exam_efp

The difference is that using the ***xmac*** command searches for macros only, whereas only entering just the name searches for a TOPSPIN command, AU program, Python program or macro of that name.

In TOPSPIN 2.0 and newer, macros are stored in a database. ***xmac*** opens the same dialog as the corresponding commands ***edmac***. For more details, see the description of this command.

SEE ALSO

edmac, delmac, xpy

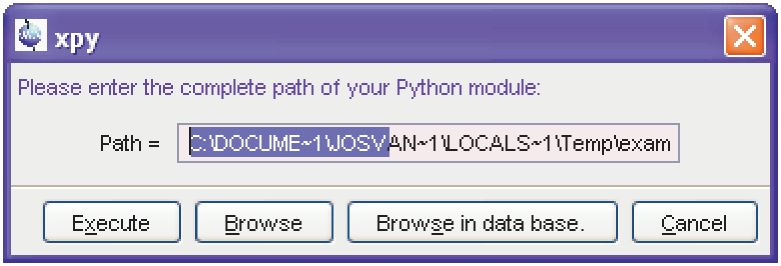
xpy

NAME

xpy - Execute Python program

DESCRIPTION

The command ***xpy*** opens a dialog where you can select the desired Python Program (see Figure 10.17).



Please enter the complete path of your Python module:

Path = C:\DOCUME~1\JOSVAN~1\LOCALS~1\Temp\exam

Figure 10.17

This dialog offer the following functions:

Path

Field where you can enter the full pathname of the Python program. Click ***Execute*** to run it.

Browse

Button to open a file browser where you can enter or select the Python program. Click ***Execute*** to run it.

Browse in data base

Button to open a dialog showing the available Python programs in the database (see Figure 10.1).Just select the desired macro and click the ***Execute*** button to run it. In TOPSPIN 2.0 and newer, Python programs can be stored in a database. ***xpy*** opens the same dialog as the corresponding commands ***edpy***. For more details, see the description of this command.

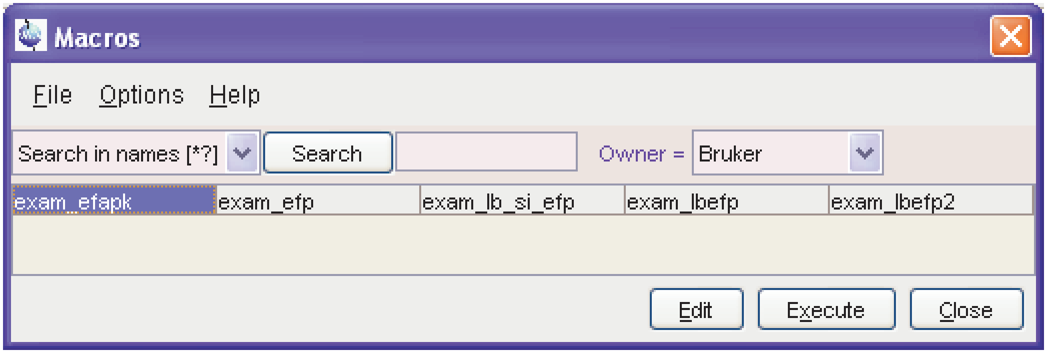


Figure 10.18

Python programs can also be executed from the command line by entering the macro name, e.g.:

ExamCmd4.py

or

xpy ExamCmd4.py

The difference is that using the ***xpy*** command searches for Python programs only, whereas only entering just the name searches for a TOPSPIN command, AU program, Python program or macro of that name.

SEE ALSO

edpy, delpy, xmac

Chapter 11

Automation

This chapter describes all TOPSPIN commands which handle parameters and parameter sets. Furthermore, you will find commands that are used to read or edit lists like pulse programs, gradient programs, frequency lists etc. and, finally, commands which are used to read, edit or run AU programs. Note that several commands in this chapter are acquisition related rather than processing related. Nevertheless they play a role in the processing part of TOPSPIN.

at

NAME

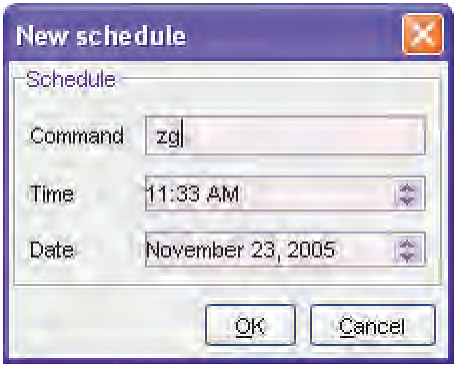
at - schedule a TOPSPIN command for execution

SYNTAX

at [HH[:mm]] [DD[.MM[.YY]]] command

DESCRIPTION

The command ***at*** performs command scheduling. When entered without arguments, it opens the dialog shown in Figure 11.1. Here you can specify the command to be scheduled, e.g. ***zg***, and the starting time and date



Command: zg

Time: 11:33 AM

Date: November 23, 2005

Figure 11.1

The **Time** and **Date** fields are initialized with the current time and date, respectively. By clicking ***OK***, the specified is scheduled for execution.

The time and date, as well as the command to be scheduled can also be specified on the command line, using the following syntax:

```
at [HH[:mm]] [DD[.MM[.YY]]] command
```

Here are some examples:

at 23:30 25.12.07 zg
will start an acquisition on the 25th of December 2007 at 23.30.

at 13 zg

will start an acquisition today at 13:00.

The command ***at*** works user specific, i.e. the scheduled command is only executed if TOPSPIN runs at the specified time and the TOPSPIN internal user is the user who scheduled the command. For more flexible time definition and user independent scheduling, you can use the command ***cron***.

Scheduled commands can be viewed in the command spooler, which can be started with the command ***spooler*** and is available in the spectrometer status bar.

SEE ALSO

cron, qu, qumulti, atmulti, spooler

atmulti

NAME

atmulti - schedule a TOPSPIN command for execution on multiple expnos

SYNTAX

atmulti [{*|1,2,3|1..7|1-7|1-7,20,21}}]

DESCRIPTION

The command ***atmulti*** schedules a command for execution on multiple experiment numbers. It works like ***at***, except that it runs on multiple expnos of the current dataset. When entered without arguments, ***atmulti*** opens the dialog shown in Figure 11.2.

Here you can enter the command to be executed, specify the time and date of execution and select the target experiments numbers. Clicking ***OK*** will then schedule the command for execution.

The command ***atmulti*** takes two arguments, the command to be executed and the target experiment number(s). The dialog will open with the specified arguments preselected. Expnos can be specified in one of the following ways:

`n` : a single experiment number

`*` : all expnos under the current dataname

`n-m` : expno n through m

`n..m` : equivalent to `n-m`

`n,m` : expno n and m

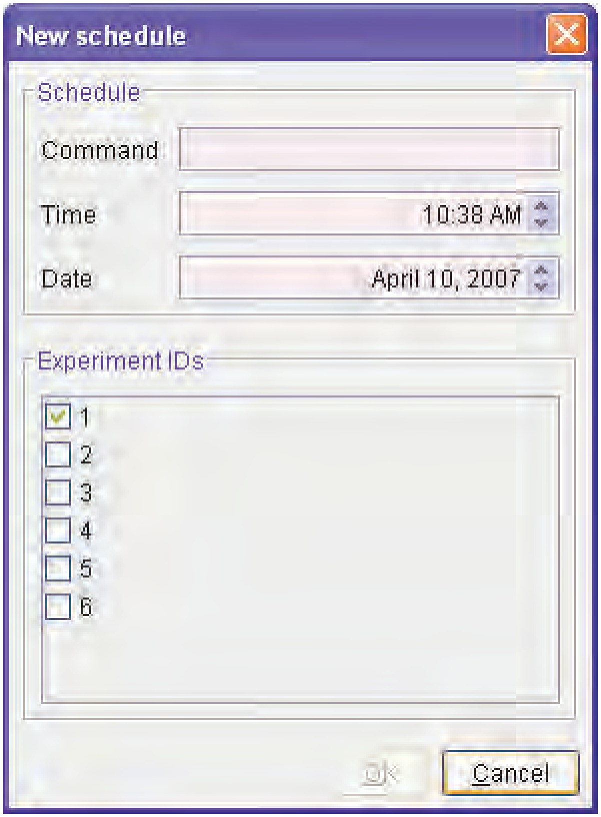
`n m` : equivalent to n,m

The command to be executed can be specified before or after the expno(s).

Examples of argument strings:

The argument:

```
efp 1,3,4-6 8 11
```



New schedule

Schedule

Command

Time 10:38 AM

Date April 10, 2007

Experiment IDs

☑ 1

□ 2

□ 3

□ 4

□ 5

□ 6

Figure 11.2

will preselect the command ***efp*** and the expnos:

1, 3, 4, 5, 6, 8 and 11

The argument:

```
1..8,10 15-20
```

will preselect the expnos:

1, 2, 3, 4, 5, 6, 7, 8, 10, 15, 16, 17, 18, 19 and 20

and leave the command field empty.

Specified expnos which do not exist are ignored. The preselected command and expnos can be modified/extended in the dialog.

To select or deselect all expnos in the opened dialog:

Right-click in the dialog and choose ***Select all*** or ***Deselect all***, respectively.

On clicking ***OK***, a delay job is created for each selected expno, starting with the lowest expno, and sent to the queue.

Scheduled commands can be viewed in the command spooler, which can be started with the command ***spooler*** and is available in the spectrometer status bar.

Note that if you try to exit TOPSPIN while a priority job is still active, you will be warned about this and requested to confirm exiting.

SEE ALSO

at, qu, qumulti, cron, spooler

compileall

NAME

compileall - Compile all Bruker and User AU programs

DESCRIPTION

The command ***compileall*** compiles all Bruker and User AU programs. In order to compile Bruker AU programs, these must have been installed. This can be done with the command ***expinstall***, with the option "Install Bruker library AU programs" enabled.

For more information on AU programs please refer to the AU reference manual.

INPUT FILES

<tshome>/exp/stan/nmr/au/src/*

AU programs (source files)

OUTPUT FILES

<tshome>/prog/au/bin/*

AU programs (executable files)

SEE ALSO

expinstall, cplbruk, cpluser, edau, xau, xaua, xaup, delau

cplbruk, cpluser

NAME

cplbruk - Compile Bruker AU programs
cpluser - Compile user defined AU programs

SYNTAX

cplbruk [<name> | all]
cpluser [<name> | all]

DESCRIPTION

The command ***cplbruk*** allows you to compile one or more Bruker AU programs. Before you can use it, the command ***expinstall*** must have been executed once, with the option "Install Bruker library AU programs" enabled. Then you can use ***cplbruk*** in three different ways:

cplbruk <name> - compile the Bruker AU program <name>
cplbruk all - compile all Bruker AU programs
cplbruk - lists Bruker AU programs; double-click one to compile it

If you specify an argument, then it may contain wildcards; for example ***cplbruk a**** compiles all Bruker AU programs which start with *a*.
cpluser works like ***cplbruk***, except that it compiles user defined AU programs.
For more information on AU programs please refer to the AU reference manual.

INPUT FILES

<tshome>/exp/stan/nmr/au/src/*
AU programs (source files)

OUTPUT FILES

<tshome>/prog/au/bin/*
AU programs (executable files)

SEE ALSO

expinstall, compileall, edau, xau, xaua, xaup, delau

cron

NAME

cron - schedule a TOPSPIN command for execution

DESCRIPTION

The command ***cron*** performs command scheduling. It allows you to executed commands periodically at predefined times. It is more versatile then the commands ***at*** and ***atmulti***.offering full flexibility in time definition, off-schedule execution and user control. When entered without arguments, it opens the dialog shown in Figure 11.1. Here you can specify the command to be scheduled, some scheduling options and the starting time and date. The following fields are available:

Command

The command to be executed.

Description

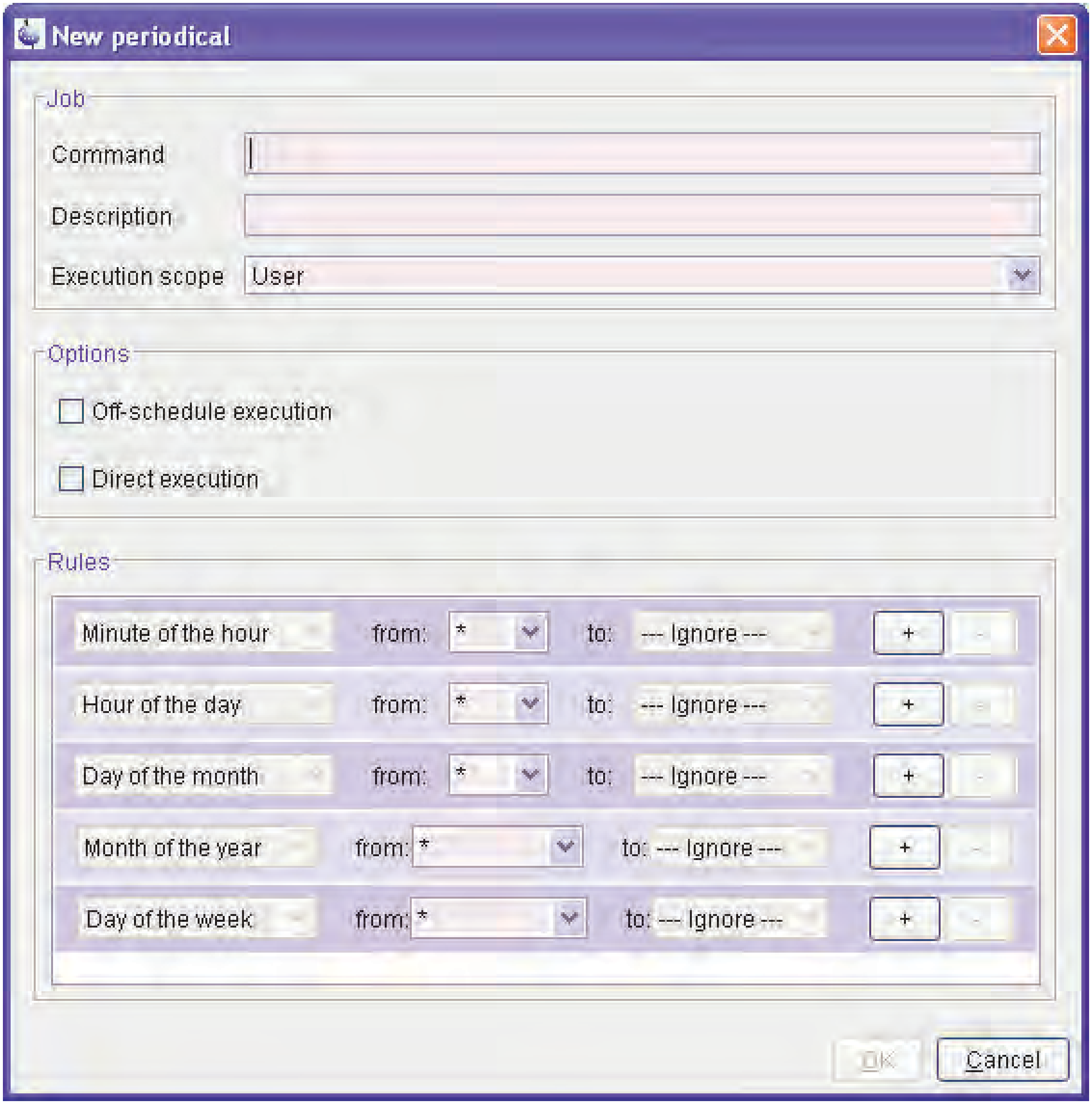
A description of the command.

Execution Scope

The scope of the command execution, *User* of *Topspin*. For scope *User*, the scheduled command will only be executed if TOPSPIN is run by the same (internal) user that is active during cron definition. If the scope is TOPSPIN, the scheduled command will be executed for any (internal) user. Scheduled command with TOPSPIN execution scope can only be defined, cancelled or modified after entering the Administration password.

Off-schedule execution

This flag allows you to executed commands that were scheduled to run at the time when TOPSPIN was not running. These commands are executed after TOPSPIN startup. Note that commands that were scheduled to run multiple times during TOPSPIN downtime are only executed once.



Job

Command

Description

Execution scope: User

Options

□ Off-schedule execution

□ Direct execution

Rules

Minute of the hour	from: *	to: --- Ignore ---	+	-
Hour of the day	from: *	to: --- Ignore ---	+	-
Day of the month	from: *	to: --- Ignore ---	+	-
Month of the year	from: *	to: --- Ignore ---	+	-
Day of the week	from: *	to: --- Ignore ---	+	-

Figure 11.3

The following time scheduling rules exist:

Minute of the hour: 00 through 59

Hour of the day: 00 through 23

Day of the month: 00 through 31

Month of the year: January through december

Day of the week: Sunday through Saturday

For each of these fields, you can define an interval by selecting a value in the **From** and a value in the **To** field. Setting the **To** field to *Ignore*, schedules the command for execution only at the time/date selected in the **From** field. An asterix (*) in the **From** field indicated all possible times. Clicking the + button to the right of a field, adds an extra field of the same type, allowing multiple interval definition. Clicking the - button removes the extra field.

SEE ALSO

at, atmulti, qu, qumulti, spooler

edau, xau, delau

NAME

edau - Edit an AU program
xau - Execute an AU program
delau - Delete an AU program

SYNTAX

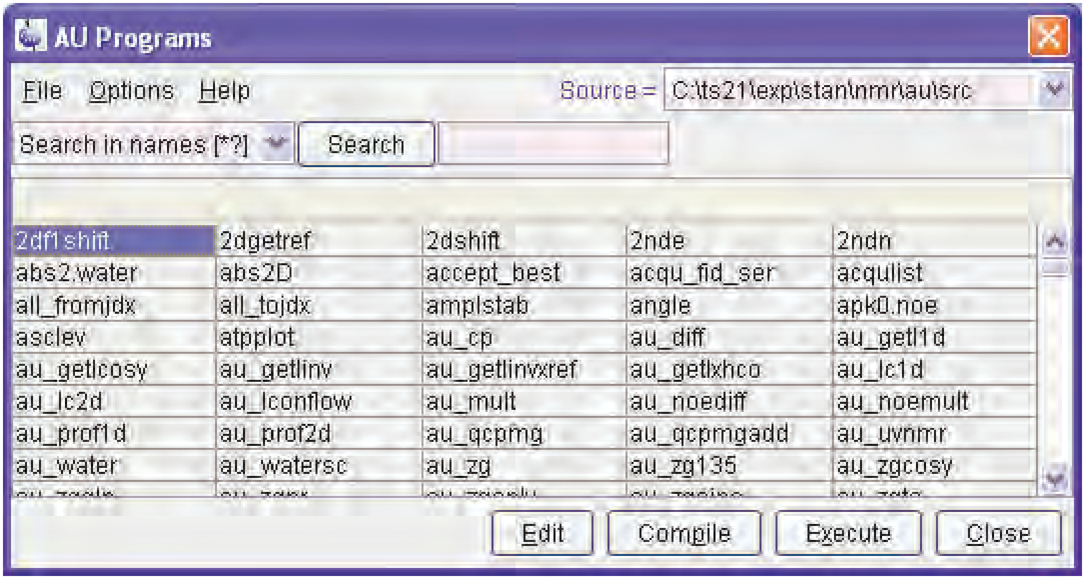
edau [<name>]

xau [<name>]

delau [<name>]

DESCRIPTION

When entered without arguments, the AU program commands ***edau***, ***xau*** and ***delau*** all open the AU program dialog box (see Figure 11.4).



