

TopSpin

Method Development

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→ **Shapes**

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→ **AU Programs**

→ **Python Programs**

→ **Macros**

→ **Pulse Programs In Python**

→ **Plot Layout Programming**

→ **User-Defined Command Panels**

Pulse Programs



Development Tools

Pulse Programs

File Options Help Source = c:\myitems\pp

Search in names [*?] Search

Class = Any Dim = Any All

c_ncanco_ia3d	c_ncanco_ia3d	c_ncbca_ia3d	c_ncbcaco_ia...	c_ncbcaco_s...
c_hcbcan_ia3d	c_hccflopsy1...	c_hnca_ia3d	c_hncaco_ia3d	c_hncaco_s3...
c_hnco_ia3d	c_hnco_ia3d	c_hncoca_ia3d	calibgp	cbcaconhgp3d
cbcaconhgpw...	cbcanhgp3d	cbcanhgpw3d	ccaconhgp2h...	ccaconhgp3d
ccaconhgp3d.2	ccanhgp2h3d	ccanhgp3d	ccanhgp3d.2	ccconhgp2h3d
ccconhgp3d	clmlevphpr	colocqf	cosycwphps	cosydcrlqf
cosydcph	cosydcphwt	cosydcqf	cosydfesgpph	cosydfesgpp...
cosydfetgp.1	cosydfetgp.2	cosydfgpph19	cosydf...	
cosydfqf	cosysetgp	cosygmfmph	cosygm...	
cosygprrqf	cosygpqf	cosyjdqf	cosylr...	
cosyphpr	cosyphtf	cosyppqf	cosypp...	
cosyqf45	cosyqf90	cosyqfr2	cosyqf...	
cosyqf45	cpmg	cpmg1d	cpmgr...	
croesyph	croesyphpr	dazzg	dec18...	
dec180pr	dec180sp	decp90	decp9...	
decp90f3	decp90sp	dept	dept1...	
dept90	deptnd	deptppnd	deptq...	
deptsp	deptsp135	deptsp45	deptsp...	
dipsi2etgp	dipsi2etgpcsix1	dipsi2etgpsi	dipsi2...	

Edit Graphical Edit

Browser

cpmg (c:\myitems\pp) *

File Edit Search

Graphical Edit

```
1 ;cpmg
2 ;avance-version (00/02/07)
3 ;T2 measurement using Carr-Purcell-Meiboom-Gil
4 #include <Avance.incl>
5
6 "p2=p1*2"
7 "d11=30m"
8
9 1 ze
10 2 d1
11   p1 ph1
12 3 d20
13   p2 ph2
14   d20
15   lo to 3 times c
16   go=2 ph31
17   d11 wr #0 if #0 ivc
18   lo to 1 times td1
19 exit
20
21 ph1=0 0 2 2 1 1 3 3
22 ph2=1 3 1 3 0 2 0 2
23 ph31=0 0 2 2 1 1 3 3
24
25 ;p1 : f1 channel - power level for pulse (def
26 ;p1 : f1 channel - 90 degree high power pulse
27 ;p2 : f1 channel - 180 degree high power pulse
28
```

24 : 1

Editor with syntax highlighting

cpmg

File Graphical assistant Edit text

Expressi Names Values L

H 1 ZE P1 ph1=[0,0...] P2 ph2=[1,3...

