



## Topspin Setup Acquisition: Bio-NMR

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TopSpin

# Setup the Acquisition: Flowchart



## TopSpin Acquisition setup

### Data set:

where to define parameters and store spectra

### Sample:

temperature, insert, eject, lock, rotate, shim

### Standard Parameter sets:

probe independent parameters

### Probe dependent parameters:

pulses and power levels

### Customize parameters:

spectral windows, number of scans,...

### Optimize parameters:

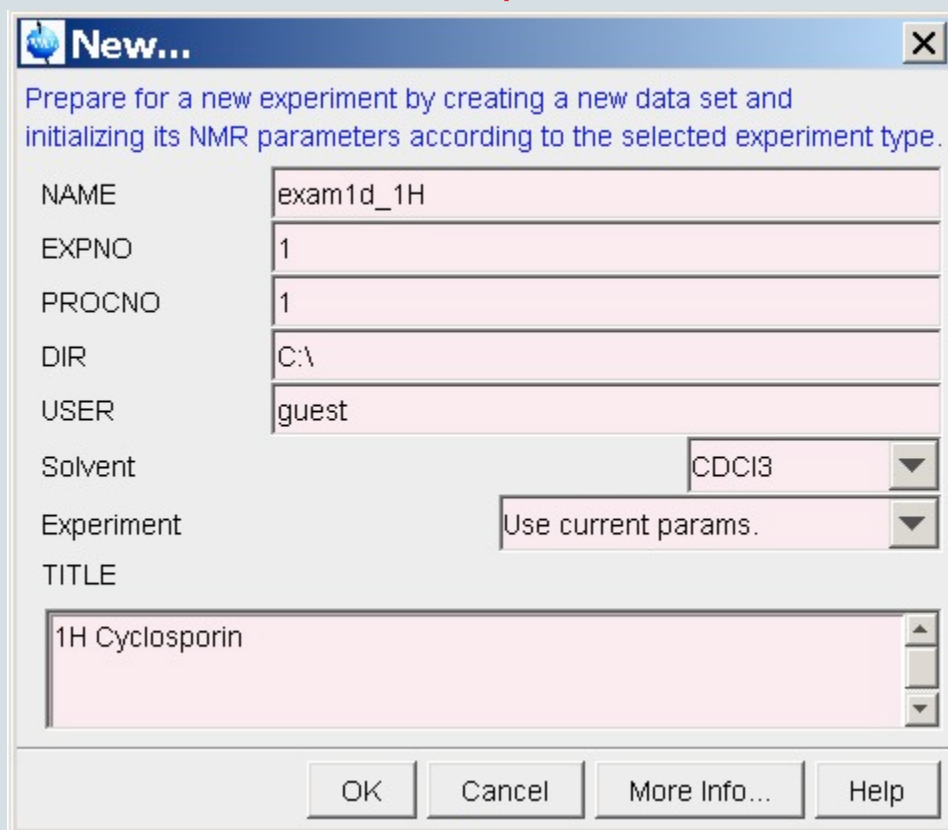
offsets, power levels, receiver gain

### Acquisition:

start and stop

## TopSpin Data set commands

Data set: where to define parameters and store spectra  
**new, edc**



**New...**

Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type.

NAME	exam1d_1H
EXPNO	1
PROCNO	1
DIR	C:\
USER	guest
Solvent	CDCl3
Experiment	Use current params.
TITLE	1H Cyclosporin

OK Cancel More Info... Help

Raw data (FID) is stored under:

