TopSpin

● TopSpin AU Programming

User Manual

Version 003

Innovation with Integrity

NMR

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Contents

1 Introduction

1.1 What is New in TopSpin 4.0

- AU-program ‘`getheliumlog`’ to copy and update helium-log file from EPU to workstation.
- AU-program method ‘`int getProbeId(char* probeId, size_t size)`’ to get the Id of the installed probe, e.g. ‘Z8157_0001’
- AU-program method ‘`int getProbeName(char* probeName, size_t size)`’ to get the name of the installed probe.
- AU-program method ‘`int isAtmaProbe()`’ to find out whether the installed probe has ATM capabilities.
- AU-program method ‘`int is SolidProbe()`’ to find out whether the installed probe is a solid state probe.
- AU-program method ‘`int getSpectrosVersion(char* cStringBuffer, const size_t bufferLength)`’ to read out version of operating system on the EPU.
- AU program function `GetTsVersionDot` to return the current version and patchlevel of TopSpin in a dotted format. For further information please refer to chapter *GetTsVersionDot [▸ 98]*.
  Please note that the former function `getxwinversion()` is deprecated.
- AU-program ``sertoint`' to convert 64-bit double ser data (Topspin 4.0 format) into 32-bit int data (Topspin 3.5 and earlier format)
- AU-program ``sertodouble`' to convert 32-bit int ser data into 64-bit double data
- new command line option **ipap2** for AU program split which makes AU program `splitipap2` obsolete

1.2 What is New in TopSpin 3.0

New AU macros `FETCHERETICPAR` and `STOREERETICPAR`.The macros `FETCHERETICPAR` and `STOREERETICPAR` can be used within AU Programs to read and write arbitrary parameters in the *eretic* file residing in the PROCNO of the current data set. Similar to the macros `FETCH1PAR` and `FETCHDOSYPAR`.

1.3 What is New in TopSpin 2.1

Changes in TopSpin 2.1 with respect to AU programs.

- The macro XAU requires two arguments, allowing you to freely choose the arguments to be propagated from the calling AU program.
- C-language argument syntax **i_argv** and **i_argc** can be used in AU programs.
- New AU macros to delete data have been added: `DELETEPROCDATA, DELETEIMAGINARYDATA, DELETERAWDATA, DELETEPROCNO, DELETEEXPNO, DELETENAME.`
- New AU macros to fetch/store nD data have been added: `FETCHPARN, FETCHPARNS, STOREPARN, STOREPARNS.`
- The functions `getParfileDirForRead` and `getParfileDirForWrite` replace the functions `getstan` and `PathXWinNMR*`.

1.4 What is New in TopSpin 2.0

Changes in TopSpin 2.0 with respect to AU programs.

- AU programs that contain a plotting command can be entered with the argument **noplot**. This argument prevents plotting.
- All AU-macros, e.g. `EF, APK, QUIT` must be specified in capital letters. In previous versions of TopSpin and its predecessor XWIN-NMR, capital letters were recommended but not required.
- New macros exist for automatic creation of Plot Editor layouts. Examples are `LAYOUT_OBJ_1D` and `LAYOUT_ADD`.

1.5 What are AU Programs?

AU programs can be considered as user defined TopSpin commands. Any repetitive task is most effectively accomplished through an AU program. All commands which can be entered on the TopSpin command line can also be entered in an AU program in the form of macros. This includes selecting and changing data sets, reading and setting parameters, starting acquisitions, processing data and plotting the result. A simple AU program is nothing else than a sequence of such macros which execute the corresponding TopSpin commands. However, AU programs may also contain C-language statements. In fact, an AU program is a C-program because all AU macros are translated to C-statements. TopSpin automatically compiles AU programs to executable binaries, using a C-compiler.

TopSpin offers three other ways of creating user defined commands: TopSpin macros (not to be confused with AU macros), Tcl/Tk scripts and Python programs. They differ from AU programs in that they do not need to be compiled.

1.6 Other Manuals Describing AU Programs/Macros

Creating and using AU programs is described and referred to in various other manuals:

- **Processing Reference Guide**: for each processing command for which an AU macro exists, this macro and its usage is specified.
- **Acquisition Reference Guide**: for each acquisition command for which an AU macro exists, this macro and its usage is specified.
- **NMR Guide**: AU programs can be sorted and listed according to their usage showing their names and short descriptions.
- **Data Publishing Manual**: chapter about AU program macros for plotting.

1.7 Quick Reference to Using AU Programs

Bruker delivers a library of standard AU programs with TopSpin. After TopSpin has been installed you must do the following in order to use them:

1. Run **expinstall** once to install all AU programs.
2. Run **compileall** once to compile all AU programs.
3. Enter the name of an AU program to execute it.

Furthermore, you can write your own AU programs in the following way:

1. Enter **edau <name>**The file <name> will be opened with a text editor.
2. Do one of the following:
   - Write your own AU program from scratch.
   - Read in an existing AU program and modify it according to your needs.

3. Click **Save, exit and compile**. If you are not using the internal editor, you have to compile the AU program in a separate step with the command **cplbruk <name>.**
4. Enter the name of the AU program to execute it.

After you have installed a new version of TopSpin, you must run **expinstall** and **compileall** again to install and compile both Bruker's and your own AU programs.

1.8 Installing and Compiling Au Programs

When you have installed a new version of TopSpin, you must install the library AU programs once by executing the TopSpin command **expinstall**. Your own AU programs which you created under a previous version of TopSpin are still available, they only need to be re-compiled.

An AU program is automatically compiled, the first time it is executed, i.e. when its name is entered on the command line.

To compile an AU program without executing it:

- Enter **cplbruk <name>**

or

- Enter **edau <name>** and click **Exit and Compile**.

To compile all Bruker AU programs:

- Enter **compileall.**

1.9 Executing AU Programs

Once an AU program has been installed, there are 3 different ways to execute it:

1. Enter the name of the AU program. This will work if:
   – No TopSpin command or macro with the same name exists. Here we refer to a TopSpin macro created with **edmac**.
2. Enter **edau**.

   A list of available AU programs will appear. Click on the AU program you want to execute and click **Execute**.

1.10 Viewing AU Programs

You can view existing AU programs in the following:

- Enter **edau**.
  – A dialog box listing all AU programs is opened. From the **Options** menu, you can choose to display **Bruker defined**, **User defined** or **All** AU programs.
- Click on an AU program in the list.
  – When you select a Bruker AU program, it is shown in *view* mode which means you cannot edit it. When you click on a user-defined AU program it is shown in *edit* mode which means you can change it.
- Enter **listall_au.**
  – A list and a short description of all library AU programs is stored in the file *listall* in the users home directory. **Note** that this list is also available in the chapter *List of Bruker AU programs [▶ 105]*of this manual.

1.11 About AU Macros

We will use the word *macro* rather often throughout this manual referring to AU macros. This should not be confused with TopSpin macros which are files containing a sequence of TopSpin commands. TopSpin macros are created with **edmac** and executed with **xmac**. An AU macro, however, is a statement in an AU program which defines one or more TopSpin commands, library functions or C-language statements. In its simplest form, an AU macro defines one TopSpin command. For example the macros `ZG` and `FT` execute the TopSpin commands **zg** and **ft**, respectively. Other macros like `FETCHPAR` and `IEXPNO` do not define TopSpin commands, their function is only relevant in the context of an AU program. More complex macros may contain several TopSpin commands and/or C-statements. All macros in AU programs should be written in capital letters. They are automatically translated to the corresponding C-code when the AU program is compiled. AU macros are defined in the file:

/tshome/prog/include/aucmd.h

1.12 About Bruker Library Functions

Bruker library functions are C-functions which are contained in Bruker libraries. They offer several features which are also used in the TopSpin interface, for example the display of a list of data sets from which the user can select one data set. If you use a Bruker library function in an AU program the corresponding library is automatically linked to the AU program during compilation. The most important and versatile Bruker library functions are described in *Macros Handling TopSpin Parameters [▶ 67]*.

1.13 Creating Your Own AU Programs

1.13.1 Writing a Simple AU Program

Before you start writing an AU program, you might want to check if an AU program already exists which (almost) meets your requirements. If this is not the case, you can write your own AU program in the following way:

1. Enter **edau <au-name>**Your preferred TopSpin text editor will be opened. To change the text editor enter **set** and click **Miscellaneous**.
2. Do one of the following:
   – Insert an existing library AU program and modify it to your needs.
   – Write a new AU program using the macros as described in this manual.
3. The last macro in an AU program should always be `QUIT` (or `QUITMSG`).
4. Click **Save, exit and compile**. If you are not using the internal editor, you have to compile the AU program in a separate step with the command **cplbruk <name>**.

1.13.2 Using Variables

Since AU programs are C programs you can use C-language variables. Several variables are already predefined for usage in AU programs. In fact, we distinguish three different types of variables:

- Predefined dedicated variables.
- Predefined general variables.
- User defined variables.

1.13.2.1 Predefined Dedicated Variables

Predefined dedicated variables have the following properties:

- They do not need to be declared in an AU program.
- Their declaration is automatically added during compilation.
- They are known to the AU main body and to possible subroutines.
- They are set implicitly by certain macros, e.g. the variable expno is set by macros like `DATA SET` and `IEXPNO`.
- They should not be set explicitly, so do **NOT** use statements like:

```
expno = 11;
FETCHPAR("NS", &expno)
```

- They can be evaluated in macros or C-statements, e.g.:

```
DATA SET(name, expno, 2, disk, "guest") i1=expno+1;
```

- Examples of different types of predefined dedicated variables are:

  char-string: `name, disk, user, name2`

  integer: `expno, procno, loopcount1, loopcount2, lastparflag`

A complete list of all predefined dedicated variables with their types can be found in *Including Header Files [▷ 16]*.

1.13.2.2 Predefined General Variables

Predefined general variables have the following properties:

- They do not need to be declared in an AU program.
- Their declaration is automatically added during compilation.
- They are known to the AU main body but not to possible subroutines.
- They can be freely used for various purposes.
- Examples of different types of predefined general variables are:

  integer: `i1, i2, i3`

  float: `f1, f2, f3`

  double: `d1, d2, d3`

  char-string: `text`

A complete list of all predefined general variables with their types and initial values can be found in *Predefined General Variables [▷ 18]*.

1.13.2.3 User Defined Variables

For simple AU programs the number of predefined general variables is sufficient, you do not need to declare any additional variables. For more complex AU programs you might need more variables or you might want to use specific names. In these cases you can define your own variables in the AU program. User defined variables have the following properties:

- They must be declared at the beginning of an AU program.
- They can be freely used for various purposes.
- They are known to the main AU program but not to possible subroutines.
- Examples of declarations are:

```
int ivar1, ivar2;
float fvar1, fvar2, fvar3;
```

```
double dvar1, dvar2, dvar3;
char cstr1[20], cstr2[200];
```

1.13.3 Using AU Macros with Arguments

Several AU macros take one or more arguments. Arguments can be constants (values) or variables. In fact, an argument can be specified in four different ways as described here for the macro `REXPNO`:

- as a constant, e.g.:

  ```
  REXPNO(3)
  ```

- as a predefined dedicated variable e.g.:

  ```
  REXPNO(expno+1)
  ```

- as predefined general variable, e.g.:

  ```
  i1 = 6; REXPNO(i1)
  ```

- as a user defined variable,e.g.:

  ```
  int my_exp;
  ....
  my_exp = 1;
  REXPNO(my_exp)
  ```

It is very important that the arguments are of the correct type. Macros can take arguments of the type integer (like `REXPNO`), float, double or character-string.

Some macros, for example `STOREPAR`, take TopSpin parameters as arguments and each parameter is of a certain type. For example, the AU statement:

```
STOREPAR("O1", d1)
```

stores the value of the variable `d1` into the parameter O1. The predefined (double) variable `d1` is used since O1 is of the type double. The second argument could also be a constant, e.g.:

```
STOREPAR("O1", 287.15)
```

A list of all TopSpin parameters and their type can be found in *TopSpin Parameter Types [▸ 117]*.

1.13.4 Using AU Programs with Arguments

An AU program can be used with arguments. Arguments are available within the AU program as C-languages variables:

`i_argc`: the number of arguments

`i_argv`: the arguments

`cmd`: all specified arguments concatenated

The first argument is the AU program path name and the second argument always `exec`. So for an AU program entered without arguments, `i_argc = 2` and `cmd` is an empty string.

For example `myau a1 a2`

```
i_argc = 4
i_argv[0] = myau
i_argv[1] = exec
i_argv[2] = a1
```

```
i_argv[3] = a2
cmd = "a1 a2"
```

Note that `cmd` is actually legacy code whose usage is discouraged. It may no longer be supported in future versions.

1.13.5 Using C-Language Statements

AU programs can contain AU macros but also C-language statements like:

- Define statements, e.g.: `#define MAXSIZE 32768`
- Include statements, e.g.: `#include <time.h>`
- Variable declarations, e.g. `int ivar;`
- Variable assignments, e.g.: `ivar = 20;`
- loop structures, e.g.: `for, while, do`
- Control structures, e.g.: `if-else`
- C-functions, e.g.: `strcpy, strcmp, sprintf`

Important: several C-language statements (including declarations of variables) are already predefined and automatically added during compilation of the AU program.

A example of an AU program using macros and C-statements is:

```
int eno, pno;
char datapath [500], dataname[50], datauser[50],
                                  datadisk[200];
(void) strcpy (dataname,name);
(void) strcpy (datauser,user);
(void) strcpy (datadisk,disk);
eno = expno;
pno = procno;
(void) sprintf (datapath,"%s/data/%s/nmr/%s/%d/pdata/%d/
         title",datadisk, datauser, dataname, eno, pno);

if ( (i1 = showfile (datapath)) < 0 )
{
  Proc_err (DEF_ERR_OPT,"Problems with
                    showfile function");

}
QUIT
```

Note that `QUIT` is an AU macro, `strcpy` and `sprintf` are C-functions and `showfile` and `Proc_err` are Bruker library functions.

For an explanation of C-functions and more information on C-language we refer to the literature on C-programming.

1.13.6 Additional Hints on C-Statements

If you are using C-language code in your AU programs, then there are a few things to be considered.

- Using C-language header files:

Several C-language header files are automatically included in your AU program during compilation. If you are using C-code which requires additional header files you must write your AU program in a special way. The main AU program should be a call to a subroutine which performs the actual task of the AU program. The *include* statements for the header file must be entered between the main AU program and the subroutine. This gives the following structure.

```
AUERR = subroutine(curdat, cmd)
QUIT
#include <headerfile.h>
static int subroutine(const char* curdat, const char* cmd) {
MACRO1
MACRO2
return 0;
}
```

Such a structure is used in several Bruker library AU programs (e.g. amplstab, decon_t1, etc.). Several Bruker library functions like `PrintExpTime`, `gethighest`, `pow_next` and `unlinkpr` also require an include statement in the AU program (see *Bruker Library Functions [▹ 87]*).

- Some macros, e.g. `IEXPNO` and `IPROCNO` change the current AU data set but do not make it available for subsequent commands. If they are followed by a `CPR_exec` or any C-statement which access the current AU data set, then you must precede that statement with `SETCURDATA` (see also the descriptions of `SETCURDATA`, `IEXPNO` etc. in *Macros Changing the Current AU Data set [▹ 45]*).
- If you are using C-languages loop statements like `for`, `do` or `while` or control statements like `if`, we strongly recommend to always put the body of such statements between {}. If the body only contains simple macros like `ZG` or `FT` you can omit them because these macro definitions already contain {}. However, more complex macros might internally define C-statements that include loop or control structures. If such a macro is used within a loop or control structure in the AU program, then you create nested loops which require the usage of {}.

1.13.7 Viewing Bruker Standard AU Programs for Macro Syntax

The syntax of many AU macros is trivial, just enter the TopSpin command in capital letters. Other macros and especially Bruker library functions are more complex. A detailed description of frequently used AU macros and functions can be found in subsequent chapters of this manual. Alternatively, you can also look for an existing AU program containing this macro or function. If, for example, you want to know the syntax of the macro `WRPA`, just search for an AU program containing the text WRPA in the directory:

<ts_home>\prog\au\src.exam

Using the Windows of Linux Search function.

1.14 How an AU Program is Translated into C-Code

This paragraph is intended for users who want to get a deeper understanding of the compilation process. If you simply want to write and use AU programs you can skip this paragraph.

TopSpin automatically translates your AU program into C-language and compiles it. Files and directories used during AU program compilation are:

/<tshome>/exp/stan/nmr/au/makeau

/<tshome>/exp/stan/nmr/au/vorspann

/<tshome>/prog/include/aucmd.h

/<tshome>/prog/include/inc

The compilation process is entirely controlled by the script *makeau* which performs the following steps.

1. The file *vorspann* is concatenated with your AU program. This file contains a variety of definitions including
   - The C-program `main` statement.
   - `#include` statements of C-header files (which in turn contain other definitions).
   - `#define` statements which define constants.
   - Predefined dedicated variables, e.g.: `name, disk, user, expno, procno`
   - Predefined general variables, e.g. : `text, i1, i2, i3, f1, f2, f3, d1, d2, d3`
2. After *vorspann* and your code have been concatenated, all macro definitions are replaced according to their definitions as described in the file *aucmd.h* and in the *inc* directory. In some cases, the name of the macro is the name of one of the files in *inc* directory and the entire content of the file represents that macro.
3. Step 2. results in a C program source file which this file is compiled and an executable program is created. By default, the compilation is done with the GNU C-compiler *gcc* which is delivered with TopSpin. The linking process is done with the native linker which is part of the native C-compiler *cc*. All AU program's source files reside in:

   /<tshome>/exp/stan/nmr/au/src

   executables will be stored into:

   /<tshome>/prog/au/bin

The following section shows the result of concatenating *vorspann* with the following AU program:

```
EFP
APK
SREF
QUIT
```

For better presentation, only a part of *vorspann* is shown. All variables declared in *vorspann* are listed in *About AU Macros [▸ 10]*.

```
#include <stdio.h>
#include <stdlib.h>
...........................
main(argc,argv)
int argc;
char **argv;
{
  char curdat[PATH_MAX];
  char arglist[BUFSIZ];
  int modret;
  ...
  (void)getcurdat(1, curdat, disk, user, type, name,
                              &expno, &procno);...

  modret = AU_program(curdat,arglist);
}
```

```
.............................
AU_program(curdat,cmd)char *curdat;
char *cmd;
{
int i1=0,i2=0,i3=0;
float f1=0,f2=0,f3=0,f998=0,f999=0;double d1=0,d2=0,d3=0;
char text[BUFSIZ/2];
GETCURDATA
EFP
APK
SREF
QUIT
```

Note that the macro `QUIT` defines the closing C-language '}'statement.

1.14.1 Using the Native gcc Compiler

By default, AU programs are compiled with the Bruker delivered gcc compiler. If you want to use the native operating system compiler, you can do that as follows.

1. From the Windows Explorer or LINUX file manager open the following file with a text editor:

   <tshome>/exp/stan/nmr/au/makeau

2. Search for the following line:

   ```
   # $opt_native = 1;
   ```

   and remove the # character at the beginning of the line.

3. Save and close the file.
4. Start TopSpin and compile your AU programs.

Now, under Windows, the Visual C++ compiler will be used.

Note that this is not a part of the standard operating system. Under LINUX, the default system GCC compiler is used.

To activate the native compiler for the current TopSpin session only, enter the following command:

env set DEBUG_MAKEAU=-native

1.15 Listing of all Predefined C-Statements

1.15.1 Including Header Files

The following C-language header files are automatically included during compilation:

stdio.h, stdlib.h, unistd.h, string.h, errno.h, math.h, limits.h, fcntl.h

Which reside in the following directory:

Under Windows: *<tshome>/GNU/usr/include*

Under LINUX: */usr/include*

and

erropt.h, brukdef.h, lib/uni.h, lib/libcb.h, lib/util.h, sample.h, aucmd.h

Which reside in the directory:

/tshome/prog/include

Note that under LINUX, the packages *glibc-kernheaders* and *glibc-devel* must be installed to be able to compile AU programs (see Installation Guide Linux).

1.15.2 Predefined Dedicated Variables

The following list contains all predefined dedicated variables, their type and the AU macros by which they are set.