Source = C:\ts21\exp\stan\nmr\au\src

2df1shift	2dgetref	2dshift	2nde	2ndn
abs2.water	abs2D	accept_best	acqu_fid_ser	acqulist
all_fromjdx	all_tojdx	amplstab	angle	apk0.noe
asclev	atpplot	au_cp	au_diff	au_getl1d
au_getlcosy	au_getlinv	au_getlinvxref	au_getlxhco	au_lc1d
au_lc2d	au_lconflow	au_mult	au_noediff	au_noemult
au_prof1d	au_prof2d	au_qcpmg	au_qcpmgadd	au_uvnmr
au_water	au_watersc	au_zg	au_zg135	au_zgcosy

Figure 11.4

The dialog offers the following buttons:

Edit
Edit the selected AU program. Equivalent to double-clicking the AU program name or entering `edau <name>` on the command line.

Compile
Compile the selected AU program. Equivalent to entering ***`cplbruk <name>`*** on the command line.

Execute
Execute the selected AU program. Equivalent to entering ***`<name>`*** or ***`xau <name>`*** on the command line.

Close

Close the dialog.

The AU programs are selected from the **Source** directory as selected at the upper right of the dialog. Note that:

`<tshome>\exp\stan\nmr\au\src`
contains all Bruker AU programs

`<tshome>\exp\stan\nmr\au\src\user`
contains all user defined AU programs

The File menu

The ***File*** menu offers the following functions:

New...
Create a new AU program. Note that new AU programs can only be stored in user defined directories.

Save as...
Save the selected AU program under a new name. A dialog will appear where you can specify the AU program name and destination directory.

Delete...
Delete the selected AU program. Note that both the source and binary AU program are deleted.

Rename...
Rename the selected AU program. Note that both the source and binary AU program are deleted.Note that only user defined AU pro-

grams can be renamed.

Export...
Export the selected AU program to an arbitrary directory. A file dialog will appear where you can select/specify the destination directory.

Import...
Import an AU program from an arbitrary directory. A file dialog will appear where you can select/specify the AU program.

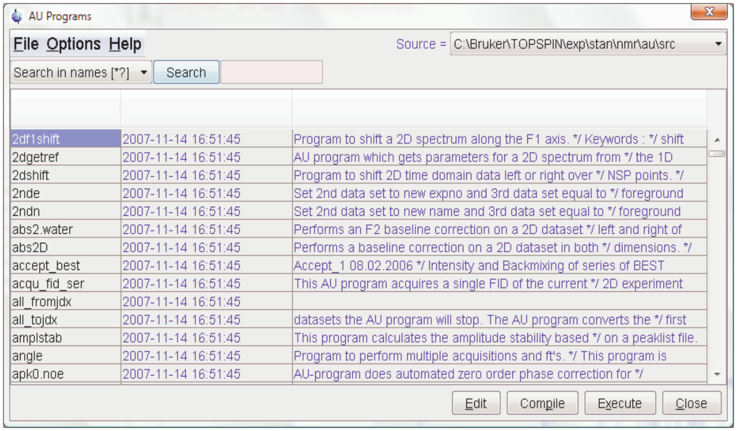
The Options menu

The ***Options*** menu offers the following functions:

Show Comment
Toggles between displaying AU programs with/without comments (see Figure 11.5)

Show Date
Toggles between displaying AU programs with/without date (see Figure 11.5).

Sort by Date
Sort AU programs by date when selected (see Figure 11.5).



Source = C:\Bruker\TOPSPIN\exp\stan\nmr\au\src

2df1shift	2007-11-14 16:51:45	Program to shift a 2D spectrum along the F1 axis. */ Keywords : */ shift
2dgetref	2007-11-14 16:51:45	AU program which gets parameters for a 2D spectrum from */ the 1D
2dshift	2007-11-14 16:51:45	Program to shift 2D time domain data left or right over */ NSP points. */
2nde	2007-11-14 16:51:45	Set 2nd data set to new expno and 3rd data set equal to */ foreground
2ndn	2007-11-14 16:51:45	Set 2nd data set to new name and 3rd data set equal to */ foreground
abs2.water	2007-11-14 16:51:45	Performs an F2 baseline correction on a 2D dataset */ left and right of
abs2D	2007-11-14 16:51:45	Performs a baseline correction on a 2D dataset in both */ dimensions. */
accept_best	2007-11-14 16:51:45	Accept_1 08.02.2006 */ Intensity and Backmixing of series of BEST
acqu_fid_ser	2007-11-14 16:51:45	This AU program acquires a single FID of the current */ 2D experiment
all_fromjdx	2007-11-14 16:51:45	
all_tojdx	2007-11-14 16:51:45	datasets the AU program will stop. The AU program converts the */ first
amplstab	2007-11-14 16:51:45	This program calculates the amplitude stability based */ on a peaklist file.
angle	2007-11-14 16:51:45	Program to perform multiple acquisitions and ft's. */ This program is
apk0.noe	2007-11-14 16:51:45	AU-program does automated zero order phase correction for */

Figure 11.5

Manage Source Directories

Add/modify AU programs source directories. AU programs will be searched for in the order of the directories specified.

Detailed information about ***Manage Source Directories*** are described in Chapter 1.9.

Export Sources...

Opens a dialog to export an entire AU program library to a user defined directory. Note the difference to the ***Export*** function under the ***File*** menu (see below).

When you edit a Bruker AU program, it is shown in view mode which means it cannot be modified. However, if you click ***Save as..*** and store it under a different name, the stored file is automatically opened in edit mode. When you edit a User defined AU program, it is opened in edit mode and can be modified.

When ***edau*** is entered on the command line with an argument, the corresponding AU program will be opened. If it does not exist it will be created. If the argument contains wildcards, the AU dialog box is opened showing the matching AU programs. For example, ***edau a**** displays all AU programs which start with *a*.

Bruker AU programs must be installed once with ***expinstall*** before they can be opened with ***edau***. The installation must be repeated when a new version of TOPSPIN is installed.

edau uses the editor which is defined in the TOPSPIN User Preferences. To change it, enter ***set***, click ***Miscellaneous*** and select or change the editor.

AU programs are usually executed simply by entering their names. The command ***xau*** is only needed in three cases:

- the AU program has not been compiled yet
- a TOPSPIN command with the same name exists
- to call an Au program from another AU program (using the macro XAU)

AU programs run in background and several of them can run simultaneously. The command ***kill*** can be used to stop a running (or hanging)

AU program.

For details on writing, compiling, and executing AU programs please refer to the AU reference manual:

click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***AU programming***

INPUT/OUTPUT FILES

`<tshome>/exp/stan/nmr/au/src/*`

AU program source files

`<tshome>/prog/au/bin/*`

AU program executable binary files

SEE ALSO

expinstall, compileall, cpluser

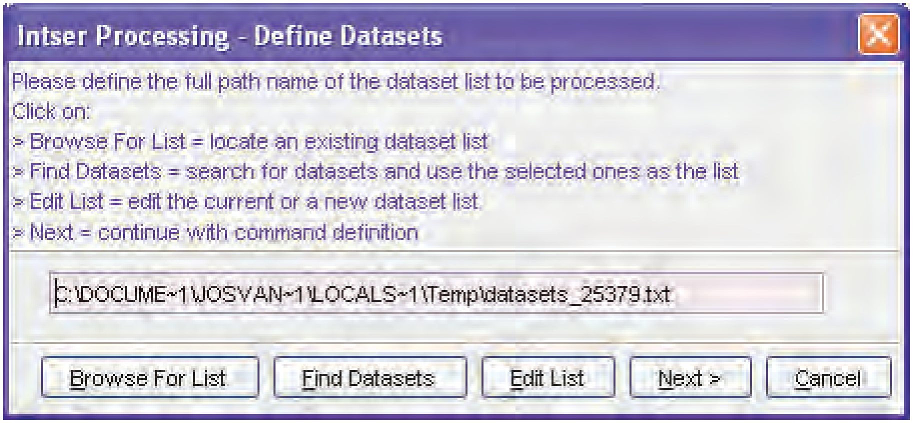
intser

NAME

intser - integrate a list of spectra (1D, 2D)

DESCRIPTION

The command ***intser*** integrates a series of 1D or 2D data. It starts by opening opens the dialog window shown in Figure 11.6.



Intser Processing - Define Datasets

Please define the full path name of the dataset list to be processed.
Click on:
> Browse For List = locate an existing dataset list
> Find Datasets = search for datasets and use the selected ones as the list
> Edit List = edit the current or a new dataset list
> Next = continue with command definition

C:\DOCUME~1\JOSVAN~1\LOCALS~1\Temp\datasets_25379.txt

Figure 11.6

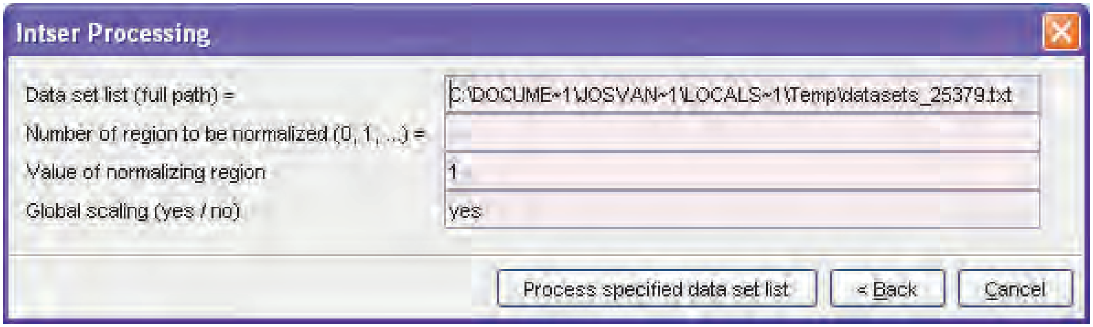
Here you can *specify*, *find* or *edit* the list of datasets to be processed. The functions of the buttons are described in the dialog.

A dataset list is a list of full pathnames, e.g.:

```
C:\bio\data\guest\nmr\exam1d_13C\1\pdata\1
C:\bio\data\guest\nmr\exam1d_13C\2\pdata\1
C:\bio\data\guest\nmr\exam1d_13C\3\pdata\1
```

The first dataset in the list serves as reference dataset. Its PROCNO directory must contain an `intrng` file with the spectral regions to be integrated. This file is created by automatic integration (command ***abs***) or by interactive integration (command ***.int***).

The ***Next*** button in the dialog allows you to go to the next dialog (see Figure 11.7)



Data set list (full path) = C:\DOCUME~1\JOSVAN~1\LOCALS~1\Temp\datasets_25379.txt

Number of region to be normalized (0, 1, ...) =

Value of normalizing region 1

Global scaling (yes / no) yes

Figure 11.7

In this dialog you have to specify the following information:

Number of region to be normalized

An integer 0, 1, 2, ...

Value of normalization region

An arbitrary floating number.

The `intrng` file contains the integral regions in the order the integrals are displayed on screen from left to right. We number them from 0 on. For example, if you specify:

Number of region to be normalized=1

Value of normalization region=37.5

then region 1 of the reference spectrum gets assigned the value 37.5.

Global scaling

Takes the value ***yes*** or ***no***. For ***yes***, all integrals of all spectra in the list will be scaled relative to the normalization region of the reference spectrum.

For ***no***, all integrals of one spectrum will be scaled relative to the normalization region of the same spectrum. The normalization region number and value are same for each spectrum (the specified values).

Clicking the button ***Process specified data set list*** will integrate the data in the specified dataset list.

The integration result is stored in a text file whose contents is shown on the screen. Its format is demonstrated by the following example. Lines beginning with a # are comment lines. The format is suitable to be imported into a spreadsheet program such as Excel for further processing. The example is the result of integrating the 3 defined regions of 3 datasets.

```
# Intser Processing Finished
# Data set list (full path) = c:\intser-list1.txt
# Result file (full path) = c:\res1.txt

# --- Integral info ---
# A 1.0 #regions in PPM
# # low field high field bias slope
# 8.44574704397792 8.322631197855793 -0.0 -0.0 # for region 1
# 7.821960090292476 7.485443444225329 -0.0 -0.0 # for region 2
# 7.345912151953584 7.206380859681841 -0.0 -0.0 # for region 3

# Spectrum number; Integral range 0; Integral range 1; Integral range 2;
0;0.307;0.587;1;
1;0.615;1.174;2;
2;1.229;2.348;4;
```

The command ***`intser`*** can also be used to integrate a series of 2D data. Note that in this case the file containing the integral regions is `int2drng`.

SEE ALSO

serial

qu

NAME

qu - queue a TOPSPIN command for execution

DESCRIPTION

The command ***qu*** queues a command for execution. It requires one argument, the command to be queued. For example, the command:

```
qu xfb
```

queues the command ***xfb*** for execution. This means that ***xfb*** is executed as soon as the currently running command and previously queued commands have finished.

Command queuing can, for example be used, to process a 2D dataset immediately after acquisition. This is done with the command sequence:

```
zg
qu xfb
```

Note that in TOPSPIN 2.0 and newer, acquisition command like ***zg***, ***go***, ***rga*** and ***atma*** are automatically queued, if *auto-spooling* is enabled in the User Preferences (command ***set***).

Queued commands can be viewed in the command spooler, which can be started with the command ***spooler*** and is available in the spectrometer status bar.

SEE ALSO

cron, at, qumulti, atmulti, spooler

qumulti

NAME

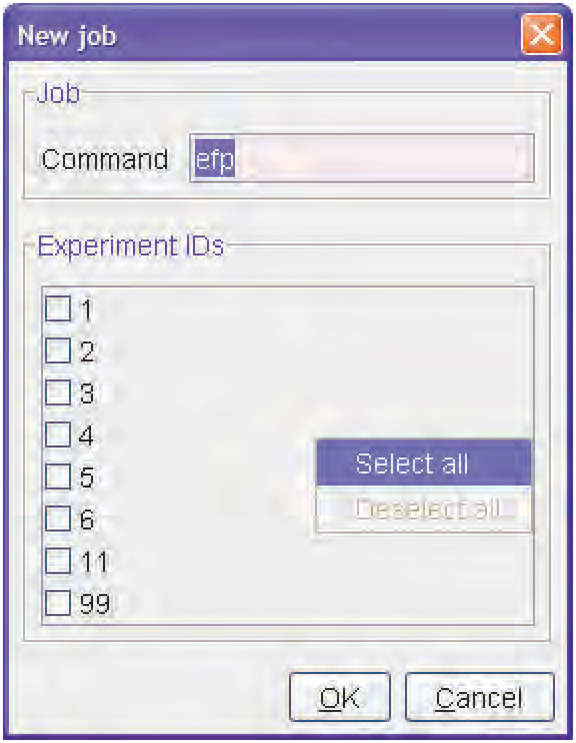
qumulti - queue a TOPSPIN command for execution on multiple expnos

SYNTAX

qumulti [{*|1,2,3|1..7|1-7|1-7,20,21}]

DESCRIPTION

The command ***qumulti*** queues a command for execution on multiple expnos of the current dataset. When entered without arguments, ***qumulti*** opens the dialog shown in Figure 11.8.



Command efp

Figure 11.8

Here you can enter the command to be executed and select the experiments numbers on which the specified command should work. The dialog shows all available expnos, with the active dataset selected.

Clicking ***OK*** queues the command for execution.

The command ***qumulti*** takes two arguments, the command to be executed and the target experiment number(s). The dialog will open with the specified arguments preselected. Expnos can be specified in one of the following ways:

`n` : a single experiment number

`*` : all expnos under the current dataname

`n-m` : expno n through m

`n..m` : equivalent to `n-m`

`n,m` : expno n and m

`n m` : equivalent to n,m

The command to be executed can be specified before or after the expno(s).

Examples of argument strings:

The argument:

```
efp 1,3,4-6 8 11
```

will preselect the command ***efp*** and the expnos:

1, 3, 4, 5, 6, 8 and 11

The argument:

```
1..8,10 15-20
```

will preselect the expnos:

1, 2, 3, 4, 5, 6, 7, 8, 10, 15, 16, 17, 18, 19 and 20

and leave the command field empty.

Specified expnos which do not exist are ignored. The preselected command and expnos can be modified/extended in the dialog.

To select or deselect all expnos in the opened dialog:

Right-click in the dialog and choose ***Select all*** or ***Deselect all***, respectively.

If ***qumulti*** is entered without argument, only the current expno is preselected.

On clicking ***OK***, a priority job is created for each selected expno, starting with the lowest expno, and sent to the queue.

Queued commands can be viewed in the command spooler, which can be started with the command ***spooler*** and is available in the spectrometer status bar.

Note that if you try to exit TOPSPIN while a priority job is still active, you will be warned about this and requested to confirm exiting.

SEE ALSO

cron, qu, at, atmulti, spooler

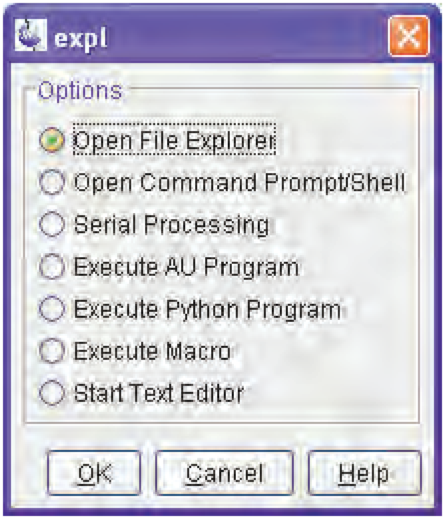
run

NAME

run - Open dialog for starting macro, AU, Python or serial

DESCRIPTION

The command ***run*** opens the run dialog window:



expl

Options

● Open File Explorer
○ Open Command Prompt/Shell
○ Serial Processing
○ Execute AU Program
○ Execute Python Program
○ Execute Macro
○ Start Text Editor

Figure 11.9

This dialog box has various options, each of which selects a certain command for execution.

Open the file explorer

This option selects the command ***expl*** for execution. It opens the File Explorer showing the processed data files (the files in the *procno* directory) of the active dataset. Under Linux the KDE konqueror will be opened. If no dataset is open in the TOPSPIN data area, the Explorer will show the users home directory. ***expl*** allows you access to the current data files as well as the entire data directory tree.

An alternative way to access data files is to right-click inside the data window and select ***Files*** in the appearing popup menu.

Open Command Prompt/Shell

This option selects the command ***shell*** for execution. It opens a Windows COmmand Prompt or Linux Shell, depending on your operating system.

Serial Processing

This option selects the command ***serial*** for execution. It opens a dialog window where you can set up and start data processing of a series of datasets using TOPSPIN commands, macros or Python programs.

Execute an AU program

This option selects the command ***xau*** for execution. It opens the AU dialog box showing a list of available AU program. Here you can select an AU program and click ***Execute*** to execute it. ***xau*** can also be entered on the command line in which case you can specify the AU program as an argument.

Execute a Python program

This option selects the command ***xpy*** for execution. It prompts you for the pathname of a Python program. Just enter this pathname and click ***OK*** to execute the Python program.