D1 D20 D20 D11

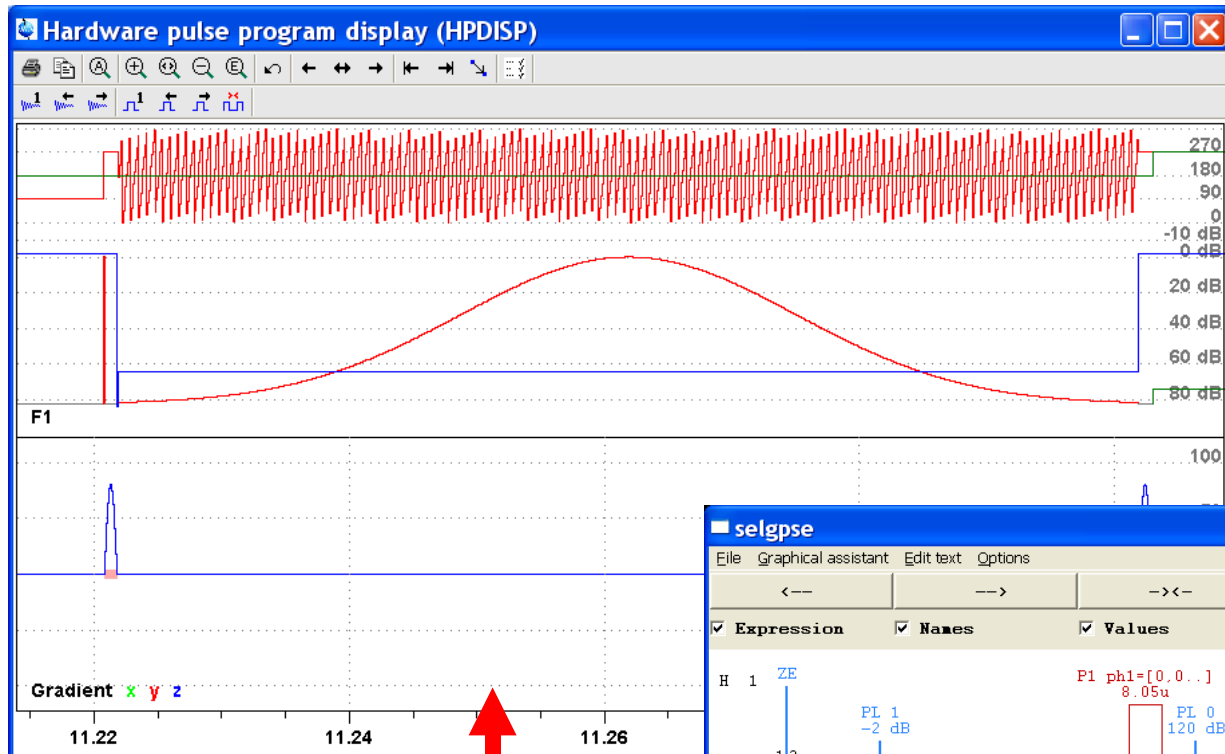
Loop VC
Go loop
Loop TD1

Symbolic display

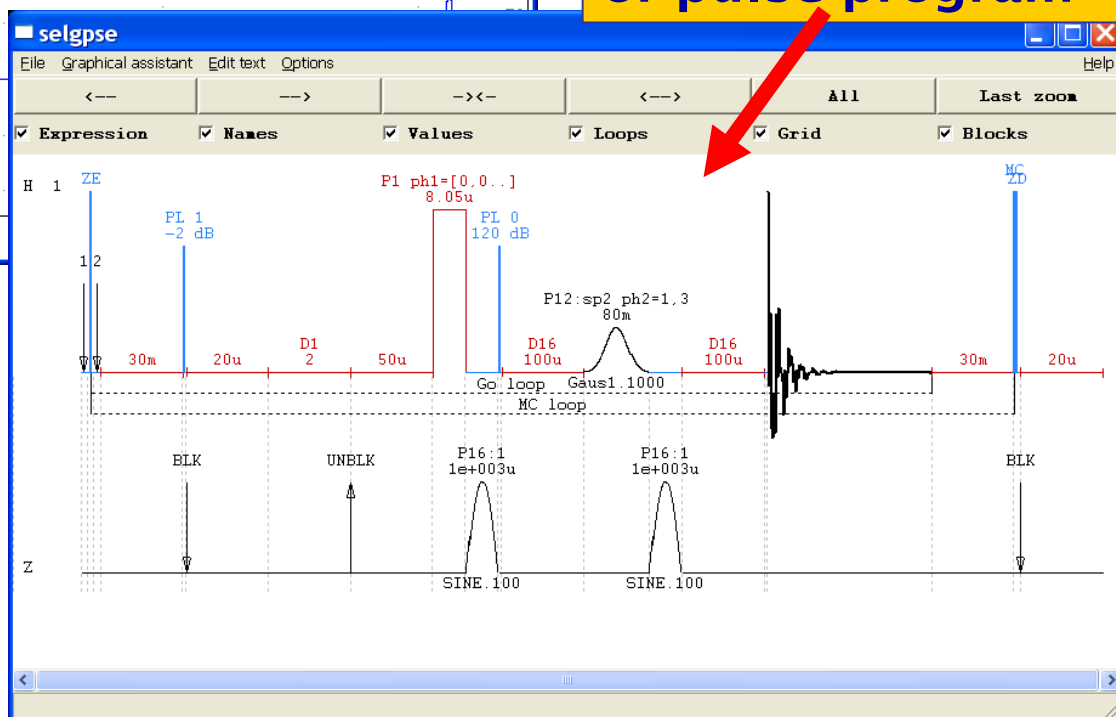
Pulse Programs



```
1 ze
2 30m
20u p11:f1 BLKGRAD
d1
50u UNBLKGRAD
p1 ph1
p16:gp1
d16 p10:f1
p12:sp2:f1 ph2:r
p16:gp1
d16
go=2 ph31
30m mc #0 to 2 F0(zd)
20u BLKGRAD
exit
```