Note that most variables are set or modified by several macros and only one or two are listed here.

type	variable	set by macros
int	lastparflag	USELASTPARS, USECURPARS
int	loopcount1	TIMES/END
int	loopcount2	TIMES2/END
int	loopcount3	TIMES3/END
int	loopcountinf	TIMESINFINITE
char	disk[256]	GETCURDATA
char	user[64]	GETCURDATA
char	type[16]	GETCURDATA
char	name[64]	GETCURDATA
int	expno	GETCURDATA, IEXPNO
int	procno	GETCURDATA, IPROCNO
char	disk2[256]	GETCURDATA2
char	user2[64]	GETCURDATA2
char	type2[16]	GETCURDATA2
char	name2[64]	GETCURDATA2
int	expno2	GETCURDATA2
int	procno2	GETCURDATA2
char	disk3[256]	GETCURDATA3
char	user3[64]	GETCURDATA3
char	type3[16]	GETCURDATA3
char	name3[64]	GETCURDATA3
int	expno3	GETCURDATA3
int	procno3	GETCURDATA3
char	namelist[10][64]	SETDATA SET

type	variable	set by macros
char	dulist[10][256]	SETDATA SET
char	userlist[10][64]	SETDATA SET
char	parsetlist[10][16]	RPARSETLIST
char	pulproglist[10][32]	RPULPROGLIST
int	expnolist[15]	SETDATA SET
int	procnolist[15]	SETDATA SET
int	loopcountlist[15]	RLOOPCOUNTLIST
float	vtlist[128]	RVTLIST
int	xloopcount	ILOOPCOUNTLIST
int	xpulprog	IPULPROGLIST
int	xparset	IPARSETLIST
int	xdata set	IDATA SETLIST
int	xvt	IVTLIST
int	listcount1	TIMESLIST
FILE	*textfilepointer	
FILE	*debug	
char	longpath[PATH_MAX]	
char	Hilfs_string[BUFSIZ/2]	

Table 1.1: Predefined Dedicated Variables

1.15.3 Predefined General Variables

The following list contains all predefined general variables, their types and initial values:

type	variable	initial value
int	i1	0
int	i2	0
int	i3	0
double	d1	0
double	d2	0
double	d3	0
float	f1	0
float	f2	0
float	f3	0
float	f998	0
float	f999	0

type	variable	initial value
`char`	`text[BUFSIZ/2 ]`	

Table 1.2: Predefined General Variables

1.16 What to do after Changing a Parameter in an AU Program?

After changing a parameter in an AU program Topspin must be updated whith the changed information. This can be done with the command `Show_meta (SM_SHOWP)`. This command also offers different arguments as following:

- `SM_RAW` ---- Update raw data.
- `SM_RAWP` ---- Update acquisition parameters.
- `SM_PROC` ---- Update processed data.
- `SM_PROCP` ---- Update processing parameters.
- `SM_ALL` ----- Update data and parameters.
- `SM_SHOWR` ---- Switch to raw data.
- `SM_SHOWP` ---- Switch to processed data.
- `SM_DEL` ---- Removed data.
- `SM_PEAK` ---- Update peaks.
- `SM_ INT` ---- Update integrals.

Please note that changing the peak list with a macro in the AU program does not require the argument `SM_PEAK`. The changings are implemented automatically.

1.17 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All what you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All what you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names Data Path Variables Table Column Names Field Names (within Dialog Windows)	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST

Type of Information	Font	Examples

Program Code
Pulse and AU Program Names
Macros
Functions
Arguments
Variables
	Courier	`go=2`
		`au_zgte`
		`edmac`
		`CalcExpTime()`
		`XAU(prog, arg)`
		`disk2, user2`

AU Macro	Courier in Capital Letters	`REX` `PNO`

Table 1.3: Font and Format Conventions

2 Inventory of AU Macros and Bruker Library Functions

2.1 Naming Conventions

This chapter lists most AU macros and Bruker library functions that are available for AU programming. Simple macros with their short description are only mentioned in this chapter. More complex macros and AU functions are mentioned here and described more extensively in the following chapters. The table below explains the macro conventions used in this chapter.

Macro	Explanation
`XXX`	The macro can be typed "as is". There is no further explanation for the macro in this manual.
`XXX(arg1,arg2)`	The macro XXX takes two arguments. Because the macro is easy to use, there is no further description in this manual.
`XXX *`	Like XXX, but there is a detailed description in one of the following chapters.
`XXX(....) *`	The macro XXX takes one or more arguments and its usage is described in one of the following chapters.

Table 2.1: Macro Conventions

Several AU macros that are described in this chapter require one or more arguments. These arguments can be constants or variables as described in *Predefined General Variables [▸ 18]*. It is very important to use the correct type of argument in a macro call. The macros described in the tables of this chapter use the following arguments:

integer : `i1, i2, i3, eno, pno`

float : `f1`

double : `d1`

char-string: `text, cmd, file, flag, mac, parm, parset,`
`prog, shim, typ, dsk, usr, nam`

Note that the arguments `i1`, `i2`, `i3`, `f1`, `d1` and `text` have the same names as the corresponding predefined general variables. The predefined general variables are easy to use because they do not need to be declared. You can, however, use your own variables as macro arguments.

2.2 Macros for Data set Handling

Macro	Description
`GETCURDATA *`	Get the foreground data set.
`SETCURDATA *`	Make the current AU data set available for subsequent AU statements.
`GETDATA SET *`	Prompt the user to specify a new data set.

Macro	Description
`DATASET(....) *`	Set the current AU data set.
`DATASET2(....) *`	Set the 2nd data set (like the TopSpin command **edc2**).
`DATASET3(....) *`	Set the 3rd data set (like **edc2**).
`GETCURDATA2`	Read the 2nd data set (like **edc2**).
`GETCURDATA3`	Read the 3rd data set (like **edc2**).
`DEXPNO *`	Decrease the experiment number by one.
`IEXPNO *`	Increase the experiment number by one.
`REXPNO(eno) *`	Set the experiment number to the value of eno.
`DPROCNO *`	Decrease the processing number by one.
`IPROCNO *`	Increase the processing number by one.
`RPROCNO(i1) *`	Set the processing number to the value of `i1`.
`GDATASETLIST`	Prompt the user to enter a data set list file name and read its contents.
`GLIST`	Prompt the user to enter the data set list file name and read its contents. In addition to the GDATA SETLIST macro, GLIST also expects a pulse program and a parameter set name in the data set list file.
`DDATASETLIST`	Decrement to the previous entry in the data set list.
`IDATASETLIST`	Increment to the next entry in the data set list.
`RDATASETLIST(i1)`	Read the data set at position `i1` of the data set list and make it the current AU data set.
`IFEODATASETLIST`	Checks if the end of the data set list is reached. The answer is true if there is no further entry.
`SETDATASET`	Set the current AU data set to the one currently defined by the data set list.
`DU(dsk)`	Set the disk unit (top level data directory) to `dsk`.
`SETUSER(usr)`	Set the user name to the user `usr`.
`RE(name)`	Read the data set name.
`WRA(eno) *`	Copy the raw data to the experiment number eno.
`WRP(pno) *`	Copy the processed data to the processing number pno.
`WRPA(....) *`	Copy the raw and processed data to the specified data set.
`VIEWDATA *`	Show the current AU program data set in a new window or activate the window that contains this data set.
`VIEWDATA_SAMEWIN*`	Show the current AU program data set in the current window.
`AUDITCOMMENTA (cmt)`	Add a user comment to the acquisition audit trail (audita.txt).
`AUDITCOMMENTP(cmt)`	Add a user comment to the processing audit trail (auditp.txt).

Macro	Description
`GDCHECK`	generate checksum, making the processing audit trail consistent.
`GDCHECKRAW`	generate checksum, making the raw audit trail consistent.
`ACQUPATH(x)`	Returns the path of the file x in the acquisition data directory (ACQU).
`PROCPATH(x)`	Returns the path of the file x in the processed data directory (PROCNO).
`DELETEPROCDATA`	Delete processed data.
`DELETEIMAGINARYDATA`	Delete imaginary processed data.
`DELETERAWDATA`	Delete raw data.
`DELETEPROCNO`	Delete processed data directory (PROCNO).
`DELETEEXPNO`	Delete raw data directory (EXPNO).
`DELETENAME`	Delete data directory (NAME).

Table 2.2: Macros for Data set Handling

2.3 Macros Prompting the User for Input

Macro	Description
`GETDOUBLE(text,d1) *`	Prompt the user to enter a double value.
`GETFLOAT(text,f1) *`	Prompt the user to enter a float value.
`GETINT(text,i1) *`	Prompt the user to enter an integer value.
`GETSTRING(text,nam) *`	Prompt the user to enter a text string.

Table 2.3: Macros Prompting the User for Input

2.4 Macros Handling TopSpin Parameters

Macro	Description
`GETPROSOL *`	Copy the probe and solvent dependent parameters to the corresponding acquisition parameters.
`FETCHPAR(par,&val) *`	Get an acquisition or processing parameter.
`FETCHPAR1(par,&val)`	Get an F1 dimension parameter (2D acquisition/ processing).
`FETCHPAR3(par,&val)`	Get an F1 dimension parameter (3D acquisition/ processing).
`FETCHPARS(par,&val) *`	Get a status parameter (acquisition and processing).
`FETCHPAR1S(par,&val)`	Get an F1 dimension status parameter (2D).
`FETCHPAR3S(par,&val)`	Get an F1 dimension status parameter (3D).
`FETCHPARN(dir,par,&val)`	Get a parameter from specified direction (nD).

Macro	Description
`FETCHPARNS(dir,par,&val)`	Get a status parameter from specified direction (nD).
`STOREPAR(par,val) *`	Store an acquisition, processing or output parameter.
`STOREPAR1(par,val)`	Store an F1 dimension parameter (2D).
`STOREPAR3(par,val)`	Store an F1 dimension parameter (3D).
`STOREPARS(par,val) *`	Store a status parameter (acquisition and processing).
`STOREPAR1S(par,val)`	Store an F1 dimension status parameter (2D).
`STOREPAR3S(par,val)`	Store an F1 dimension status parameter (3D).
`STOREPARN(dir,par,&val)`	Store a parameter to specified direction (nD).
`STOREPARNS(dir,par,&val)`	Store a status parameter to specified direction (nD).
`FETCHPARM(par,&val)`	Get a tomography measurement parameter.
`STOREPARM(par,val)`	Store a tomography measurement parameter.
`FETCHT1PAR(par,&val)`	Get a T1 parameter.
`STORET1PAR(par,val)`	Store a T1 parameter.
`FETCHDOSYPAR(par,&val)`	Get a dosy (**eddosy**) parameter.
`STOREDOSYPAR(par,val)`	Store a dosy (**eddosy**) parameter.
`RPAR(parset,typ) *`	Read a parameter set to the current data set.
`WPAR(parset,typ) *`	Write the current data set parameters to a parameter set.
`DELPAR(parset)`	Delete the parameter set *parset.*

Table 2.4: Macros Handling TopSpin Parameters

PARSET is not used in any AU program

2.5 Acquisition Macros

Macro	Description
`ZG`	Start acquisition; if raw data already exist, they are overwritten.
`GO`	Continue the acquisition on already existing raw data by adding to them.
`II`	Initialize acquisition interface.
`RGA`	Automatic receiver gain adjustment.
`MAKE_ZERO_FID`	Create an empty FID.
`DEG90`	Determine 90° pulse automatically.
`GPULPROGLIST`	Prompt the user to enter the name of a pulse program list file and read its contents.
`DPULPROGLIST`	Decrement to the previous name in the pulse program list.
`IPULPROGLIST`	Increment to the next name in the pulse program list.

Macro	Description
`RPULPROGLIST(i1)`	Read the pulse program name in position `i1` of the pulse program list and write it to the acquisition parameters.
`SETPULPROG`	Store the current pulse program name from the pulse program list.
`IFEOPULPROGLIST`	Check if the end of the pulse program list is reached. The answer is true if there is no further entry.

Table 2.5: Acquisition Macros

2.6 Macros Handling the Shim Unit and the Sample Changer

Macro	Description
`AUTOGAIN`	Optimize lock gain.
`AUTOPHASE`	Optimize lock phase.
`AUTOSHIM_ON`	Turn autoshim on.
`AUTOSHIM_OFF`	Turn autoshim off.
`EJ`	Eject sample from the magnet.
`IJ`	Insert sample into the magnet.
`LOCK_ON`	Turn lock on.
`LOCK_OFF`	Turn lock off.
`ROT`	Turn rotation on (use value RO from acquisition parameters).
`ROTOFF`	Turn rotation off and wait until rotation was turned off.
`LOPO`	Set the lock parameters (lock power, lock gain, loop filter, loop time and loop gain).
`LFILTER(i1)`	Set the loop filter to the value of `i1`.
`LG`	Auto-adjust the lock gain.
`LGAIN(f1)`	Set the loop gain to the value of `f1`.
`LO(f1)`	Set the lock power to the value of `f1`.
`LTIME(f1)`	Set the loop time to the value of `f1`.
`LOCK`	Lock according to the parameters LOCNUC and SOLVENT using the lock parameters from the **edlock** table.
`RSH(file)`	Read the shim values from the specified file.
`SETSH(shim,i1)`	Set one shim to the value of `i1`.
`SWEEP_ON`	Turn the lock-sweep on.
`SWEEP_OFF`	Turn the lock-sweep off.
`WSH(file)`	Write the shim values to the specified file.
`TUNE(file)`	Start autoshimming with the specified tune file.

Macro	Description
`TUNESX`	Start autoshimming with the tune file defined by the currently defined probe and solvent.

Table 2.6: Macros Handling the Shim Unit and the Sample Changer

2.7 Macros Handling the Temperature Unit

Macro	Description
`TESET`	Set the temperature on the temperature unit to the value of the acquisition parameter TE.
`TEGET`	Get the temperature from the temperature unit and store it in the acquisition status parameter TE
`TE2SET`	Set the temperature on the second regulator of the temperature unit to the value of the acquisition parameter TE2.
`TE2GET`	Get the temperature from the second regulator of the temperature unit and store it in the acquisition status parameter TE2.
`TEREADY(i1,f1)`	After the temperature is set, wait until it is accurate to `f1` degrees for at least 10 sec., then wait `i1` seconds for stabilization.
`TE2READY(i1,f1)`	After the second temperature is set, wait until it is accurate to `f1` degrees for at least 10 sec., then wait `i1` seconds for stabilization.
`TEPAR(file)`	Read a file with parameter settings for the temperature unit.
`GVTLIST`	Prompt the user to enter the variable temperature list name and read its contents.
`RVTLIST`	Read the contents of the variable temperature list file defined by the acquisition parameter VTLIST.
`DVTLIST`	Decrement to the previous value in the vtlist.
`IVTLIST`	Increment to the next value in the vtlist.
`VT`	Read and set the temperature according to the current value of the vtlist.

Table 2.7: Macros Handling the Temperature Unit

2.8 Macros Handling the MAS Unit

Macro	Description
`MASE`	Eject sample from MAS unit.
`MASI`	Insert sample into MAS unit.
`MASR`	Set spinning rate according to the acquisition parameter MASR.
`MASRGET`	Get spinning rate from the MAS unit and store it in the status acquisition parameters.
`MASG(i1)`	Start spinning of sample in MAS with at the most `i1` retries.

Macro	Description
`MASH`	Halt spinning of sample in MAS.

Table 2.8: Macros Handling the MAS Unit

2.9 1D Processing Macros

Macro	Description
`ABS`	Automatic baseline correction (creates intrng file).
`ABSD`	Automatic baseline correction with DISNMR algorithm (creates intrng file).
`ABSF`	Automatic baseline correction between limits ABSF1 and ABSF2.
`APK`	Automatic phase correction.
`APK0`	Zero order automatic phase correction.
`APK1`	First order automatic phase correction.
`APKF`	Automatic phase correction using the spectral region determined by ABSF2 and ABSF1 for the calculation of the phase values.
`APK0F`	Zero order automatic phase correction using the spectral region determined by ABSF2 and ABSF1 for the calculation of the phase values.
`APKS`	Automatic phase correction especially suitable for polymer spectra.
`BC`	Baseline correction of FID (DC correction).
`BCM`	User defined spectrum baseline correction.
`CONVDTA(eno)`	Convert digitally filtered FID into analogue (conventional) form.
`EF`	Exponential window multiplication + Fourier transform.
`EFP`	Exponential window multiplication + Fourier transform + phase correction using the processing parameters PHC0 and PHC1.
`EM`	Exponential window multiplication of FID.
`FMC`	Fourier Transform + magnitude calculation.
`FP`	Fourier Transform + phase correction using the processing parameters PHC0 and PHC1.
`FT`	Fourier Transform.
`GENFID(eno)`	Create FID from processed data.
`GF`	Gaussian window multiplication + Fourier Transform.
`GFP`	Gaussian window multiplication + Fourier Transform + phase correction using the processing parameters PHC0 and PHC1.
`GM`	Gaussian window multiplication.
`HT`	Hilbert Transform.
`IFT`	Inverse Fourier Transform.

Macro	Description
MC	Magnitude calculation.
PK	Phase correction using the processing parameters PHC0 and PHC1.
PS	Power spectrum calculation.
QSIN	Squared sine window multiplication.
SAB	Spline baseline correction using base_info file.
SINM	Sine window multiplication.
SINO	Calculate signal to noise ratio.
SREF	Automatic spectral referencing using 2Hlock parameters.
TM	Trapezoidal window multiplication.
TRF	Processing of the raw data according to the currently defined processing parameters.
TRFP	Processing of the processed data according to the currently defined processing parameters.
UWM	User-defined window multiplication.

Table 2.9: 1D Processing Macros

Note that 1D processing macros which access raw data, execute the corresponding command with the option **same**. For example, FT executes the command **ft same**.

2.10 Peak Picking, Integration and Miscellaneous Macros

Macro	Description
PP	Peak picking according to currently set processing parameters.
PPH	Like PP, but with a peak histogram along the listing.
PPP	Like PP, but the output is written to the file peaklist in the current processing data directory (PROCNO).
PPJ	Like PP, but store peaks in JCAMP-DX format
LI	List integrals according to the currently defined intrng file. The macro ABS can be used to create an intrng file.
LIPP	List integrals and all peaks in the integral ranges.
LIPPF	Like LIPP, but works always on the full spectrum.
PP2D	Perform peak picking on a 2D data set.
RMISC(typ,file)	Read a file from one of the following list types: base_info, baslpnts, intrng, peaklist or reg.
WMISC(typ,file)	Write a base_info, baslpnts, intrng, peaklist or reg file to its lists directory.

Table 2.10: Peak Picking, Integration and Miscellaneous Macros

2.11 Macros for Algebraic Operations on Data sets

Macro	Description
`ADD`	Add 2nd and 3rd data set and put the result into the current data set. The 3rd data set is multiplied by DC.
`ADDFID`	Add two FIDs multiplying one of them with DC.
`ADDC`	Add the constant DC to the current data set.
`AND`	Put logical "and" of 2nd and 3rd data set into the current data set.
`DIV`	Divide 2nd and 3rd data set and put the result into the current data set. The 3rd data set is multiplied by DC.
`DT`	Calculate the first derivative of the data set.
`FILT`	Apply a software digital filter to the current data set.
`LS`	Left shift spectrum or FID by NSP points.
`MUL`	Multiply 2nd and 3rd data set and put the result into the current data set. The 3rd data set is multiplied by DC.
`MULC`	Multiply the current data set with DC.
`NM`	Negate current spectrum.
`RS`	Right shift spectrum or FID by NSP points.
`RV`	Reverse the spectrum.
`ZF`	Zero the spectrum (1r,1i).
`ZP`	Zero the first NZP points of the spectrum or FID.

Table 2.11: Macros for Algebraic Operations on Data sets

2.12 Deconvolution Macros

Macro	Description
`GDCON`	Gaussian deconvolution of the peaks automatically picked according to the currently set processing parameters.
`LDCON`	Lorentzian deconvolution of the peaks automatically picked according to the currently set processing parameters.
`MDCON`	Mixed Gaussian/Lorentzian deconvolution of the peaks in the peaklist file. The peaklist file can be created with the **ppp** command and it can be modified using the **edmisc** command.

Table 2.12: Deconvolution Macros

2.13 2D Processing Macros

Macro	Description
`ABS1`	Baseline correction in F1 dimension.
`ABS2`	Baseline correction in F2 dimension.
`ABSD1`	Baseline correction in F1 dimension using the DISNMR algorithm.

Macro	Description
ABSD2	Baseline correction in F2 dimension using the DISNMR algorithm.
ABSOT1	Trapezoidal baseline correction in F1 dimension using a slightly different algorithm than abst1.
ABSOT2	Trapezoidal baseline correction in F2 dimension using a slightly different algorithm than abst2.
ABST1	Trapezoidal baseline correction in F1 dimension using the processing parameters ABSF1, ABSF2, SIGF1, SIGF2.
ABST2	Trapezoidal baseline correction in F2 dimension using the processing parameters ABSF1, ABSF2, SIGF1, SIGF2.
ADD2D	Add the processed data of the 2nd data set to the current data set.
ADDSER	Add the raw data of the 2nd data set to the current data set.
BCM1	Baseline correction of all columns using the coefficients that were obtained with a manual 1D baseline correction.
BCM2	Baseline correction of all rows using the coefficients that were obtained with a manual 1D baseline correction.
INVSF	Interchange the frequencies of the two dimensions.
LEVCALC	Calculate the levels for the contour representation of the 2D matrix.
PTILT	Tilt the 2D matrix by an arbitrary angle.
PTILT1	Tilt the 2D matrix along its central vertical line.
REV1	Reverse the spectrum in F1 dimension.
REV2	Reverse the spectrum in F2 dimension.
SUB1	Subtract 1D spectrum in F1 dimension (no change in sign).
SUB2	Subtract 1D spectrum in F2 dimension (no change in sign).
SUB1D1	Subtract 1D spectrum in F1 dimension.
SUB1D2	Subtract 1D spectrum in F2 dimension.
SYM	Symmetrize COSY spectrum.
SYMA	Symmetrize phase sensitive COSY spectrum.
SYMJ	Symmetrize J-resolved spectrum.
TILT	Tilt J-resolved spectrum by an internally calculated angle.
XF1	Fourier transform in F1 dimension.
XF1P	Phase correction in F1 dimension using the processing parameters PHC0 and PHC1.
XF2	Fourier transform in F2 dimension.
XF2P	Phase correction in F2 dimension using the processing parameters PHC0 and PHC1.
XFB	Fourier transform in both dimensions.
XFBP	Phase correction in both dimensions.
XF1M	Magnitude calculation in F1 dimension.
XF2M	Magnitude calculation in F2 dimension.