Execute a Macro

This option selects the command ***xmac*** for execution. It opens the Macro dialog box showing a list of available macros. Here you can select macro and click ***Execute*** to execute it. ***xmac*** can also be entered on the command line in which case you can specify the macro as an argument.

Open a text editor

This option selects the command ***edtext*** for execution. It opens an empty text file with the TOPSPIN editor. The file can be stored in any directory.

SEE ALSO

expl, shell, xau, xpy, xmac, edtext

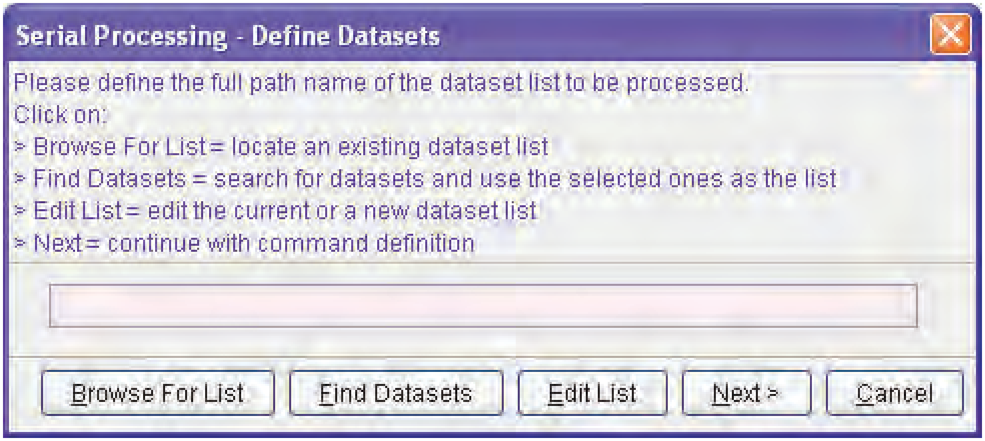
serial

NAME

serial - Serial processing with macro or Python script

DESCRIPTION

The command ***serial*** opens the dialog window shown in Figure 11.10.



Serial Processing - Define Datasets

Please define the full path name of the dataset list to be processed.
Click on:
> Browse For List = locate an existing dataset list
> Find Datasets = search for datasets and use the selected ones as the list
> Edit List = edit the current or a new dataset list
> Next = continue with command definition

Figure 11.10

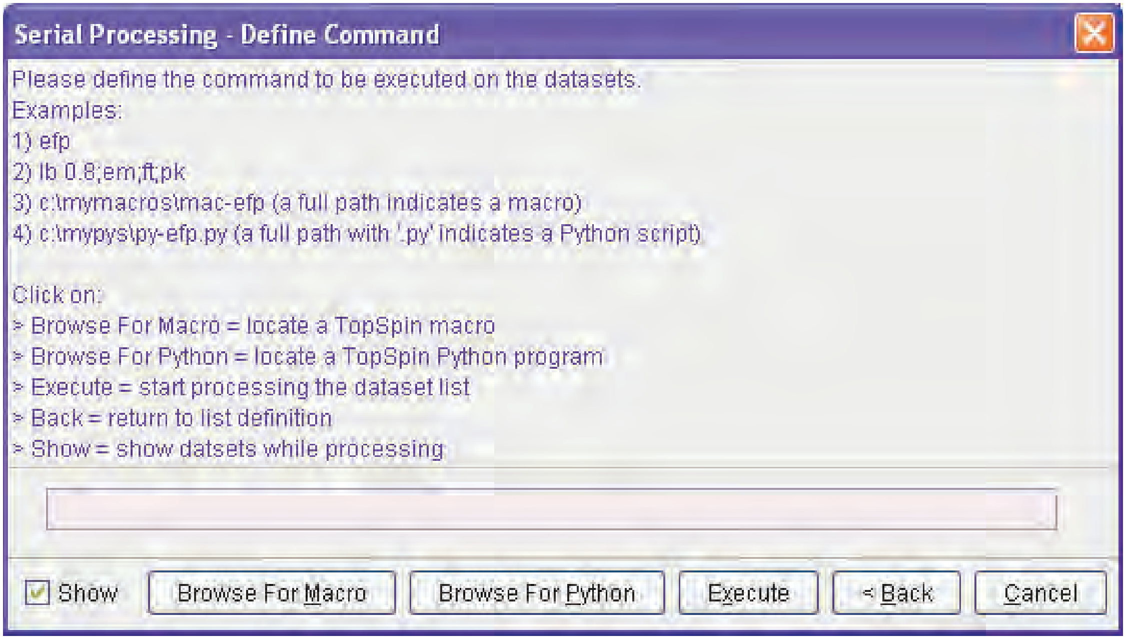
Here you can specify, find or edit the list of datasets to be processed. The functions of the buttons are described in the dialog.

A dataset list is a list of full pathnames, e.g.:

```
C:\bio\data\guest\nmr\exam1d_13C\1\pdata\1
C:\bio\data\guest\nmr\exam1d_13C\2\pdata\1
C:\bio\data\guest\nmr\exam1d_13C\3\pdata\1
```

The ***Next*** button in the dialog allows you to go to the next dialog (see Figure 11.11) where you can specify the command(s), macro or Python program to be executed. The functions of the buttons are described in the dialog. The ***Browse*** button not only allow you to browse for macros/Python programs but also to create new ones.

Clicking the ***Execute*** button will actually start the execution.



Please define the command to be executed on the datasets.
Examples:
1) efp
2) lb 0.8;em;ft;pk
3) c:\mymacros\mac-efp (a full path indicates a macro)
4) c:\mypys\py-efp.py (a full path with '.py' indicates a Python script)

Click on:
> Browse For Macro = locate a TopSpin macro
> Browse For Python = locate a TopSpin Python program
> Execute = start processing the dataset list
> Back = return to list definition
> Show = show datsets while processing

Figure 11.11

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* → *Manuals* → [Programming Manuals] *Python programming

Note that serial processing also be started as follows:

- click ***Processing* → *Serial Processing...***

or

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

INPUT/OUTPUT FILES

`<tshome>/exp/stan/nmr/py`

`<tshome>/exp/stan/nmr/py/user`

`ser_*.py` - Python programs for serial processing

`<tshome>/exp/stan/nmr/lists/mac/`

`<tshome>/exp/stan/nmr/lists/mac/user`

`ser_*` - Macros for serial processing

SEE ALSO

edpy, edmac, intser

spooler

NAME

spooler - display queued, scheduled and cron jobs

DESCRIPTION

The command ***`spooler`*** displays the spooler jobs. It opens a dialog showing:

- Queued jobs (jobs started with the command ***`qu`*** or ***`qumulti`***)
- Scheduled jobs (jobs started with the command ***`at`*** or ***`atmulti`***)
- Cron jobs (jobs started with the command ***`cron`***)

For each job the dialog shows the command to be executed, the target data object, the owner and, depending on the job various other information.

The Spooler dialog offer the following menus:

Spooler

Allows you to suspend or remove all queued, scheduled or cron jobs.

Queue

Allows you to:

- Create new jobs
- Suspend all jobs.
- Remove all jobs.

for priority, delayed and cron jobs, separately.

Job

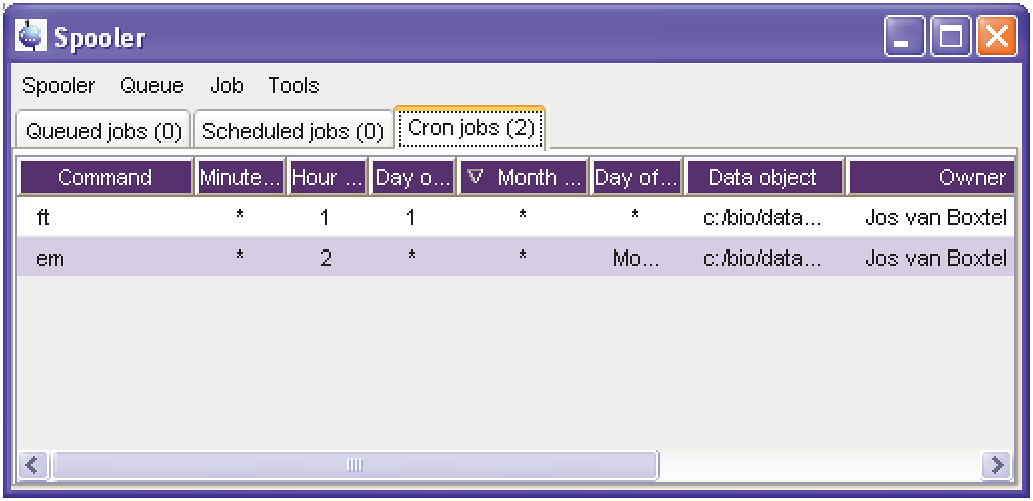
Allows you to:

- Create new jobs
- Stop, restart or delete selected jobs.
- Open the job properties dialog from here (also available by double click on the job entry).

for the selected job type.

Tools

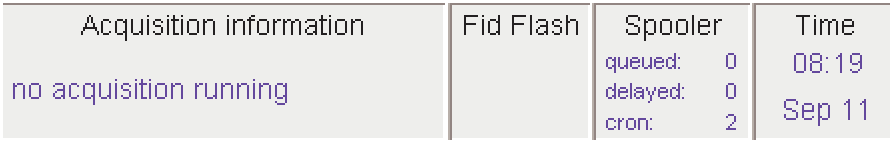
Allows you show the spooler log file and spooler report.



Command	Minute...	Hour ...	Day o...	Month ...	Day of...	Data object	Owner
ft	*	1	1	*	*	c:/bio/data...	Jos van Boxtel
em	*	2	*	*	Mo...	c:/bio/data...	Jos van Boxtel

Figure 11.12

•



Acquisition information	Fid Flash	Spooler	Time
no acquisition running		queued: 0 delayed: 0 cron: 2	08:19 Sep 11

Figure 11.13

Spooler Report

To show the spooler report:

Click ***Tools*** → ***Show spooler report***

To delete entries from the spooler report:

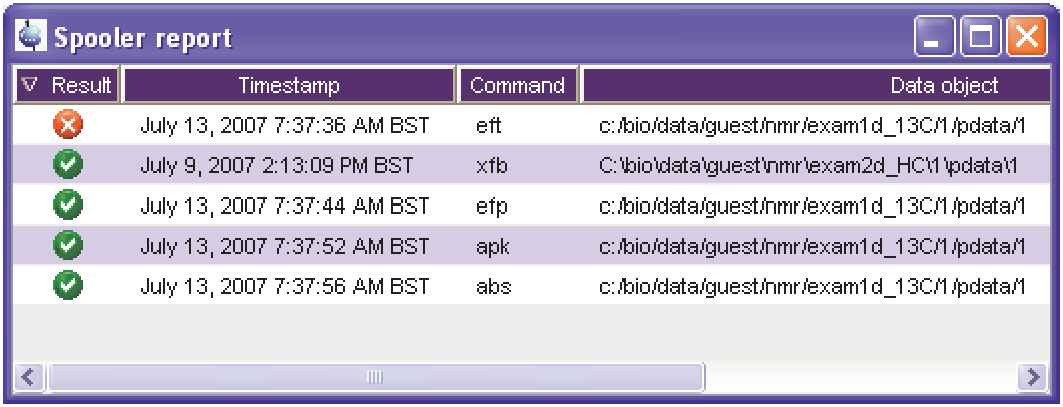
1. Mark the entries to be deleted
2. Right-click in the dialog and choose ***Delete***.

To open datasets from the spooler report:

Double-click the respective entry

or

Right-click the respective entry and choose ***Display***



▽ Result	Timestamp	Command	Data object
✗	July 13, 2007 7:37:36 AM BST	eft	c:/bio/data/guest/nmr/exam1d_13C/1/pdata/1
✓	July 9, 2007 2:13:09 PM BST	xfb	C:\bio\data\guest\nmr\exam2d_HC\1\pdata\1
✓	July 13, 2007 7:37:44 AM BST	efp	c:/bio/data/guest/nmr/exam1d_13C/1/pdata/1
✓	July 13, 2007 7:37:52 AM BST	apk	c:/bio/data/guest/nmr/exam1d_13C/1/pdata/1
✓	July 13, 2007 7:37:56 AM BST	abs	c:/bio/data/guest/nmr/exam1d_13C/1/pdata/1

Figure 11.14

Note that the spooler report can also be opened from Spooler field (if enabled) in the Acquisition Status Bar by right-clicking the word **Spooler** and choosing ***Show spooler report***.

INPUT/OUTPUT FILES

<tshome>/conf/globals

`spoolerprotocol.xml` - system spooler report

<userhome>/.topspin-<hostname>/prop/

`spoolerprotocol.xml` - user spooler report

SEE ALSO

cron, qu, qumulti, at, atmulti

Chapter 12

Conversion commands

This chapter describes all TOPSPIN conversion commands. These are commands which convert one data format to another. Described are the conversion of Bruker Aspect 2000/3000, WINNMR, Varian, Jeol and Felix data to TOPSPIN. Furthermore, the conversion to and from JCAMP-DX, ZIP and TXT format.

conv

NAME

conv - Convert Aspect 2000/3000 data to TOPSPIN format (1D,2D,3D)

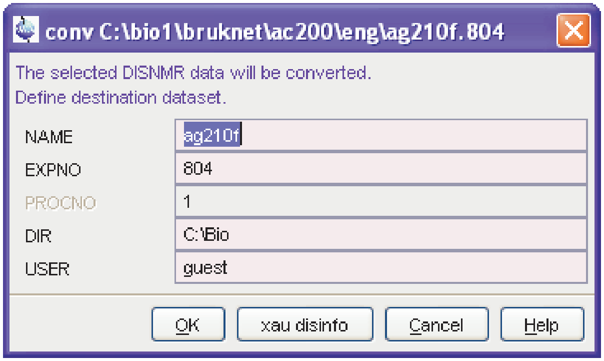
DESCRIPTION

The command ***conv*** converts DISNMR/DISMSL data (data from an Aspect 2000/3000) to the TOPSPIN format. It opens a file browser where you can:

1. Navigate to the input directory where the DISNMR/DISMSL data reside.
2. Select the datafile to be converted and click ***convert***
3. In the appearing dialog box (see Figure 12.1)

   Specify the output TOPSPIN dataset. Note that the datapath variables are initialized as follows:

   - NAME is the filename of the DISNMR input data
   - EXPNO is the extension of the DISNMR input dataset. If the extension is not numeric or if it is missing, EXPNO is initialized with 1.
   - PROCNO is set to 1 and cannot be changed
   - DIR is the <DIR> value of the current TOPSPIN datapath
   - USER is the <USER> value of the current TOPSPIN datapath



conv C:\bio1\bruknet\ac200\eng\ag210f.804

The selected DISNMR data will be converted.
Define destination dataset.

NAME	ag210f
EXPNO	804
PROCNO	1
DIR	C:\Bio
USER	guest

Figure 12.1

The command ***conv*** executes the AU program ***disconv***. This means the command ***expinstall*** must have been executed once, installing the Bruker AU programs, before you can use ***conv***.

The dialog box in Figure 12.1 shows the button ***xau disinfo***. Clicking this button executes the corresponding AU program showing the relevant dataset parameters.

Please note that the TOPSPIN command ***conv*** does not need the `disnmr.conf` or `dismsl.conf` files which were needed by TOPSPIN's predecessor XWIN-NMR. Therefore, the XWIN-NMR command ***convsys*** does not exist in TOPSPIN.

INPUT FILES

<input directory>/* - A2000/3000 data

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - Avance type 1D raw data
`ser` - Avance type 2D or 3D raw data
`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`1r`, `1i` - converted processed 1D data
`2rr`, `2ir`, `2ri`, `2ii` - converted processed 2D data
`proc` - processing parameters
`procs` - processing status parameters

For 2D data, the additional parameter files `acqu2`, `acqu2s`, `proc2` and `proc2s` will be created. For 3D data, the additional parameter files `acqu2`, `acqu2s`, `proc2` and `proc2s` and `acqu3`, `acqu3s`, `proc3` and `proc3s` will be created.

SEE ALSO

winconv, convdta, vconv, jconv, fconv

convdta

NAME

convdta - Convert Avance type raw data to AMX type (1D,2D,3D)

DESCRIPTION

The command ***`convdta`*** converts Avance type raw data to AMX type raw data. It can handle 1D, 2D and 3D data. This is useful if you want to process data that have been acquired on an Avance spectrometer on an AMX or ARX spectrometer.

`convdta` takes up to six arguments and can be used as follows:

1. ***`convdta`***
   You will be prompted for an *expno* under which the raw data must be stored
2. ***`convdta <expno>`***
   The raw data will be stored under the specified *expno*.
3. ***`convdta <expno> <name> y`***
   The output will be stored under the specified *name* and *expno*. The last argument (*y*) causes ***`convdta`*** to overwrite existing data without a warning.
4. ***`convdta <expno> <name> <user> <dir> y n`***
   The output will be stored under the specified *expno*, *name*, *user* and *dir*. The second last argument (*y*) causes ***`convdta`*** to overwrite existing data without a warning. The last argument (*n*) causes the display to remain on the current dataset rather than change to the output dataset.

You can use any other combination of arguments as long they are entered in the correct order. The processed data number (*procno*) of the new dataset cannot be chosen, it is always set to 1.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - Avance type 1D raw data
`ser` - Avance type 2D or 3D raw data

`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`proc` - processing parameters
`procs` - processing status parameters

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<*expno*>/

`fid` - AMX type 1D raw data
`ser` - AMX type 2D or 3D raw data
`acqu` - acquisition parameters
`acqus` - acquisition status parameters
`audita.txt` - acquisition audit trail

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

`proc` - processing parameters
`procs` - processing status parameters

For 2D data, the additional parameter files `acqu2`, `acqu2s`, `proc2` and `proc2s` will be used. For 3D data, the additional parameter files `acqu2`, `acqu2s`, `proc2` and `proc2s` and `acqu3`, `acqu3s`, `proc3` and `proc3s` will be used.

USAGE IN AU PROGRAMS

CONVDTA(expno)

SEE ALSO

conv, vconv, jconv, fconv

convertpeaklist

NAME

convertpeaklist - Convert XML-format peaklist to TXT-format peaklist

DESCRIPTION

The command ***convertpeaklist*** converts an XML-format peaklist to various other formats. The output format can be controlled with the argument:

txt - text format (TOPSPIN 2.0 and older and XWIN-NMR), file `peak.txt`

peaklist - Mixed Shape Deconvolution format, file `peaklist`

ml - AUREMOL format, file `1r.ml` (1D), `masterlist.ml` (2D)

peaks - XEASY format, file xeasy.peaks)

INPUT FILES

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

`peaklist.xml` - peak list for the Plot Editor in XML format

OUTPUT FILES

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

`peak.txt` - peak list for the Plot Editor in TXT format

SEE ALSO

pps, pp, mdcon

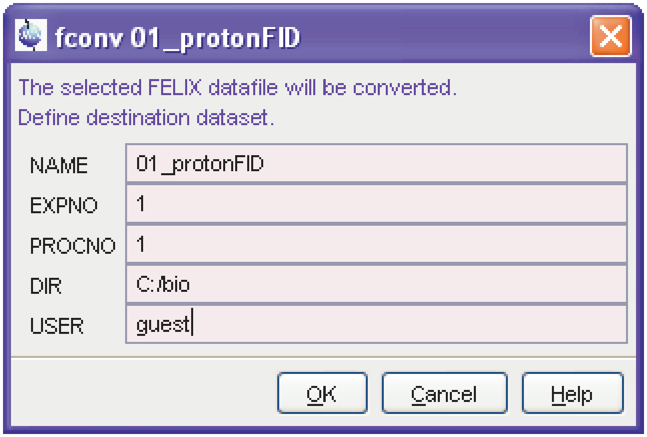
fconv

NAME

fconv - Convert Felix type data to Bruker TOPSPIN type data (1D)

DESCRIPTION

The command ***fconv*** converts Felix data to TOPSPIN format. It opens a dialog window where you can navigate to the Felix input data file. Just select the desired file and click ***convert***. This will open the dialog box shown in Figure 12.2.



fconv 01_protonFID

The selected FELIX datafile will be converted.
Define destination dataset.