C:\data\guest\nmr\exam1d\_1H\1

↓ ↓ ↓  
**USER NAME/PROJECT EXPNO**

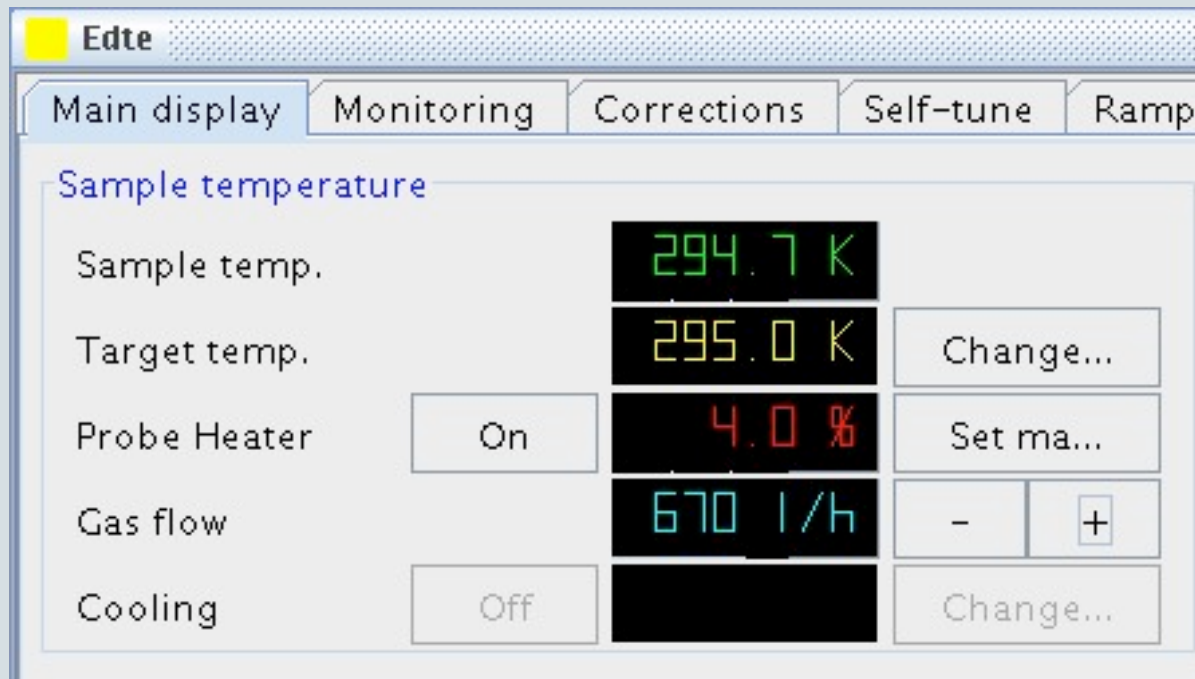
Processed data stored under:

C:\data\..\exam1d\_1H\1\pdata\1

↓  
**PROCNO**

## TopSpin Sample

Sample: temperature, insert, eject, lock, rotate, shim  
**edte (te and treset)**



Edte			
Main display   Monitoring   Corrections   Self-tune   Ramp			
Sample temperature			
Sample temp.		294.7 K	
Target temp.		295.0 K	Change...
Probe Heater	On	4.0 %	Set ma...
Gas flow		670 l/h	-   +
Cooling	Off		Change...

Note for CryoProbe:

- Temperature range: 0° – 50° C (temperature has to be calibrated!)
- Gas flow: 670 l/h

## TopSpin Sample

Sample: temperature, insert, eject, lock, rotate, shim  
**bsmsdisp:** for all functions  
**ej, ij:** eject, insert sample  
**ro:** start, stop rotation  
**lock:** lock  
**lock -noauto:** lock on solvent with multiple solvent signals (MeOD)

## TopSpin Sample

Sample: temperature, insert, eject, lock, rotate, shim  
**lock:** for all functions



A dialog box titled "Solvents table" with a close button (X) in the top right corner. It contains a table with two columns: "Solvent" and "Description". The table lists various solvents and their corresponding descriptions. The row for "H2O+D2O" is highlighted in red, with the description "90%H2O and 10%D2O" also in red. At the bottom right of the dialog box are "OK" and "Cancel" buttons.

Δ Solvent	Description
Acetic	acetic acid-d4
Acetone	acetone-d6
C6D6	benzene-d6
CD2Cl2	methylenechloride-d2
CD3CN	acetonitrile-d3
CDCl3	chloroform-d
CH3CN+D2O	HPLC Solvent (Acetonitril/D2O)
CH3OH+D2O	HPLC Solvent (Methanol/D2O)
D2O	deuteriumoxide
DEE	diethylether-d10
Dioxane	dioxane-d8
DME	dimethylether-d6
DMF	dimethylformamide-d7
DMSO	dimethylsulfoxide-d6
EtOD	ethanol-d6
<b>H2O+D2O</b>	<b>90%H2O and 10%D2O</b>
MeOD	methanol-d4
Pyr	pyridine-d5
THF	tetrahydrofurane-d8
Tol	toluene-d8



## TopSpin Sample

Sample: temperature, insert, eject, lock, rotate,

shim

**topshim:** latest gradient shimming tool  
**gradshim:** alternative gradient shimming tool





## TopSpin Experiment definitions

Standard Parameter sets: probe independent parameters

Probe dependent parameters: pulses and power levels



## TopSpin Standard Parameter files

Standard Parameter sets: probe independent parameters

*rpar* (example: *rpar HNCOGP3D all*)

Standard parameter files contain:

Default parameters for an experiment: pulse program, number of scans, spectra windows, time domain data points, window functions for processing etc.