Macro	Description
`XFBM`	Magnitude calculation in both dimensions.
`XF1PS`	Power spectrum in F1 dimension.
`XF2PS`	Power spectrum in F2 dimension.
`XFBPS`	Power spectrum in both dimensions.
`XHT1`	Hilbert Transform in F1 dimension.
`XHT2`	Hilbert transform in F2 dimension.
`XIF1`	Inverse Fourier transform in F1 dimension.
`XIF2`	Inverse Fourier transform in F2 dimension.
`XTRF`	2D processing according to processing parameter flags (starts always on the raw data).
`XTRF2`	2D processing according to F2 processing parameter flags only (starts always on the raw data).
`XTRFP`	2D Processing according to the processing parameter flags.
`XTRFP1`	2D processing according to the F1 processing parameter flags only.
`XTRFP2`	2D processing according to the F2 processing parameter flags only.
`ZERT1`	Zero a region of each column (F1). The region is determined by ABSF1/ ABSF2 (first column) and SIGF1/SIGF2 (last column).
`ZERT2`	Zero a region of each row (F1). The region is determined by ABSF1/ ABSF2 (first row) and SIGF1/SIGF2 (last row).
`GENSER(eno)`	Create a 2D series file from the processed data.

Table 2.13: 2D Processing Macros

Note that 2D processing macros which access raw data, execute the corresponding command with the option **same**. For example, XFB executes the command **xfb same**.

2.14 Macros Reading and Writing Projections etc.

Macro	Description
`F1SUM(i1,i2,pno)`	Read sum of columns from `i1` to `i2` into the 1D processing number `pno`.
`F2SUM(i1,i2,pno)`	Read sum of rows from `i1` to `i2` into the 1D processing number `pno`.
`F1DISCO(i1,i2,i3,pno)`	Read disco projection between `i1` and `i2` columns with reference row `i3` into the 1D processing number `pno`.
`F2DISCO(i1,i2,i3,pno)`	Read disco projection between `i1` and `i2` rows with reference column `i3` into the 1D processing number `pno`.

Macro	Description
F1PROJN(i1,i2,pno)	Read partial negative projection between columns i1 and i2 into the 1D processing number pno.
F1PROJP(i1,i2,pno)	Read partial positive projection between columns i1 and i2 into the 1D processing number pno.
F2PROJN(i1,i2,pno)	Read partial negative projection between rows i1 and i2 into the 1D processing number pno.
F2PROJP(i1,i2,pno)	Read partial positive projection between rows i1 and i2 into the 1D processing number pno.
RHNP(pno)	Read horizontal (F2) negative projection into the 1D processing number pno.
RHPP(pno)	Read horizontal (F2) positive projection into the 1D processing number pno.
RSC(i1,pno) *	Read column i1 of 2D into the 1D processing number pno.
RSR(i1,pno) *	Read row i1 of 2D into the 1D processing number pno.
RVNP(pno) *	Read vertical (F1) negative projection into the 1D processing number pno.
RVPP(pno) *	Read vertical (F1) positive projection into the 1D processing number pno.
RSER(i1,eno,pno) *	Read row i1 of 2D raw data into the eno and pno.
RSER2D(direc, i1,eno) *	Read plane number i1 in direction direc of 3D raw data into the eno.
WSC(i1,pno,eno,nam,usr,dsk) *	Write a column back into position i1 of a 2D data set defined by pno, eno, nam, usr and dsk.
WSR(i1,pno,eno,nam,usr,dsk) *	Write a row back into position i1 of a 2D data set defined by pno, eno, nam, usr and dsk.
WSER(i1,nam,eno,pno,dsk,usr)*	Write an FID back into position i1 of a 2D raw data defined by eno, pno, nam, dsk and usr.
WSERP(i1,nam,eno,pno,dsk,usr)	Write a processed FID back into position i1 of a 2D raw data defined by eno, pno, nam, dsk and usr.

Table 2.14: Macros Reading and Writing Projections etc.

2.15 3D Processing Macros

Macro	Description
`TF3(flag,dsk)`	Fourier transform in F3 dimension. The `flag` can be "y" or "n" and determines whether the imaginary parts are stored or not. The processed are stored on disk unit `dsk`.
`TF2(flag)`	Fourier transform in F2 dimension (`flag` as in TF3).
`TF1(flag)`	Fourier transform in F1 dimension (`flag` as in TF3).
`TF3P(flag)`	Phase correction in F3 dimension (`flag` as in TF3).
`TF2P(flag)`	Phase correction in F2 dimension (`flag` as in TF3).
`TF1P(flag)`	Phase correction in F1 dimension (`flag` as in TF3).
`TABS3`	Automatic baseline correction in F3 dimension.
`TABS2`	Automatic baseline correction in F2 dimension.
`TABS1`	Automatic baseline correction in F1 dimension.
`R12(i1,pno)`	Read F1-F2 plane into a new `procno`.
`R13(i1,pno)`	Read F1-F3 plane into a new `procno`.
`R23(i1,pno)`	Read F2-F3 plane into a new `procno`.

Table 2.15: 3D Processing Macros

2.16 Spectral Width Calculation Macros

Macro	Description
`GETLIM`	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of the 1D spectrum to the difference + 10%.
`GETLCOSY`	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of a COSY spectrum to the difference + 10%.
`GETLXHCO`	Get frequency of leftmost and rightmost peak from two 1D spectra and adjust the sweep width of an X-H correlation spectrum to the difference + 10%.
`GETLJRES`	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of a J-RESolved spectrum to the difference + 10%.
`GETLINV`	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of an INVerse spectrum to the difference + 10%.

Table 2.16: Spectral Width Calculation Macros

2.17 Plot Editor Related Macros

`XWP_LP *`	Create a parameter listing for a plot with the plot editor.

`XWP_PP *`	Create a peak picking listing for a plot with the plot editor.
`AUTOPLOT *`	Plot the current data set according to the plot editor layout defined by the processing parameter LAYOUT.
`AUTOPLOT_TO_FILE(file name) *`	as AUTOPLOT except that the plot is not sent to the printer but store in the postscript file `file name`.
`DECLARE_PORTFOLIO *`	Initialize the usage of other TopSpin portfolio AU macros. Required in XWIN-NMR and TopSpin ≤ 1.2. Obsolete in TopSpin ≥ 1.3.
`CREATE_PORTFOLIO(file name) *`	Create the TopSpin portfolio `file name`.
`ADD_TO_PORTFOLIO(disk, user, name, expno, procno) *`	Add the data set that is specified with the arguments to the portfolio created with CREATE_PORTFOLIO.
`ADD_CURDAT_TO_PORTFOLIO *`	Add the current data set to the portfolio created with CREATE_PORTFOLIO
`CLOSE_PORTFOLIO *`	Close the definition for the portfolio created with CREATE_PORTFOLIO. Must be used before AUTOPLOT_* macros.
`AUTOPLOT_WITH_PORTFOLIO *`	Plot the data set(s) defined in the portfolio created with CREATE_PORTFOLIO according to the layout defined by the parameter LAYOUT.
`AUTOPLOT_WITH_PORTFOLIO_TO_FILE(file name) *`	as AUTOPLOT_WITH_PORTFOLIO except that the plot is not sent to the printer but store in the postscript file `file name`.
`LAYOUT_ADD`	Add object to current layout.
`LAYOUT_ADD_1D_OBJECT`	Add 1D object to current layout.
`LAYOUT_ADD_PARAMETERS`	Add parameter object to current layout.
`LAYOUT_BEGIN_FILE`	Open layout file.
`LAYOUT_BEGIN_FILE`	Close layout file.
`LAYOUT_END_FILE`	Define layout format.
`LAYOUT_FORMAT`	Define 1D object.
`LAYOUT_OBJ_1D`	Define parameter object.
`LAYOUT_OBJ_PARAMETERS`	Define title object.
`LAYOUT_OBJ_TITLE`	Add object to current layout.

Table 2.17: Plot Editor Related Macros

2.18 Macros Converting Data sets

Macro	Description
`FROMJDX(....) *`	Convert a JCAMP-DX file to TopSpin data format.
`TOJDX(....) *`	Convert a data set to JCAMP-DX 6.0 format.
`TOJDX5(....) *`	Convert a data set to JCAMP-DX 5.0 format.
`JCONV(....) *`	Convert a Jeol data set to Bruker TopSpin format.
`VCONV(....) *`	Convert a Varian data set to Bruker TopSpin format.

Table 2.18: Macros Converting Data sets

2.19 Macros to Execute Other AU Programs, TopSpin Macros or Commands

Macro	Description
`CPR_exec(....) *`	C-function for executing special TopSpin commands.
`WAIT_UNTIL(....) *`	Hold the AU program until the specified date and time.
`XAUA`	Execute the acquisition AU program stored in AUNM (**eda**). The next line in the AU program is executed after the AU program AUNM has finished.
`XAUP`	Execute the processing AU program stored in AUNMP (**edp**). The next line in the AU program is immediately executed after the AU program AUNMP has been started.
`XAUPW`	Execute the processing AU program stored in AUNMP (**edp**). Like XAUP, but now the next line in the AU program is executed after the AU program AUNMP has finished.
`XAU(prog, arg)`	Execute the AU program `prog` with the wait option.
`XCMD(cmd) *`	Execute the TopSpin command for which no dedicated macro exists.
`XMAC(mac)`	Execute a TopSpin macro `mac`.

Table 2.19: Macros to Execute Other AU Programs, TopSpin Macros or Commands

2.20 Bruker Library Functions

Macro	Description
`CalcExpTime() *`	Calculate the experiment time for the current experiment.
`PrintExpTime(....) *`	Print the experiment time for the current experiment.
`check_pwd(usr) *`	Prompt the user `usr` to enter a password.
`GetNmrSuperUser() *`	Get the name of the current TopSpin superuser.
`getdir(....) *`	Get all file names and/or directory names within a directory.

Macro	Description
`freedir(....) *`	Free memory allocated by `getdir`.
`dircp(....) *`	Copy a file.
`dircp_err(i1) *`	Return the error message that corresponds to the error return value of a `dircp` function call.
`fetchstorpl(....) *`	Read or store one or several plot parameters.
`FileSelect(....) *`	Display a list of files and allow to select a file.
`gethighest(....) *`	Return the next highest unused experiment number of a data set.
`getParamDirs(...)`	List all directories specified for key.
`getParfileDirForRead(...) *`	Determines path name of list file to be read.
`getParfileDirForWrite(..) *`	Determines path name of list file to be written.
`getstan(....) *`	Return the path name to the user's current experiment directory.
`GetTsVersionDot(....) *`	Return the current version and patchlevel of TopSpin.
`mkudir(....) *`	Create a complete directory path.
`PathXWinNMR() *`	A class of functions which return path names to certain TopSpin directories.
`pow_next(i1) *`	Round `i1` to the next larger power of two.
`Proc_err(....) *`	Show a message in a TopSpin dialog window.
`Show_status(text) *`	Show a string in the status line of TopSpin.
`showfile(file) *`	Show the contents of a `file` in a TopSpin window.
`ssleep(i1) *`	Pause in an AU program for `i1` seconds.
`unlinkpr(....) *`	Delete all processed data files (1r, 1i, 2rr, 2ii etc.) of a data set.

Table 2.20: Bruker Library Functions

2.21 Macros for Loop Control

Macro	Description
`TIMES(n)`	Execute the statements in the loop `n` times.
`TIMES2(n)`	Execute the statements in the loop `n` times. Normally used for the second level of nested loops.
`TIMES3(n)`	Execute the statements in the loop `n` times. Normally used for the second level of nested loops.
`END`	End of a loop.
`STOP`	Stop the AU program with the return value of AUERR.

Macro	Description
`STOPMSG("text")`	Stop the AU program with the return value of AUERR and display the message `"text"`.

Table 2.21: Macros for Loop Control

2.22 Macros to Return from an AU Program

Macro	Description
`ABORT`	Abort the AU program or any of its subroutines with the return value of -1.
`ERRORABORT`	Return from an AU program or any of its subroutines with the value of AUERR if it is less than 0.
`QUIT`	Return from an AU program with the value of AUERR. QUIT is usually the last statement of the AU program code.
`QUITMSG(text)`	Print the text message and then return from the AU program with the value of AUERR. This is an alternative to QUIT.
`STOP`	Stop the AU program with the return value of AUERR.
`STOPMSG("text")`	Stop the AU program with the return value of AUERR and display the message `"text"`.

Table 2.22: Macros to Return from an AU Program

3 General AU Macros

This chapter contains a description of all general AU macros which can be used for various purposes.

3.1 CPR_exec

NAME

`CPR_exec` - Generic function for executing TopSpin commands.

SYNTAX

```
CPR_exec(const char *command, int mode);
```

DESCRIPTION

`CPR_exec` is a generic function which can be used for executing TopSpin commands in AU. The first argument of `CPR_exec` is a string containing a TopSpin command. The second argument must be one of the following values:

`WAIT_TERM` - Waits for the command to finish, then start the next command.

`WAIT_START` - Waits for the command to start, then start the next command.

`CONT_EX` - Starts the command and immediately start the next command.

Practically all dedicated macros which execute a TopSpin command call `CPR_exec` with `WAIT_TERM`. For example, the macro FT is defined as:

```
FT {SETCURDATA AUERR=CPR_exec( "ft same",WAIT_TERM);}
```

The `CPR_exec` return value allows you to check for successfully execution. The return value of `CPR_exec` is `NORM_TERM` (=0) for normal termination or `ERR_TERM` (=-1) for error termination.

`WAIT_START` or `CONT_EX` can be used if asynchronous execution is required. For example, the AU macro `XAUP` uses `WAIT_START` to allow data simultaneous processing and acquisition in automation.

Note that using `WAIT_START` and `CONT_EX` does not allow you to check the return value for successful execution.

For most commands a dedicated AU macro is available, like `ZG` for **zg** and `FT` for **ft**. If you want to use TopSpin commands for which no dedicated macro exist, e.g. editor commands or commands with special arguments, then you can use the generic macro `XCMD` which takes only one argument, the TopSpin command and is started with `WAIT_TERM`. `XCMD` is defined as:

```
XCMD(cmd) {SETCURDATA AUERR=CPR_exec(cmd,WAIT_TERM);}
```

In fact, the only reason to use `CPR_exec` explicitly is to start a command with `WAIT_START` or `CONT_EX`, i.e. to run commands simultaneously.

Note that dedicated macros and XCMD call SETCURDATA before they do their actual task. This ensures that they operate on the current AU data set. If you use CPR_exec explicitly, it is recommended to precede it with SETCURDATA.

Note that in the example below, CPR_exec is preceded by the macro ZG which implicitly calls SETCURDATA.

In summary:

- Use dedicated AU macros whenever you can.
- Use XCMD when no dedicated macro is available.
- Use CPR_exec when you want to use WAIT_START or CONT_EX.

CPR_exec is part of the uni library which is delivered with TopSpin.

EXAMPLE

The following AU program gets the foreground data set, runs an acquisition, starts the Fourier Transform and, after this has started, continues an acquisition on the next experiment number:

```
TIMES(10)
  ZG
  CPR_exec("ft", WAIT_START);
  IEXPNO
END
QUIT
```

SEE ALSO

XCMD [▸ 41] - Generic macro to execute commands for which no dedicated macro exists
SETCURDATA - make the current AU data set available for subsequent AU statements.

3.2 XAU

NAME

XAU - Generic function for executing AU programs.

SYNTAX

```
XAU(prog, arg)
```

DESCRIPTION

XAU is a general macro to execute (and, if necessary compile) AU programs. The macro takes two arguments:

1. prog - The AU program to be executed.
2. arg – Arguments.

The second argument can be:

- Any character string in """ containing one or more arguments.
- cmd - To transfer all arguments from calling AU program.

- `""` - No arguments are propagated.

In TopSpin 2.0 and older, XAU requires only one argument, the AU program to be executed, automatically propagates all arguments.In TopSpin 2.1 and newer, you can freely choose the arguments to be transferred.

User defined AU programs containing XAU macros must be modified. You could simply extend an XAU call with the extra argument cmd. As such, your AU program behaves exactly the same as in your previous version, namely propagating all caller arguments. The reason, however, that XAU was modified is that you normally do not want to propagate all arguments. In this case, you can replace XAU by XCMD, in which case the AU program can still be used with TopSpin 2.0 and older.

- **To propagate no arguments**
  - Replace `XAU("auprog")` with `XCMD("auprog")` or `XAU("auprog", "")`.
- **To propagate all arguments**
  - Replace `XAU(auprog)` with `XAU("auprog", cmd)`.
- **To specify new arguments arg1 and arg2.**
  - Use `XCMD("auprog arg1 arg2")` or `XAU("auprog", "arg1 arg2")`.

SEE ALSO

XCMD [▸ 41] - Generic function for executing TopSpin commands.

3.3 XCMD

NAME

`XCMD` - Generic function for executing TopSpin commands.

SYNTAX

```
XCMD(const char* command)
```

DESCRIPTION

`XCMD` is a general macro to execute TopSpin commands for which no dedicated macro exists. For most TopSpin commands a dedicated macro does exist and we strongly recommend to:

Use dedicated macros whenever available!

Note that `XCMD` executes `CPR_exec` with the option `WAIT_TERM`. If you want to use the options `CONT_EX` or `WAIT_START`, you must use `CPR_exec`.

If you want to check whether or not `XCMD` was executed successfully, you can check the value of `AUERR (NORM_TERM` or `ERR_TERM)`.

EXAMPLE

The following AU program gets the foreground data set, opens the acquisition parameter editor (**eda**) and runs an acquisition and Fourier transform:

```
XCMD("sendgui eda")
ZG
```

```
  FT
  QUIT
```

SEE ALSO

CPR_exec [▸ 39] - C-function for executing special TopSpin commands.

3.4 WAIT_UNTIL

NAME

`WAIT_UNTIL` - Hold the AU program until the specified date and time.

SYNTAX

```
int WAIT_UNTIL(int hour, int minute, int day, int month)
```

DESCRIPTION

The function `WAIT_UNTIL` waits in an AU program until the specified date has been reached. The variables are internally converted to seconds. Every sixty seconds, the function checks whether the current date matches with the selected date. This function basically allows to program an event or command to start at a certain date rather than waiting for a certain time until something is executed.

EXAMPLE

Wait in the AU program until the 31st of October, 6 pm, and then continue:

```
  WAIT_UNTIL(18,0,31,10)
```

SEE ALSO

ssleep [▸ 103] - Pause in an AU program for a certain number of seconds.

4 TopSpin Interface Functions

AU programs are normally used to execute a series of acquisition or processing commands. For these commands you can use dedicated AU macros like `ZG` and `FT`. Less common is the use of TopSpin Java interface commands in AU programs. You can, however, do that with the `XCMD` or `CPR_exec` macros and the command **sendgui**. Two examples:

- Display the acquisition parameters
  - `XCMD("sendgui eda")`
- Perform a vertical reset of the current data set
  - `CPR_exec("sendgui .vr", WAIT_START)`

Note that `XCMD` is the same as `CPR_exec` with `WAIT_TERM`.

This can be used for all TopSpin interface commands like data window tabs, menu entries and toolbar buttons. Here are some examples:

TopSpin Interface	TopSpin Command	AU statement
Menus		
File => reopen	**reopen**	`XCMD("sendgui reopen")`
File => Close	**close**	`XCMD("sendgui close")`
Window => New Window	**newwin**	`XCMD("sendgui newwin")`
Data Window Tabs		
Spectrum	**spec**	`XCMD("sendgui spec")`
ProcPars	**edp**	`XCMD("sendgui edp")`
Title	**edti**	`XCMD("sendgui edti")`
Toolbar buttons		
	.vr	`XCMD("sendgui .vr")`
	.zi	`XCMD("sendgui .zi")`
	.ov	`XCMD("sendgui .ov")`

Table 4.1: TopSpin interface commands

5 Macros Changing the Current AU Data set

This chapter contains a description of all AU macros which can be used to change the current AU data set, i.e. the data set on which subsequent AU statements operate.

5.1 SETCURDATA

NAME

`SETCURDATA` - Makes the current AU data set available for subsequent AU statements .

SYNTAX

```
SETCURDATA
```

DESCRIPTION

`SETCURDATA` makes the current AU data set, i.e. the data set defined by the data path variables *disk*, *user*, *type*, *name*, *expno* and *procno*, available for subsequent AU commands. Normally, you do not need to enter `SETCURDATA` because it is automatically called by macros which operate on data sets **before** they perform their actual task. Furthermore, the macros `DATA SET` and `GETDATA SET`, which change the current AU data set, automatically call `SETCURDATA` **after** they performed their actual task. In some cases, however, `SETCURDATA` must be specified explicitly in the AU program. For example, the macros `IEXPNO` and `IPROCNO` change the current AU data set, but do not call `SETCURDATA`. If they are followed by a `CPR_exec` or any C-statement which access the current AU data set, then you must precede that statement with `SETCURDATA`.