NAME	01_protonFID
EXPNO	1
PROCNO	1
DIR	C:/bio
USER	guest

Figure 12.2

Her you can specify the TOPSPIN destination dataset and click ***OK*** to start the conversion.

The ***fconv*** source and destination data can also be entered on the command line. Here are some examples:

fconv <path>/fdata
When the specified input data are found, the dialog window shown in Figure 12.2 will appear. Here, you can specify the output dataset.

vconv fdata <name> <expno> <dir> <user>
Here, the destination dataset is specified as command line arguments. The *procno* is automatically set to 1. If the dataset specification

is incomplete, the dialog window shown in Figure 12.2 will appear.

fconv can convert raw and processed Felix data.

Note that ***fconv*** converts 1D data only.

INPUT FILES

`<fdata_name>` - Felix data file

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - TOPSPIN 1D raw data
`acqu` - TOPSPIN acquisition parameters
`acqus` - TOPSPIN acquisition status parameters
`audita.txt` - acquisition audit trail

<dir>/data/<user>/nmr/<name>/<expno>/pdata/1/

`proc` - TOPSPIN processing parameters
`procs` - TOPSPIN processing status parameters

SEE ALSO

vconv, jconv, conv, winconv, convdta

fromjdx

NAME

fromjdx - Convert a JCAMP-DX datafile to TOPSPIN format (1D,2D)

SYNTAX

fromjdx [<pathname> [<path-variable>] [y]]

DESCRIPTION

The command ***fromdjx*** converts a JCAMP-DX data file to a TOPSPIN dataset. JCAMP-DX is a standard ascii exchange format for spectroscopic data.

fromdjx supports the conversion of 1D data (raw or processed) and 2D data (raw or processed-real).

fromjdx takes up to three arguments and can be used as follows:

fromjdx
prompts for the pathname of the JCAMP-DX input file, converts it and stores it under the lowest empty *expno* and *procno* 1.

fromjdx <pathname>
converts the JCAMP-DX file specified by the pathname and stores it under the lowest empty *expno* and *procno* 1

fromjdx <pathname> y
converts the JCAMP-DX file specified by the pathname and stores it under *expno* 1 and *procno* 1. Possibly existing data are overwritten (y).

In the examples above, ***fromjdx*** stores the output dataset in the directory:

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

where

<dir> - the data directory of the current dataset
<user> - the user of the currently current dataset
<name> - the name of the JCAMP-DX file but without the extension

`.dx`

Further examples:

`fromjdx <pathname> du`
converts the JCAMP-DX file specified by the pathname and stores it under the *dir* (=*du*), *user*, *name*, *expno* and *procno* as specified in the input JCAMP-DX file.

`fromjdx <pathname> user`
converts the JCAMP-DX file specified by the pathname and stores it under the *dir* of the current dataset and the *user*, *name*, *expno* and *procno* as specified in the input JCAMP-DX file.

`fromjdx <pathname> name`
converts the JCAMP-DX file specified by the pathname and stores it under the *dir* and user of the active dataset and the name, *expno* and *procno* as specified in the input JCAMP-DX file.

`fromjdx <pathname> expno`
converts the JCAMP-DX file specified by the pathname and stores it under the *dir*, *user* and *name* of the active dataset and the *expno* and *procno* as specified in the input JCAMP-DX file.

`fromjdx <pathname> procno`
converts the JCAMP-DX file specified by the pathname and stores it under the *dir*, *user* and *name* of the active dataset, *expno* 1 and the *procno* as specified in the input JCAMP-DX file.

All the above examples can be used with the ***y*** option to overwrite possibly existing data.

INPUT FILES

<pathname>/<mydata.dx> - TOPSPIN data in JCAMP-DX format

OUTPUT FILES

For 1D and 2D data:

<tshome>/prog/curdir/<user>/

`curdat` - current data definition

<dir>/data/<user>/nmr/<name>/<expno>/

`audita.txt` - acquisition audit trail (if input file contains raw data)

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

`auditp.txt` - processing audit trail (if input file contains processed data)
`outd` - output device parameters
`title` - title file (see ***`edti`***)

For 1D data:

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data (if input file contains 1D raw data)
`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`1r` - real processed 1D data (if input file contains 1D real processed data)
`1i` - imaginary processed 1D data (if input file contains 1D imaginary data)
`proc` - processing parameters
`procs` - processing status parameters

For 2D data:

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - 2D raw data (input if Output Data = raw)
`acqu` - F2 acquisition parameters
`acqu2` - F1 acquisition parameters
`acqus` - F2 acquisition status parameters
`acqu2s` - F1 acquisition status parameters

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

`2rr` - real processed 2D data (if input file contains 2D real processed data)
`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters
`clevels` - 2D contour levels

USAGE IN AU PROGRAMS

FROMJDX(name)
for example FROMJDX("/tmp/mydata.dx")

SEE ALSO

tojdx, totxt, tozip, fromzip

fromzip

NAME

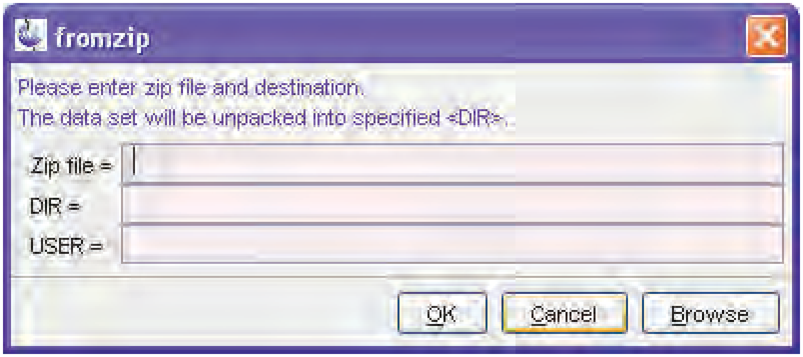
fromzip - Unzip/display a zipped TOPSPIN dataset (nD)

SYNTAX

fromzip [<pathname> <dir> <user>]

DESCRIPTION

The command ***fromzip*** opens a dialog box to unzip a ZIP TOPSPIN dataset.



Please enter zip file and destination.
The data set will be unpacked into specified <DIR>.

Zip file =

DIR =

USER =

Figure 12.3

Here you can enter the ZIP file (pathname) and the DIR and USER part of the output data path.

fromzip takes up to three arguments and can be used as follows:

fromzip
opens the above dialog box.

fromzip <pathname> <dir> <user>
converts the ZIP file specified by the pathname and stores it under the specified <dir> and <user> and the *name*, *expno* and *procno* as stored in the ZIP archive.

In the examples above, ***fromzip*** stores the output dataset in the directory:

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

The TOPSPIN dataset created by ***fromzip*** becomes the active dataset.

INPUT FILES

<pathname>/<mydata.bnmr.zip> - TOPSPIN data as stored by ***tozip***

OUTPUT FILES

For 1D and 2D data:

<tshome>/prog/curdir/<user>/

`curdat` - current data definition

<dir>/data/<user>/nmr/<name>/<expno>/

`audita.txt` - acquisition audit trail (if input file contains raw data)

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

`auditp.txt` - processing audit trail (if input file contains processed data)
`outd` - output device parameters
`title` - title file (see ***edti***)

For 1D data:

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data (if input file contains 1D raw data)
`acqu` - acquisition parameters
`acqus` - acquisition status parameters

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

`1r` - real processed 1D data (if input file contains 1D real processed data)
`1i` - imaginary processed 1D data (if input file contains 1D imaginary data)
`proc` - processing parameters
`procs` - processing status parameters

For 2D data:

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - 2D raw data (input if Output Data = raw)
`acqu` - F2 acquisition parameters
`acqu2` - F1 acquisition parameters
`acqus` - F2 acquisition status parameters
`acqu2s` - F1 acquisition status parameters

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

`2rr` - real processed 2D data (if input file contains 2D real processed data)
`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters
`clevels` - 2D contour levels

For 3D data, the additional parameter files `acqu3`, `acqu3s`, `proc3` and `proc3s` will be created.

SEE ALSO

tozip, tojdx, totxt, fromjdx

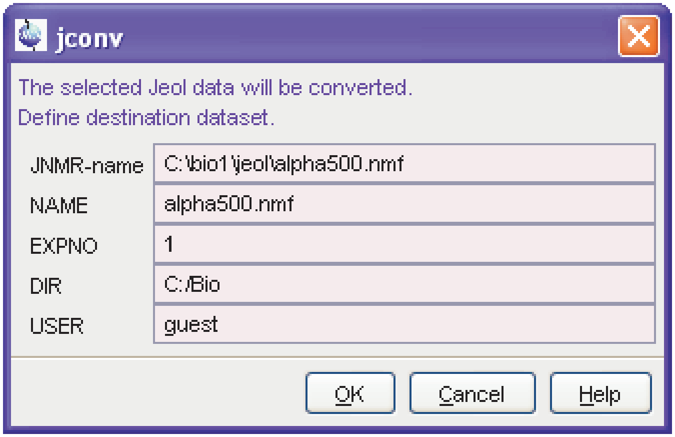
jconv

NAME

jconv - Convert Jeol type data to Bruker TOPSPIN data (1D,2D,3D)

DESCRIPTION

The command ***jconv*** converts Jeol raw data to TOPSPIN format. It opens a dialog window where you can navigate to the Jeol input data file. Just select the desired file and click ***JNMR data conversion***. This will open the dialog box shown in Figure 12.4.



The selected Jeol data will be converted.
Define destination dataset.

JNMR-name: C:\bio1\jeol\alpha500.nmf
NAME: alpha500.nmf
EXPNO: 1
DIR: C:/Bio
USER: guest

Figure 12.4

Her you can specify the TOPSPIN destination dataset and click ***OK*** to start the conversion.

The ***jconv*** source and destination data can also be entered on the command line. Here are some examples:

> ***jconv jdata.<ext>***
> searches for *jdata.<ext>* in the directory defined by the environment variable JNMR [1]. When the specified input data are found, the dialog window shown in Figure 12.4 will appear. Here, you can specify the output dataset.

[1] Can be set with the TOPSPIN command ***env set JNMR=<path>***

vconv <path>/jdata.<ext>
as above, except that the source data are searched for in the directory *<path>*

vconv jdata.<ext> <name> <expno> <dir> <user>
Here, the destination dataset is specified as command line arguments. The *procno* is automatically set to 1. If the dataset specification is incomplete, the dialog window shown in Figure 12.4 will appear.

jconv can handle Jeol EX, GX and ALPHA raw data and works on 1D, 2D and 3D data. Processed data cannot be converted. The conversion of FX FID data has been implemented. FX data must have a numerical extension (like in proton.1) and the name must be specified on the command line, e.g. ***jconv proton.1***. No parameter file is needed for the conversion, the most relevant parameters are extracted from the header of the data file.

Data type	extension of data file	extension of parameter file
EX	.gxd	.gxp
GX	.gxd	.gxp
ALPHA	.nmf	.txt
DELTA	.bin	.hdr
FX	.num (an integer number)	no parameter file

Table 12.1

jconv converts all JNMR parameters which have a TOPSPIN equivalent. First, the JNMR parameter EXMOD is interpreted. If it is set to a certain name, ***jconv*** checks the existence of a TOPSPIN parameter set with that name. If it exists, it is copied to the destination dataset. If it does not exist, a standard parameter set (*standard1D* for 1D data) is copied. Then ***jconv*** converts all JNMR parameters which have a TOPSPIN equivalent and overwrites the values of the parameter set which was previously copied. The parameters of the TOPSPIN parameter set which do not have a JNMR equivalent keep their original values. If you frequently convert Jnmr data, with typical values of EXMOD, you might want to create the TOPSPIN parameter sets with the corresponding names. This can be done by reading a standard parameter set with ***rpar***, modify it with ***eda*** and ***edp*** and then store it with ***wpar***.

INPUT FILES

`<jdata.ext>` - Jeol raw data

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - TOPSPIN 1D raw data
`acqu` - TOPSPIN acquisition parameters
`acqus` - TOPSPIN acquisition status parameters
`audita.txt` - acquisition audit trail

<dir>/data/<user>/nmr/<name>/<expno>/pdata/1/

`proc` - TOPSPIN processing parameters
`procs` - TOPSPIN processing status parameters
`jnm` original Jeol parameter file

For 2D and 3D data, the raw data are stored in the file `ser` and the additional parameter files `acqu2(s)`, `acqu3(s)`, `proc2(s)` and `proc3(s)`are created.

USAGE IN AU PROGRAMS

JCONV(jname,uxname,uxexp,uxdisk,uxuser)

SEE ALSO

vconv, fconv, conv, winconv, convdta

tojdx

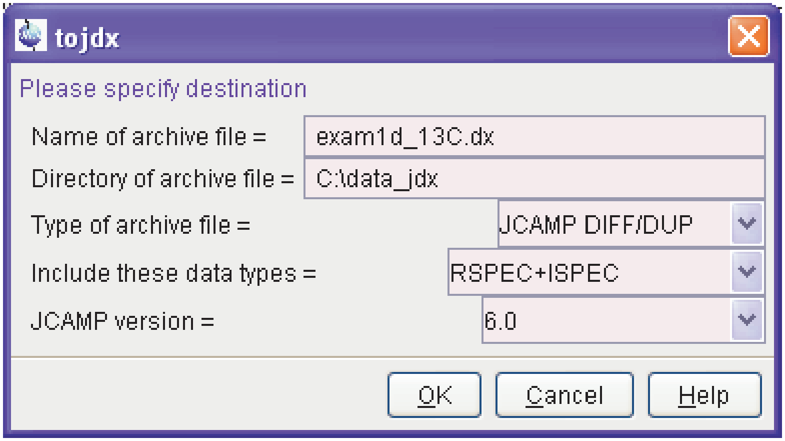
NAME

tojdx - Convert dataset to JCAMP-DX format (1D,2D)

DESCRIPTION

The command ***todjx*** converts a TOPSPIN dataset to JCAMP-DX format. JCAMP-DX is a standard ascii exchange format for spectroscopic data.

When ***tojdx*** is entered without argument, it will open a dialog box.



Please specify destination

Name of archive file = exam1d_13C.dx
Directory of archive file = C:\data_jdx
Type of archive file = JCAMP DIFF/DUP
Include these data types = RSPEC+ISPEC
JCAMP version = 6.0

Figure 12.5

in which you can enter the required information. This includes:

Name of the archive file

The filename should have the extension **.**dx. This allows you to open it in TOPSPIN with drop & drag. Default is the dataset name with the extension **.**dx.

Directory of the archive file

Any directory. Default is the users home directory.

Type of archive file

For JCAMP format, you can choose between the following archive types:

- *FIX* (=0) : table format
- *PACKED* (=1) : no spaces between the intensity values
- *SQUEEZED* (=2) : the sign of the intensity values is encoded in the first digit
- *DIFF/DUP* (=3) : the difference between successive values is encoded, suppressing repetition of successive equal values

The default value is *DIFF/DUP*.

Include these data types

For the included data types, you have the following choices:

- FID (=0)
  raw data
- RSPEC (=1)
  real processed data
- RSPEC+ISPEC (=2)
  real and imaginary processed data
- PARAMS (=3)
  parameter files
- FID+RSPEC+ISPEC (=4)
  raw data + real and imaginary processed data
- FID+ALL_PROCNOS (=5)
  Raw data +real and imaginary processed data of all PROCNO's under the current EXPNO
- ALL_EXPNOS_DIM_1_2 (=6)
  Raw data +real and imaginary processed data of all EXPNO's under the current NAME

The default value is RSPEC+ISPEC (=2)

The above information can be entered as arguments of ***tojdx*** as follows:

```
tojdx <path> <data> <file> <title> <origin> <owner>
```

Note that in this case three extra arguments are required. The arguments have the following meaning:

- <path>: name and directory of the archive file
- <data>: data types included
- <file>: type of archive file
- <title>: the title as it appears in the output file: enter a character string
- <origin>: the origin as it appears in the output file: enter a character string
- <owner>: the owner as it appears in the output file: enter a character string

The default *title* is the plot title as defined with ***edti***. If no plot title is defined the data name is taken as default. The default *origin* and *owner* are taken from the acquisition status parameter files (`acqus`). If you enter an * character as argument, the default value will be used.

Here are some examples are:

```
tojdx C:\temp\mydata.dx 0 2 mytitle BRUKER guest
tojdx D:\nmr\mydata.dx 0 2 mytitle * *
tojdx * 1 * mytitle MYORIGIN joe
tojdx F:\users\guest\mydata.dx * * * * *
```

INPUT FILES

For 1D and 2D data:

<tshome>/prog/curdir/<user>/

`curdat` - current data definition

For 1D data:

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data
`acqus` - acquisition status parameters

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

`1r` - real processed 1D data
`1i` - imaginary processed 1D data
`proc` - processing status parameters

`procs` - processing status parameters

For 2D data:

<dir>/data/<user>/nmr/<name>/<expno>/

`ser` - 2D raw data
`acqus` - F2 acquisition status parameters
`acqu2s` - F1 acquisition status parameters

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

`2rr` - real processed 2D data
`proc` - F2 processing parameters
`proc2` - F1 processing parameters
`procs` - F2 processing status parameters
`proc2s` - F1 processing status parameters

OUTPUT FILES

<pathname>/<mydata.dx> - TOPSPIN data in JCAMP-DX format

USAGE IN AU PROGRAMS

TOJDX(name, data, mode, title, origin, owner)
for example TOJDX("/tmp/mydata.dx", 0, 2, "mytitle", "BRUKER", "joe")

SEE ALSO

fromjdx, tozip, totxt

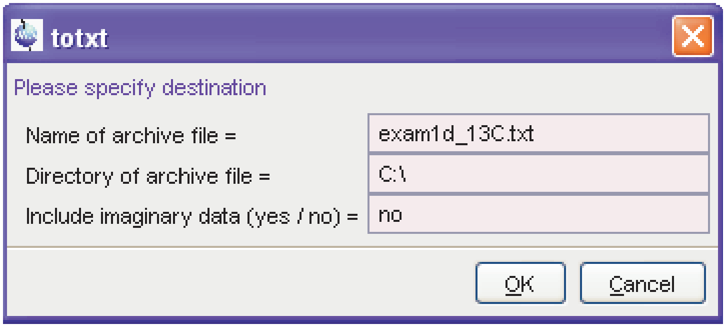
totxt

NAME

totxt - Save the currently displayed region as a text file (1D,2D)

DESCRIPTION

The command ***totxt*** saves the currently displayed spectral region as text file. It will open the following dialog box.