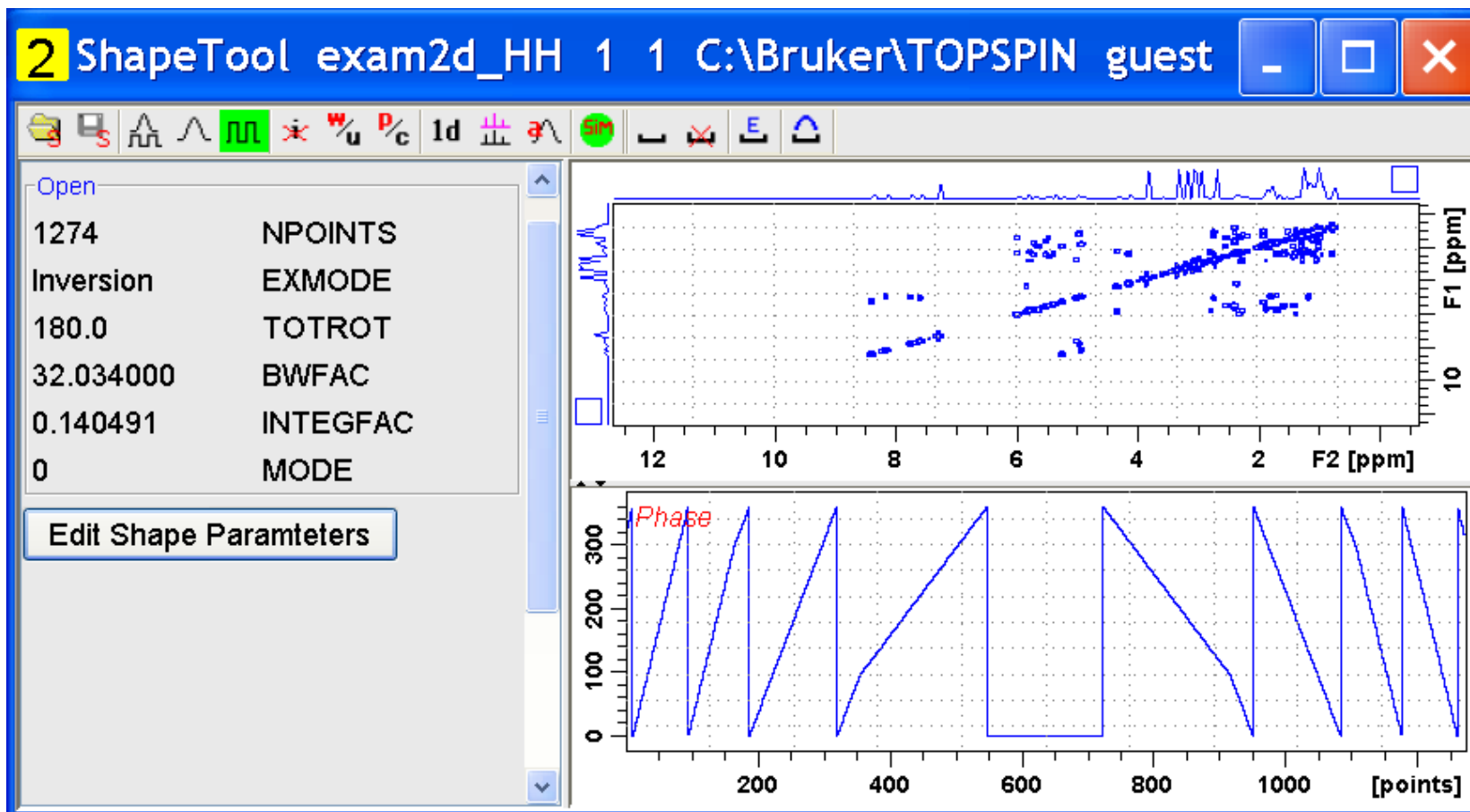


Symbolic display
of pulse program



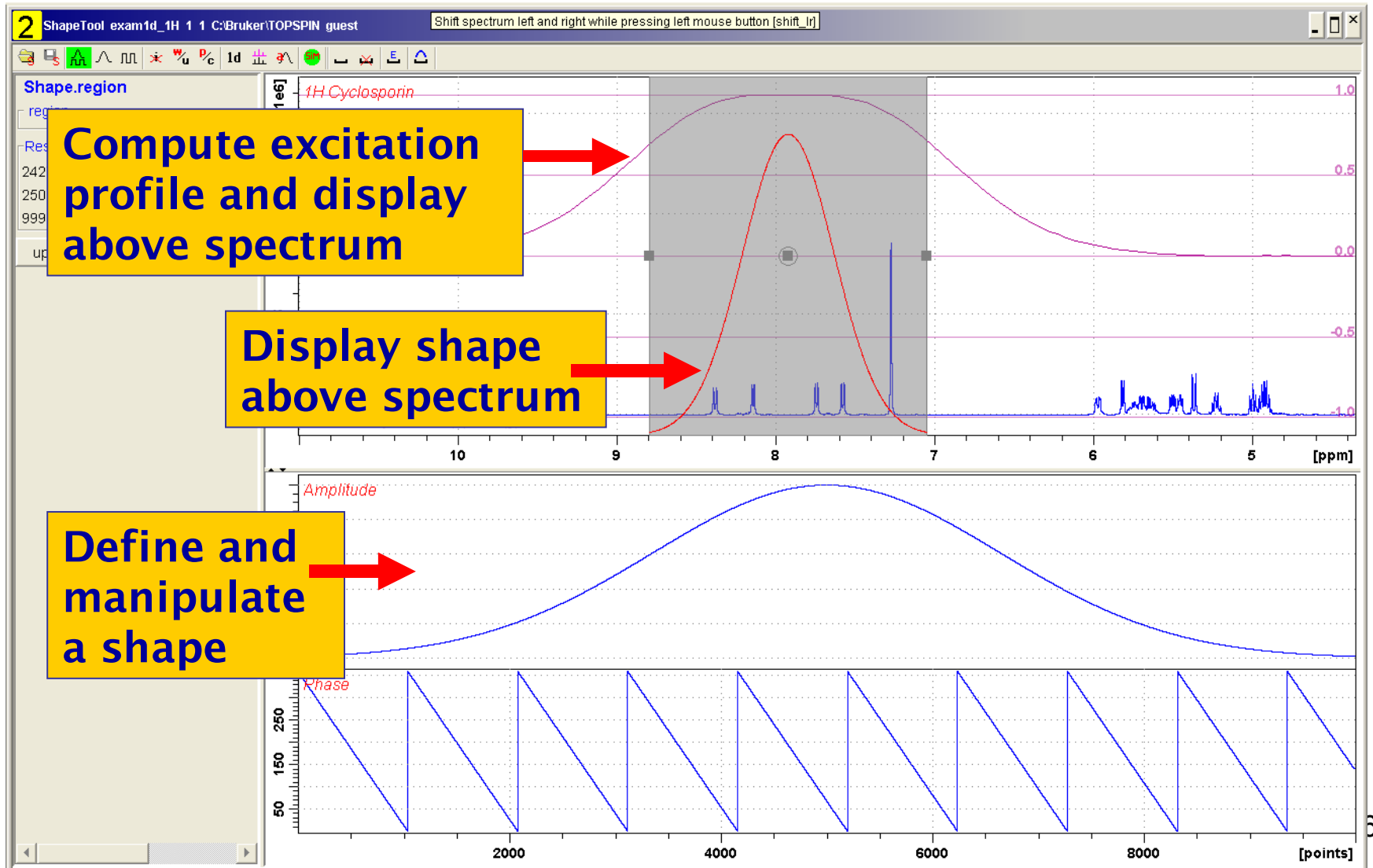
Simulation of
pulse generator
output for pulse
program
development &
testing