EXAMPLE

This example shows the part of the library AU program `multizg` which calculates the total experiment time of all acquisitions performed by this AU program:

```
int expTime;
static void PrintExpTime();
....
expTime = 0;
TIMES(i1)
  SETCURDATA;
  expTime += CalcExpTime() + 4;
  IEXPNO;
ENDDEXPNO;
....
QUIT
```

Note that `IEXPNO` is followed by `SETCURDATA` in the next cycle of the loop.

SEE ALSO

DATA SET [▸ 46] - Sets the current AU data set.

IEXPNO [▸ 48] - Increases the experiment number by one.

5.2 DATASET

NAME

`DATASET` - Sets the current AU data set.

SYNTAX

```
DATASET(char *name, int expno, int procno, char *disk, char *user )
```

DESCRIPTION

The macro `DATASET` sets the current AU data set. All data path variables *name*, *expno*, *procno*, *disk* and *user* must be specified as arguments. Subsequent AU commands will operate on this dataset.

EXAMPLE

The following AU program first gets the foreground data set, then selects a new dataset and runs an acquisition:

```
char newname[20];
strcpy(newname, "glycerine");
DATASET(newname, expno, 3, disk, "peter")
ZG
QUIT
```

The data path variables in this example are entered in the following way:

- *expno* and *disk* keep the values of the current data set.
- *name* gets the value of `newname`, a variable defined in this AU program.
- *procno* and *user* get the values `3` and `peter`, respectively, which are entered as constants.

SEE ALSO

GETDATASET [▸ 47] - Prompts the user to specify a new data set.

DATASET2 [▸ 47] - Sets the second data set.

IEXPNO [▸ 48] - Increases the experiment number by one.

5.3 DATASET2, DATASET3

NAME

`DATASET2` - Sets the second AU dataset `DATASET3` - set the third AU data set.

SYNTAX

```
DATASET2(char *name, int expno, int procno, char *disk, char *user)
DATASET3(char *name, int expno, int procno, char *disk, char *user)
```

DESCRIPTION

The macro `DATASET2` sets the second AU data set. The current (first) AU dataset is not affected by this macro. `DATASET2` is typically used in combination with algebra macros, like ADD or `MUL`, which operate on the second and third data set.

EXAMPLE

The following AU program gets the foreground dataset, adds the spectra of the next processing number and the one after that and stores the result into the current dataset:

```
DATASET2(name, expno, procno+1, disk, user)
DATASET3(name, expno, procno+2, disk, user)
ADD
QUIT
```

SEE ALSO

DATASET [▸ 46] - Sets the current AU data set.

GETDATASET [▸ 47] - Prompts the user to specify a new data set.

5.4 GETDATASET

NAME

`GETDATASET` - Prompts the user to specify a new dataset.

SYNTAX

```
GETDATASET
```

DESCRIPTION

The macro `GETDATASET` prompts the user to specify a new dataset. A dialogue is opened and the user is requested to enter the data path variables *name*, *expno*, *procno, user* and *disk*. Subsequent AU commands will operate on this data set. GETDATASET can be used anywhere in an AU program but, since it requires user input, should not be used in fully automated sequences.

NOTE

`GETDATASET` is not used very often. In AU programs, data sets are usually changed without user interaction, e.g. with the macros DATASET, IEXPNO etc.

EXAMPLE

The following AU program gets the foreground data set, prompts the user to specify a new data set and then processes this data set:

```
GETDATASET
EFP
QUIT
```

SEE ALSO

DATASET [▹ 46] - Sets the current AU data set.

IEXPNO [▹ 48] - Increase the experiment number by one.

IPROCNO [▹ 50] - Increase the processing number by one.

5.5 IEXPNO

NAME

`IEXPNO` - Increases the experiment number by one.

SYNTAX

```
IEXPNO
```

DESCRIPTION

The macro `IEXPNO` increases the experiment number of the current AU data set by one. In fact, the value of the data path variable *expno* is incremented by one. Subsequent macros will operate on this new *expno*. `IEXPNO` is typically used in AU programs which run a series of acquisitions on data sets with the same *name* and successive *expnos.*

EXAMPLE

The following AU program gets the foreground data set and runs acquisitions on eight successive *expnos*:

```
TIMES(8)
  ZG
  IEXPNO
END
QUIT
```

NOTE

`IEXPNO` must be followed by a `SETCURDATA` if the AU program continues with an explicit `CPR_exec` or C-statement (see *SETCURDATA [▹ 45]*).

SEE ALSO

DEXPNO [▸ 49] - Decreases the experiment number by one.

REXPNO [▸ 50] - Sets the experiment number to the specified value.

IPROCNO [▸ 50] - Increases the processing number by one.

DATA SET [▸ 46] - Sets the current AU data set.

5.6 DEXPNO

NAME

`DEXPNO` - Decreases the experiment number by one.

SYNTAX

```
DEXPNO
```

DESCRIPTION

The macro `DEXPNO` decreases the experiment number of the current AU data set by one. In fact, the value of the data path variable *expno* is decremented by one. Subsequent macros will operate on this new *expno*. `DEXPNO` is typically used after a loop which includes an `IEXPNO` at the end, to revert the effect of the last (unnecessary) `IEXPNO`.

EXAMPLE

The following AU program gets the foreground data set, runs acquisitions on eight successive *expnos* and displays the data of the last *expno*:

```
TIMES(8)
  ZG
  IEXPNO
END
DEXPNO
VIEWDATA
QUIT
```

Note that `DEXPNO` must be followed by a `SETCURDATA` if the AU program continues with an explicit `CPR_exec` or C-statement (see *SETCURDATA [▸ 45]*).

SEE ALSO

IEXPNO [▸ 48] - Increases the experiment number by one.

REXPNO [▸ 50] - Sets the experiment number to the specified value.

DPROCNO [▸ 51] - Decreases the processing number by one.

5.7 REXPNO

NAME

`REXPNO` - Sets the experiment number to the specified value.

SYNTAX

```
REXPNO(int number )
```

DESCRIPTION

The macro `REXPNO` sets the experiment number of the current AU data set to the specified value. In fact, the value of the data path variable *expno* is set. Subsequent macros will operate on this new *expno*.

EXAMPLE

The following AU program gets the foreground data set, runs acquisitions on eight successive *expnos* then sets the current AU data set back to the first *expno* and Fourier transforms it:

```
i1 = expno;
TIMES(8)
  ZG
  IEXPNO
END
REXPNO(i1)
FT
QUIT
```

Note that `REXPNO` must be followed by a `SETCURDATA` if the AU program continues with an explicit `CPR_exec` or C-statement (see *SETCURDATA [▸ 45]*).

SEE ALSO

IEXPNO [▸ 48] - Increases the experiment number by one.

DEXPNO [▸ 49] - Decreases the experiment number by one.

RPROCNO [▸ 52] - Sets the processing number to the specified value.

5.8 IPROCNO

NAME

`IPROCNO` - Increases the processing number by one.

SYNTAX

```
IPROCNO
```

DESCRIPTION

The macro `IPROCNO` increases the processing number of the current AU data set by one. In fact, the value of the data path variable *procno* is incremented by one. Subsequent macros will operate on this new *procno*. `IPROCNO` is typically used in an AU program which processes a series of data sets with same *name* and *expno* and successive *procnos*.

EXAMPLE

The following AU program runs Fourier transforms on eight successive *procnos*:

```
TIMES(8)
  FT
  IPROCNO
END
QUIT
```

Note that `IPROCNO` must be followed by a `SETCURDATA` if the AU program continues with an explicit `CPR_exec` or C-statement (see *SETCURDATA [▸ 45]*).

SEE ALSO

DPROCNO [▸ 51] - Decreases the processing number by one.

RPROCNO [▸ 52] - Sets the processing number to the specified value.

IEXPNO [▸ 48] - Increases the experiment number by one.

5.9 DPROCNO

NAME

`DPROCNO` - Decreases the processing number by one.

SYNTAX

```
DPROCNO
```

DESCRIPTION

The macro `DPROCNO` decreases the processing number of the current AU data set by one. In fact, the value of the data path variable *procno* is decremented by one. Subsequent macros will operate on this new *procno*. `DPROCNO` is typically used after a loop which includes an `IPROCNO` at the end, to revert the effect of the last (unnecessary) `IPROCNO`.

EXAMPLE

The following AU program gets the foreground data set, runs a Fourier transform on eight successive *procnos* and displays the data of the last *procno*:

```
TIMES(8)
  FT
  IPROCNO
END
```

```
  DPROCNO
  VIEWDATA
  QUIT
```

Note that `DPROCNO` must be followed by a `SETCURDATA` if the AU program continues with an explicit `CPR_exec` or C-statement (see *SETCURDATA [▸ 45]*).

SEE ALSO

IPROCNO [▸ 50] - Decreases the experiment number by one.

RPROCNO [▸ 52] - Sets the processing number to specified value.

DEXPNO [▸ 49] - Decreases the experiment number by one.

5.10 RPROCNO

NAME

`RPROCNO` - Sets the processing number to the specified value.

SYNTAX

```
RPROCNO(int number )
```

DESCRIPTION

The macro `RPROCNO` changes the current AU data set by setting the processing number to the specified value. In fact, the value of the data path variable *procno* is set. Subsequent macros will then operate on this new *procno*.

EXAMPLE

The following AU program gets the foreground data set and runs a Fourier transform on eight successive *procnos.*Then the current AU data set is set back to the first *procno* which is then phase corrected:

```
  i1 = procno;
  TIMES(8)
    FT
    IPROCNO
  END
  RPROCNO(i1)
  APK
  QUIT
```

Note that `RPROCNO` must be followed by a `SETCURDATA` if the AU program continues with an explicit `CPR_exec` or C-statement (see *SETCURDATA [▸ 45]*).

SEE ALSO

IPROCNO [▸ 50] - Increases the processing number by one.

DPROCNO [▸ 51] - Decreases the processing number by one.

REXPNO [▸ 50] - Sets the experiment number to the specified value.

5.11 VIEWDATA

NAME

`VIEWDATA` - Shows the current AU program data set in new window .

SYNTAX

```
VIEWDATA
```

DESCRIPTION

The macro `VIEWDATA` shows the current AU program data set in a new window or activates the window that contains this data set. `VIEWDATA` is used whenever the current AU data set is changed within the AU program, i.e. with `DATA SET`, `IEXPNO` etc. and this data set must be shown in TopSpin.

EXAMPLE

The following AU program gets the foreground data set, increases the processing number and performs a Fourier transform storing the spectrum in this processing number. The spectrum is then shown in TopSpin:

```
IPROCNO
FT
VIEWDATA
QUIT
```

SEE ALSO

VIEWDATA_SAMEWIN [▸ 53] - Shows the current data set in the current window.

GETDATA SET [▸ 47] - Prompts the user to specify a new data set.

DATA SET [▸ 46] - Sets the current AU data set.

IEXPNO [▸ 48] - Increases the experiment number by one.

IPROCNO [▸ 50] - Increases the processing number by one.

5.12 VIEWDATA_SAMEWIN

NAME

`VIEWDATA_SAMEWIN` - Shows the current AU program data set in the current window.

SYNTAX

```
VIEWDATA_SAMEWIN
```

DESCRIPTION

The macro `VIEWDATA_SAMEWIN` shows the current AU program data set in the current window that contains this data set. It is used as an alternative to `VIEWDATA`.

EXAMPLE

The following AU program gets the foreground data set, increases the processing number and performs a Fourier transform storing the spectrum in this processing number. The spectrum is then shown in TopSpin:

```
IPROCNO
FT
VIEWDATA_SAMEWIN
QUIT
```

SEE ALSO

VIEWDATA [▸ 53] - Shows the current data set in new window.

GETDATA SET [▸ 47] - Prompts the user to specify a new data set.

DATA SET [▸ 46] - Sets the current AU data set.

IEXPNO [▸ 48] - Increases the experiment number by one.

IPROCNO [▸ 50] - Increases the processing number by one.

6 Macros Copying Data sets

This chapter contains a description of all AU macros which can be used to copy the current AU data set or parts of it to a new data set.

6.1 WRA

NAME

`WRA` - Copies the raw data to the specified experiment number.

SYNTAX

```
WRA(int expno)
```

DESCRIPTION

The macro `WRA` copies the raw data, including the acquisition and processing parameters of the current AU data set to a new experiment number. It does not copy the processed data.

EXAMPLE

The following AU program gets the foreground data set and copies the raw data to eight successive experiment numbers , starting with *expno* 11:

```
i1 = 11;
TIMES(8)
  WRA(i1)
  i1++;
END
QUIT
```

SEE ALSO

WRP [▸ 55] - Copies the processed data to the specified processing number.

WRPA [▸ 56] - Copies the raw and processed data to the specified data set.

6.2 WRP

NAME

`WRP` - Copies the processed data to the specified processing number.

SYNTAX

```
WRP(int procno)
```

DESCRIPTION

The macro `WRP` copies the processed data, including the processing parameters of the current AU data set, to the specified processing number.

EXAMPLE

The following AU program gets the foreground data set and copies the processed data to eight successive processing numbers, starting with *procno* 11:

```
i1 = 11;
TIMES(8)
  WRP(i1)
  i1++;
END
QUIT
```

SEE ALSO

WRA [▸ 55] - Copies the raw data to the specified experiment number.

WRPA [▸ 56] - Copies the raw and processed data to the specified data set.

6.3 WRPA

NAME

`WRPA` - Copies the raw processed data to the specified data set.

SYNTAX

```
WRPA(char *name, int expno, int procno, char *disk, char *user)
```

DESCRIPTION

The macro `WRPA` copies the raw and processed data of the current AU data set to the specified data set. `WRPA` takes 5 arguments, *name*, *expno*, *procno*, *disk* and *user*, i.e. the data path variables which define the data set path. You can set one, several, or all of these variables to new values in order to define the destination data set. You can, for instance, archive your data to an external medium by changing the value of the variable `disk` and leaving the other path variables the same.

EXAMPLE

The following AU program copies the current data set to an external disk drive E:/:

```
WRPA(name, expno, procno, "E:/", user)
QUIT
```

SEE ALSO

WRA [▸ 55] - Copies the raw data to the specified experiment number.

WRP [▸ 55] - Copies the processed data to the specified processing number.

7 Macros Handling Rows/Columns

This chapter contains a description of all AU macros which can be used to read (write) rows or columns from (to) a 2D data set and AU macros that can be used to read rows or planes from 3D raw data.

7.1 RSR

NAME

`RSR` - Reads a row from a 2D spectrum and store it as a 1D spectrum.

SYNTAX

```
RSR(int row, int procno)
```

DESCRIPTION

The macro `RSR` reads a row from a 2D spectrum and stores it as a 1D spectrum. It can be used in the following ways:

- Specified with procno > 0, executed on a 2D data set.

  The specified row is stored under the current data name, the current expno and the specified procno.
- Specified with procno = -1, executed on a 2D data set.

  The specified row is stored under data set ~TEMP/1/pdata/1
- Specified with procno > 0, executed on a 1D data set.

  The specified row is read from a 2D data set that resides under the current data name, the current expno and the specified procno.
- Specified with procno = -1, executed on a 1D data set.

  The specified row is read from the 2D data set from which the current 1D data set was extracted (as defined in the file *used_from*).

EXAMPLE

The following AU program gets a 2D data set and processes it. Then it reads row 16 and stores that under *procno 999*:

```
DATA SET("my_2D_data", 1, 1, "C:/bio", "guest")
XFB
RSR(16, 999)
QUIT
```

SEE ALSO

RSC [▸ 58] - Reads a column from a 2D spectrum and store it as a 1D spectrum.

7.2 RSC

NAME

RSC - Reads column from a 2D spectrum and store it as a 1D spectrum.

SYNTAX

```
RSC(int column, int procno)
```

DESCRIPTION

The macro RSC reads a column from a 2D spectrum and stores it as a 1D spectrum. It can be used in the following ways:

- Specified with procno > 0, executed on a 2D data set the specified column is stored under the current data name, the current expno and the specified procno.
- Specified with procno = -1, executed on a 2D data set the specified column is stored under data set ~TEMP/1/pdata/1
- Specified with procno > 0, executed on a 1D data set the specified column is read from a 2D data set that resides under the current data name, the current expno and the specified procno.
- Specified with procno = -1, executed on a 1D data setthe specified column is read from the 2D data set from which the current 1D data set was extracted (as defined in the file *used_from*).

EXAMPLE

The following AU program gets a 2D data set and processes it in the F2 dimension. Then it reads column 128 and processes the resulting 1D data set:

```
DATA SET("my_2D_data", 1, 1, "C:/bio", "guest")
XF2
RSC(128, 10)
RPROCNO(10)
EF
QUIT
```

SEE ALSO

RSR [▸ 57] - Reads a row from a 2D spectrum and store it as a 1D spectrum.

WSC [▸ 59] - Replaces a column of a 2D spectrum by a 1D spectrum.

7.3 WSR

NAME

WSR - Replaces a row of a 2D spectrum by a 1D spectrum.

SYNTAX

```
WSR(int row, int procno, int expno, char *name, char *user, char
*disk)
```

DESCRIPTION

The macro `WSR` replaces a row of a 2D spectrum by a 1D spectrum. It can be used in the following ways:

- Executed on a 1D dataset.

  The specified row of the specified dataset (must 2D data) is replaced by the current 1D data.
- Executed on a 2D dataset.

  The specified row of the current 2D dataset is replaced by the specified data set (must be 1D data).

EXAMPLE

The following AU program gets a 2D dataset, reads row 16, phase corrects this row and writes it back to the 2D data:

```
DATASET("my_2D_data", 1, 1, "C:/bio", "guest")
XFB
RSR(16, 999)
RPROCNO(999)
APK
WSR(16, 1, expno, name, user, disk)
QUIT
```

SEE ALSO

WSC [▸ 59] - Replaces a column of a 2D spectrum by a 1D spectrum.

RSR [▸ 57] - Reads a row from a 2D spectrum and store it as a 1D spectrum.

7.4 WSC

NAME

`WSC` - Replaces a column of a 2D spectrum by a 1D spectrum.

SYNTAX

```
WSC(int column, int procno, int expno, char *name, char *user, char
*disk)
```

DESCRIPTION

The macro `WSC` replaces a column of a 2D spectrum by a 1D spectrum. It can be used in the following ways:

- Executed on a 1D data set.

  The specified column of the specified data set (must 2D data) is replaced by the current 1D data.
- Executed on a 2D data set.

  The specified column of the current 2D data set is replaced by the specified data set (must be 1D data).

EXAMPLE

The following AU program gets a 2D data set, reads column 16, phase corrects this column and writes it back to the 2D data:

```
DATA SET("my_2D_data", 1, 1, "C:/bio", "guest")
RSC(16, 999)
RPROCNO(999)
APK
WSC(16, 1, expno, name, user, disk)
QUIT
```

SEE ALSO

WSR [▸ 58] - Replaces a row of a 2D spectrum by a 1D spectrum.

RSC [▸ 58] - Reads a column from a 2D spectrum and store it as a 1D spectrum.

7.5 RSER

NAME

`RSER` - Reads a row from 2D or 3D raw data and store it as a 1D FID.

SYNTAX

```
RSER(int row, int expno, int procno)
```

DESCRIPTION

The macro `RSER` reads a row from 2D or 3D raw data and stores it as a 1D fid. It can be used in the following ways:

- Specified with expno > 0, executed on a 2D data set the specified row is stored under the current data name and the specified expno. Processing parameters are stored under procno 1.
- Specified with expno = -1, executed on a 2D data set the specified row is stored under data set ~TEMP/1/pdata/1
- Specified with expno > 0, executed on a 1D data set the specified row is read from a 2D raw data that resides under the current data name and the specified expno. Processing parameters are read from procno 1.
- Specified with expno = -1, executed on a 1D data set the specified row is read from the 2D data set from which the current 1D data set was extracted (as defined in the file *used_from*).

EXAMPLE

The following AU program splits 2D raw data into single fids that are stored in successive expnos:

```
int td;
FETCHPAR1S("TD",&td)
i1=0;
TIMES(td)
```

```
    i1 ++;
    RSER(i1,i1+expno,1)
  END
  QUITMSG("--- splitser finished ---")
```

Note that this is the AU program `splitser` that is delivered with TopSpin.

SEE ALSO

WSER [▸ 61] - Replaces a row of 2D raw data by 1D raw data.
RSER2D [▸ 62] - Reads a plane from 3D raw data and store it as 2D raw data.
RSR [▸ 57] - Reads a row from a 2D spectrum and store it as a 1D spectrum.

7.6 WSER

NAME

`WSER` - Replaces a row of 2D raw data by 1D raw data.

SYNTAX

```
WSER(int row, char *name, int expno, int procno, char *disk, char
*user)
```

DESCRIPTION

The macro `WSER` replaces a row of 2D raw data by 1D raw data. It can be used in the following ways:

- Executed on a 1D data set.

  The specified row of the specified data set (must be 2D data) is replaced by the current 1D data.
- Executed on a 2D data set.

  The specified row of the current 2D data set is replaced by the specified data set (must be 1D data).

EXAMPLE

The following AU program writes a number of 1D FIDs that are stored under the same data name and incremental expnos to 2D raw data.:

```
  int ne, exp1, proc1;
  char nm1[20];
  ne=1; exp1=1; proc1=1;
  strcpy(nm1, name);
  GETSTRING("Enter name of 1D series: ", nm1)
  GETINT("Enter starting EXPNO: ", exp1)
  GETINT("Enter starting PROCNO: ", proc1)
  GETINT("Enter # of Fids: ", ne)
```

```
USECURPARS
TIMES(ne)
  WSER(loopcount1+1, nm1, exp1, proc1, disk, user)
  exp1++;
END
QUIT
```

Note that this is the AU program `fidtoser` that is delivered with TopSpin.