Name of archive file = exam1d_13C.txt
Directory of archive file = C:\
Include imaginary data (yes / no) = no

in which you can enter the text filename and directory.
totxt works on 1D and 2D datasets and only stores the real processed data. The 1D file format is:

```
# File created = Wednesday, March 3, 2004 11:52:01 AM CET
# Data set = exam1d_13C  1  1  C:\bio  guest
# Spectral Region:
# LEFT = 145.2549493926 ppm. RIGHT = 116.58206350384 ppm.
# SIZE = 3940 ( = number of points)
# In the following ordering is from the 'left' to the
'right' limits!
# Lines beginning with '#' must be considered as comment..
#
1.4612096E7
3084512.0
4615664.0
1.6594048E7
4898192.0
-4555792.0
...
```

INPUT FILES

For 1D data:

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

`1r` - real processed 1D data

For 2D data:

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

`2rr` - real processed 2D data

OUTPUT FILES

<pathname>/<mydata.txt> - text file containing displayed region

SEE ALSO

tojdx, tozip

tozip

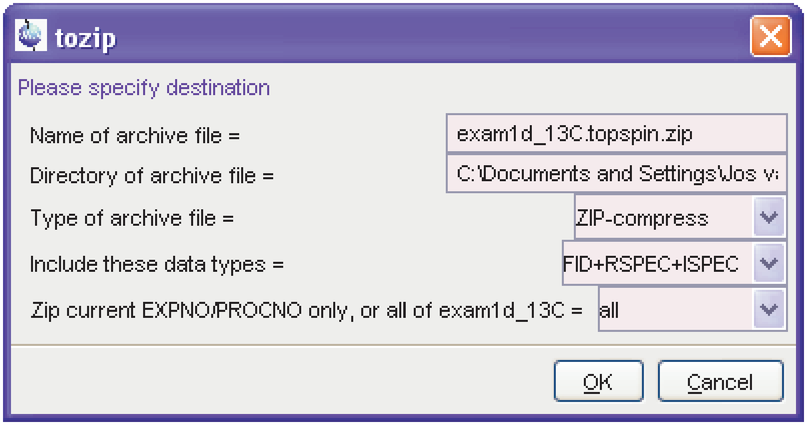
NAME

tozip - Store current dataset in ZIP file (nD)

DESCRIPTION

The command ***tozip*** converts a TOPSPIN dataset to ZIP format.

It opens a dialog box where you can enter the required information



Please specify destination

Name of archive file = exam1d_13C.topspin.zip

Directory of archive file = C:\Documents and Settings\Jos v

Type of archive file = ZIP-compress

Include these data types = FID+RSPEC+ISPEC

Zip current EXPNO/PROCNO only, or all of exam1d_13C = all

Figure 12.6

This information includes:

Name of archive file: output file name and extension (default .topspin.zip)

Directory of archive file: directory where output file is stored

Type of archive:

- ZIP-compress
- ZIP-no compress

Data types included:

- FID+RSPEC+ISPEC: raw + real and imaginary processed data
- FID+RSPEC: raw + real processed data

- FID: raw data
- RSPEC+ISPEC: real and imaginary processed data
- RSPEC: real processed data

Zip current EXPNO/PROCNO only, or all of ...: archive current expno/procno or all expnos/procnos in current dataset.

In TOPSPIN 2.1 and newer, the command ***tozip*** takes one argument, the destination pathname, e.g.:

tozip c:/xzy.zip

This command will store the raw and processed data in the current expno/procno, uncompressed, in the file `C:\xyz.zip`. Without argument, tozip will open it's dialog showing the default destination file `<dataname>.topspin.zip`. You can change this default as follows:

1. Enter ***expl prop***

   to open the file explorer in the user properties directory.
2. Edit the file `globals.prop`
3. Add the line:

   TOZIP_CONFIG=option1|option2

   where the options must be separated by the character "|" and

   option1= N, NE or NEP, for name, name, name-expno or name-expno-procno, respectively.
   option2 = any string, e.g. “-mycompany.zip“

Example:

Dataset: "exam1d_13C 102 1 c:\bruker\topspin guest"

option2=.bruker.zip

If option1=N, the default name is: exam1d_13C.bruker.zip.

If option1= NE, the default name is exam1d_13C-102.bruker.zip

If option1 was NEP, the default name is exam1d_13C-102-1.bruker.zip

INPUT FILES

If Data type includes FID

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - 1D raw data
`ser` - 2D or 3D raw data

If Data type includes RSPEC

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

`1r` - real processed 1D data
`2rr` - real processed 2D data
`3rrr` - real processed 3D data

If Data type includes ISPEC

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

`1i` - imaginary processed 1D data
`2ir`, `2ri`, `2ii` - imaginary processed 2D data
`3irr`, `3rir`, `3iii` - imaginary processed 3D data

The parameter files `acqu*` and `proc*` are stored for all data types.

OUTPUT FILES

<pathname>/<mydata.bnmr.zip> - TOPSPIN data in ZIP format

SEE ALSO

fromzip, tojdx, totxt

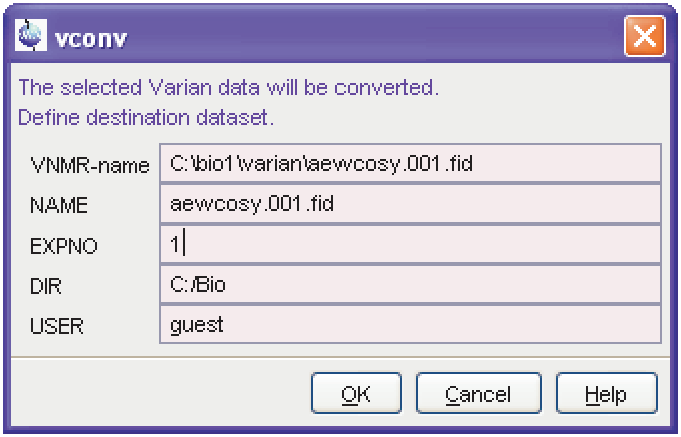
vconv

NAME

vconv - Convert Varian type data to TOPSPIN data (1D,2D,3D)

DESCRIPTION

The command ***vconv*** converts Varian data, which were measured with the VNMR program, to TOPSPIN format. It opens a browser where you can navigate to the Varian input data file. Just select the desired file and click ***VNMR data conversion***. This will open the dialog box shown in Figure 12.7.



vconv

The selected Varian data will be converted.
Define destination dataset.

VNMR-name	C:\bio1\varian\aewcosy.001.fid
NAME	aewcosy.001.fid
EXPNO	1
DIR	C:/Bio
USER	guest

Figure 12.7

Here you can specify the TOPSPIN destination dataset and click ***OK*** to start the conversion.

The ***vconv*** source and destination data can also be entered on the command line. Here are some examples:

vconv vdata.fid
searches for *vdata.fid* in the directory defined by the environment variable VNMR [1]. When the specified input data are found, the dialog window shown in Figure 12.7 will appear. Here, you can specify the

[1] Can be set with the TOPSPIN command ***env set VNMR=<path>***

output dataset.

vconv <path>/vdata.fid
as above, except that the source data are searched for in the directory *<path>*

vconv vdata.fid <name> <expno> <dir> <user>
Here, the destination dataset is specified as command line arguments. The *procno* is automatically set to 1. If the dataset specification is incomplete, the dialog window shown in Figure 12.7 will appear.

Note that the extension `.fid` of the Vnmr dataset is not obligatory.

vconv converts all VNMR parameters which have a TOPSPIN equivalent. First, the VNMR parameter SEQFIL is interpreted. If it is set to a certain name, ***vconv*** checks the existence of a TOPSPIN parameter set with that name. If it exists, it is copied to the destination dataset. If it does not exist, a standard parameter set (*standard1D* for 1D data) is copied. Then ***vconv*** converts all VNMR parameters which have a TOPSPIN equivalent and overwrites the values of the parameter set which was previously copied. The parameters of the TOPSPIN parameter set which do not have a VNMR equivalent keep their original values. If you frequently convert Vnmr data, with typical values of SEQFIL, you might want to create the TOPSPIN parameter sets with the corresponding names. This can be done by reading a standard parameter set with ***rpar***, modify it with ***eda*** and ***edp*** and then store it with ***wpar***.

VNMR	XWIN-NMR	VNMR	XWIN-NMR
ct	NS(status)	rfl/rfp	OFFSET
d1	D1	rfl1/rfp1	OFFSET(2D)
date	DATE	rfl2/rfp2	OFFSET(3D)
dfrq	BF2	rp	PHC0
dfrq2	BF3	rp/lp	PHC0/PHC1
dmf	P31	rp1/lp1	PHC0/PHC1(2D)
dn	DECNUC	rp2/lp2	PHC0/PHC1(3D)
dn2	DECBNUC	seqfil	PULPROG
dof	O2	sfrq	BF1
dof2	O3	solvent	SOLVENT
fb	FW	spin	RO
fn	SI	ss	DS
lp	PHC1	sw	SW_h
np	TD	sw1	SW_h(2D)
nt	NS(foreground)	sw2	SW_h(3D)
pp	P3	temp	TE
pslabel	AUNM	tn	NUCLEUS
pw	P0	tof	O1
pw90	P1		

Table 12.2

The original VNMR parameter file `procpar` is stored in the TOPSPIN processed data directory. You can check this ascii file for possible parameters which could not be converted.

Table 12.2 shows the Varian parameters and there TOPSPIN equivalent.

vconv can handle Unity and Gemini data acquired with VNMR 4.1 or newer. Data from older Varian spectrometers or acquired with older software versions might also work, but have not been tested by Bruker.

INPUT FILES

<dir>/data/<user>/nmr/<vdata>.fid

or

<VNMR>/<vdata>.fid/

`fid` - the VNMR raw data
`procpar` - the parameters
`text` - title file

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - TOPSPIN 1D raw data
`acqu` - TOPSPIN acquisition parameters
`acqus` - TOPSPIN acquisition status parameters
`audita.txt` - acquisition audit trail

<dir>/data/<user>/nmr/<name>/<expno>/pdata/1

`proc` - TOPSPIN processing parameters
`procs` - TOPSPIN processing status parameters
`procpar` - VNMR parameter file

For 2D and 3D data, the raw data are stored in the file `ser` and the additional parameter files `acqu2(s)`, `acqu3(s)`, `proc2(s)` and `proc3(s)`are created.

USAGE IN AU PROGRAMS

VCONV(vname, xwname, xwexpno, xwdisk, xwuser)

SEE ALSO

jconv, fconv, conv

winconv

NAME

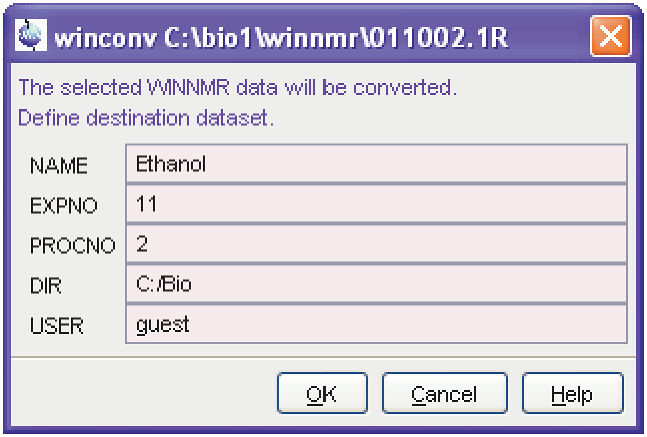
winconv - Convert WINNMR type data to TOPSPIN data (1D)

DESCRIPTION

The command ***winconv*** converts Bruker WIN-NMR data to TOPSPIN format. It opens a browser where you can navigate to the WIN-NMR input datasets. A WIN-NMR dataset is a directory with several files. Each file has:

- a number as filename
- the extension `.FID`, `.1R`, `.1I`, `.AQS` or `.FQS` for raw data, processed real data, processed imaginary data, acquisition parameters and processing parameters, respectively.

Just select any of these files and click ***convert***. This will open the dialog box shown in Figure 12.8.



winconv C:\bio1\winnmr\011002.1R

The selected WINNMR data will be converted.
Define destination dataset.

NAME	Ethanol
EXPNO	11
PROCNO	2
DIR	C:/Bio
USER	guest

Figure 12.8

Here you can specify the TOPSPIN destination dataset. The datapath fields are initialized as follows:

NAME - the WIN-NMR data directory
EXPNO - the first three digits of the WIN-NMR data name
PROCNO - the second three digits of the WIN-NMR data name

DIR - DIR of the active TOPSPIN dataset
USER - USER of the active TOPSPIN dataset

Specify a the datapath or accept the initial values and click ***OK*** to start the conversion. To display the dataset, just open it from the TOPSPIN browser or use the command ***`re`***.

INPUT FILES

`<name>/`

`num.FID` - WIN-NMR raw data
`num.1R` - WIN-NMR real processed data
`num.1I` - WIN-NMR imaginary processed data
`num.1I` - WIN-NMR imaginary processed data
`num.AQS` - WIN-NMR acquisition parameters
`num.FQS` - WIN-NMR processing parameters
`num.TIT` - WIN-NMR title

OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`fid` - TOPSPIN 1D raw data
`acqu` - TOPSPIN acquisition parameters
`acqus` - TOPSPIN acquisition status parameters

<dir>/data/<user>/nmr/<name>/<expno>/pdata/1

`1r` - real processed data
`1i` - imaginary processed data
`proc` - TOPSPIN processing parameters
`procs` - TOPSPIN processing status parameters

SEE ALSO

conv, fconv, jconv, vconv, convdta

Chapter 13

TOPSPIN Interface/Processes

This chapter describes commands which are related to the User interface and TOPSPIN processes. Each user can set up his/her own interface including the TOPSPIN menu, colours, printer usage etc. Commands are described for following processes on the screen, storing them in the history file or killing them. Online help is described as far as it can be started from the command line.

about

NAME

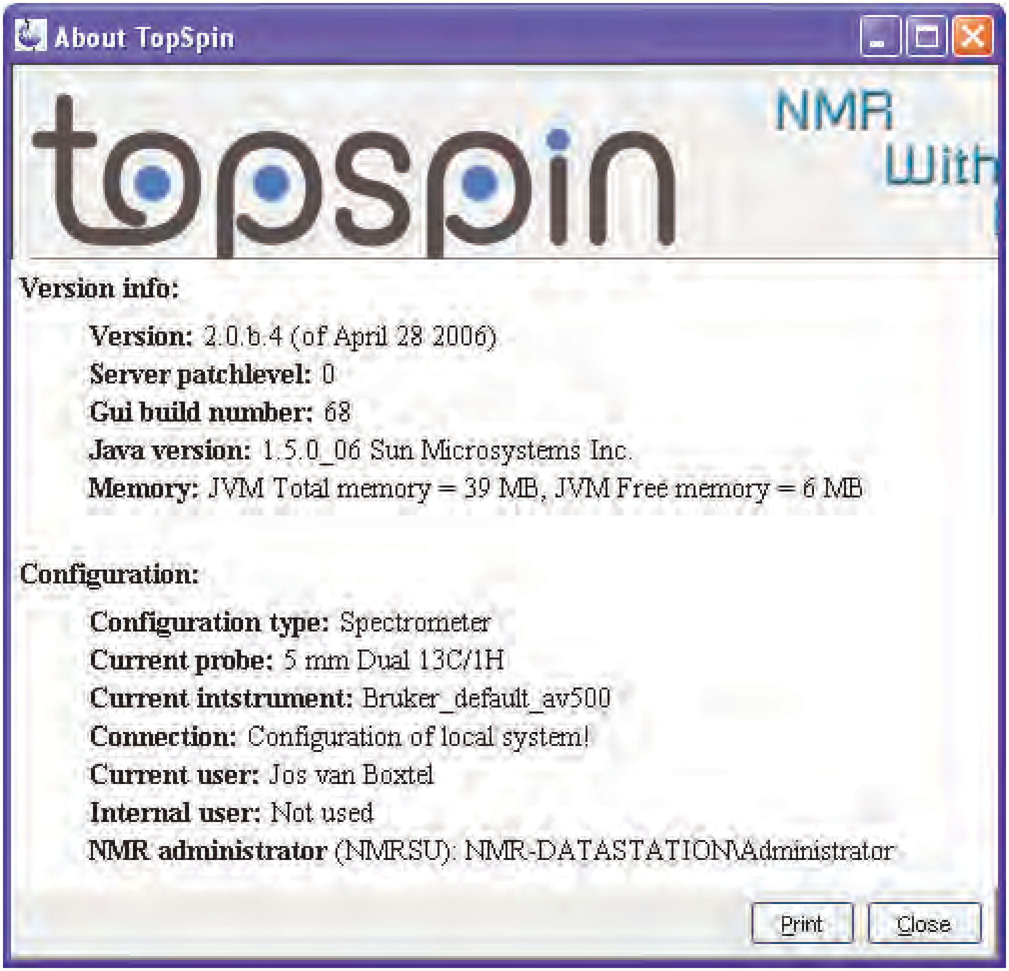
about - Show TOPSPIN version and configuration information.

DESCRIPTION

The command ***about*** shows various TOPSPIN version and configuration information (see Figure 13.1).

This command can also be started as follows:

Click ***Help → Version Info***



Version info:

Version: 2.0.b.4 (of April 28 2006)
Server patchlevel: 0
Gui build number: 68
Java version: 1.5.0_06 Sun Microsystems Inc.
Memory: JVM Total memory = 39 MB, JVM Free memory = 6 MB

Configuration:

Configuration type: Spectrometer
Current probe: 5 mm Dual 13C/1H
Current intstrument: Bruker_default_av500
Connection: Configuration of local system!
Current user: Jos van Boxtel
Internal user: Not used
NMR administrator (NMRSU): NMR-DATASTATION\Administrator

Figure 13.1

bpan

NAME

bpan - Open a user defined button panel (nD)

DESCRIPTION

The command ***bpan*** opens a user defined button panel. It prompts you for the name the desired panel.

A button panel is a window with user-defined buttons for executing TOPSPIN commands, AU programs, Python programs or macros. It appears as an integral part of the active data window and act on that. Bruker delivers a few standard button panels like ***bnmr***. To create your own button panels, you can modify one of these or write them from scratch.

In this description we will create a very simple button panel with some 1D processing commands and print/export buttons (see Figure 13.2)

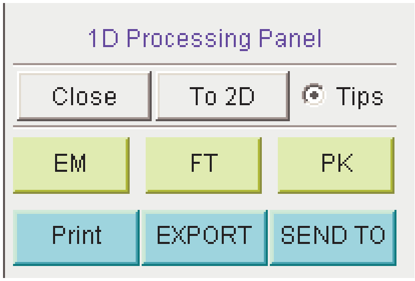


Figure 13.2

To write this button panel, take the following steps:

1. Open the File Explorer and navigate to the subdirectory:

```
userdefined
```

of the users properties directory [1].

2. Create a text file with the name

```
buttonpanel_<name>.prop
```

[1] To locate this, enter ***hist*** and look for the entry "User properties directory=".

where <name> is the name of the button panel.

3. Enter the button definitions including *Panel title*, *Colors*, *Toggle buttons*, *Top buttons*, *Panel layout*, *Panel buttons* and *Tooltips*.
4. Save the file. Make sure the extension of the file is `.prop` and not `.txt`, `.prop.txt` or anything else.
5. Enter ***`bpan <name>`*** on the command line to open the button panel.