ShapeTool to define shaped pulses



Shapes

Calculation and display of excitation profiles



Simulates a wide range of NMR experiments

Simulation result is a 1D, 2D, ... fid

Simulates the behaviour of *general homo- and heteronuclear* spin systems (up to quantum number 2)

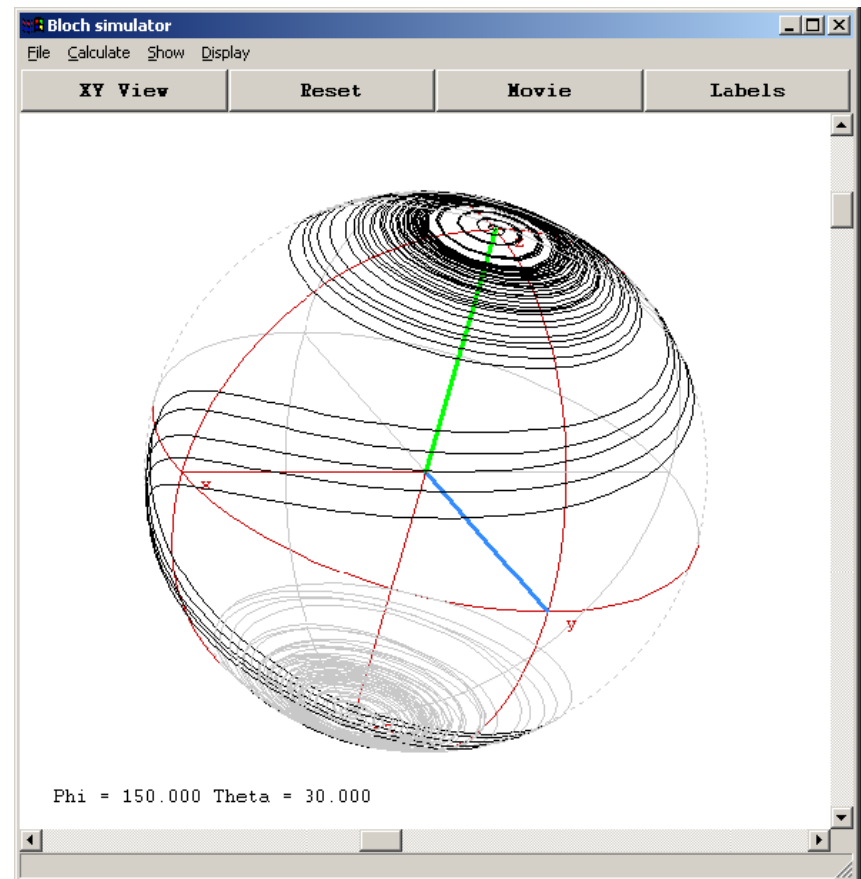
Supports simulation of rotating frame magnetization transfer experiments (TOCSY or HOHAHA)

Supports simulation gradient enhanced exp.

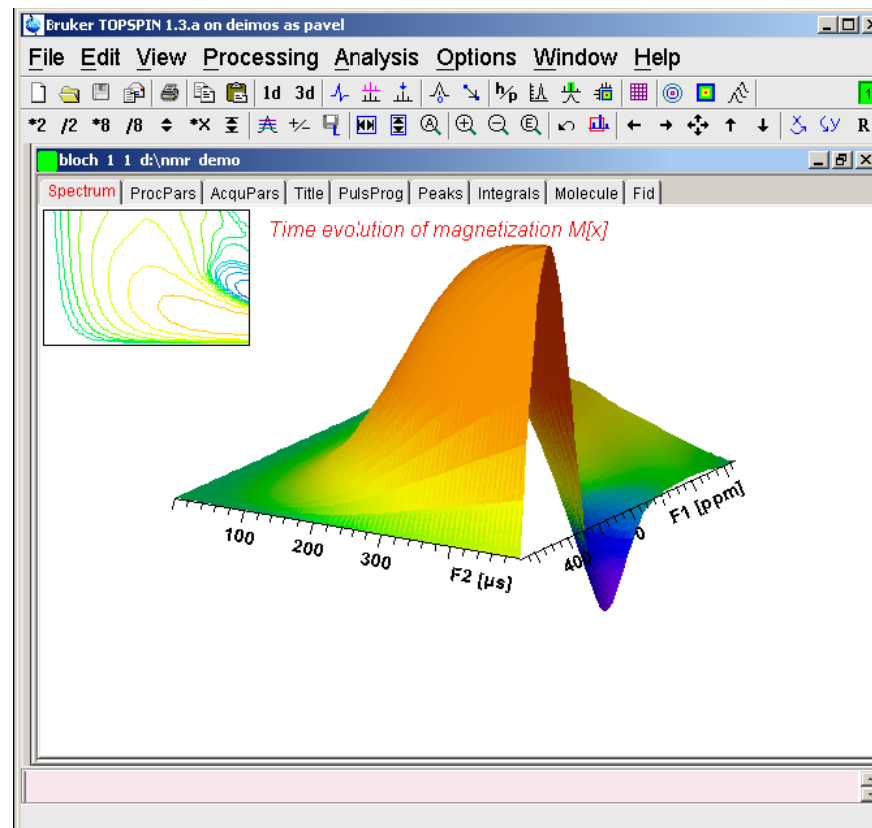
Solves the quantum mechanical Liouville equation

The Bloch module lets you visualize the time development of the nuclear magnetization during various experiments.