SEE ALSO

RSER [▸ 60] - Reads a row from 2D or 3D raw data and store it as a 1D FID.
WSR [▸ 58] - Replaces a row of a 2D spectrum by a 1D spectrum.
WSC [▸ 59] - Replaces a column of a 2D spectrum by a 1D spectrum.

7.7 RSER2D

NAME

`RSER2D` - Reads a plane from 3D raw data and store it as 2D pseudo raw data.

SYNTAX

```
RSER2D(char *direction, int plane, int expno, int procno)
```

DESCRIPTION

The macro `RSER2D` reads a plane from 3D raw data and stores it as 2D pseudo raw data. The first argument, the plane direction can be "s23" or "s13" for the F2-F3 or F1-F3 direction, respectively. The specified plane is stored under the current data name, the specified expno and the specified procno.

EXAMPLE

The following AU program gets a 3D data set, reads the F2-F3-plane 64 and stores that under expno 11. It then switches to the output 2D data set and processes it.

```
DATA SET("my_3D_data", 1, 1, "C:/bio", "guest")
RSER2D("s23", 64, 11)
REXPNO(11)
XFB
QUIT
```

SEE ALSO

RSER [▸ 60] - Reads a row from 2D or 3D raw data and store it as a 1D FID.
WSER [▸ 61] - Replaces a row of 2D raw data by 1D raw data.

8 Macros Converting Data sets

This chapter contains a description of all AU macros which can be used to convert TopSpin data. This includes the conversion of Bruker Aspect 2000/3000 data, Varian data and Jeol data to TopSpin data format as well as the conversion of TopSpin data to JCAMP-DX.

8.1 TOJDX, TOJDX5

NAME

`TOJDX` - Converts a data set to JCAMP-DX 6.0 format .

`TOJDX5` - Converts a data set to JCAMP-DX 5.0 format.

SYNTAX

```
TOJDX(char *path, int type, int mode, char *title, char *origin,
char *owner)
```

```
TOJDX5(char *path, int type, int mode, char *title, char *origin,
char *owner)
```

DESCRIPTION

The macro `TOJDX` converts the current AU data to standard JCAMP-DX 6.0 format. It takes 6 arguments:

1. The path name of the output file, e.g. */tmp/data1.dx*
2. The output type: enter a number between 0 and 6, where:
   - 0 = FID (default).
   - 1 = Real spectrum.
   - 2 = Complex spectrum.
   - 3 = Parameter files.
   - 4 = Raw data + real and imaginary processed data.
   - 5 = Raw data +real and imaginary processed data of all PROCNO’s under the current EXPNO.
   - 6 = Raw data +real and imaginary processed data of all EXPNO’s under the current NAME.
3. The compression mode: enter `0, 1, 2` or `30=FIX`, `1=PACKED`, `2=SQUEEZED`, `3=DIFF/DUP` (default).
4. The title as it appears in the output file: enter a character-string.
5. The origin as it appears in the output file: enter a character-string.
6. The owner as it appears in the output file: enter a character-string.

If "*" is entered as an argument, then the default value is used.

Note that the macro TOJDX5 only supports the output types 0, 1, 2 and 3.

EXAMPLE

The following AU program gets the foreground data set and performs a conversion to JCAMP on 5 successive experiment numbers. The name of the JCAMP file contains the *name* and *expno* of the corresponding TopSpin data set.

```
TIMES(5)
  sprintf(text,"C:/TEMP/%s_%d.dx", name, expno);
  TOJDX(text, 0, 3, "*", "*", "*")
  IEXPNO
END
QUIT
```

SEE ALSO

FROMJDX [▸ 64] - Converts a JCAMP-DX file to TopSpin data format.

8.2 FROMJDX

NAME

`FROMJDX` - Converts a JCAMP-DX file to TopSpin data format.

SYNTAX

```
FROMJDX(char *input-file)
```

DESCRIPTION

The macro `FROMJDX` converts a JCAMP-DX file to TopSpin data format. It takes one argument; the path name of the input file, e.g. */tmp/data1.dx*

`FROMJDX` can convert 1D and 2D data.

EXAMPLE

The following AU program converts all files with the extension *.dx* in the directory *C:/TEMP* to a TopSpin data set:

```
char **listfile;
i1 = getdir ("C:/TEMP",&listfile,"*.dx");
TIMES(i1)
  sprintf(text, "C:/TEMP/%s", listfile[i1]);
  FROMJDX(text)
END
QUIT
```

SEE ALSO

TOJDX [▸ 63] - Converts a data set to JCAMP-DX format.

getdir [▸ 91] - Gets all file names and/or directory names within a directory.

8.3 VCONV

NAME

`VCONV` - Converts a Varian data set to Bruker TopSpin format.

SYNTAX

```
VCONV(char *v_name, char *x_name, int expno, char *disk, char *user)
```

DESCRIPTION

The macro `VCONV` converts a Varian data set to TopSpin data format. It takes 5 parameters:

1. The name of the input Varian data set.
2. The name of the output TopSpin data set.
3. The experiment number of the output TopSpin data set.
4. The disk unit of the output TopSpin data set.
5. The user of the output TopSpin data set.

EXAMPLE

The following AU program converts a Varian data set to TopSpin format:

```
VCONV("pinen_h.fid", "pinen_h", 1, "C:/bio", "joe")
QUIT
```

Note that `VCONV` searches for the input data file in the directory defined by the environment variable `VNMR`.

Assume the file resides in *C:/bio*. You can set `VNMR` from the TopSpin command line with:

env set VNMR=c:/bio

or inside the AU program with:

```
CPR_exec("env set VNMR=C:/bio", WAIT_TERM);
```

SEE ALSO

JCONV [▸ 65] - Converts a Jeol data set to Bruker TopSpin format.

8.4 JCONV

NAME

`JCONV` - Converts a Jeol data set to Bruker TopSpin format.

SYNTAX

```
JCONV(char *j_name, char *x_name, int expno, char *disk, char *user)
```

DESCRIPTION

The macro `JCONV` converts a Jeol data set to TopSpin data format. It takes 5 parameters:

- The name of the input Jeol data set.
- The name of the output TopSpin data set.
- The experiment number of the output TopSpin data set.
- The disk unit of the output TopSpin data set.
- The user of the output TopSpin data set.

Note that `JCONV` searches for the input data file in the directory defined by the environment variable `JNMR`.

Assume the file resides in *C:/bio*. You can set JNMR from the TopSpin command line with:

env set JNMR=c:/bio

Or inside the AU program with:

```
CPR_exec("env set JNMR=C:/bio", WAIT_TERM);
```

EXAMPLE

The following AU program converts a Jeol data set to TopSpin format:

```
JCONV("gx400h.gxd", "gx400h", 1, "C:/bio", "joe")
QUIT
```

SEE ALSO

VCONV [▸ 65] - Converts a Varian data set to Bruker TopSpin format.

9 Macros Handling TopSpin Parameters

This chapter contains a description of AU macros which can be used to get and store TopSpin parameters. Parameters are subdivided in acquisition, processing, output and plot parameters. Furthermore, they exist in two different forms; as foreground and status parameters. Finally, multi-dimensional data sets have parameter sets for each dimension. Different AU macros are available for getting and storing parameters of all categories, forms or dimensions.

9.1 FETCHPAR

NAME

`FETCHPAR` - Gets an acquisition, processing or output parameter.

SYNTAX

```
FETCHPAR(par, &val)
```

DESCRIPTION

The macro `FETCHPAR` gets the value of a foreground parameter and stores it into an AU variable. This AU variable can then be used in subsequent AU statements. `FETCHPAR` allows to get acquisition parameters (**eda**) and processing parameters (**edp**). It is typically used to check or modify a parameter prior to an acquisition or processing statement.

The macro `FETCHPAR` takes two arguments:

1. The name of the parameter.
2. The AU variable into which the parameter value will be stored.

There are two important things to be considered:

1. The type of the AU variable must be the same as the type of the parameter (see *TopSpin Parameter Types [▸ 117]*).
2. The second argument must be specified as the variable's address, i.e. it must be prepended with the '&' character. This, however, does not count for a text variable since a text variable is already an address.

`FETCHPAR` works on 1D, 2D or 3D data sets and always gets a parameter of the first dimension (F2 for 1D, F2 for 2D and F3 for 3D).

The handling of the macros `FETCHPAR1, FETCHPAR3, FETCHPARM, FETCHT1PAR` and `FETCHDOSYPAR` is equivalent to the handling of `FETCHPAR`.

EXAMPLES

The following AU program gets the value of the processing parameter SI and processes the data 4 times, each time doubling the spectrum size and storing the data in successive processing numbers:

```
FETCHPAR("SI", &i1)
TIMES(4)
```

```
    EFP
    IPROCNO
    i1 = i1*2;
    STOREPAR("SI", i1)
  END
  QUIT
```

The following AU statements get the values of the acquisition parameter DW and the processing parameter STSI and stores them in the predefined variables `f1` and `i1`, respectively. Then it gets value of the parameter ABSF1 and stores it in the user defined variable `leftlimit`.

```
float leftlimit;
...
FETCHPAR("DW", &f1 )
FETCHPAR("STSI", &i1)
FETCHPAR("ABSF1", &leftlimit )
```

SEE ALSO

FETCHPARS [▸ 68] - Gets a status parameter.

FETCHPARN [▸ 70] - Gets a parameter from specified direction.

STOREPAR [▸ 69] - Stores an acquisition, processing or output parameter.

9.2 FETCHPARS

NAME

`FETCHPARS` - Gets a status parameter (acquisition and processing) .

SYNTAX

```
FETCHPARS(par, &val)
```

DESCRIPTION

The macro `FETCHPARS` gets the value of a status parameter and stores it into an AU variable. This AU variable can then be used in subsequent AU statements. Acquisition status parameters are set by acquisition commands and describe the status of the data set after acquisition.

Note that the status parameters (**dpa**) describe what really happened and that this is sometimes different from what was set up before the acquisition as acquisition parameters (**eda**). For example, the status NS is smaller than originally specified when an acquisition was halted prematurely. Any AU program statement which follows an acquisition command and evaluates acquisition parameters must read status parameters. Therefore, `FETCHPARS` is typically used after acquisition or processing statements, for example for error or abort conditions (see example below).

The macro `FETCHPARS` takes two arguments:

1. The name of the parameter.

2. The AU variable into which the value is value will be stored.

There are two important things to be considered:

1. The type of the AU variable must be the same as the type of the parameter (see *TopSpin Parameter Types [▸ 117]*).
2. The second argument must be specified as the variable's address, i.e. it must be prepended with the '&' character. This, however, does not count for a text variable since a text variable is already an address.

The handling of the macros `FETCHPARS1` and `FETCHPARS3` is equivalent to the handling of `FETCHPARS`.

EXAMPLE

The following AU program performs a series of acquisitions on the same data set until a minimum signal/noise is reached. In a loop 8 scans are acquired, Fourier transformed and phase corrected. Then the signal/noise of the spectrum is calculated and compared with the minimum value. If the minimum signal/noise was not reached yet, 8 more scans are accumulated etc. A maximum of 8000 scans is acquired. After the acquisition has been stopped, the total number of actually acquired scans is displayed.

```
STOREPAR("NS", 8)
GETFLOAT("Please enter the minimum signal/noise", f1)
ZG
TIMES(1000)
  FT
  APK
  SINO
  FETCHPARS("SINO", f2)
  if (f1 >= f2)
    break;
  GO
END
FETCHPARS("NS", i1)
Proc_err (DEF_ERR_OPT,"Acquisition stopped
                      after %d scans", i1);
QUIT
```

SEE ALSO

FETCHPAR [▸ 67] - Gets an acquisition, processing or output parameter.

FETCHPARNS - Gets a status parameter from specified direction.

STOREPARS [▸ 71] - Stores a status parameter (acquisition and processing).

9.3 STOREPAR

NAME

`STOREPAR` - Stores an acquisition, processing or output parameter.

SYNTAX

```
STOREPAR(par, val)
```

DESCRIPTION

The macro `STOREPAR` stores the value of an AU variable into a parameter. This AU variable can then be used in subsequent AU statements. `STOREPAR` can be used for acquisition parameters (**eda**) and processing parameters (**edp**). It is typically used to set parameters prior to an acquisition or processing statement. `STOREPAR` takes two arguments:

1. The name of the parameter.
2. The value to be stored which can specified in two different forms:
   - As a constant.
   - As the name of an AU variable.

Important: the type of the parameter must be the same as the type of the constant or variable. (see *TopSpin Parameter Types [▸ 117]*).

NOTES

`STOREPAR` works on 1D, 2D or 3D data sets and always stores a parameter of the first dimension (F2 for 1D, F2 for 2D and F3 for 3D).

The handling of the macros `STOREPAR1`, `STOREPAR3`, `STORET1PAR` and `STOREDOSYPAR` is equivalent to the handling of `STOREPAR`.

EXAMPLE

The following AU program reads a standard parameter set, sets the pulse program and power level and asks the user for the number of scans. Then a data set is acquired and processed according to these parameters.

```
RPAR("PROTON", "all")
STOREPAR("PULPROG", "zg30" )
STOREPAR("PL 1", 10.0)
GETINT("Please enter the number of scans:", i1)
STOREPAR("NS", i1 )
ZG
EFP
QUIT
```

SEE ALSO

STOREPARS [▸ 71] - Stores a status parameter.

STOREPARN [▸ 70] - Stores a parameter to specified direction.

FETCHPAR [▸ 67] - Gets an acquisition, processing or output parameter.

9.4 STOREPARN

NAME

`STOREPAR` - Stores a parameter to the specified direction.

SYNTAX

```
STOREPARN(dir, par, val)
```

DESCRIPTION

TopSpin 2.1 and newer offers the macro `STOREPARN`. It works like `STOREPAR` except that it can be used for any direction of an n-dimensional data set. `STOREPARN` takes three arguments:

1. The direction of the data set.
2. The name of the parameter.
3. The value to be stored which can specified in two different forms:
   – As a constant.
   – As the name of an AU variable.

`STOREPARN` works on nD data sets of any dimension.

TopSpin 2.0 and older only supported AU parameter storage up to 3D, using the macros STOREPAR, STOREPAR1 and STOREPAR3. In TopSpin 2.1 and newer, these macros can still be used or they can be replaced by STOREPARN.

Note that the direction specification for STOREPARN is different from STOREPAR/1/3.

For a 2D data set:

- F2 direction (acquisition direction):
  – `STOREPAR(par, val)` or `STOREPARN(2, par, val)`
- F1 direction:
  – `STOREPAR1(par, val)` or `STOREPARN(1, par, val)`

For a 3D data set:

- F3 direction (acquisition direction):
  – `STOREPAR(par, val)` or `STOREPARN(3, par, val)`
- F2 direction:
  – `STOREPAR1(par, val)` or `STOREPARN(2, par, val)`
- F1 direction:
  – `STOREPAR3(par, val)` or `STOREPARN(1, par, val)`

SEE ALSO

STOREPAR [▸ 69] - Stores a parameter in acquisition direction.

STOREPARN [▸ 70] - Stores a status parameter to specified direction.

9.5 STOREPARS

NAME

`STOREPARS` - Stores a status parameter (acquisition and processing)

SYNTAX

```
STOREPARS(par, val)
```

DESCRIPTION

The macro STOREPARS stores the value of an AU variable into a status parameter. This AU variable can then be used in subsequent AU statements. Status parameters are set by an acquisition or processing command and describe the status of the data set after this acquisition or processing command. If the data are now manipulated by AU statements which do not update the status parameters, these must be set explicitly with STOREPARS. For example, if you add two fid's with **addfid**, the total number of scans of the resulting data set is not automatically updated. This must be done explicitly with STOREPARS.

The handling of the macros STOREPAR1S and STOREPAR3S is equivalent to the handling of STOREPARS.

EXAMPLE

The following AU program reads the foreground data set, adds the fid of the next experiment number and the experiment number after that and stores the result in the foreground data set. The number of scans of the original FID's are added and stored in the status parameter NS of the resulting data set.

```
int expno_save;
DATA SET2(name, expno+1, procno, disk, user)
DATA SET3(name, expno+2, procno, disk, user)
expno_save = expno;
IEXPNO
FETCHPARS("NS", &i1)
IEXPNO
FETCHPARS("NS", &i2)
REXPNO(expno_save)
ADDFID
STOREPARS("NS", i1+i2)
QUIT
```

SEE ALSO

FETCHPARS [▹ 68] - Gets a status parameter (acquisition and processing).

STOREPAR [▹ 69] - Stores an acquisition, processing or output parameter.

9.6 RPAR

NAME

RPAR - Reads a parameter set to the current AU data set.

SYNTAX

```
RPAR(char *parset, char *typ)
```

DESCRIPTION

The macro `RPAR` reads a parameter set to the current AU data set. This can be a standard Bruker parameter set or a user defined parameter set which was stored with `WPAR`. `RPAR` takes two arguments:

1. The name of the parameter set.
2. The type of parameters which are to be read.

The second argument can be:

- *acqu* for acquisition parameters (**eda**).
- *proc* for processing parameters (**edp**).
- *outd* for output parameters (**edp**).
- *all* for acquisition, processing, plot and output parameters.

EXAMPLE

The following AU program reads the standard Bruker parameter set PROTON, sets the number of scans to 1024 and runs an acquisition:

```
RPAR("PROTON", "all")
STOREPAR("NS", 1024)
ZG
QUIT
```

SEE ALSO

WPAR [▸ 73] - Writes the current data set parameters to a parameter set.

9.7 WPAR

NAME

`WPAR` - Writes the current data set parameters to a parameter set.

SYNTAX

```
WPAR(char *parset, char *typ)
```

DESCRIPTION

The macro `WPAR` writes the parameters of the current AU data set to a parameter set. You can only write to user defined parameter sets. Bruker standard parameters sets cannot be overwritten. `WPAR` is typically used in AU programs to store a temporary parameter set. It takes two arguments:

- The name of the parameter set.
- The type of parameters which are to be stored.

The second argument can be:

- *acqu* for acquisition parameters (**eda**).
- *proc* for processing parameters (**edp**).
- *outd* for output parameters.
- *all* for acquisition, processing, plot and output parameters.

EXAMPLE

The following AU program reads the acquisition parameters of the Bruker standard parameter set PROTON, sets the number of scans, the frequency offset and time domain data size and writes the acquisition parameters to a temporary parameter set. It then performs 8 successive acquisitions with these parameters.

```
RPAR("PROTON", "all")
STOREPAR("NS", 16)
STOREPAR("O1", 766.23)
STOREPAR("TD",8192)
WPAR("partemp", "acqu")
TIMES(8)
  ZG
  IEXPNO
  RPAR("partemp", "acqu")
END
QUIT
```

SEE ALSO

RPAR [▸ 72] - Reads a parameter set to the current AU data set.

10 Macros for Plot Editor/Autoplot

This chapter contains a description of AU macros which can be used to plot data using Plot Editor portfolios and layouts. These include macros for the creation and definition of portfolios and for plotting to the printer, to a postscript file or enhanced metafile.

TopSpin 2.0 and newer also offer macros for automatic creation of Plot Editor layouts. Examples are `LAYOUT_OBJ_1D` and `LAYOUT_ADD`. These are described in a separate manual (see **Help** => **Manuals** => [**Programming Manuals**] **Plot Layout Programming**).

10.1 AUTOPLOT

NAME

`AUTOPLOT` - Plots the current data set according a Plot Editor layout.

SYNTAX

```
AUTOPLOT
```

DESCRIPTION

The macro `AUTOPLOT` plots the current data set according to the Plot Editor layout that is defined by the parameter LAYOUT.

The Plot Editor layout can be:

- A standard layout that was delivered with TopSpin.
- A user defined layout that was setup and stored from Plot Editor.

Processing AU programs that contain the `AUTOPLOT` macro can be used with one of the options **a**, **e**, **h** or **t**. They cause `AUTOPLOT` to store the plot as a postscript file. For example, the AU program `proc_1d` can be entered as:

`proc_1d` – Prints to the printer defined in the layout.

`proc_1d a` – Prints to a PDF file in the data set procno.

`proc_1d e` – Also prints to a postscript file in the data set procno.

`proc_1d h` – Also prints to a postscript file in the users home directory.

`proc_1d t` – Also prints to a postscript file in the TEMP directory.

Furthermore, you can use multiple arguments, e.g.:

`proc_1d a e` - Prints to a PDF file and to a postscript file in the data set procno.

(see also the header of the AU program `plot_to_file`).

EXAMPLE

This AU program processes the current 1D data set and plots it according to the Plot Editor layout specified in **edp**:

```
EF
APK
SREF
ABS
```

```
AUTOPLOT
QUIT
```

SEE ALSO

AUTOPLOT_TO_FILE [▸ 76]
AUTOPLOT_WITH_PORTFOLIO [▸ 79]
AUTOPLOT_WITH_PORTFOLIO_TO_FILE [▸ 80]

10.2 AUTOPLOT_TO_FILE

NAME

`AUTOPLOT_TO_FILE` - as AUTOPLOT but store the output into a file

SYNTAX

```
AUTOPLOT_TO_FILE(file name)
```

DESCRIPTION

The macro `AUTOPLOT_TO_FILE` plots the current data set according to the Plot Editor layout defined by the parameter LAYOUT. The output is not sent to the printer but stored in the file that is specified as an argument. The argument is normally a full path name. If it is not, the file is stored in the TopSpin home directory.