Here is the contents of the properties file for the button panel above:

```
# Color definitions used in this file (RGB)

BLUE1=51$ 204$ 255
YELLOW1=255$ 255$ 0
GREEN1=84$ 196$ 20

# Title definition

TITLE=1D Processing Panel
TITLE_COLOR=0$ 0$ 255

# Toggle button definition

TOGGLE_BUTTON=To 2D
TOGGLE_CMD=bpan bproc2d
TOGGLE_TIP=Switch to 2D processing

# Top row button definition

TOP_BUTTONS=EM$ $FT$ $PK$ $
TOP_COLORS=YELLOW1$ YELLOW1$ YELLOW1
TOP_CMDS=em$ ft$ pk
TOP_TIPS=Exponential multiplication $\
Fourier transform$\
Phase correction

# Panel button definitions

# LAYOUT format: rows columns hgap vgap
PAN_LAYOUT=1$ 3$ 8$ 8

PAN_BUTTONS=Print$ $ EXPORT$ $SEND TO$ $
PAN_COLORS=BLUE1$ BLUE1$ BLUE1
PAN_CMDS=prnt$ exportfile$ smail
PAN_TIPS=Print the spectrum<br>\
as it appears on the screen$\
Export the dataset<br>\
to png, jpg, bmp etc.$\
Send the dataset by email
```

Note that:

- the *Close* button and *Tips* switch are automatically created. You don't need to specify them.
- The TOGGLE button is typically, but not necessarily, used to call another button panel. In this example it calls the panel ***bproc2d***.
- items must be separated with the "$" character, button items with "$ $"
- a "\" followed by "end of line" continues an item on the next line
- tooltips may use html tags for text formatting
- commands may be specified as single commands like "em" or as composite commands like "em\nft\npk". Note that in the latter case, the commands must be separated by "\n".

INPUT FILES

<userhome>/<.topspin-hostname>/prop/userdefined/cmdpanel_<name>.prop

SEE ALSO

bnmr

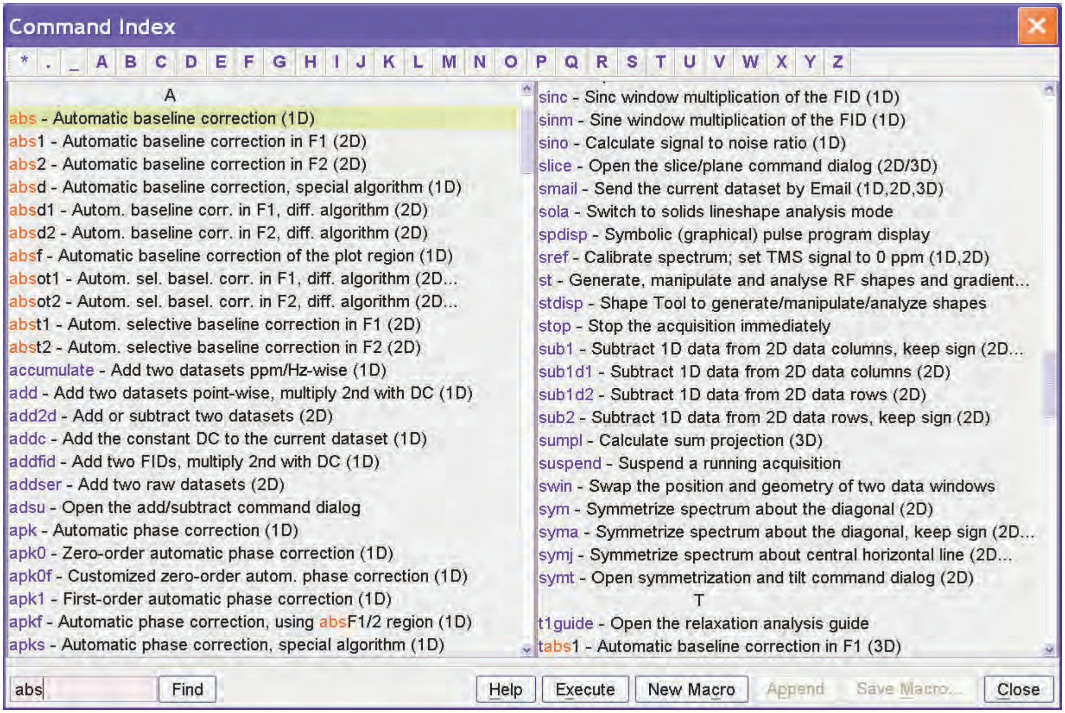
cmdindex

NAME

cmdindex - Open the command index

DESCRIPTION

The command ***cmdindex*** opens a command index dialog box (see Figure 13.3).



A

abs - Automatic baseline correction (1D)
abs1 - Automatic baseline correction in F1 (2D)
abs2 - Automatic baseline correction in F2 (2D)
absd - Automatic baseline correction, special algorithm (1D)
absd1 - Autom. baseline corr. in F1, diff. algorithm (2D)
absd2 - Autom. baseline corr. in F2, diff. algorithm (2D)
absf - Automatic baseline correction of the plot region (1D)
absot1 - Autom. sel. basel. corr. in F1, diff. algorithm (2D...
absot2 - Autom. sel. basel. corr. in F2, diff. algorithm (2D...
abst1 - Autom. selective baseline correction in F1 (2D)
abst2 - Autom. selective baseline correction in F2 (2D)
accumulate - Add two datasets ppm/Hz-wise (1D)
add - Add two datasets point-wise, multiply 2nd with DC (1D)
add2d - Add or subtract two datasets (2D)
addc - Add the constant DC to the current dataset (1D)
addfid - Add two FIDs, multiply 2nd with DC (1D)
addser - Add two raw datasets (2D)
adsu - Open the add/subtract command dialog
apk - Automatic phase correction (1D)
apk0 - Zero-order automatic phase correction (1D)
apk0f - Customized zero-order autom. phase correction (1D)
apk1 - First-order automatic phase correction (1D)
apkf - Automatic phase correction, using absF1/2 region (1D)
apks - Automatic phase correction, special algorithm (1D)

sinc - Sinc window multiplication of the FID (1D)
sinm - Sine window multiplication of the FID (1D)
sino - Calculate signal to noise ratio (1D)
slice - Open the slice/plane command dialog (2D/3D)
smail - Send the current dataset by Email (1D,2D,3D)
sola - Switch to solids lineshape analysis mode
spdisp - Symbolic (graphical) pulse program display
sref - Calibrate spectrum; set TMS signal to 0 ppm (1D,2D)
st - Generate, manipulate and analyse RF shapes and gradient...
stdisp - Shape Tool to generate/manipulate/analyze shapes
stop - Stop the acquisition immediately
sub1 - Subtract 1D data from 2D data columns, keep sign (2D...
sub1d1 - Subtract 1D data from 2D data columns (2D)
sub1d2 - Subtract 1D data from 2D data rows (2D)
sub2 - Subtract 1D data from 2D data rows, keep sign (2D)
sumpl - Calculate sum projection (3D)
suspend - Suspend a running acquisition
swin - Swap the position and geometry of two data windows
sym - Symmetrize spectrum about the diagonal (2D)
syma - Symmetrize spectrum about the diagonal, keep sign (2D...
symj - Symmetrize spectrum about central horizontal line (2D...
symt - Open symmetrization and tilt command dialog (2D)

T

t1guide - Open the relaxation analysis guide
tabs1 - Automatic baseline correction in F1 (3D)

Figure 13.3

It shows all TOPSPIN commands which can be entered from the command line with a one-line description for each command. You can select one or more commands for further actions. The following actions are available:

Help

Open the HTML Help page of the selected command. This is equivalent to double-clicking the command.

Execute

Execute the selected command or commands.

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 the name on the command line.

Find

Find a character string in the command index.

INPUT FILES

`<tshome>/classes/prop`

`cmdindex_main.prop` - command index properties file

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

`*.html` - TOPSPIN command help files

OUTPUT FILES

`<tshome>/exp/stan/nmr/lists/mac/`

`*` - Macros (created by ***cmdhist*** → ***Save as..***)

SEE ALSO

cmdhist

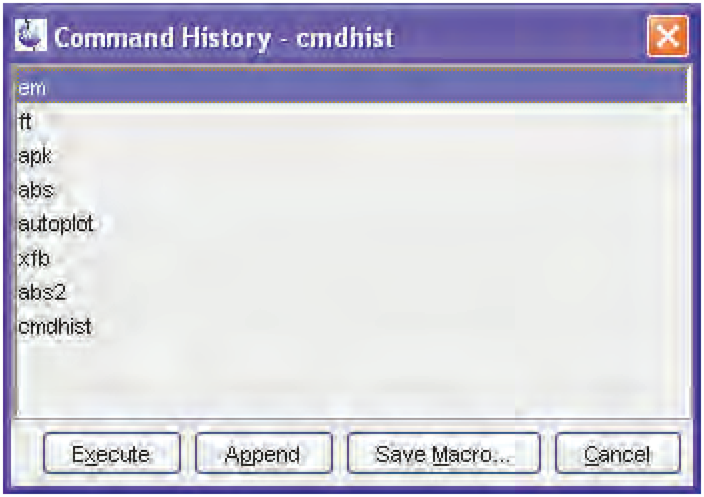
cmdhist

NAME

cmdhist - Open command history

DESCRIPTION

The command ***cmdhist*** opens a command history control window (see Figure 13.4).



```
em
ft
apk
abs
autoplot
xfb
abs2
cmdhist
```

Figure 13.4

It shows all commands that have been entered from the command line since TOPSPIN was started. You can select one or more commands. Furthermore, the following buttons are available:

Execute

Execute the selected command or commands.

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 Macro...

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 the name on the command line.

The command history control window can also be started as follows:

- Click ***View → Command Line History***

or

- Right-click in the command line and select ***Command Line History***

OUTPUT FILES

`<tshome>/exp/stan/nmr/lists/mac/`

* - Macros (created by ***`cmdhist`*** → ***Save as..***)

SEE ALSO

hist, edmac

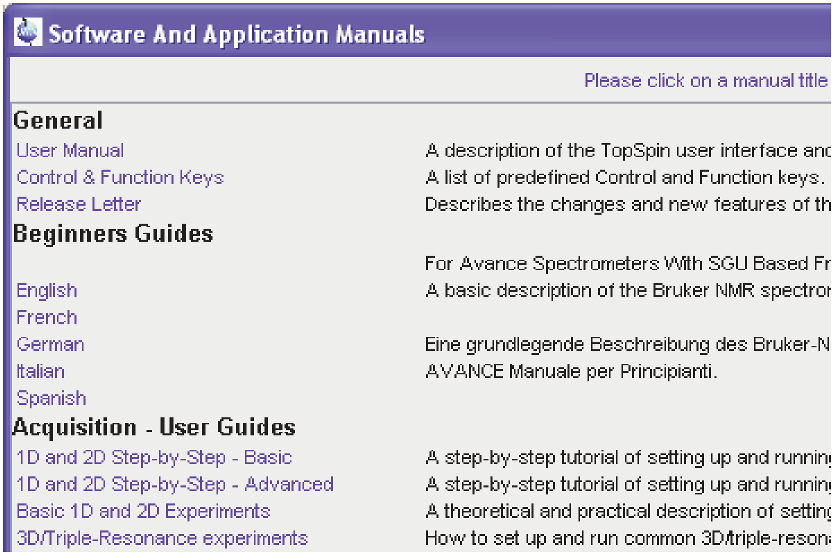
docs

NAME

docs - Open Manual list

DESCRIPTION

The command ***docs*** opens a list of available documents. This list shows all Bruker manuals delivered on the TOPSPIN DVD (Figure 13.5).



Software And Application Manuals

Please click on a manual title

General	
User Manual	A description of the TopSpin user interface anc
Control & Function Keys	A list of predefined Control and Function keys.
Release Letter	Describes the changes and new features of th
Beginners Guides	
	For Avance Spectrometers With SGU Based Fr
English	A basic description of the Bruker NMR spectror
French	
German	Eine grundlegende Beschreibung des Bruker-N
Italian	AVANCE Manuale per Principianti.
Spanish	
Acquisition - User Guides	
1D and 2D Step-by-Step - Basic	A step-by-step tutorial of setting up and runnin
1D and 2D Step-by-Step - Advanced	A step-by-step tutorial of setting up and runnin
Basic 1D and 2D Experiments	A theoretical and practical description of settin
3D/Triple-Resonance experiments	How to set up and run common 3D/triple-reson

Figure 13.5

The manuals are divided in the topics TopSpin, Beginners Guides, etc.... Just click the manual name to open it. Furthermore, the Manual dialog offer the following buttons:

- ***Close this dialog when a manual is opened***
- ***Books*** - list available hardcopy (printed) manuals
- ***Close*** - close the Manuals dialog

SEE ALSO

help

edtext

NAME

edtext - Open an empty text file with an editor

DESCRIPTION

The command ***edtext*** open an empty text file with the TOPSPIN editor. The file can be stored in any directory.

SEE ALSO

nbook

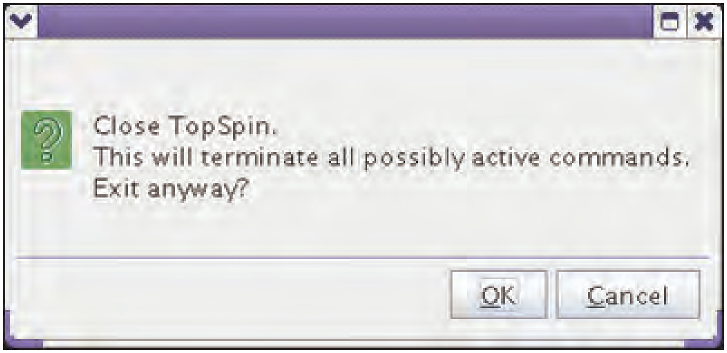
exit

NAME

exit - Exit TOPSPIN

DESCRIPTION

The command ***exit*** exits TOPSPIN and terminates all running processes. Before this happens, the following warning is displayed.

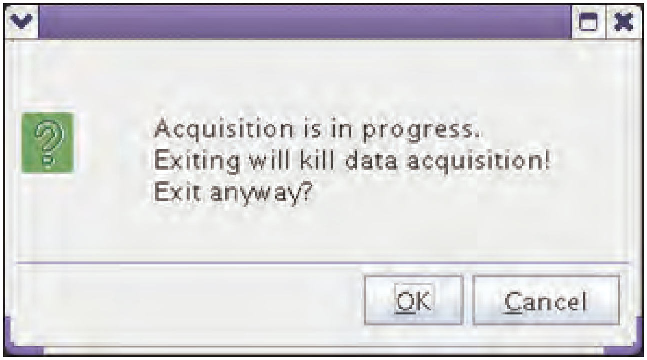


Close TopSpin.
This will terminate all possibly active commands.
Exit anyway?

Figure 13.6

Furthermore TopSpin 2.1 and newer displays different warnings and error messages, depending on the actual TopSpin use, before exiting the programm:

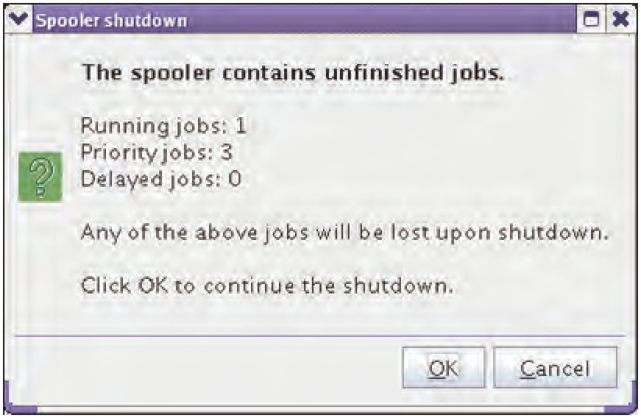
1.) If Acquisition is running (see Figure 13.7)..



Acquisition is in progress.
Exiting will kill data acquisition!
Exit anyway?

Figure 13.7

2.) If the spooler contains unfinished jobs (see Figure 13.8).



The spooler contains unfinished jobs.

Running jobs: 1
Priority jobs: 3
Delayed jobs: 0

Any of the above jobs will be lost upon shutdown.

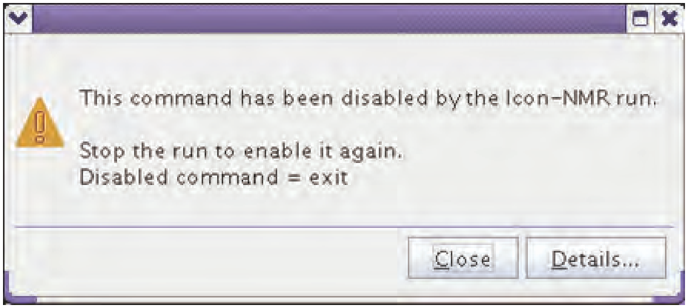
Click OK to continue the shutdown.

Figure 13.8

Click ***OK*** in the respectively of the three dialogs above to exit TOPSPIN.

3.) If ICON-NMR runs actively at the exit-moment, TopSpin cannot be closed (see Figure 13.9).

.



This command has been disabled by the Icon-NMR run.

Stop the run to enable it again.
Disabled command = exit

Figure 13.9

Entering ***`exit`*** on the command line is equivalent to clicking ***File*** → ***Exit***.

SEE ALSO

close

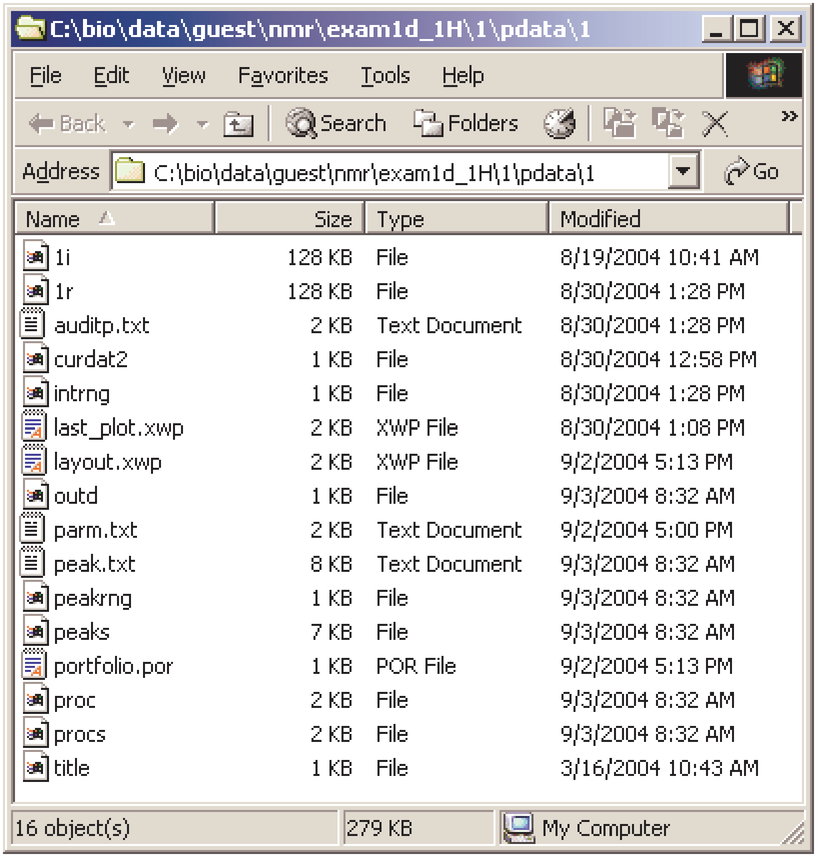
expl

NAME

expl - Open File Explorer, show current processing folder

DESCRIPTION

The command ***expl*** opens the Explorer (Windows) or Konqueror/Nautilus (Linux) showing the processed data files (the files in the *procno* directory) of the active dataset (see Figure 13.10).