Standard parameter files do **NOT** contain:

Parameters for pulses and power levels

## TopSpin Standard Parameter files

How do I interpret the meaning of the parameter file name?:  
*example: rpar HNCOGP3D all*

### edpul Pulprog.info

;Pulprog.info

;The two-character codes used are the following:

ar	experiment for aromatic residues
at	adiabatic TOCSY
bi	with bird pulse for homonuclear J-decoupling
bp	using bipolar gradients
cc	cross correlation experiment
cp	with composite pulse
ct	constant time
cw	decoupling using cw command
cx	using CLEANEX_PM
dc	decoupling using cpd

.....

## TopSpin Probe dependent parameters

Probe dependent parameters: pulses and power levels  
`getprosol`

`getprosol`: load default pulses and power levels according to the current **probe** and **solvent**

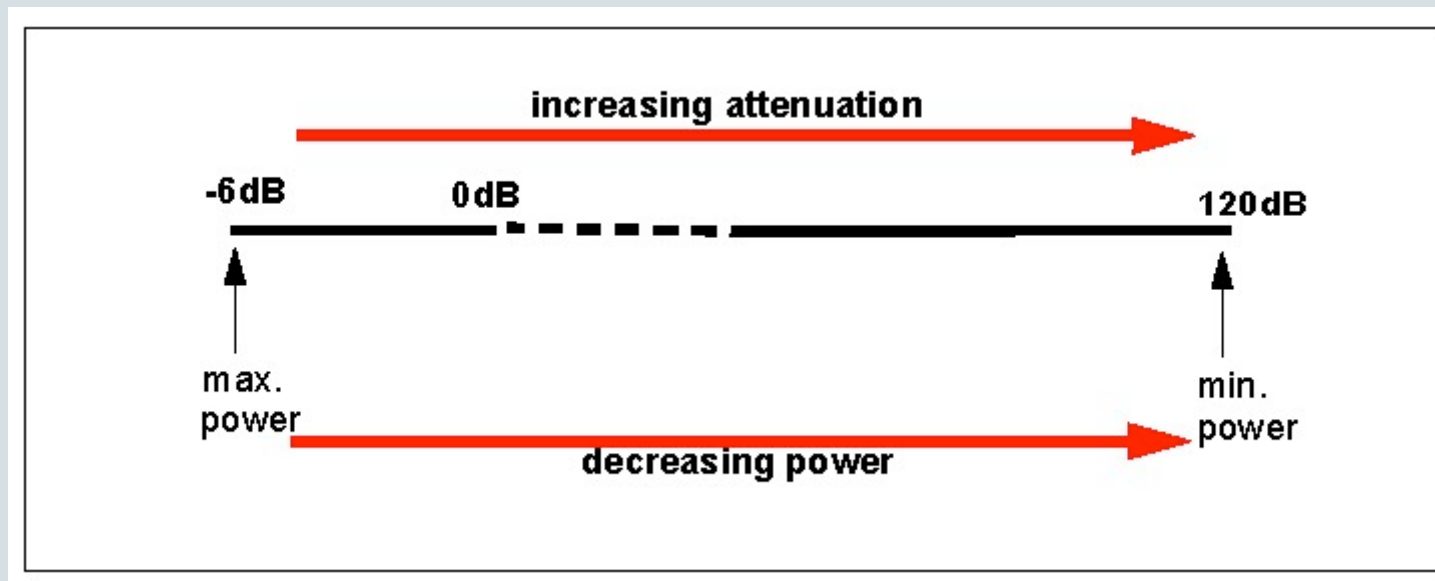
When a pulse does not correspond to the default value, all power levels for pulses of that nucleus can be recalculated for the current data set:

EXAMPLE!: `getprosol 1H 10.5us -2.3db`

for a 1H pulse of 10.5 usec at -2.3 dB

## TopSpin Power level definitions

Power levels are defined as attenuation values in dB:



## TopSpin Customizing parameters

Customize parameters: spectral windows, number of scans, ..