If the file name has the extension *.ps*, the output is stored as a postscript file. If (under Windows) it has the extension *.emf*, as in the example below, the output will be stored as an enhanced metafile.

`AUTOPLOT_TO_FILE` is actually a composite macro that consists of several `PORTFOLIO*/AUTOPLOT*` macros. This, however, is transparent to the user.

EXAMPLE

This AU program processes the current 1D data set and plots it according to the Plot Editor layout specified in **edp**. The result is stored in an enhanced metafile.

```
EF
APK
SREF
ABS
AUTOPLOT_TO_FILE("C:/mydata.emf")
QUIT
```

SEE ALSO

AUTOPLOT [▸ 75]
AUTOPLOT_WITH_PORTFOLIO [▸ 79]

10.3 CREATE_PORTFOLIO

NAME

`CREATE_PORTFOLIO` - Creates a Plot Editor portfolio.

SYNTAX

`CREATE_PORTFOLIO(name)`

DESCRIPTION

The macro `CREATE_PORTFOLIO` creates the Plot Editor portfolio that is specified as an argument. It takes one argument; the file name of the portfolio.

The argument is normally specified as a full path name. If it is not, the portfolio is stored under the TopSpin home directory. If the specified file already exists, it is overwritten.

Note that `CREATE_PORTFOLIO` creates the portfolio but does not insert any data set specifications.

EXAMPLE

This AU program plots the current data set according to the Plot Editor layout specified in **edp**. It is just a simple demonstration of the use of `PORTFOLIO` macros.

```
CREATE_PORTFOLIO(“C:/temp/myPortfolio.por”)
ADD_CURDAT_TO_PORTFOLIOCLOSE_PORTFOLIO
AUTOPLOT_WITH_PORTFOLIO
QUIT
```

Note that this AU program does the same as the command **autoplot**.

SEE ALSO

ADD_TO_PORTFOLIO [▸ 78]
CLOSE_PORTFOLIO [▸ 79]

10.4 ADD_CURDAT_TO_PORTFOLIO

NAME

`ADD_CURDAT_TO_PORTFOLIO` - Adds the current data set to the portfolio.

SYNTAX

`ADD_CURDAT_TO_PORTFOLIO`

DESCRIPTION

The macro `ADD_CURDAT_TO_PORTFOLIO` adds the current data set to the Plot Editor portfolio that was previously create with `CREATE_PORTFOLIO`.

EXAMPLE

This AU program plots two data sets, the current and next processing number of the current data name, according to the Plot Editor layout.

```
CREATE_PORTFOLIO("C:/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO
IPROCNO
ADD_CURDAT_TO_PORTFOLIO
CLOSE_PORTFOLIO
AUTOPLOT_WITH_PORTFOLIOQUIT
```

SEE ALSO

CREATE_PORTFOLIO [▸ 77]
CLOSE_PORTFOLIO [▸ 79]

10.5 ADD_TO_PORTFOLIO

NAME

`ADD_TO_PORTFOLIO` - Adds the specified data set to the portfolio.

SYNTAX

```
ADD_TO_PORTFOLIO(disk,user, name, expno, procno)
```

DESCRIPTION

The macro `ADD_TO_PORTFOLIO` adds a data set to the portfolio that was previously created with `CREATE_PORTFOLIO`. The data set to be added is completely specified by the five arguments of `ADD_TO_PORTFOLIO`.

Note that these arguments can be constants (values) or variables.

EXAMPLE

This AU program plots two data sets according to the TopSpin layout.

Note that the first data set to be plotted is the so called second data set (**edc2**), specified by the predefined dedicated variables `disk2`, `user2` etc.

```
CREATE_PORTFOLIO("/temp/myPortfolio.por")
GETCURDATA2
```

```
ADD_TO_PORTFOLIO(disk2, user2, name2, expno2, procno2)
ADD_TO_PORTFOLIO("C:/ts", "guest", "mydata", 1, 3)
CLOSE_PORTFOLIO
AUTOPLOT_WITH_PORTFOLIO
QUIT
```

SEE ALSO

ADD_CURDAT_TO_PORTFOLIO [▸ 77]

10.6 CLOSE_PORTFOLIO

NAME

`CLOSE_PORTFOLIO` - Closes the portfolio definition.

SYNTAX

`CLOSE_PORTFOLIO`

DESCRIPTION

The macro `CLOSE_PORTFOLIO` closes the definition of the portfolio that was previously created with `CREATE_PORTFOLIO`. It must be used after the last `ADD_CURDAT_TO_PORTFOLIO` or `ADD_TO_PORTFOLIO` macro and before the first `AUTOPLOT*` macro.

EXAMPLE

This AU program plots the current data set according to the TopSpin layout. It is just a simple demonstration of the use of `PORTFOLIO` macros.

```
CREATE_PORTFOLIO("C:/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIOCLOSE_PORTFOLIO
AUTOPLOT_WITH_PORTFOLIO
QUIT
```

Note that this AU program does the same as the command **autoplot**.

SEE ALSO

CREATE_PORTFOLIO [▸ 77]
ADD_TO_PORTFOLIO [▸ 78]

10.7 AUTOPLOT_WITH_PORTFOLIO

NAME

`AUTOPLOT_WITH_PORTFOLIO` - Plots the data set(s) of the current portfolio.

SYNTAX

```
AUTOPLOT_WITH_PORTFOLIO
```

DESCRIPTION

The macro `AUTOPLOT_WITH_PORTFOLIO` plots the data set(s) defined in the portfolio created with `CREATE_PORTFOLIO` according to the Plot Editor layout defined by the **edp** parameter LAYOUT.

EXAMPLE

This AU program plots the current data set according to the TopSpin layout. It is just a simple demonstration of the use of PORTFOLIO macros.

```
CREATE_PORTFOLIO("C:/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIOCLOSE_PORTFOLIO
AUTOPLOT_WITH_PORTFOLIO
QUIT
```

Note that this AU program does the same as the command **autoplot**.

SEE ALSO

AUTOPLOT [▶ 75]
AUTOPLOT_WITH_PORTFOLIO_TO_FILE [▶ 80]

10.8 AUTOPLOT_WITH_PORTFOLIO_TO_FILE

NAME

`AUTOPLOT_WITH_PORTFOLIO_TO_FILE` - Plots the data set(s) of the current portfolio and store the output into a file.

SYNTAX

```
AUTOPLOT_WITH_PORTFOLIO_TO_FILE(file name)
```

DESCRIPTION

The macro `AUTOPLOT_WITH_PORTFOLIO_TO_FILE` plots the data set(s) defined in the Plot Editor portfolio that was previously created with `CREATE_PORTFOLIO`. The plot is made according to the layout defined by the parameter LAYOUT. The output is stored in the file that is specified as an argument to the macro. The argument is normally a full path name. If it is not, the portfolio is stored under the TopSpin home directory.

If the file name has the extension *.ps*, as in the example below, the output will be stored as a postscript file. If (under Windows) it has the extension *.emf*, the output is stored as an enhanced metafile.

EXAMPLE

This AU program plots the current data set according to the Plot Editor layout specified in **edp** and stores the result into a postscript file.

```
CREATE_PORTFOLIO(“C:/temp/myPortfolio.por”)
ADD_CURDAT_TO_PORTFOLIOCLOSE_PORTFOLIO
AUTOPLOT_WITH_PORTFOLIO_TO_FILE("/users/guest/mydata.ps")
QUIT
```

SEE ALSO

AUTOPLOT_WITH_PORTFOLIO [▸ 79]
AUTOPLOT_TO_FILE [▸ 76]

11 Macros Prompting the User for Input

This chapter contains a description of all AU macros which can be used to prompt the user for input and store the input into an AU variable. Different macros are available for requesting integer, float, double or text values.

11.1 GETINT

NAME

`GETINT` - Prompts the user to enter an integer value.

SYNTAX

```
GETINT("Please enter an integer value : ", i1)
```

DESCRIPTION

The macro `GETINT` prompts the user to enter an integer value and stores this value into an integer variable. It can be used for various purposes, for example to set the value of a TopSpin (integer) parameter or to specify the number of cycles in an AU program loop. `GETINT` takes two arguments:

- A text string which prompts the user to enter an integer value.
- An integer variable into which the value is stored.

EXAMPLE

The following AU program prompts the user for the number of scans per acquisition and the number of experiments to be done:

```
GETINT("Please enter the number of scans:", i1)
GETINT("Please enter the number of experiments:", i2 )
TIMES(i2)
  STOREPAR("NS", i1 )
  ZG
  IEXPNO
END
QUIT
```

SEE ALSO

GETFLOAT [▸ 84] - Prompts the user to enter a float value.

GETDOUBLE [▸ 84] - Prompts the user to enter a double value.

GETSTRING [▸ 84] - Prompts the user to enter a text string.

11.2 GETFLOAT, GETDOUBLE

NAME

`GETFLOAT` - prompt the user to enter a float value.

`GETDOUBLE` - prompt the user to enter a double value.

SYNTAX

```
GETFLOAT(text, f1)
GETDOUBLE(text, d1)
```

DESCRIPTION

The macro `GETFLOAT` prompts the user to enter a float value and stores this value into a float AU variable. It is used to get the value for a TopSpin (float) parameter which can then be stored with `STOREPAR`. GETFLOAT takes 2 arguments:

1. A text string which prompts the user to enter a float value.
2. The float variable into which the value is store.

The description for `GETDOUBLE` is equivalent, except that it is used for TopSpin (double) parameters.

EXAMPLE

The following AU program prompts the user for the *frequency offset* and *Gaussian broadening*, stores these values into the parameters O1 and GB respectively and then runs an acquisition, Gaussian multiplication and Fourier transform:

```
GETDOUBLE("Please enter the frequency offset:", d1 )
STOREPAR("o1", d1 );
GETFLOAT("Please enter the Gaussian broadening:", f1)
STOREPAR("GB", f1)
ZG
GM
FT
QUIT
```

SEE ALSO

GETINT [▸ 83] - Prompts the user to enter an integer value.

GETSTRING [▸ 84] - Prompts the user to enter a text string.

11.3 GETSTRING

NAME

`GETSTRING` - Prompts the user to enter a text string.

SYNTAX

```
GETSTRING(text, cval)
```

DESCRIPTION

The macro `GETSTRING` prompts the user to enter a text string which is then stored into an AU variable. It can be used for various purposes, for example to ask the user a question or prompt the user to enter a name. `GETINT` takes two arguments:

1. A text string which prompts the user to enter a text string.
2. The character-string variable into which the value is stored.

EXAMPLE

The following AU program asks the user if an integration must be done and, if yes, which intrng file must be used. Then the integrals are calculated and listed:

```
char answer[8];
GETSTRING("Do you want to do an integration (yes/no)?", answer )
if ( !strcmp(answer,"yes") )
{
  GETSTRING("Which intrng file must be used?", text)
  RMISC("intrng", text)
  LI
}
QUIT
```

SEE ALSO

GETINT [▸ 83] - Prompts the user to enter an integer value.

GETFLOAT [▸ 84] - Prompts the user to enter a float value.

GETDOUBLE [▸ 84] - Prompts the user to enter a double value.

12 Bruker Library Functions

This chapter contains a description of various C functions which are available as part of Bruker libraries. Several of them concern the handling of data set lists or directory lists. You can, for instance, get a list of file names, display it, select a file from the list and then copy the file to a different directory. The functions described in this chapter are particularly useful for files located in the directories */<tshome>/conf* and */<tshome>/exp*. For copying data sets, we recommend to use the macros described in *Macros Changing the Current AU Data set [▸ 45]*.

12.1 CalcExpTime, PrintExpTime

NAME

`CalcExpTime` - Calculates the experiment time for the current experiment.

`PrintExpTime` - Prints the experiment time for the current experiment.

SYNTAX

```
static void PrintExpTime();
int CalcExpTime ();
void PrintExpTime (int exptime, int expno);
#include<inc/exptutil>
```

DESCRIPTION

The function `CalcExpTime` calculates the experiment time for the current experiment. The return value is the experiment time in seconds. The function `PrintExpTime` can be used to print the experiment time in the form "days hours minutes seconds".

EXAMPLE

The following AU program calculates and prints the experiment time of a sequence of 10 experiments starting with the foreground data set.

```
  static void PrintExpTime();
  TIMES(10)
    PrintExpTime (CalcExpTime(),loopcount1);
    IEXPNO
  END
  QUIT
#include<inc/exptutil>
```

Note that the declaration of `PrintExpTime` must appear at the beginning of the AU program and the #include statement at the end of the AU program.

SEE ALSO

multiexpt [▸ 105] - A standard Bruker library AU program.

12.2 CheckSumFile

NAME

`CheckSumFile` - Creates a checksum of a data file .

SYNTAX

```
CheckSumFile( filnam, 0, dest, 0, verb, bytord, dtyp, dim, siz0,
siz, xdim)
```

DESCRIPTION

The function `CheckSumFile` generates a checksum of a data file. The output consist of a checksum preceded by hash type and data sizes, e.g:

```
data hash MD5: 512 * 256
16 A5 E9 14 FB 66 8B 48 09 8B E3 CA 86 D2 68 A2
```

Which are stored in a destination character string. The input data file can be a TopSpin raw or processed data file or any other integer data file. The data size, storage mode and dimensionality must be specified as arguments.

The arguments of the function have the following meaning:

- `const char* filnam`

  Full path name of the input data file.
- `char* dest`

  Destination character string for function output. Must at least be 128 byte.
- `int verb`

  Verbose error if the input file does not exist (0=no, 1=yes).
- `int bytord`

  Byteorder of the input data (parameter BYTORDA for raw data or BYTORDP for processed data).
- `int dtyp`

  Data type of the input data (parameter DTYPA for raw data and DTYPP for processed data).
- `int dim`

  Data dimensionality (1 for 1D data, 2 for 2D data, ... etc.).
- `int siz0`

  For raw data, siz0 must be set to TD in the acquisition direction. For processed data, siz0 must be set to SI in the first direction.
- `const int* siz`

  Array of sizes. For processed data, siz must be set to SI in the successive directions. For example, for 2D data, `siz = (F2-SI, F1-SI)`. For raw data, `siz` must be set to TD in the successive directions.

Attention: in the acquisition direction, `siz` must be TD rounded to the next multiple of 256.

- `const int* xdim`

  For raw data, `xdim = siz`. For processed data, `xdim` is the array of submatrix sizes of successive directions. For example, for 2D processed data `xdim = (F2-XDIM, F1-XDIM).`

`CheckSumFile` can have the following return values:

> 0 : successful operation.

= 0 : parameter inconsistency or I/O problems.

< 0 : all other cases.

The return value can be used as an argument of the function `CheckSumError()` which generates an error string.

The output of `CheckSumFile` can be appended to the audit file with the function `AuditAppend` as shown in the example below.

EXAMPLE

The following AU statements will generate a data checksum of the current processed 2D data and store it in the current data auditp.txt file. It is part of the Bruker AU program `xfshear`.

```
int bytordp, dtypp, size[2], xdim[2];
char name2rr[PATH_MAX], nameaudit[PATH_MAX],
                             audittext[512];
char* auditp = audittext + sprintf(audittext,
                   "processing description");
FETCHPARS("BYTORDP",&bytordp)
FETCHPARS("DTYPP",&dtypp)
FETCHPARS("SI",&size[0])
FETCHPARS("XDIM", &xdim[0])
FETCHPAR1S("SI",&size[1])
FETCHPAR1S("XDIM", &xdim[1])
sprintf(name2rr,"%s/data/%s/nmr/%s/%d/pdata/%d/2rr",
                   disk, user, name, expno, procno);
if (CheckSumFile(name2rr, 0, auditp, 0, 1, bytordp,
  dtypp, 2, size[0], size, xdim) > 0)
{
  sprintf(nameaudit,"%s/data/%s/nmr/%s/%d/pdata/%d/
       auditp.txt",disk, user, name, expno, procno);
  AuditAppend(nameaudit, audittext);
}
QUIT
```

SEE ALSO

AuditAppend [▸ 89]

AuditCreate [▸ 90]

12.3 AuditAppend

NAME

`AuditAppend` - Appends a new entry to an existing audit file .

SYNTAX

```
AuditAppend(const char* auditn, const char* what).
```

DESCRIPTION

The function `AuditAppend` appends a new entry to an existing audit file. An audit file entry consists of the following fields:

NUMBER, WHEN, WHO, WHERE, PROCESS, VERSION, WHAT

All of these are automatically set by `AuditAppend`, except for the WHAT field which is specified as the second argument. It can be any character string.

Note that `AuditAppend` does not create an audit file if this does not exist yet.

EXAMPLE

See the example of the function *CheckSumFile [▸ 88]*.

SEE ALSO

CheckSumFile [▸ 88]

AuditCreate [▸ 90]

12.4 AuditCreate

NAME

`AuditCreate` - Creates a new audit file .

SYNTAX

```
AuditCreate(const char* auditn, const char* what).
```

DESCRIPTION

The function `AuditCreate` creates a new audit file with a single entry. This is, for example, useful when new data are created. An audit trail entry consists of the following fields:

NUMBER, WHEN, WHO, WHERE, PROCESS, VERSION, WHAT

All of these are automatically set, except for the WHAT field which is specified as the second argument.

Caution: `AuditCreate` overwrites a possibly existing audit file.

EXAMPLE

Please look at the Bruker AU program `split3d` for an example of using `AuditCreate`.

SEE ALSO

CheckSumFile [▸ 88]

AuditAppend [▸ 89]

12.5 FileSelect

NAME

`FileSelect` - Displays a list of directory entries and allow to select entries.

SYNTAX

```
FileSelect(sourcedir, flist, &num, type );
```

DESCRIPTION

The function `FileSelect` opens a directory, shows a list of all file and directory entries and allows you to select one or more entries. The list is stored in a 2 dimensional character-string variable which can be evaluated by subsequent AU statements. `FileSelect` takes four arguments:

1. The source directory.
2. The variable into which the list is stored.
3. The variable into which the number of selected entries is stored.
4. A flag which determines whether files (0) or directories (1) are listed.

`FileSelect` replaces the functions `uxselect` and `getdir` which were used by TopSpin's predecessor XWIN-NMR.

EXAMPLES

The following AU program will make a list of all shim files and will display this list in a selection window. If an entry is selected, then the corresponding shim file is read with the macro RSH. If no entries were found or selected, the AU program aborts.

```
char sourcedir[200];
int num= 100;
char flist[128][128];
               sprintf(sourcedir, "%s/nmr/lists/bsms",
                                PathXWinNMRExpStan());

if (i1 = FileSelect(sourcedir, flist, &num, 0)< 0)
{
  Proc_err(DEF_ERR_OPT, "Error: No shim files selected!");
}
else
{
  RSH(flist[0])
}
QUIT
```

12.6 getdir

NAME

`getdir` - Gets all file names and/or directory names within a directory.

SYNTAX

```
int getdir (char *directory, char ***filelist, const char
*match_code );
```

DESCRIPTION

The function `getdir` opens a directory and gets all file and directory names in that directory. This list is stored in a 2 dimensional character-string variable which can be evaluated by subsequent AU statements. The list can be limited by specifying a match_code; only names matching this string are entered into the list. `getdir` takes three arguments:

1. The source directory.
2. The variable into which the list of names is stored.
3. The match_code; an arbitrary string of characters.

The third argument can also be `/files` to get all files but not directories, or `/dir` to get all directories but not files.

The return value of `getdir` is the number of successfully matched file names and/or directory names.

`getdir` internally allocates memory for the list of names. Officially, you must free this memory with the Bruker library function `freedir`. In practice, however, you can omit `freedir` because all memory allocated by the AU program is automatically freed when the AU program finishes.

EXAMPLES

The following AU statements will create a list of experiment directories from a TopSpin data set. All entries are returned because no match_code was specified.

```
char sourcedir[200], **listfile;
sprintf (sourcedir, "%s/data/%s/%s/%s/",
                      disk,user,type,name);

i1 = getdir (sourcedir,&listfile,NULL);
```

The following AU statements will create a list of shim files starting with the letters a to p from the bsms directory.

```
char sourcedir[200], **listfile;
sprintf(sourcedir, "%s/nmr/lists/bsms",
                    PathXWinNMRExpStan());

i1 = getdir (sourcedir,&listfile,"[a-p]*");
```

The following AU statement will create a list of all files but not directories from the users home directory.

```
i1 = getdir (PathSystemHome(),&listfile,"/files");
```

The following AU statement will return a list of all directory names from the users home directory.

```
i1 = getdir (PathSystemHome(),&listfile,"/dir");
```

SEE ALSO

freedir [▸ 93] - Free memory allocated by getdir.

12.7 freedir

NAME

`freedir` - Free memory allocated by `getdir`.

SYNTAX

```
void freedir(char **listfile );
```

DESCRIPTION

The function `freedir` frees the memory that was allocated by a `getdir` function call.

EXAMPLE

See the example under the function `FileSelect`.

SEE ALSO

getdir [▸ 91] - Gets all file names and/or directory names within a directory.

FileSelect [▸ 91] - Displays a list from which an entry can be selected by mouse-click.

12.8 dircp, dircp_err

NAME

`dircp` - Copy a file.