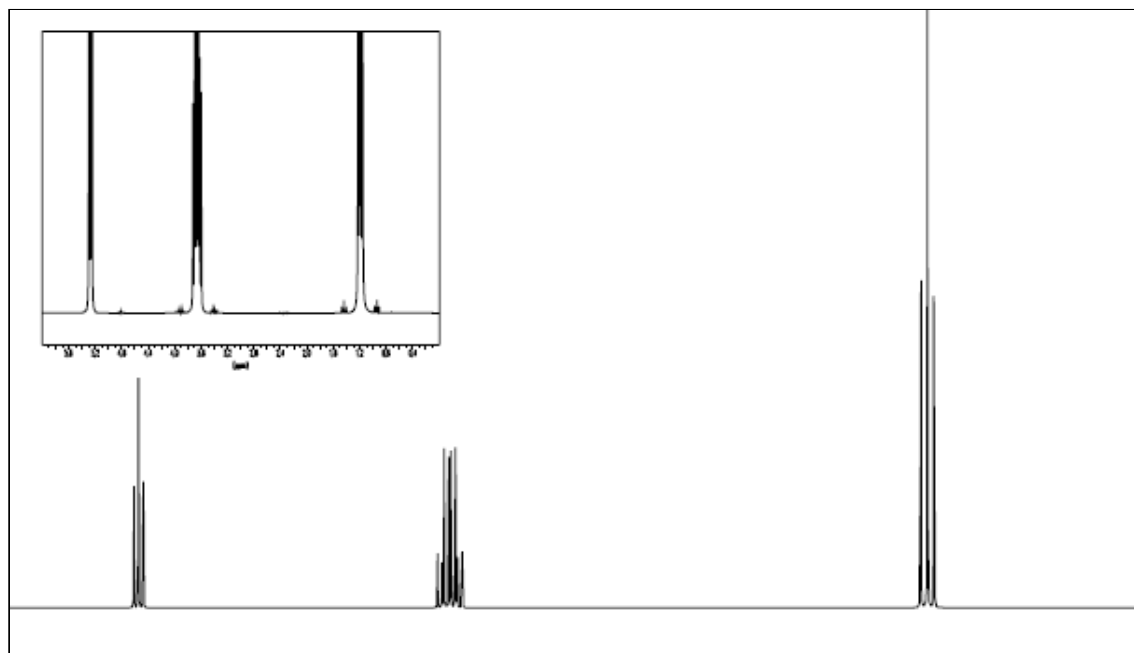
The time evolution of a nuclear magnetization vector during an adiabatic pulse, calculated for several offsets, is shown as a projection on the sphere



**Time evolution of
the magnetization
shown in TOPSPIN**



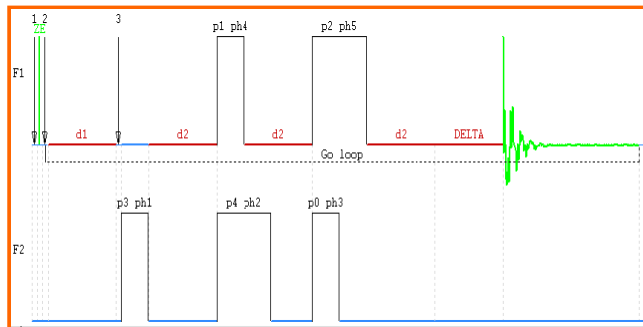
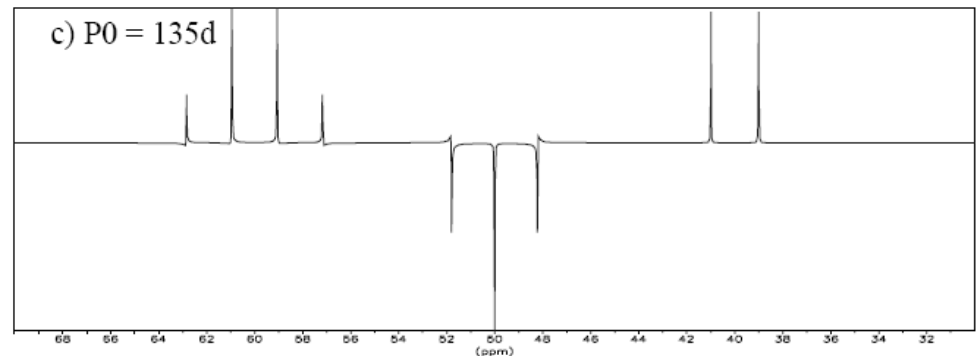
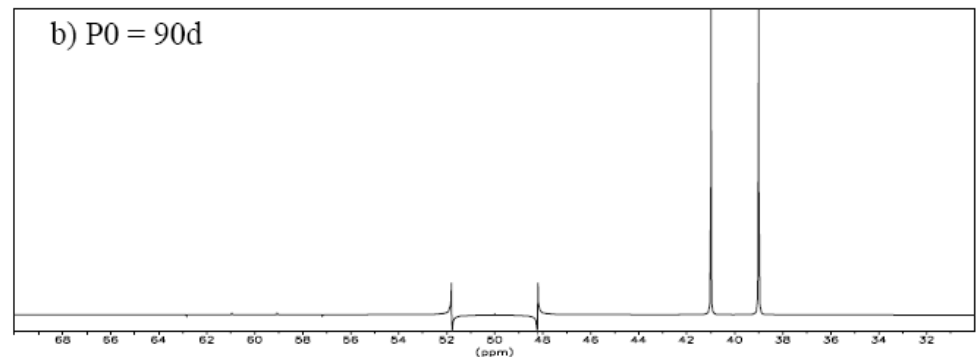
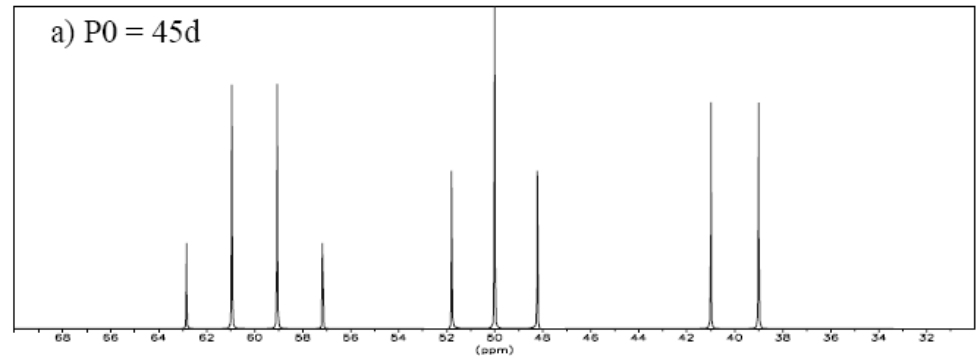
The proton spectrum of ethanol at 200 MHz. The inset shows the C13 satellites (vertical scale with 8 times magnification).