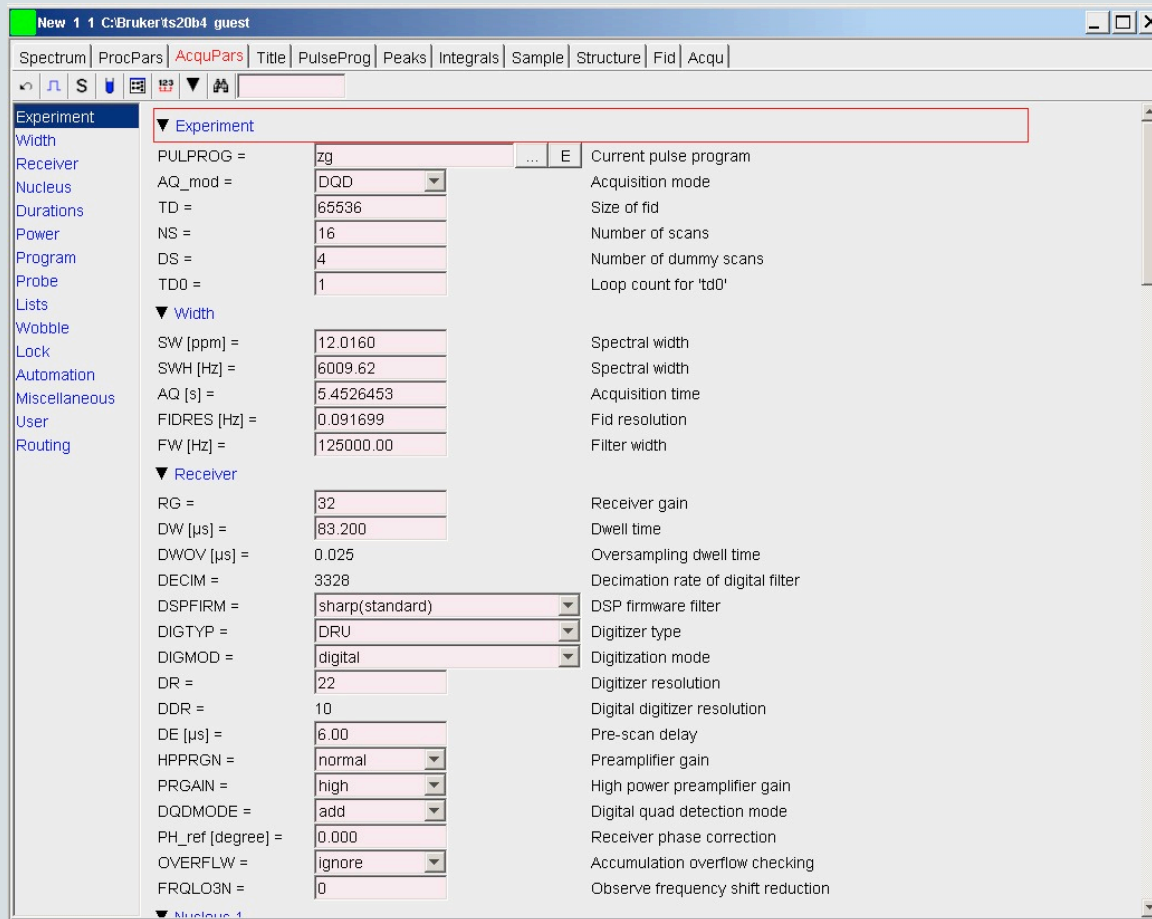
Acquisition:

**eda:** show all parameters

**ased:** show parameters related to current pulse program

# TopSpin Customizing parameters

eda: show all parameters



The screenshot shows the 'AcquPars' window in the Bruker TopSpin software. The window title is 'New 1 1 C:\Bruker\ts20b4 guest'. The interface includes a menu bar with options like 'Spectrum', 'ProcPars', 'AcquPars', 'Title', 'PulseProg', 'Peaks', 'Integrals', 'Sample', 'Structure', 'Fid', and 'Acqu'. A left-hand navigation pane lists categories such as 'Experiment', 'Width', 'Receiver', 'Nucleus', 'Durations', 'Power', 'Program', 'Probe', 'Lists', 'Wobble', 'Lock', 'Automation', 'Miscellaneous', 'User', and 'Routing'. The main area displays a list of parameters with their current values and descriptions:

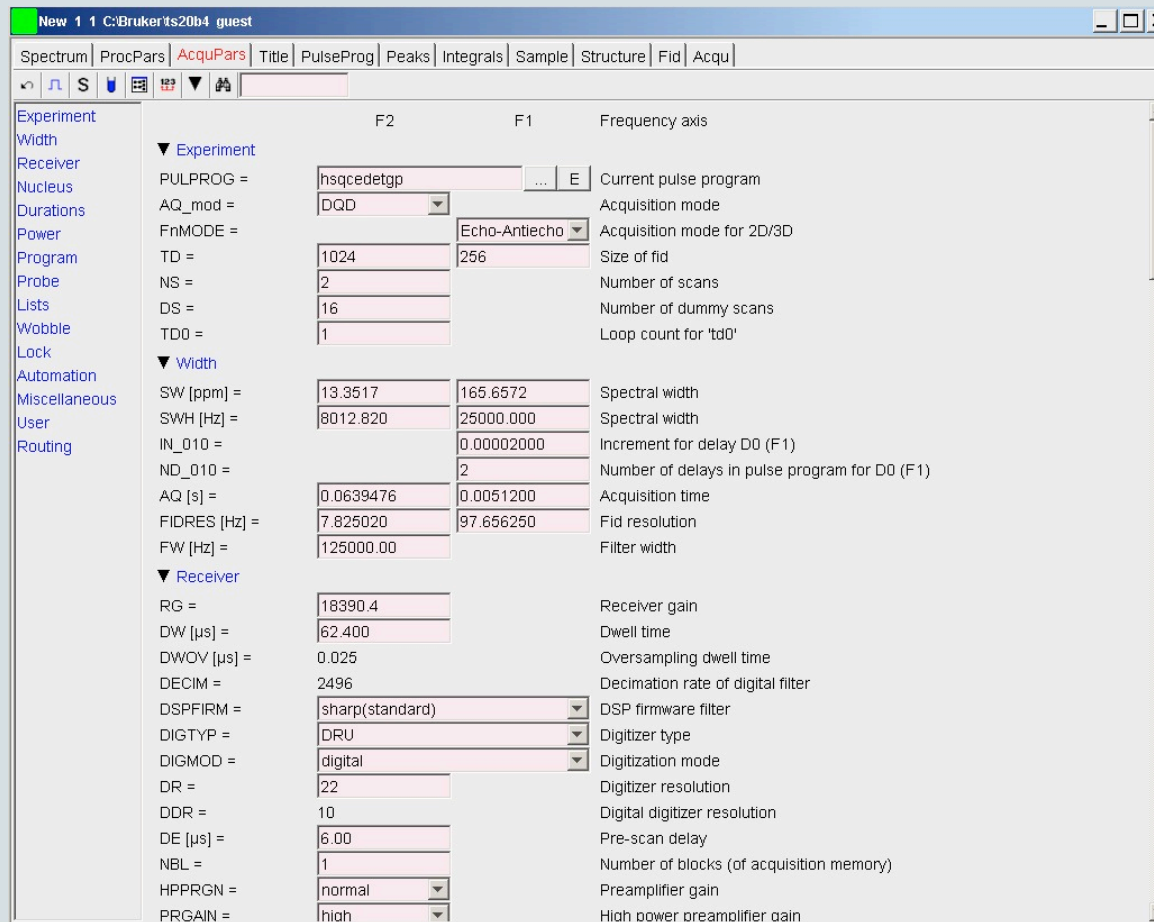
Parameter	Value	Description
PULPROG	zg	Current pulse program
AQ_mod	DQD	Acquisition mode
TD	65536	Size of fid
NS	16	Number of scans
DS	4	Number of dummy scans
TD0	1	Loop count for 'td0'
<b>Width</b>		
SW [ppm]	12.0160	Spectral width
SWH [Hz]	6009.62	Spectral width
AQ [s]	5.4526453	Acquisition time
FIDRES [Hz]	0.091699	Fid resolution
FW [Hz]	125000.00	Filter width
<b>Receiver</b>		
RG	32	Receiver gain
DW [μs]	83.200	Dwell time
DWOV [μs]	0.025	Oversampling dwell time
DECIM	3328	Decimation rate of digital filter
DSPFIRM	sharp(standard)	DSP firmware filter
DIGTYP	DRU	Digitizer type
DIGMOD	digital	Digitization mode
DR	22	Digitizer resolution
DDR	10	Digital digitizer resolution
DE [μs]	6.00	Pre-scan delay
HPPRGN	normal	Preamplifier gain
PRGAIN	high	High power preamplifier gain
DQDMODE	add	Digital quad detection mode
PH_ref [degree]	0.000	Receiver phase correction
OVERFLW	ignore	Accumulation overflow checking
FRQLO3N	0	Observe frequency shift reduction