`dircp_err` - Returns the error message that corresponds to the error return value of a `dircp` function call.

SYNTAX

```
dircp (char *sourcefile, char *targetfile );
char *dircp_err (int return_value );
```

DESCRIPTION

The function `dircp` copies the sourcefile into the targetfile. If the targetfile exists, it will be overwritten. A negative number is returned if copying was not possible. The function `dircp_err` will return the corresponding C error message. A return value of 0 indicates successful execution.

EXAMPLE

The following AU program copies the *title* file of the foreground data set to the user's home directory.

```
  char sourcefile[200], targetfile[200];
  sprintf (targetfile, "%s/title",PathSystemHome());
  if ( (i1 = dircp (PROCPATH("title"),targetfile)) < 0 )
    Proc_err (DEF_ERR_OPT, dircp_err (i1));
```

```
QUIT
```

Note that PROCPATH uses a static buffer for building the path name, which means it cannot be used to build more than one path name at a time, e.g. it cannot be used in both `dircp` arguments.

12.9 gethighest

NAME

`gethighest` - Returns the next highest unused experiment number of a data set.

SYNTAX

```
int gethighest (char *directory);
#include <inc/sysutil>
```

DESCRIPTION

The function `gethighest` scans a directory for all subdirectories whose name is a number and then returns the next highest unused number. `gethighest` is typically used to scan a data set name directory of a TopSpin data set. In that case, it returns the highest unused experiment number. If, for example, the highest used experiment number is 56, the function will return the value 57. The function can also be used to return the highest unused processing number of a data set.

EXAMPLE

The following AU program will copy the current TopSpin experiment into the next highest unused experiment data set.

```
(void) sprintf (text,"%s/data/%s/nmr/%s",disk,user,name);
i1 = gethighest (text);
WRA(i1)
QUIT
#include <inc/sysutil>
```

Note that the #include statement must be included **at the end** of the AU program.

12.10 getParfileDirForRead

NAME

`getParfileDirForRead` - Determines the path name of a list file to be read.

SYNTAX

```
int getParfileDirForRead (const char *file name, const char *key,
char *path);
```

DESCRIPTION

The function `getParfileDirForRead` determines the path name of a list file to be read. The function has three arguments:

1. The file name of the list file.
2. The type (key) of the list file: `PP_DIRS`, `VD_DIRS` etc. (see *Bruker Library Functions [▷ 87]*).
3. The path name of the list file.

The third argument contains the result of the function. For determining this path name, the function searches for the specified file name in all source directories that are set up for the specified list type, for the current user. The first source directory in which the file is found determines the output path name. To view or change the list of source directories:

1. Click **Options** => **Preferences** [**set**].
2. Click **Miscellaneous** in the left part of the dialog box.
3. Click the **Change** button of the entry *Manage source directories....*

The functions `getParfileDirForRead` and `getParfileDirForWrite` are only implemented in TopSpin 2.1 and newer. This replaces the functions `getstan` and `PathXWinNMR`*.

EXAMPLE

The following AU statements are an example of the usage of the function `getParfileDirForRead`. They are part of the AU program `proc_intrng`.

```
char intrngfilePath name[PATH_MAX];
if (getParfileDirForRead("testrng", INTRNG_DIRS,
                        intrngfilePath name) < 0)
{
  Proc_err(DEF_ERR_OPT, "testrng: %s",
                  intrngfilePath name);
  ABORT
}
RMISC("intrng", intrngfilePath name)
```

SEE ALSO

getParfileDirForWrite [▷ 96] - Determines path name of list file to be written.

Directory Token	File Type
`PP_DIRS`	Pulse programs.
`CPD_DIRS`	cpd programs.
`MAC_DIRS`	Macros.
`PY_DIRS`	Python programs.
`GP_DIRS`	Gradient programs.
`SHAPE_DIRS`	Shape files.
`SP_DIRS`	Shape lists.
`AU_DIRS`	AU programs.

Directory Token	File Type
`PAR_DIRS`	Parameter sets.
`VD_DIRS`	Delays.
`VP_DIRS`	Pulses.
`VC_DIRS`	Loop counters.
`VT_DIRS`	Temperatures.
`VA_DIRS`	Amplitudes.
`F1_DIRS`	Frequency channel 1.
`DS_DIRS`	Data sets.
`SCL_DIRS`	Solvent scaling region.
`PHASE_DIRS`	Phase programs.
`INTRNG_DIRS`	intrng files.
`PEAKRNG_DIRS`	Peakrng files.
`BASLPNTS_DIRS`	Baslpnts files.
`BASE_INFO_DIRS`	Base_info files.
`PEAKLIST_DIRS`	Peaklist files.
`CLEVELS_DIRS`	C levels files.
`REG_DIRS`	Region files.
`INT2DRNG_DIRS`	int2drng files.

Table 12.1: Directory Tokens in an AU Program and Respective File Types

12.11 getParfileDirForWrite

NAME

`getParfileDirForWrite` - Determines the path name of a list file to be written.

SYNTAX

```
int getParfileDirForWrite (const char *file name, const char *key,
char *path);
```

DESCRIPTION

The function `getParfileDirForWrite` determines the path name of a list file to be read. The function has three arguments:

1. The file name of the list file.
2. The type (key) of the list file: `PP_DIRS`, `VD_DIRS` etc. (see *Bruker Library Functions [▸ 87]* at the description of getParfileDirForRead).
3. The path name of the list file.

The third argument contains the result of the function. For determining this path name, the function searches through all source directories that are set up for the specified list type, for the current user. The first source directory that actually exists on disk (usually the first specified source directory) determines the output path name. To view or change the list of source directories:

1. Click **Options** => **Preferences** [**set**].
2. Click **Miscellaneous** in the left part of the dialog box.
3. Click the **Change** button of the entry *Manage source directories....*

The functions `getParfileDirForRead` and `getParfileDirForWrite` are only implemented in TopSpin 2.1 and newer. The replace the functions `getstan` and `PathXWinNMR*`.

EXAMPLE

The following AU statements are an example of the usage of the function `getParfileDirForWrite`. They are part of the AU program `sysgenpar`.

```
char vdpath[PATH_MAX];
if (getParfileDirForWrite("syst1list", VD_DIRS,
                                            vdpath) < 0)
{
  Proc_err(DEF_ERR_OPT, "syst1list: %s", vdpath);
  ABORT
}
```

SEE ALSO

getParfileDirForRead [▶ 94] - Determines path name of list file to be read.

12.12 getstan

NAME

`getstan` - Returns the path name to the user's current experiment directory.

SYNTAX

```
char * getstan (char *path name, const char *subdir);
```

DESCRIPTION

The function `getstan` returns the path name to the user's current experiment directory. The returned path name can be concatenated with a known subdirectory path name as a part of the same `getstan` function call.

Please note: in TopSpin 2.1 and newer the functions `getstan` and `PathXWinNMR*` have become obsolete and can be replaced by the functions `getParfileDirForRead` and `getParfileDirForWrite`.

EXAMPLE

The following AU program will get the pulse program of the current AU data set. It will then prompt the user to confirm the name of the pulse program or to enter a new name. Finally, the pulse program will be shown in a TopSpin window.

```
char pulprog[80];
FETCHPAR("PULPROG",pulprog)
GETSTRING ("Enter the name of the pulse program: ",
                                         pulprog);
(void) sprintf (text,"%s/%s",getstan (NULL,
                     "lists/pp"),pulprog);
showfile (text);
QUIT
```

Note that in the above example, the function call `getstan (NULL,"lists/pp")` returns the path name */<tshome>/exp/stan/nmr/lists/pp*. The function call `getstan(NULL,NULL)` returns */<tshome>/exp/stan/nmr/.*

SEE ALSO

*PathXWinNMR [▸ 99]** - A class of functions which return path names to certain TopSpin directories.

getParfileDirForRead [▸ 94] - Determines path name of list file to be read.

getParfileDirForWrite [▸ 96] - Determines path name of list file to be written.

12.13 GetTsVersionDot

NAME

`GetTsVersionDot` - Returns the current version and patchlevel of TopSpin in a dotted format.

SYNTAX

```
const char* GetTsVersionDot(void);
```

DESCRIPTION

The function `GetTsVersionDot` returns the version and patchlevel of the currently running TopSpin program. This variable can then be printed out.

NOTE: There are similar functions to find out parts of the version:

- `int GetTsVersionMajor(void)` returns the major version as number. e.g. 4.
- `int GetTsVersionMinor(void)` returns the minor version as number, e.g. 0.
- `int GetTsVersionPl(void)` returns the patch level as number, e.g. 1.
- `int GetTsVersionBeta(void)` returns 1 if TopSpin is a beta version, or 0 if TopSpin is a release version.
- `const char* GetTsVersionName(void)` returns the program name, as a string, i.e. TopSpin.

- `const char* GetTsVersionProduct(void)` returns the product name, version and patch level as a string.

EXAMPLE

The following AU program prints the current version and patchlevel in the status line of TopSpin.

```
const char* curversion =
GetTsVersionProduct();
Show_status (curversion);
QUIT
```

12.14 mkudir

NAME

`mkudir` - Creates a complete directory path.

SYNTAX

```
int mkudir (char *directory);
```

DESCRIPTION

The function `mkudir` scans the specified directory for the last /. Then it checks recursively for the existence of all components of the directory path and creates them if necessary. The function returns -1 if an error occurs, otherwise 0.

If the full path name is to be created, then the directory must end with *a /* (see the example below). Possible characters behind the last slash are discarded.

EXAMPLE

The following AU program will create a data set directory tree which has an experiment number one higher than the current foreground data set.

```
 (void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/%d/",
disk,user,name,expno+1,procno);
if (mkudir(text) < 0)
  Proc_err (DEF_ERR_OPT, "could not create :\n%s",text);
QUIT
```

12.15 PathXWinNMR

NAME

`PathXWinNMR` - A class of functions which return path names to certain TopSpin directories.

SYNTAX

```
char *PathXWinNMRConf ();
char *PathXWinNMRCurDir ();
char *PathXWinNMRDotXWinNMR ();
char *PathXWinNMRExp ();
char *PathXWinNMRPlot ();
char *PathXWinNMRProg ();
```

DESCRIPTION

The above functions return path names to certain TopSpin mostly subdirectories of the TopSpin directory <*tshome*>. For a standard installation, <*tshome*> is:

On LINUX systems: */opt/topspin*

On Windows systems: *C:\Bruker*

Please note: in TopSpin 2.1 and newer the functions `getstan` and `PathXWinNMR*` have become obsolete and can be replaced by the functions `getParfileDirForRead` and `getParfileDirForWrite`.

For a user-defined installation, <*tshome*> can be any directory. The following table lists the directory path names returned by the above functions. For examples, please check the Bruker AU program library.

`char * PathXWinNMRConf`	: returns */<tshome>/conf*
`char * PathXWinNMRCurDir`	: returns */<tshome>/prog/curdir*
`char * PathXWinNMRDotXWinNMR`	: returns *$HOME/.xwinnmr-hostname*
`char * PathXWinNMRExp`	: returns */<tshome>/exp*
`char * PathXWinNMRPlot`	: returns */<tshome>/plot*
`char * PathXWinNMRProg`	: returns */<tshome>/prog*

SEE ALSO

getParfileDirForRead [▸ 94] - Determines path name of list file to be read.

getParfileDirForWrite [▸ 96] - Determines path name of list file to be written.

12.16 pow_next

NAME

`pow_next` - Rounds to the next larger power of two

SYNTAX

```
int pow_next (int i1);
#include <inc/sysutil>
```

DESCRIPTION

The function `pow_next` takes `i1` and rounds it to the next larger integer value which is a power of two. The return value of the function is this power of two values. The function has no error handling. If `i1` is smaller than 1, then the function will return 1.

EXAMPLE

The following AU program will return 8192 in `i2` because this is the next larger number (compared to `i1`) which is a power of two.

```
i1 = 7000;
i2 = pow_next(i1);
QUIT
#include <inc/sysutil>
```

Note that the #include statement must be included **at the end** of the AU program.

12.17 Proc_err

NAME

`Proc_err` - Shows an error message in a TopSpin dialog window.

SYNTAX

```
int Proc_err (int flag, char *format);
int Proc_err (int flag, char *format, varargs);
```

DESCRIPTION

The function `Proc_err` can be used to construct a error message which will be displayed in a TopSpin dialog window. The function takes two or three arguments:

1. A flag which determines the type and the number (2 or 3) of buttons in the error window.
2. The error message to be displayed. If this argument contains `%d`, `%f`, or `%s` statements, then `Proc_err` needs a third argument which provides the corresponding variables.
3. Variables whose values replace the corresponding `%d`, `%f`, or `%s` statements of the second argument.

The first argument (flag) can have the following values:

- `DEF_ERR_OPT`

  The error window has one button (**OK**). The AU program holds until the user clicks **OK**.
- `INFO_OPT`

  The error window has one button (Seen). The AU program continues but the error window remains on the screen until it is cleared by another error window or the user clicks **Seen**.
- `QUESTION_OPT`

  The error window has two buttons, **OK** and **CANCEL**. `Proc_err` returns `ERR_OK (0)` if the **OK** button is clicked and `ERR_CANCEL (-1)` if the **CANCEL** button is clicked. The return value is normally used by subsequent control statements to decide whether or not to continue the AU program.

Note that the message in the `Proc_err` window is constructed in the same way as the C function `sprintf` constructs its strings.

EXAMPLE

The following examples show several possibilities of constructing error messages for the `Proc_err` function call.

Example for DEF_ERR_OPT :

```
 (void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/%d/",
    disk,user,name,expno+1,procno);
Proc_err (DEF_ERR_OPT, "Could not create :\n%s",text);
```

Example for QUESTION_OPT :

```
i1 = Proc_err(QUESTION_OPT,"Continue with the AU program?
             \n\ Click OK to continue, click cancel stop");

if ( i1 == ERR_OK )
{
  /* Further AU statements */
}
if ( i1 == ERR_CANCEL )
{
  ABORT
}
```

Example for INFO_OPT :

```
i1 = 7;
i2 = 5;
Proc_err(INFO_OPT,"%d is bigger than %d",i1,i2);
```

SEE ALSO

Show_status [▸ 102] - Shows a string in the status line of TopSpin.

All AU programs from the Bruker AU program library which use `Proc_err`.

12.18 Show_status

NAME

`Show_status` - Shows a string in the TopSpin status line.

SYNTAX

```
void Show_status (char *text);
```

DESCRIPTION

The function `Show_status` displays the specified text in the TopSpin status line. This function can be used as an alternative to the `Proc_err` function. One difference to `Proc_err` is that there is no window that needs to be acknowledged.

EXAMPLE

The following AU program will display the line "The AU program test has started" in the status line of TopSpin:

```
 (void) strcpy(text,"The AU program test has started");
Show_status (text);
```

```
QUIT
```

SEE ALSO

Proc_err [▸ 101] - Shows a message in a TopSpin dialog window

12.19 showfile

NAME

`showfile` - Shows the contents of a file in a TopSpin window.

SYNTAX

```
int showfile (char *file);
```

DESCRIPTION

The function `showfile` reads the specified file and displays it in a TopSpin window. This display is a read-only display, so the file cannot be changed.

EXAMPLE

The following AU program will show the title file in a TopSpin window.

```
(void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/
         %d/title",disk, user,name,expno,procno);
i1 = showfile (text);
QUIT
```

12.20 ssleep

NAME

`ssleep` - Pauses in an AU program for a certain number of seconds.

SYNTAX

```
int ssleep (int seconds);
```

DESCRIPTION

The function `ssleep` will cause the AU program to wait with the execution of the next statement until the specified number of seconds has elapsed.

EXAMPLE

The following AU program will wait for 3 minutes before it resumes execution.

```
i1 = ssleep (180);
EFP
QUIT
```

SEE ALSO

WAIT_UNTIL [▸ 42] - Holds the AU program until the specified date and time.

12.21 unlinkpr

NAME

`unlinkpr` - Deletes all processed data files (1r, 1i, 2rr, 2ii etc.) of a data set.

SYNTAX

```
int unlinkpr (char *directory);
#include <inc/sysutil>
```

DESCRIPTION

The function `unlinkpr` deletes all processed data files (*1r*, *1i*, *2rr*, *2ii*, *2ri*, *2ir*, *dsp*, *dsp.hdr*, *dsp_low*) in the specified data set directory. There is no error check whether the files could be deleted; the return value of the function is always 0 and can be ignored.

EXAMPLE

The following AU program will delete the processed data files of the foreground data set.

```
(void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/%d",
                        disk,user,name,expno,procno);
i1 = unlinkpr (text);
QUIT
#include <inc/sysutil>
```

Note that the #include statement must be included **at the end** of the AU program.

13 List of Bruker AU programs

This chapter contains a list with the names and short-descriptions of all Bruker library AU programs.

Program	Description
abs2.water	Performs an F2 baseline correction on a 2D data set left and right of the water peak.
abs2D	Performs a baseline correction on a 2D data set in both dimensions.
acqu_fid_ser	Acquires a single FID of the current 2D experiment and replaces the old fid in the ser file.
acqulist	Set up and start acquisitions using f1, f2, f3, vt, vc, vd, vp lists.
amplstab	Calculates the amplitude stability based on a peaklist file.
angle	Perform multiple acquisitions and ft’s. This program is particularly interesting when you want to adjust the magic angle for MAS type experiments.
asclev	Converts the level file in the current processed data directory to ASCII and writes it to the file.
atpplot	Create a plot and a pdf file within ATP. Execute when the ATP button 'Print actual spectrum' is clicked.
au_cp	Acquisition with adjustment of decoupling power to acquisition time .
au_getl1d	Acquire sweep width optimized 1D spectra.
au_getlcosy	Acquire sweep width optimized COSY spectra.
au_getlinv	Acquire sweep width optimized 2D inverse spectra.
au_getlxhco	Acquire sweep width optimized XH correlated spectra.
au_mult	AU program for C13 multiplicity analysis.
au_noediff	noe difference spectroscopy using different expnos.
au_noemult	noe difference spectroscopy with multiple irradiation points for each multiplet using different expnos.
au_water	Acquire water-suppression spectra for use in foreground (xau,xaua).
au_watersc	Acquire water-suppression spectra for use in automation, e.g., with sample changer.
au_zg	General AU program for data acquisition.
au_zg135	Acquire DEPT135 type spectra.
au_zgcosy	Acquire COSY type spectra.
au_zgglp	Automatic data evaluation according to GLP standards. This AU program takes O1, SW and O2 as arguments and then works like au_zg.
au_zgnr	Acquisition with rotation switched off.

Program	Description
au_zgonly	General AU program for data acquisition.
au_zgsino	Acquisition with signal to noise break up.
au_zgte	Acquisition with temperature setting.
aunmp_tojdx	Used in LIMS automation to process data. First, AUNMP is executed, then, if specified, the command given on the command line.
autoflist	Automatic generation of a frequency list for the peaks in the plot region of the spectrum.
autot1	Automatic processing of a 2D T1/T2 experiment with subsequent T1/T2 calculation.
bsms_exam	Example AU program which shows how to use low level functions to read or write BSMS parameters.
bsms_getlock	Read current LockLevel from BSMS Unit.
butselau	AU program for selective experiments in **bnmr**.
buttonau	AU program for basic experiments in **bnmr**.
butsel90	AU program for calibrating selective 90 pulse **bnmr**.
calcphhomo	Calculate the phase correction for the F2 and F1 dimension of homonuclear 2D experiments.
calcphinv	Calculate the phase correction for the F1 dimension in HMQC/ HSQC type experiments.
calcplen	Calculate the pulse length according to the power level.
calcpowlev	Calculate the power level according to the pulse length.
calctemp	Calculate the temperature in the probe using the chemical shift difference between the aliphatic and OH protons.
calfun	Calculates an FID from an arbitrary function. This AU program is especially useful when you want to create a user defined window function for the 'uwm' command.
calibo1p1o3	Calibrate O1 and P1 for H2O samples .
check-vtu	Updates TE variable from the actual temperature and store it in a separate file (edte) in the data set.
clev	Automatically calculate levels for 2D data.
clspec	Cleans spectra from the effects of solvent suppression. Multiple Regions can filtered or deleted from the spectrum. Entries for these regions can be deleted from peak lists and integrals. Regions are requested interactively.
coiltemp	Read the Shim Coil Temperature.
convbin2asc	Writes a 1D spectrum, with or without imaginary data points, into a file in ASCII table format. Each line in the file corresponds to one data point. The resulting file, named ascii-spec.txt, can be used to import a 1D spectrum into third party software, like Matlab.