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

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

Name	Size	Type	Modified
1i	128 KB	File	8/19/2004 10:41 AM
1r	128 KB	File	8/30/2004 1:28 PM
auditp.txt	2 KB	Text Document	8/30/2004 1:28 PM
curdat2	1 KB	File	8/30/2004 12:58 PM
intrng	1 KB	File	8/30/2004 1:28 PM
last_plot.xwp	2 KB	XWP File	8/30/2004 1:08 PM
layout.xwp	2 KB	XWP File	9/2/2004 5:13 PM
outd	1 KB	File	9/3/2004 8:32 AM
parm.txt	2 KB	Text Document	9/2/2004 5:00 PM
peak.txt	8 KB	Text Document	9/3/2004 8:32 AM
peakrng	1 KB	File	9/3/2004 8:32 AM
peaks	7 KB	File	9/3/2004 8:32 AM
portfolio.por	1 KB	POR File	9/2/2004 5:13 PM
proc	2 KB	File	9/3/2004 8:32 AM
procs	2 KB	File	9/3/2004 8:32 AM
title	1 KB	File	3/16/2004 10:43 AM

16 object(s) | 279 KB | My Computer

Figure 13.10

If no dataset is open in the TOPSPIN data area, the users home directory will be shown.

expl allows you to access to the current data files as well as the entire data directory tree. An alternative way to access the processed data files is to right-click in the data window and select ***Files...***

The command can also be used with one argument:

expl top
shows the contents of the TOPSPIN home directory

expl home
shows the contents of the User home directory

expl spect
shows the contents of the directory <tshome>/conf/instr/<curinst<

expl prop
shows the contents of the User properties directory

expl <absolute_path>
shows the contents of directory <absolute_path>

SEE ALSO

run

hist

NAME

hist - Show the TOPSPIN history and protocol

DESCRIPTION

The command ***hist*** shows the TOPSPIN protocol and history files. These files only contain information if the protocol function is active. You can switch on this function as follows:

1. Click ***Options → Preferences*** [**set**]
2. Click ***Miscellaneous*** in the left part of the dialog box.
3. Check the item *Record commands in protocol file*

The protocol file contains TOPSPIN startup information and command information on interface level. The history file contains command information on the level of the command interpreter and application modules. It also contains error messages.
Note that the files `history` and `protocol` are emptied when you restart TOPSPIN which means the history of the previous TOPSPIN session is lost. In case of problems, you should first make a copy of these files before you restart TOPSPIN. Note that a long TOPSPIN session, especially with automation can create very large `history` and protocol files. Therefore, it is useful to regularly check the size of the files or simply restart TOPSPIN after each (automation) session.

OUTPUT FILES

<tshome>/prog/curdir/<user>/
`history` - TOPSPIN history file
`history_i.txt` - TOPSPIN protocol file

<userhome>/<.topspin-hostname>/prop/
`protocol.txt` - TOPSPIN protocol file (if TOPSPIN was started as **`topspin -client`**)

SEE ALSO

ptrace

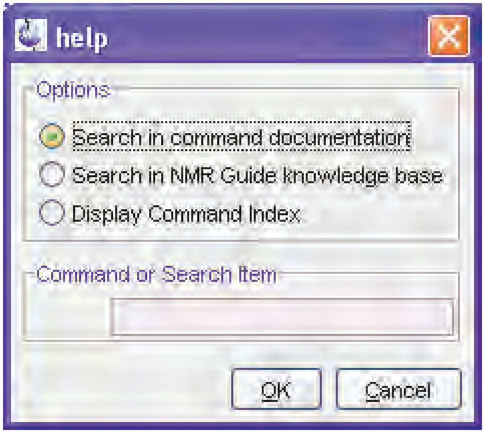
help, ghelp

NAME

help - Search for keywords in command help
ghelp - Search for keywords in command in NMR Guide

DESCRIPTION

The command ***help*** opens a search dialog (see Figure 13.11).



help
Options
○ Search in command documentation
○ Search in NMR Guide knowledge base
○ Display Command Index
Command or Search Item
OK
Cancel

Figure 13.11

This dialog box has several options, each of which selects a certain command for execution.

Search in command documentation

This option activates the command ***help***. It allows you to search for the specified item in the command help documents.

Search in NMR Guide knowledge base

This option activaytes the command ***ghelp***. It allows you to search for the specified item in the NMR Guide knowledge base.

Search in NMR Guide knowledge base

This option activaytes the command ***cmdindex***. It opens the command index dialog, irrespective of the specified command.

Entering ***help*** on the command line is equivalent to clicking ***Help → Advanced Search*** or hitting the ***F1*** key.

INPUT FILES

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

`*.html` - TOPSPIN command help files

<tshome>/guide/

* - NMR Guide files and directories

SEE ALSO

docs

kill, show

NAME

kill, show - Show active TOPSPIN commands and allow to kill them

DESCRIPTION

The command ***kill*** displays a list of all active TOPSPIN commands. To kill a command:

- click a command entry
- click the button ***Kill...***

The command ***show*** is equivalent to ***kill***.

A running acquisition should not be stopped with ***kill*** because this would leave an inconsistent dataset. Instead, the commands ***halt*** or ***stop*** should be used for this purpose.

nbook

NAME

nbook - Open the user notebook

DESCRIPTION

The command ***nbook*** opens a user specific notebook. Each user can create and keep his/her own notebook for individual notes, information, settings etc.

INPUT AND OUTPUT FILES

<userhome>/<.topspin-hostname/prop/

`notebook.txt` - notebook text file

SEE ALSO

peakw

newtop

NAME

newtop - Open a new Topspin interface

DESCRIPTION

The command ***newtop*** opens a new additional TOPSPIN interface. The additional interface is completely equivalent to the one it was started from. Entering ***newtop*** in the second or in the initial TOPSPIN interface opens another interface etc. The number of TOPSPIN interfaces is only limited by the available computer memory.

When single dataset is displayed in multiple TOPSPIN interfaces, the display in each interface is completely independent from the others. As such, you can display different regions, scalings and data objects. When the dataset is (re)processed from one interface, its display is automatically updated in all TOPSPIN interfaces.

The command ***exit*** closes the current Topspin interface. Interfaces that were opened from that 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.

SEE ALSO

exit, newwin, hist

newwin, nextwin, close, closeall

NAME

newwin - Open a new (empty) data window
nextwin - Select the next data window
close - Close the current data window
closeall - Close all data windows

DESCRIPTION

The command ***newwin*** opens a new empty data window. It is equivalent to clicking ***Window* → *New Window***

The command ***nextwin*** activates the next open data window. It is equivalent to clicking ***Window* → *Next Window*** or hitting the ***F6*** key

The command ***close*** closes the current data window. It is equivalent to clicking ***File* → *Close*** or hitting ***Ctrl-w***.

The command ***closeall*** closes the current data window. It is equivalent to clicking ***File* → *Closeall***.

SEE ALSO

newtop

ptrace

NAME

ptrace - Display messages from various log files time sorted

DESCRIPTION

The command ***ptrace*** shows the TOPSPIN protocol and history files time sorted (see Figure 13.12). These files only contain valuable information if the protocol function is active. You can switch on this function as follows:

1. Click ***Options → Preferences*** [**`set`**]
2. Click ***Miscellaneous*** in the left part of the dialog box.
3. Check the item *Record commands in protocol file*

The protocol file contains TOPSPIN startup information and command information on interface level. The history file contains command information on the level of the command interpreter and application modules. It also contains error messages.

Note that the files `history` and `protocol` are emptied when you restart TOPSPIN which means the history of the previous TOPSPIN session is lost. In case of problems, you should first make a copy of these files before you restart TOPSPIN. Note that a long TOPSPIN session, especially with automation can create very large `history` and protocol files. Therefore, it is useful to regularly check the size of the files or simply restart TOPSPIN after each (automation) session.

OUTPUT FILES

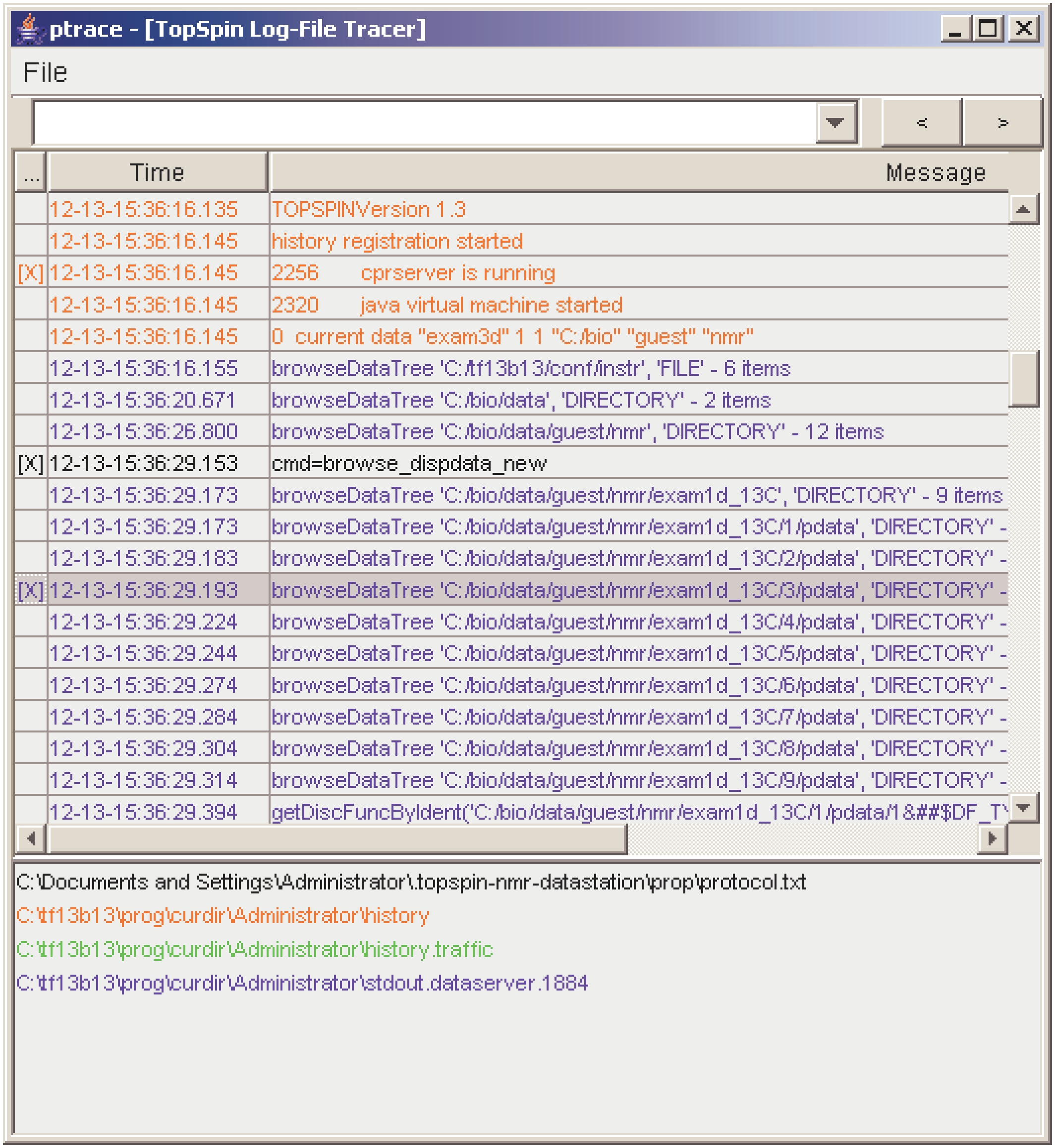
<tshome>/prog/curdir/<user>/

`history` - TOPSPIN history file
`history_i.txt` - TOPSPIN protocol file
`history.traffic.txt` - network traffic log
`stdout.dataserver.<number>.txt` - dataserver output file

<userhome>/<.topspin-hostname>/prop/

`protocol.txt` - TOPSPIN protocol file (if TOPSPIN was started as

topspin -client)



```
   12-13-15:36:16.135 TOPSPINVersion 1.3
   12-13-15:36:16.145 history registration started
[X]12-13-15:36:16.145 2256     cprserver is running
   12-13-15:36:16.145 2320     java virtual machine started
   12-13-15:36:16.145 0  current data "exam3d" 1 1 "C:/bio" "guest" "nmr"
   12-13-15:36:16.155 browseDataTree 'C:/tf13b13/conf/instr', 'FILE' - 6 items
   12-13-15:36:20.671 browseDataTree 'C:/bio/data', 'DIRECTORY' - 2 items
   12-13-15:36:26.800 browseDataTree 'C:/bio/data/guest/nmr', 'DIRECTORY' - 12 items
[X]12-13-15:36:29.153 cmd=browse_dispdata_new
   12-13-15:36:29.173 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C', 'DIRECTORY' - 9 items
   12-13-15:36:29.173 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/1/pdata', 'DIRECTORY' -
   12-13-15:36:29.183 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/2/pdata', 'DIRECTORY' -
[X]12-13-15:36:29.193 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/3/pdata', 'DIRECTORY' -
   12-13-15:36:29.224 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/4/pdata', 'DIRECTORY' -
   12-13-15:36:29.244 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/5/pdata', 'DIRECTORY' -
   12-13-15:36:29.274 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/6/pdata', 'DIRECTORY' -
   12-13-15:36:29.284 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/7/pdata', 'DIRECTORY' -
   12-13-15:36:29.304 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/8/pdata', 'DIRECTORY' -
   12-13-15:36:29.314 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/9/pdata', 'DIRECTORY' -
   12-13-15:36:29.394 getDiscFuncByIdent('C:/bio/data/guest/nmr/exam1d_13C/1/pdata/1&##$DF_T

C:\Documents and Settings\Administrator\.topspin-nmr-datastation\prop\protocol.txt
C:\tf13b13\prog\curdir\Administrator\history
C:\tf13b13\prog\curdir\Administrator\history.traffic
C:\tf13b13\prog\curdir\Administrator\stdout.dataserver.1884
```

Figure 13.12

SEE ALSO

hist

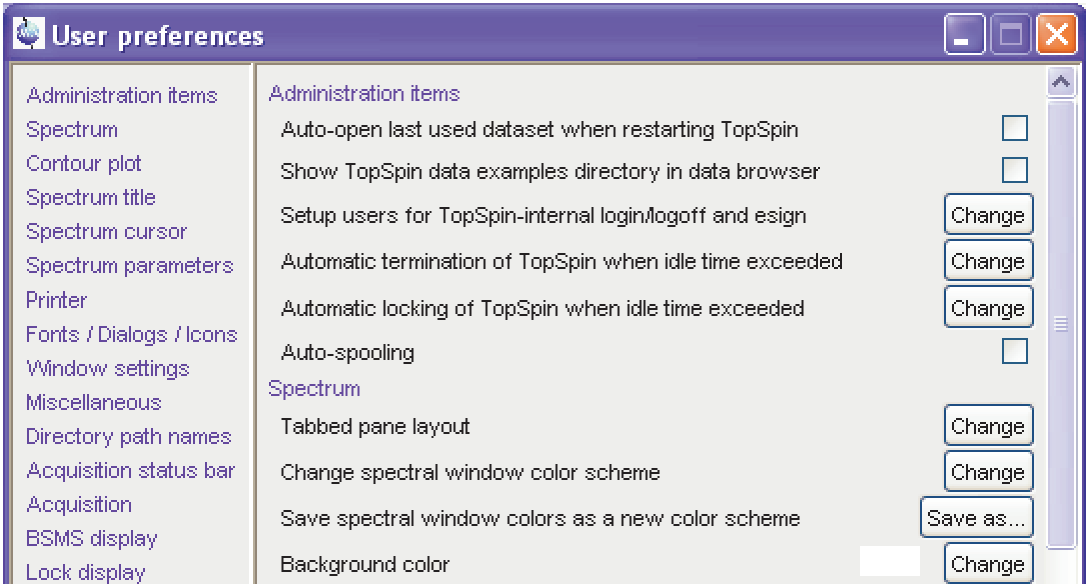
set

NAME

set - Open the user preferences window

DESCRIPTION

The command ***set*** allows you to set user preferences. It opens the dialog box shown in Figure 13.13.



Administration items

Auto-open last used dataset when restarting TopSpin □

Show TopSpin data examples directory in data browser □

Setup users for TopSpin-internal login/logoff and esign Change

Automatic termination of TopSpin when idle time exceeded Change

Automatic locking of TopSpin when idle time exceeded Change

Auto-spooling □

Spectrum

Tabbed pane layout Change

Change spectral window color scheme Change

Save spectral window colors as a new color scheme Save as...

Background color Change

Figure 13.13

In the left part of the dialog window, you find various cathegories of objects. Click the cathegory of which you want to view/change certain objects. It will become highlighted and the corresponding objects will be displayed at the right part of the dialog box. Some objects can be changed by entering a value, others can be changed by clicking the ***Change*** button to the right of the object entry.

INPUT AND OUTPUT FILE

<home>/.topspin-<hostname>/prop

`globals.prop` - ascii file containing User Interface settings

`view.prop` - colors fonts etc.

where

<home> is the users home directory
<hostname> is the hostname of the computer

setdef

NAME

setdef - Switch error message acknowledgment on/off

DESCRIPTION

The command ***setdef*** is mainly used to switch the error message acknowledgement function on or off. It takes two arguments and can be used as follows:

setdef ackn no - commands continue without acknowledgment

setdef ackn ok - commands require acknowledgment before continuing

Note that (re)starting TOPSPIN always sets ***setdef ackn*** to its default value which is ***ok***.

setdef can also be used to switch the storage of standard output and standard error message off or on. In this case it must be entered in the form:

setdef stdout on - store standard output message

setdef stdout off - do not store standard output messages

The equivalent for standard error messages is ***setdef stderr ok/no***.

OUTPUT FILES

<tshome>/prog/curdir/<user>

`stdout.num` - standard TOPSPIN output file for ***setdef stdout ok***
`stderr.num` - standard TOPSPIN error file for ***setdef stderr ok***

shell

NAME

shell - Open a Windows Command Prompt or Linux Shell

DESCRIPTION

The command ***`shell`*** opens a Command Prompt (under Windows) or a shell (under Linux).

swin

NAME

swin - Swap the position and geometry of two data windows

DESCRIPTION

The command ***swin*** swaps the position of two data windows. If the layout contains exactly two data windows, ***swin*** simple swaps their position and geometry. If the layout contains more than two data windows, ***swin*** allows you to swap the currently selected (active) data window with any of the other data windows. The latter can be selected from a list.

swin is typically used after reading a window layout with more than one data window.

SEE ALSO

close, newwin, nextwin

Chapter 14

TOPSPIN User Management

This chapter describes commands which are related to TOPSPIN audit trail and user management. The audit trail contains a record of all acquisition and processing activities, data checksums and electronic signatures. The can be included by TOPSPIN internal users, which can be set up by the NMR administrator. Internal users are required to log in to TOPSPIN before they can use it or exit it.