Experiment Simulation (NmrSim)



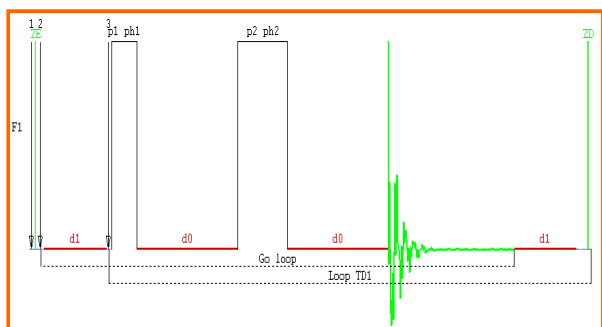
Comparison of simulated ^{13}C DEPT spectra for three different leading pulses P0.



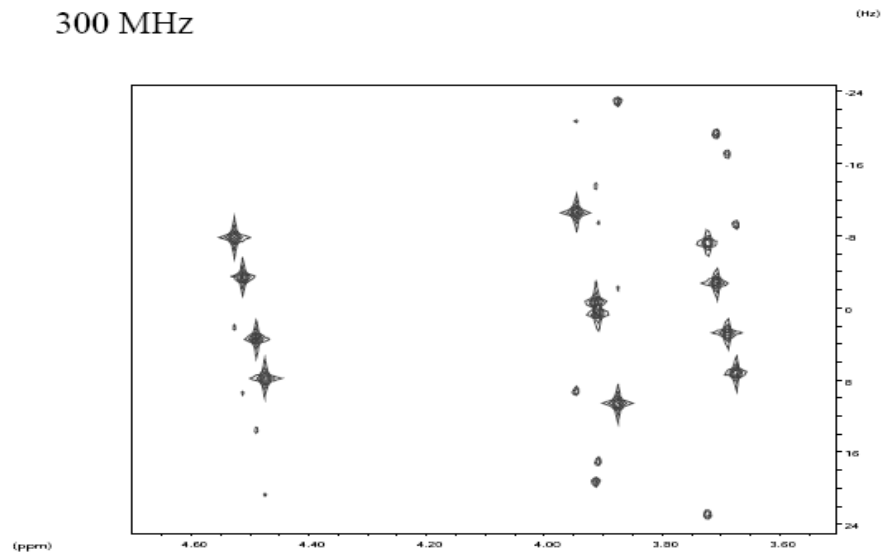
Experiment Simulation (NmrSim)



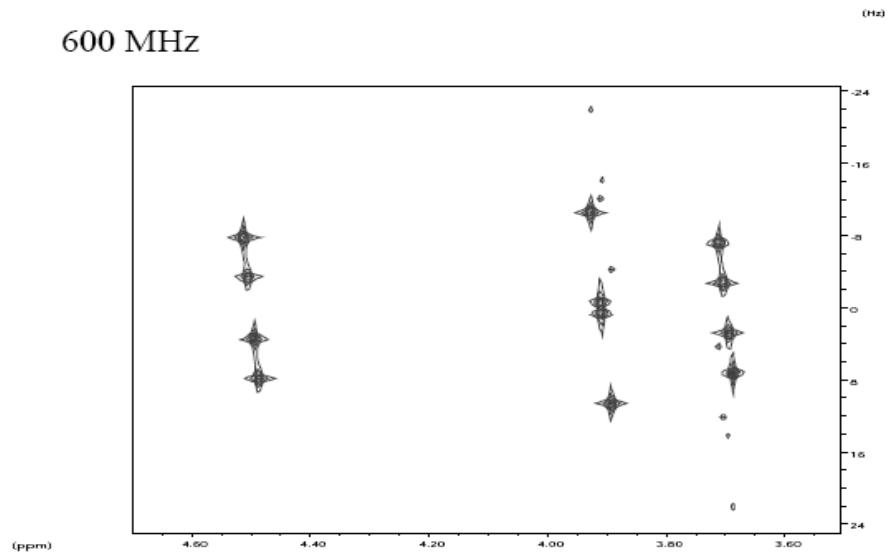
Comparison of J-resolved spectra on 300 MHz and 600 MHz shows the significant reduction of *strong coupling artifacts* for the higher resonance frequency



300 MHz



600 MHz



What is an AU (Automation) program?