Program	Description
convfidtoasc	AU program to convert an fid data file into an ascii table containing point number and intensity values. The output file is stored in the same directory as the fid. It can be used for calculations in spread-sheet programs or other third-party software.
convto1d	Converts a 2D spectrum to 1D format.
covariance	Processes data according to Covariance NMR
dcorr	Enables/disables the automatic DC-offset correction procedure of the software in case of a DRU installed.
decon_t1	Automatic deconvolution of a 2D T1/T2 experiment.
deptcyc	Creates 3 DEPT experiments from 13C experiment with CPD and then performs multiple cycles of NS scans (times 2 for DEPT90).
depthalt	Halt "deptcyc" AU program.
diffe	Calculate the difference spectra between expnos.
diffp	Calculate the difference spectra between procnos.
dosy	Setup for diffusion/DOSY experiments linear gradient amplitude ramp.
elim_ints	Eliminates regions from the intrng file that contain the solvent and/or reference signals. The result will be an intrng file where the integral trails have a more reasonable scaling and smaller integrals are better resolved.
f1ref	Corrects the referencing in F1 for inverse type experiments.
fidadd	Add up FID’s in incremented expno’s.
fidtoser	Writes a number of fids that are stored under the same NAME and incremental EXPNOs to a ser file.
getphsum	Reads the total phase values from the status parameters and stores them back to the actual parameters.
gifadosy	Gifa starter AU program.
goalternate	Acquire alternated X/Y measurements. N averages are acquired alternatingly in two experiments.
graderror	Shows error messages generated by the gradshim gradient shimming procedure.
gontp	Starts an ntp test program.
gradratio	Calculates gradient ratios for common inverse gradient pulse programs.
gradratiogs	Calculates gradient ratios for common inverse gradient pulse programs.
gradshimau	Start gradshim gradient shimming procedure.
gsau	Program to start the gradshim gradient shimming procedure
gssel_setup	AU program to determine the transmitter offset for 1H selective gradient shimming using 1H as observe nucleus.
heater	Switch the heater on/off.

Program	Description
humpcal	Performs the 'hump test'. Measures the width of a peak at 0.55% and 0.11% of its signal height.
hwcal	Calculate the width of a peak at half height.
iexpno	Program to change to a new experiment number.
ift3d	Inverse Fourier transform of 3 dimensional data.
interleave	Perform interleaved acquisitions.
ilhalt	Stop an interleaved acquisition which was started with the AU program interleave.
jconv_aufx	Converts Jeol FX data in a loop. The data must be stored with increasing extensions like proton.1, proton.2, ... etc.
listall_au	Scans all AU programs and extracts the name and the short description. This information is then copied into the file listall in your home directory. This list corresponds to the list you are currently reading.
loadshimZ	Reads the on-axis shim values from disk and loads them to the BSMS.
lock_off	Switch off the lock to start data acquisition on the lock channel.
lock_on	Switch on the lock if it has been disabled.
loopadj	Parameter optimization au program which calculates the lock parameters loop filter, loop gain and loop time for optimal long-time stability after adjusting lock phase and lock gain to optimal.
make2d	Create a new 2D data set from the current 1D data set. Can be used for 2D spectroscopy and relaxation experiments. F2 parameters are copied from the 1D data, F1 parameters are set to reasonable values.
mkflist	Automatically generates a frequency list file.
mulabel	Processing AU program for determination of 13C multiplicity.
multanal	Processing AU program for determination of 13C multiplicity.
multi_decon	Automatic deconvolution of a series of 1D spectra with AI calibration.
multi_integ	Automatic integration of a series of 1D spectra with AI calibration.
multi_integ2	Automatic integration of a series of 1D spectra with calibration of the integral values.
multi_integ3	Automatic integration of a series of 1D spectra with AI calibration. The output is written in a format suitable for import in excel or similar desktop publishing programs.
multi_zgvd	Performs multiple acquisitions on increasing expnos with delays that are read from a vdlist file. Alternatively, a fixed delay can be entered.
multi_zgvt	Performs multiple acquisitions on increasing expnos with temperatures that are read from a vtlist file.
multicmd	Performs multiple commands on increasing expnos.
multicom	Executes a TopSpin command in increasing expnos.

Program	Description
multicyc	Cycles through a series of acquisitions of increasing expnos.
multiefp	Performs multiple "efp" on increasing expnos.
multiexpt	Calculates experimental time for multizg.
multifp	Performs multiple "fp" on increasing expnos.
multiftapk	Performs multiple "ft;apk" on increasing expnos.
multihalt	Halt "multicyc" AU program.
multimas	Performs multiple MAS experiments on increasing expnos.
multipcom	Executes a TopSpin command in increasing procnos.
multiwinpro	Performs multiple processing on increasing expnos. The program asks for the window function and its parameters.
multixfb	Performs multiple "xfb" on increasing expnos.
multizg	Performs multiple acquisitions on increasing expnos.
noediff	noe difference spectroscopy using different expnos.
noeflist	Automatic generation of a frequency list with the peaks from the current plot region for noe.
noemult	noe difference spectroscopy with multiple irradiation points for each multiplet using different expnos.
paropt	Parameter optimization au program.
parray	Parameter optimization au program using parameter arrays. Derived from ’paropt’, but several parameters may now be changed per experiment. In addition, parameters are not changed via constant increments. Instead, the values are taken from an array.
pass2d	Perform a PASS experiment with 5 Pi-pulses and 16 increments (samples up to 16 spinning side bands).
pecosy	Program to pre-process P.E.COSY raw data before 2D-FT.
phtran	Transfer phase correction parameters PHC0 and PHC1 into acquisition parameters PH_ref and DE.
plintfac	Plot integrals with different scaling factors.
plot_sino	Plot spectrum, scaling depends on Signal/Noise.
plot_to_file	Creates a postscript file of the desired plot.
plotx	Plots individually scaled integral regions as separate objects.
popt au	Parameter optimization au program using parameter arrays. Derived from 'paropt' but several parameters can be optimized. The parameters are changed according to the parameter arrays.The AU program will be started from user interface 'popt' (parameter editor).
popthalt	Halt "popt" AU program.
proc_1H	Processes and plots 1D spectra. Does not perform baseline correction.
proc_1d	Processes and plots 1D spectra.

Program	Description
proc_1dapks	Processes and plot 1D spectra. Uses 'apks' for phase correction.
proc_1dconlf	Processes and plots 1D spectra. Plots an additional spectrum on the same plot if there are integrals in the lowfield range outside delta > 11.
proc_1dconlf_pr	Processes and plots 1D spectra. Plots an additional spectrum on the same plot if there are integrals in the lowfield range outside the plot limits.
proc_1dglp	Processing AU program with automatic data evaluation according to GLP standards. This AU program takes CY as an argument and then works like proc_1d.
proc_1dlf	Processes and plot 1D spectra. Plots an additional lowfield plot.
proc_1dpppti	Processes and plots 1D spectra. Creates a special peaklist file (frequency (Hz) and half width) and prints this on the plot.
proc_1dppti	Processes and plots 1D spectra. Creates a peak picking list and prints this on the plot.
proc_2d	Processing AU program for 2D spectra without plotting.
proc_2dhom	Processes and plots 2D homonuclear type spectra.
proc_2dhom_2pp	Processes and plots 2D homonuclear type spectra with two positive projections.
proc_2dinv	Processes and plots 2D inverse type spectra.
proc_2dinv_2p	Processes and plots 2D inverse type spectra. Plots two projections.
proc_2dphf2het	Determines phase correction in F2 for heteronuclear spectra.
proc_2dphf2hom	Determines phase correction in F2 for homonuclear spectra.
proc_2dpl	Processes and plots 2D type spectra.
proc_2dsym	Processes and symmetrizes 2D type spectra.
proc_2dt1	Automatic processing of one 2D T1/T2 experiment with subsequent T1/T2 calculation.
proc_cpd135	Processes and plots 13C CPD and DEPT135 spectra that were acquired with the AU program au_zg135.
proc_glp	Automatic GLP data evaluation.
proc_intrng	Processes and plots 1D spectra. Uses the predefined integral range file 'testrng' for integration.
proc_MAS	Processes and plot 1D MAS spectra.
proc_no	AU program which does no processing.
proc_noe	Processes and plots noediff spectra.
proc_t1	Semi-automatic processing of multiple 2D T1/T2 experiment with subsequent T1/T2 calculation.
proc_tecalib	Evaluation of previous temperature calibration experiments.
psys180f1t1	Processing AU program for the 180° pulse calibration tests.

Program	Description
psysamp1s39	Processing AU program for the amplitude stability tests - with shaped pulse - with 30 ° pulse - with 90° pulse - after gradient echo (5msec, 30 G/cm) - after gradient echo (5msec, 10 G/cm) - after gradient pulse (1msec, 10G/cm).
psysb1hom	Processing AU program for the B1 homogeneity test.
psysb2hom	Processing AU program for the B2 homogeneity test.
psyscancel	Processing AU program for the - phase cycling cancellation test - phase cycling cancellation test after gradient pulse.
psysdante1	Processing AU program for the dante type turn on test.
psysdecpro1	Processing AU program for the decoupler profile test.
psysexpro1	Processing AU program for the - excitation profile (16 usec gauss shape) test - excitation profile (6 msec gauss shape) test.
psysglitch	Processing AU program for the glitch test.
psysgrreco1	Processing AU program for the gradient recovery test.
psysgrzpro	Processing AU program for the z-gradient profile.
psysmodl1	Processing AU program for the - modulator linearity test - shaped pulse modulator linearity test.
psysmultl1	Processing AU program for the amplitude linearity test (1dB power level steps).
psysphas1st	Processing AU program for the - phase stability test ("13° test") - shaped pulse phase stability test (16 usec gaussian shape, "13° test").
psysphasf1	Processing AU program for the - phase propagation test - phase shifting test.
psyspullin1	Processing AU program for the - amplitude linearity test - shaped pulse amplitude linearity test (pulse length *2, power level +6).
psysquadim	Processing AU program for the quad image suppression test.
psysrgtest	Processing AU program for the receiver gain test (analog and digital).
psyssoftp1	Processing AU program for the shaped pulse comparison (rectangular, gaussian, eburp1).
psystestab	Automatic processing of a 2D Temperature stability experiment, evaluation of temperature and statistic of temperature stability. Can be used to process data obtained with the AU program systestab.
psysturnon	Processing AU program for the turn on test.
pulse	Program to calculate attenuation value for given pulse length or nutation frequency, or vice versa.
pulsecal	Single scan pulse calibration via stroboscopic nutation experiment.
pulsecalib	Offset/Pulsecalibration H2O/D2O and Offset/Pulsecalibration 13C, 15N probe.

Program	Description
qnpset	Define the QNP parameter according to the currently defined probe.
quadplot	First plots a 2D overview spectrum and then the 4 quadrants of the 2D spectrum.
queue	Queue data acquisition.
queue_init	Initialise data acquisition with the AU program queue.
queuerga	Queue data acquisition.
r23mplot	Read 2D slices from a 3D data set and plot them.
r23mult	Repeatedly reads slices from a 3D data set (3rrr) into successive experiment numbers.
rampXY	3D gradient shimming with the BSMS RCB board.
remproc	Automatic conversion and processing of data sets transferred via BRUKNET, LIGHTNET, NMR-LINK or TCP-LINK.
repeat	Repeat an acquisition with exactly the same parameters, pulse program and other lists.
rescale	Applies intensity scaling, for direct comparison of spectra acquire with different RG, NS and flip angle.
secplot	Generate a section plot. The overview spectrum is plotted together with a vertical expansion of a smaller part of the spectrum on top of it.
set2hdecgp	Setup AU program for standard 3D parameter sets.
setccnh3dgp	Setup AU program for standard 3D parameter sets.
setdiffparm	Extracts diffusion sequence parameters and stores parameters for "vargrad" simfit fitting (T1/T2) or DOSY processing.
seteditedgp	Setup AU program for standard 3D parameter sets.
sethccc3dgp	Setup AU program for standard 3D parameter sets.
setpar3dgp	Setup AU program for standard 3D parameter sets.
set_sreglist	Set SREGLST parameter from NUC1 and SOLVENT.
simplex	AU program for autoshimming. It is suitable for adjustment of strongly coupled shim groups which may be far from the optimum position.
simtoseq	Converts data which have been recorded in digital and qsim mode to data which appear to be acquired in qseq mode.
sinocal	Calculates the signal to noise ratio.
split	Separate data obtained with interleaved acquisition.
split2D	Splits a processed 2D file into single 1D spectra.
split3D	Separate interleaved 3D data.
splitcomb	Combine, shift and add 2D/3D data recorded with an interleaved single or double InPhase/AntiPhase or S3E scheme.
splitcrin	AU program to separate interleaved 3D data
splitcrinept	AU program to separate interleaved 3D data.

Program	Description
splitdqzq	Combine DQ/ZQ data.
splithb	Separate and combine H-bond experiments.
splithmsc	Separate the 1J and nJ component of the HMSC experiment.
splitinvnoe	Separate NOE and NONOE data obtained with a pulse program like invinoef3gpsi.
splitipap	Create separate InPhase and AntiPhase data sets.
splitipap2	Create separate InPhase and AntiPhase data sets for DSSE experiments.
splitipap3d	Separate Inphase/Antiphase data from 3D data sets.
splitpfids	Separate decoupled/non-decoupled data obtained with a pulse program like pfidsetgpsi.
splitser	Splits a ser file into single fids, starting with the expno which follows the ser file.
splitxf	Separate and combine double half filtered data.
ssd	Set the 2nd and 3rd data set from the commandline.
stack1d	Generates a stacked plot of 1D spectra from increasing or decreasing EXPNOs or PROCNOs.
stack2d	Generate a 2D stack plot.
stackp1d	Generates a stacked plot of 3 to 12 1D spectra from increasing or decreasing EXPNOs or PROCNOs.
stdsplit	Splits STD pseudo 2D data sets.
suppcal	Calculates the width of the Water peak at 100% and 50% of the DSS signal height. The result is referred to as the ’water suppression test’.
sys180f1t1	Acquisition AU program for the 180° pulse calibration test with different phases.
sys180f1t2	Acquisition AU program for the 180° pulse calibration test with different flip angles.
sysamp1sp9	Acquisition AU program for the shaped pulse amplitude stability test.
sysamp1st	Acquisition AU program for the amplitude stability tests - with 30° pulse - with 90° pulse.
sysb1hom	Acquisition AU program for the B1 homogeneity test.
sysb2hom	Acquisition AU program for the B2 homogeneity test.
syscancel	Acquisition AU program for the phase cycling cancellation test.
sysdante1	Acquisition AU program for the dante type turn on test.
sysdecpro1	Acquisition AU program for the decoupler profile test .
sysexpro1	Acquisition AU program for the - excitation profile (16 usec gauss shape) test - excitation profile (6 msec gauss shape) test.
sysgenpar	Preparation AU program for all HWT test programs.
sysglitch	Acquisition AU program for the glitch test.

Program	Description
sysgrcan	Acquisition AU program for the phase cycling cancellation test after gradient pulse.
sysgrecho	Acquisition AU program for the amplitude stability test after gradient echo (5msec, 30 G/cm and 5msec, 10 G/cm).
sysgrreco1	Acquisition AU program for the gradient recovery test.
sysgrstab	Acquisition AU program for the amplitude stability test after gradient pulse (1msec, 10G/cm).
sysgrzpro	Acquisition AU program for the z-gradient profile.
sysmodl1	Acquisition AU program for the modulator linearity test.
sysmodls1	Acquisition AU program for the shaped pulse modulator linearity test.
sysmultl1	Acquisition AU program for the amplitude linearity test (1dB power level steps).
sysphas1sp	Acquisition AU program for the shaped pulse phase stability test (16 usec gaussian shape, "13 degree test").
sysphas1st	Acquisition AU program for the phase stability test ("13 degree test").
sysphasf1	Acquisition AU program for the - phase propagation test - phase shifting test.
syspullin1	Acquisition AU program for the amplitude linearity test (pulse length *2, power level +6).
sysquadim	Acquisition AU program for the quad image suppression test.
sysrgtest	Acquisition AU program for the receiver gain test (analog and digital).
syssoftp1	Acquisition AU program for the shaped pulse comparison (rectangular, gaussian, eburp1).
syssplin1	Acquisition AU program for the shaped pulse amplitude linearity test (pulse length *2, power level +6).
systestab	AU program for a temperature stability experiment performed as pseudo 2D experiment including evaluation of temperature and statistics of temperature stability.
systurnon	Acquisition AU program for the turn on test.
tecalib	AU program to determine the temperature calibration curve.
testsuite	Test the general functionality of a TopSpin release version. Basic functionality is given if this program is completed without error messages.
tmscal	Performs a peak picking around the TMS signal. If the two satellites from the 29Si - 1H coupling can be detected, the resolution is OK.
tune	Tune a probe.
update_layout	Sets the parameter 'LAYOUT' in all parameter sets.
update_aunmp	Sets the parameter AUNMP in all parameter sets.
vtu_airflow	Switch the VTU air flow.

Program	Description
`vtu_exam`	Example AU program which shows how to use low level functions to read or write VTU (BVT1000/BDTC) parameters.
`vtu_heater`	Switch the VTU heater.
`writeshimZ`	Reads the on-axis shim values and writes a pseudo shim file.
`xfshear`	Program for shearing of 2D MQMAS spectra of odd half integer quadrupolar nuclei. Data need to be acquired in States Mode
`zeroim`	Zero the imaginary data of a 1D or 2D data set.
`zg_2Hoffon`	General AU program for data acquisition. The lock is switched off before the acquisition is started.
`zgchkte`	Starts acquisition with zg and monitors the temperature. The experiment is halted if the current temperature differs too much from the target temperature.
`zg_dfs`	Calculates shape file for double frequency sweep and subsequent data-acquisition.
`2df1shift`	Shift a 2D spectrum along the F1 axis.
`2dgetref`	Gets parameters for a 2D spectrum from the 1D reference spectra: Nucleus, Frequencies, Spectral Width, and reference plot data set names. The F2 reference is taken from the second data set. The F1 reference is taken from the third data set.
`2dshift`	Shift 2D time domain data left or right over NSP points.
`2nde`	Set 2nd data set to new *expno* and 3rd data set equal to foreground data set.
`2ndn`	Set 2nd data set to new name and 3rd data set equal to foreground data set.

Table 13.1: Bruker Library Au Programs

14 TopSpin Parameter Types

This chapter contains a list of all TopSpin parameters grouped by their type. The type of a parameter can be integer, float, double or character-string. Several AU macros read TopSpin parameters into AU variables or store the value of AU variables into TopSpin parameters. In both cases it is important that the type of the AU variable is the same as the parameter type.

14.1 Integer Parameters

The following TopSpin parameters are of the type integer:

ABSG	AQORDER	AQSEQ	AQ_mod
BC_mod	BYTORDA	BYTORDP	DATMOD
DIGMOD	DIGTYP	DS	EXPNO2
EXPNO3	FnMODE	FT_mod	HGAIN[4]
HOLDER	HPMOD[33]	HPPRGN	INTBC
L[32]	LOCSHFT	LPBIN	MASR
MC2	ME_mod	NBL	NC
NCOEF	NC_proc	NLEV	NS
NSP	NZP	OVERFLW	PARMODE
PH_mod	PKNL	POWMOD	PPARMOD
PRGAIN	PSCAL	PSIGN	PROCNO2
PROCNO3	QNP	REVERSE	RO
RSEL[25]	SI	STSI	STSR
SYMM	TD	TD0	TDeff
TDoff	TILT	WBST	WDW
XDIM	XGAIN[4]	YMAX_p	YMIN_p

Table 14.1: TopSpin Parameters of Type Integer

14.2 Float Parameters

The following TopSpin parameters are of the type float:

ABSF1	ABSF2	ABSL	ALPHA
ASSFAC	ASSFACI	ASSFACX	ASSWID
AZFE	AZFW	BCFW	CNST[64]
DC	DE	D[64]	FCOR
FW	GAMMA	GB	GPX[32]
GPY[32]	GPZ[32]	ISEN	LB
LEV0	LOCPHAS	MAXI	MI
NOISF1	NOISF2	OFFSET	PC

PCPD[10]	PHC0	PHC1	PHCOR[32]
PH_ref	PL[64]	P[64]	RECPH
RG	SIGF1	SIGF2	SINO
SPOAL[64]	SPOFFS[64]	SP[64]	SSB
S_DEV	TE	TE2	TM1
TM2	TOPLEV	V9	WBSW[8]

Table 14.2: TopSpin Parameters of Type Float

14.3 Double Parameters

The following TopSpin parameters are of the type double:

BF1	BF2	BF3	BF4
BF5	BF6	BF7	BF8
COROFFS	CY	F1P	F2P
INP[64]	IN[64]	INTSCL	LFILTER
LGAIN	LOCKPOW	LTIME	O1
O2	O3	O4	O5
O6	O7	O8	SF
SFO1	SFO2	SFO3	SFO4
SFO5	SFO6	SFO7	SFO8
SW	YMAX_a	YMIN_a	

Table 14.3: TopSpin Parameters of Type Double:

14.4 Character-string Parameters

The following TopSpin parameters are of the type character-string:

AUNM[32]	AUNMP[32]	CPDPRG[9][32]	DFILT[16]
DU[256]	DU2[256]	DU3[256]	EXP[64]
FQ1LIST[32]	GPNAM[32][64]	INSTRUM[64]	LAYOUT[256]
LOCNUC[8]	MASRLST[16]	NAME[96]	NUC1[8]
PROBHD[64]	PULPROG[32]	SOLVENT[32]	SPNAM[64][64]
SREGLST[40]	TI[72]	TYPE[16]	USER[64]
USERA1[80]	USERP1[80]	VCLIST[32]	VDLIST[32]
VPLIST[32]	VTLIST[32]		

Table 14.4: TopSpin Parameters of Type Character-String:

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Manufacturer

Bruker BioSpin GmbH
Silberstreifen 4
D-76287 Rheinstetten
Germany
http://www.bruker.com

WEEE DE43181702

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E-mail: *nmr-support@bruker.com*

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Bruker Corporation

info@bruker.com
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