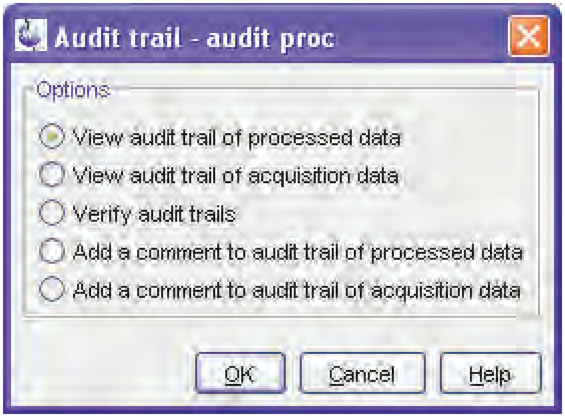
audit, auditcheck

NAME

audit - Open audit trail dialog box (nD)
auditcheck - Check data consistency (nD)

DESCRIPTION

The command ***audit*** opens the audit trail dialog box.



Audit trail - audit proc

Options

● View audit trail of processed data
○ View audit trail of acquisition data
○ Verify audit trails
○ Add a comment to audit trail of processed data
○ Add a comment to audit trail of acquisition data

Figure 14.1

This dialog box has several options, each of which selects a certain command for execution.

View audit trail of the processed data

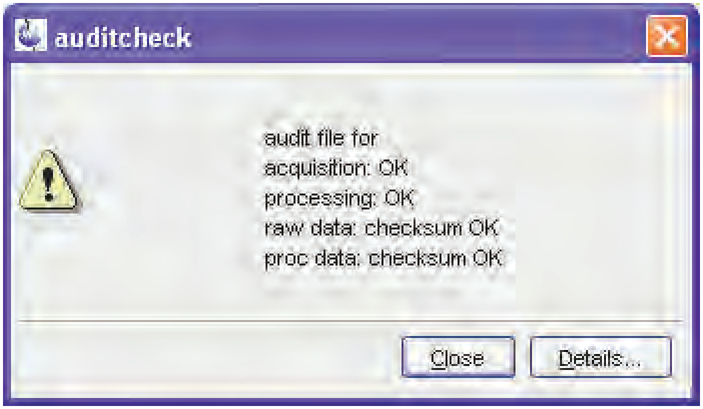
This option selects the command ***audit proc*** for execution. It shows the processing audit trail file `auditp.txt`. This file is created by the processing command that creates the processed data, e.g. ***em***. Any processing command that modifies/updates the processed data, e.g. ***ft***, makes an additional entry. Furthermore, any command that changes one or more processing status parameters makes an additional entry.

View audit trail of the acquisition data

This option selects the command ***audit acqu*** for execution. It shows the acquisition audit trail file `audita.txt`. This file is created by the acquisition command that creates the raw data, e.g. ***zg***. Any acquisition command that modifies/updates the raw data, e.g. ***go***, makes an additional entry. Furthermore, any command that changes one or more acquisition status parameters makes an additional entry.

Verify audit trails

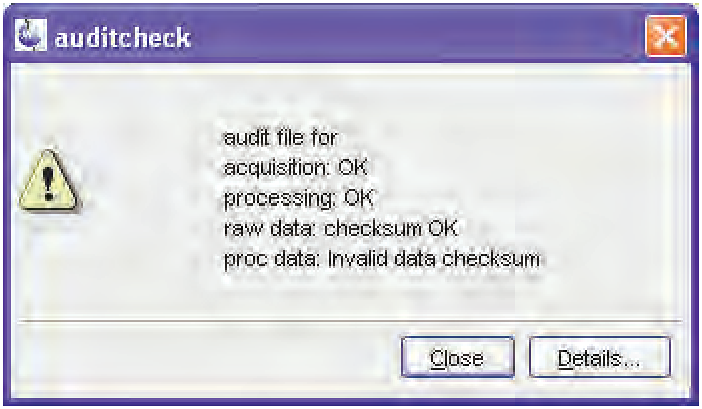
This option selects the command ***audit check*** for execution. It performs an audit trail check, i.e. a data consistency check. If both raw and processed data are consistent, you will get the following message:



audit file for
acquisition: OK
processing: OK
raw data: checksum OK
proc data: checksum OK

Figure 14.2

If the data have been manipulated, e.g. with third party software or by changing certain status parameters (e.g. SI), the checksum will be inconsistent. Figure 14.3 shows the message for inconsistent processed data.



audit file for
acquisition: OK
processing: OK
raw data: checksum OK
proc data: Invalid data checksum

Figure 14.3

Add a comment to audit trail

This option selects the command ***audit com*** for execution. It allows you to add a comment to one of the audit trail files (raw or processed).

Each audit trail file entry contains the following elements:

- *Number*: the entry number (1, 2, 3,...)
- *When* : starting date and time of the command
- *Who* : user who starts the command (the user that started TOPSPIN)
- *Where* : location where the command started (the computer host name)
- *What* : command and associated parameters, e.g. <em LB = 0.3 SI = 16384>

The last line of the file is a checksum which looks like:

$$ 24 EB 5D 82 76 AD F2 2B 7E D2 A1 35 7B B5 C4 D5

The command ***auditcheck*** uses this line for the consistency check.

INPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`audita.txt` - acquisition audit trail

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

`auditp.txt` - processing audit trail

Note that these are also the output files for ***audit com***.

SEE ALSO

gdcheck

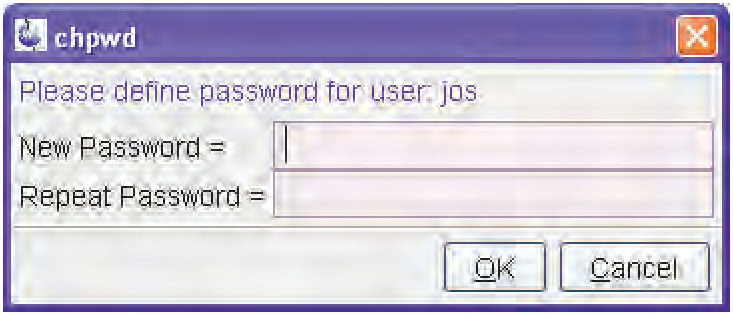
chpwd

NAME

chpwd - Exit TOPSPIN

DESCRIPTION

The command ***chpwd*** allows you to change the password of the internal user. It opens the following dialog:



chpwd

Please define password for user: jos

New Password =

Repeat Password =

Figure 14.4

Enter the new password twice and click OK

The command can also be started as follows:

click ***Options* → *Administration* → *Change internal user password***

SEE ALSO

uadmin, esign, logoff

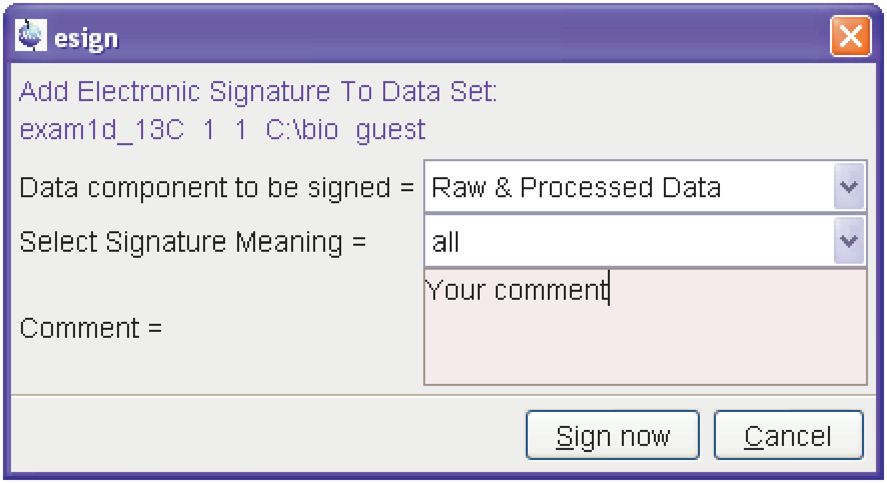
esign

NAME

esign - Exit TOPSPIN

DESCRIPTION

The command ***esign*** adds an electronic signature to the raw data and/or to the processed data of a dataset. It opens the following dialog:



esign

Add Electronic Signature To Data Set:
exam1d_13C 1 1 C:\bio guest

Data component to be signed = Raw & Processed Data

Select Signature Meaning = all

Comment = Your comment

Figure 14.5

Just select the data component to be signed, the signature meaning and, optionally, add a comment.Then click ***Sign now***.

The signature will appear with the parameters on the plot (commands ***plot***, ***autoplot***) and in the Audit file (command ***audit proc***). It consists of four lines, e.g.:

USER ID	larry
USER NAME	Larry Hill
MEANING	approval
COMMENT	Spectrum quality is OK.

The command ***esign*** can also be started as follows:

Click ***Options*** → ***Administration*** → ***E-Sign Data Set***

esign requires that the NMR administrator has set up a list of users who are allowed to sign a data set, along with definitions of signature *meanings* (e.g. review, approval).

INPUT FILES

<tshome>/conf/

`topspin-users.prop` - TOPSPIN users properties file

OUTPUT FILES

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

`auditp.txt` - processing audit trail

SEE ALSO

uadmin, chpwd, logoff, lockgui

gdcheck

NAME

gdcheck - Generate data checksum

DESCRIPTION

The command ***gdcheck*** generates a data checksum. It updates the audit trail files. It takes one argument and can be used as follows:

gdcheck
make the processing audit trail consistent

gdcheck raw
make the acquisition audit trail consistent

gdcheck is, for example, required if a dataset has been manipulated with third party software. In that case the audit trail would be inconsistent, i.e. the command ***auditcheck*** would report an inconsistency error. ***gdcheck*** updates the audit trail file with a new data checksum and adds the entry:

Unknown data manipulation detected

After this, ***auditcheck*** would report:

Unknown data manipulation

For 2D and 3D data, ***gdcheck*** adds a data checksum. For 1D data, a data checksum is automatically created by processing commands. In 2D and 3D, however, processing commands do not create a data checksum because this would be too time consuming. If it is required ***gdcheck*** allows you to create it.

INPUT AND OUTPUT FILES

<dir>/data/<user>/nmr/<name>/<expno>/

`audita.txt` - acquisition audit trail

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

`auditp.txt` - processing audit trail

USAGE IN AU PROGRAMS

GDCHECK

GDCHECK_RAW

executes the command ***`gdcheck raw`***

AUDITCOMMENTA("user comment")

adds a user comment to the `audita.txt` file.

AUDITCOMMENTP("user comment")

adds a user comment to the `auditp.txt` file.

SEE ALSO

audit, auditcheck

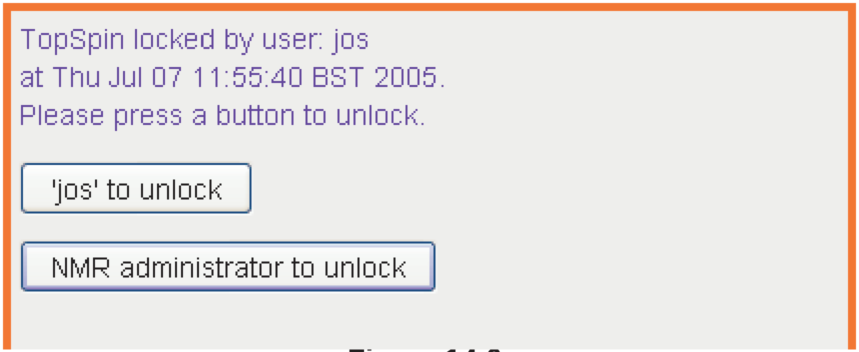
lockgui

NAME

lockgui - Lock the TOPSPIN interface

DESCRIPTION

The command ***lockgui*** allows you to logoff the internal user. It opens the dialog shown in Figure 14.6.



TopSpin locked by user: jos
at Thu Jul 07 11:55:40 BST 2005.
Please press a button to unlock.

Figure 14.6

This indicates the locked status and offers buttons to unlock. Note that only the current internal user and the NMR Administrator can unlock the interface

The command can also be started as follows:

click ***Options*** → ***Administration*** → ***Lock TopSpin user interface***

INPUT FILES

<tshome>/conf/

`topspin-users.prop` - TOPSPIN users properties file

SEE ALSO

uadmin, esign, chpwd, login, logoff

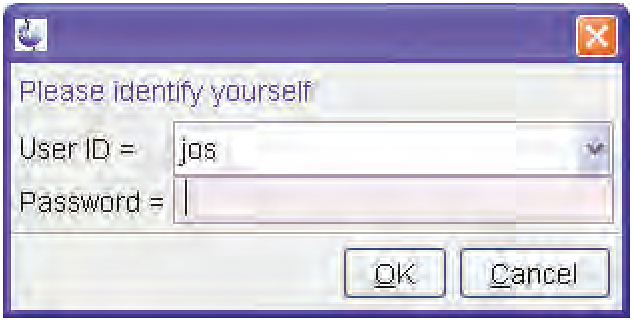
login

NAME

login - Exit TOPSPIN

DESCRIPTION

The command ***login*** allows you to login as a (different) TOPSPIN internal user. It opens the following dialog:



Please identify yourself

User ID = jos

Password =

Figure 14.7

Enter the user name of the internal user and enter the password.

The command can also be started as follows:

click ***Options*** → ***Administration*** → ***Login As Internal User***

INPUT FILES

<tshome>/conf/

`topspin-users.prop` - TOPSPIN users properties file

SEE ALSO

logoff, uadmin, esign, chpwd, lockgui

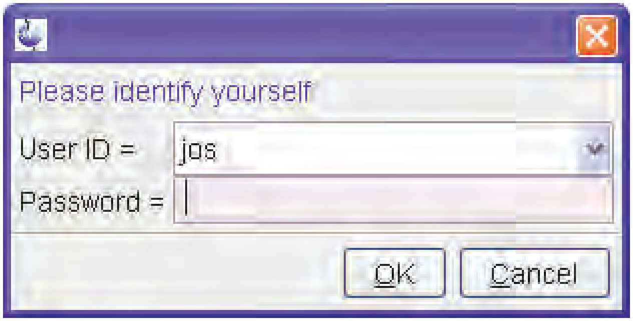
logoff

NAME

logoff - Exit TOPSPIN

DESCRIPTION

The command ***logoff*** allows you to logoff the internal user. It opens the following dialog:



Please identify yourself

User ID = jos

Password =

Figure 14.8

Enter the current user name and enter the password.

The command can also be started as follows:

click ***Options*** → ***Administration*** → ***Log Off From Internal User***

INPUT FILES

<tshome>/conf/

`topspin-users.prop` - TOPSPIN users properties file

SEE ALSO

login, uadmin, esign, chpwd, lockgui

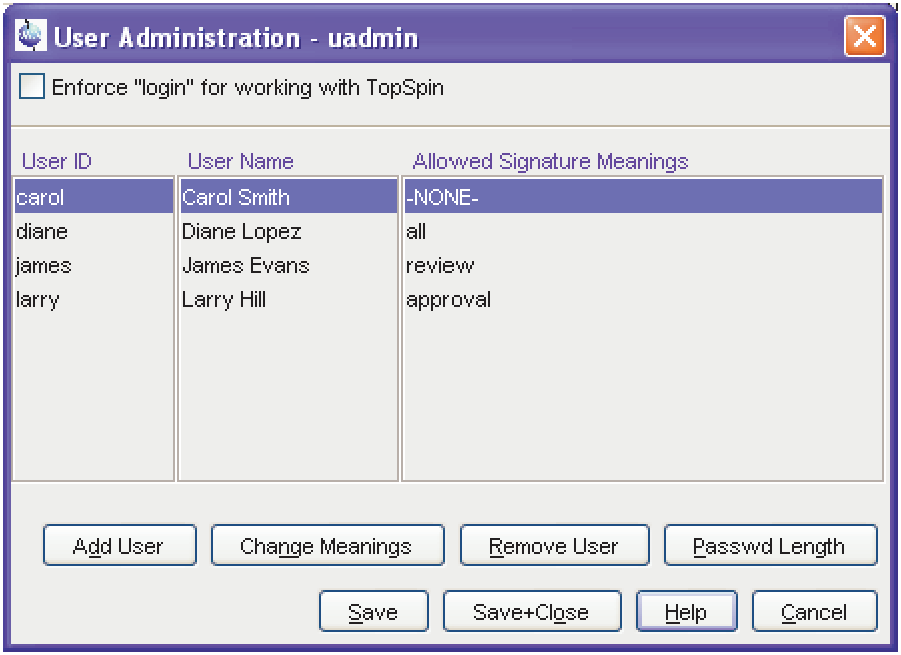
uadmin

NAME

uadmin - TOPSPIN internal user administration

DESCRIPTION

The command ***uadmin*** allows you to administer TOPSPIN internal users. It opens the dialog shown in Figure 14.9.



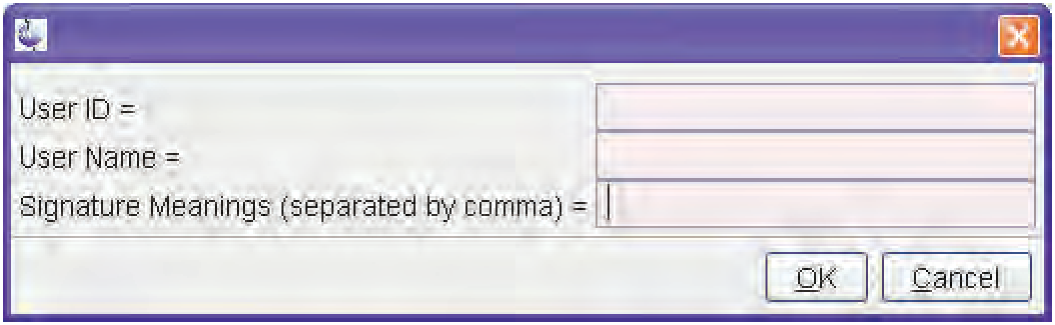
□ Enforce "login" for working with TopSpin

User ID	User Name	Allowed Signature Meanings
carol	Carol Smith	-NONE-
diane	Diane Lopez	all
james	James Evans	review
larry	Larry Hill	approval

Figure 14.9

To add a new user, click the button ***Add User***, which will open the following dialog: shown in Figure 14.10. Here you can enter the User-Id, full user name and Signature meaning.

The Signature meaning can be chosen userspecifically. This freedom is offered by Bruker TopSpin Software because normally the Signature meaning is acted in accordance to the guidelines of your concern (e. g. ISO 9001).



User ID =

User Name =

Signature Meanings (separated by comma) =

Figure 14.10

The ***uadmin*** dialog also offer the following buttons:

- ***Change Meaning*** - change the signature meaning of the marked user
- ***Remove User*** - remove the marked user entry
- ***Passwd Length*** - change the minimum password length
- ***Save*** - save the user administration
- ***Save+Close*** - save the user administration and close the dialog
- ***Cancel*** - Close the dialog discarding any changes

The command can also be started as follows:

click ***Options*** → ***Administration*** → ***Change internal user password***

INPUT/OUTPUT FILES

<tshome>/conf/

`topspin-users.prop` - TOPSPIN users properties file

SEE ALSO

esign, logoff, chpwd, lockgui

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