A C program automatically interfaced to TopSpin

Purpose:

Extending TopSpin with user-defined functionalities, programmed in C

Example:

*Requests LB,
performs em,ft,pk
on the current
dataset*

```
double lb = 0.3;  
|  
GETCURDATA  
GETDOUBLE ("Enter LB: ", lb)  
STOREPAR ("LB", lb)  
EM  
FT  
PK  
QUIT
```

AU Programs



AU development tools delivered with TopSpin

AU Programs

File Options Help irce = C:\Bruker\TOPSPIN\exp\stan\nmr\au\src

Search in names [*?] Search

lcp90	lcprep	lcsetsup	lcshlrn	lcsino
lctshim	lcwetcalc	lcwetset	lczshim	ldshim
list_pp	listall_au	loadshimZ	lock_off	lock_on
loopadj	make2d	mkflist	mulabel	multana
multext	multi_decon	multi_integ	multi_integ2	multi_in
multi_zgvd	multi_zgvt	multicmd	multicom	multicyc
multiefp	multiexpt	multifp	multiftapk	multigo
multihalt	multimas	multimser	multipcom	multiwir
multixfb	multizg	nmr_save	noediff	noeflist
	_1d	p_1dapks	p_1dcor	
	_1dppti	p_2dnom	p_2dinv	
	_cpd135	p_intrng	p_noe	
	_paropt	parray	parray2	
parray3	parray4	pass2d	pecosy	phtran
plintfac	plot_3d	plot_sino	plot_to_file	plotx

Edit Compile Execute

**AU Browser
AU Library**

**GNU C Compiler
For Windows or Linux**

parbg (C:\Bruker\TOPSPIN\exp\stan\nmr\au\src)

File Edit Search

Compile Execute

```
124 storeregion(curexp, mprocno, offset1, npoints, ncdiff, filsiz, specbuf)
125 int curexp, mprocno, offset1, npoints, ncdiff, filsiz, *specbuf;
126 {
127 int ret, fd, regbuf[REGSIZ], reim, i1, i2;
128 char fnam[200], spec[5];
129 /****** read plot region in buffer ******/
130 for(reim=0; reim<=1; reim++)
131 {
132 (void)strcpy(spec, "1r");
133 if(reim==1) (void)strcpy(spec, "1i");
134 (void)sprintf(fnam, "%s/data/%s/nmr/%s/%d/pdata/%d/%s",
135 disk, user, name, expno, procno, spec); /* make source file name */
136
137 fd=open(fnam, 0); /* open source file for read */
138 if(fd==-1)
139 {
140 Proc_err(DEF_ERR_OPT, "File does not exist:\n%s", fnam);
141 return(-1);
142 }
143
144 lseek(fd, (long)(offset1*4), 0); /* position of plot region */
145 if(npoints > REGSIZ)
146
```

AU Editor

1 : 1

TopSpin supports: *Python programs automatically interfaced to TopSpin*

Purpose:

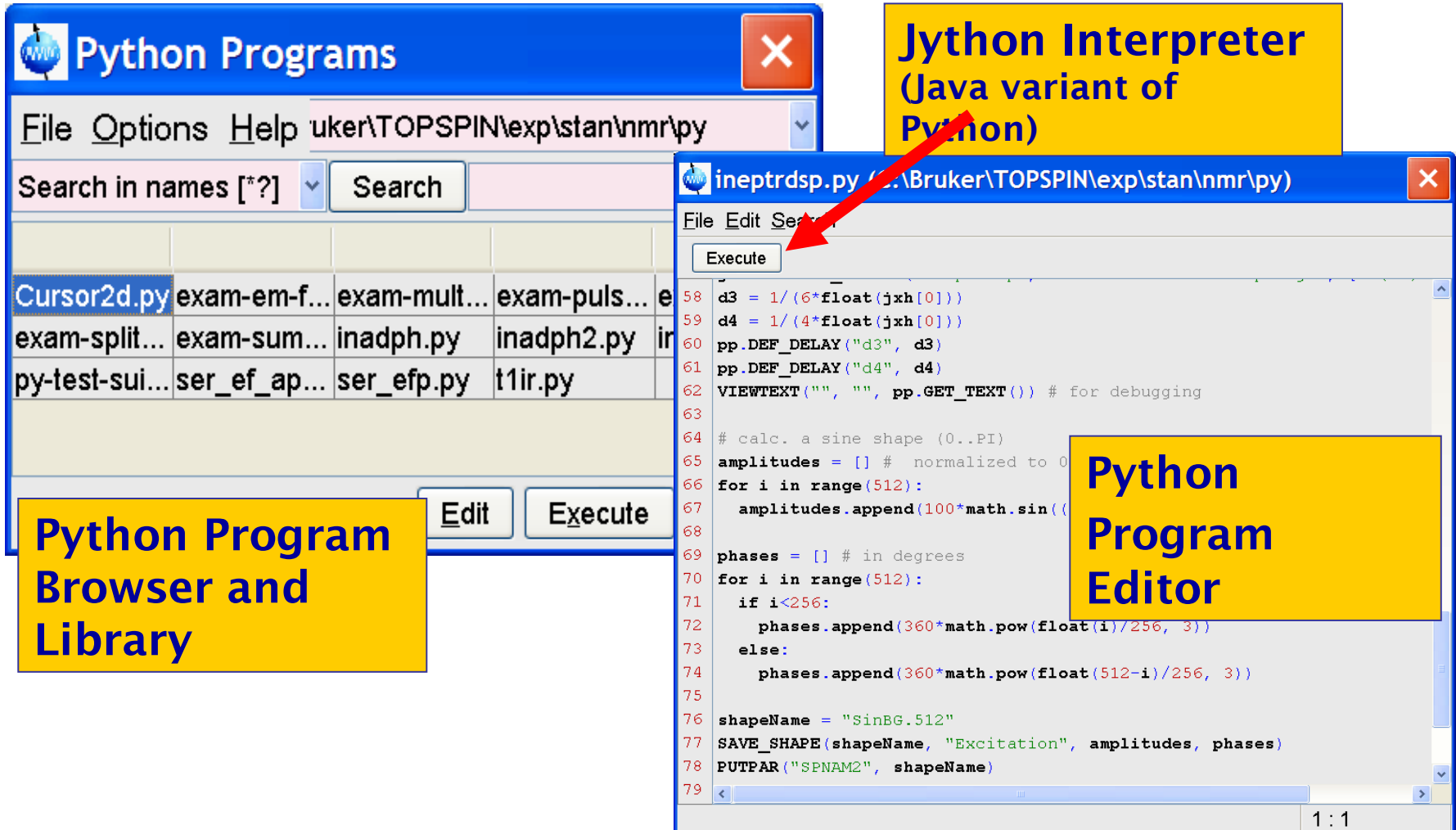
Extending TopSpin with user-defined functionalities, programmed in Python (“Jython”)

Example:

*Requests LB,
performs em,ft,pk
on the current
dataset*

```
lb = INPUT_DIALOG("", "", \
    ["Please enter LB: "], ["0.3"])
if lb == None:
    EXIT()
PUTPAR("LB", lb[0])
EM()
FT()
PK()
```

Python development tools delivered with TopSpin



The screenshot displays two windows from the TopSpin software. The left window, titled "Python Programs", is a file browser showing a directory of Python files. The right window, titled "ineptrdsp.py", is a code editor showing Python code for generating a sine wave shape. A red arrow points from the "Execute" button in the code editor to the "Execute" button in the file browser.

Python Programs

File Options Help uker\TOPSPIN\exp\stan\nmr\py

Search in names [*?] Search

Cursor2d.py	exam-em-f...	exam-mult...	exam-puls...	e
exam-split...	exam-sum...	inadph.py	inadph2.py	ir
py-test-sui...	ser_ef_ap...	ser_efp.py	t1ir.py	

Edit Execute

Python Program Browser and Library

Jython Interpreter (Java variant of Python)

Python Program Editor

```
58 d3 = 1/(6*float(jxh[0]))
59 d4 = 1/(4*float(jxh[0]))
60 pp.DEF_DELAY("d3", d3)
61 pp.DEF_DELAY("d4", d4)
62 VIEWTEXT("", "", pp.GET_TEXT()) # for debugging
63
64 # calc. a sine shape (0..PI)
65 amplitudes = [] # normalized to 0
66 for i in range(512):
67     amplitudes.append(100*math.sin((
68
69 phases = [] # in degrees
70 for i in range(512):
71     if i<256:
72         phases.append(360*math.pow(float(i)/256, 3))
73     else:
74         phases.append(360*math.pow(float(512-i)/256, 3))
75
76 shapeName = "SinBG.512"
77 SAVE_SHAPE(shapeName, "Excitation", amplitudes, phases)
78 PUTPAR("SPNAM2", shapeName)
79
```

Execute

1:1

What is a Macro?

A sequence of TopSpin commands

Purpose:

Extending TopSpin with user-defined functionalities, built from existing commands

Example:

*Sets LB,
performs em,ft,pk
on the current
dataset*

```
LB 0.3  
em  
ft  
pk
```

What is a Python Pulse Program?

A Python program acting as a Pulse Program

Purpose:

Computing pulse program parameters such as delays, shapes, phases using Python statements for the contained pulse program

Example:

*Computes phase list **ph1** using Python and starts acquisition*

```
PPTEXT = """
1 ze
2 d1
   p1 ph1
   go=2 ph31
exit
ph31=0 2 2 0 1 3 3 1
"""

pulsprog=DEF_PULSPROG (PPTEXT)
ph1 = [0,0,4,4]*2 + [2,2,6,6]*2
phlinc = 360/4
for i in range(16):
    ph1[i] = float(ph1[i])*phlinc
pulsprog.DEF_PHASE_LIST(1, ph1, phlinc)
PUTPAR ("PULPROG", "bgzg")
pulsprog.SAVE_AS ("bgzg")
ZG ()
```

What is a command panel?

A panel containing user-defined buttons to execute commands, AU programs, macros, etc.

Purpose:

Defining application specific user interfaces

Examples:

```
BLUE1=51$ 204$ 255
YELLOW1=255$ 255$ 0
GREEN1=84$ 196$ 20
# Title definition
TITLE=1D Processing Panel
TITLE_COLOR=0$ 0$ 255
# Toggle button definition
TOGGLE_BUTTON=To 2D
TOGGLE_CMD=bpan bproc2d
TOGGLE_TIP=Switch to 2D processing
# Top row button definition
TOP_BUTTONS=EM$ $FT$ $PK$ $
TOP_COLORS=YELLOW1$ YELLOW1$ YELLOW1
TOP_CMDS=em$ ft$ pk
TOP_TIPS=Exponential multiplication $\\
Fourier transform$\\
Phase correction
```

script *result*