1D-experiments

# TopSpin Customizing parameters

eda: show all parameters

2D-experiments

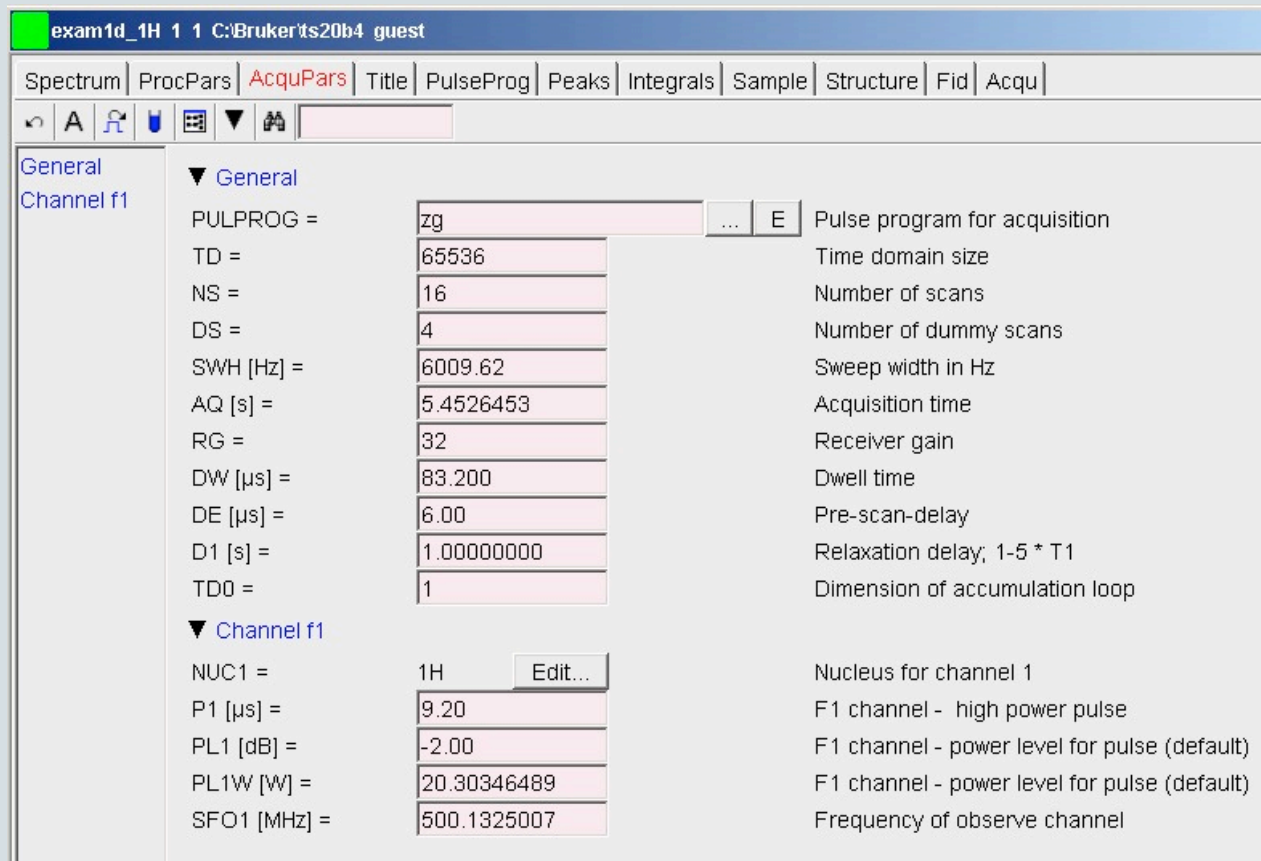


Parameter	F2	F1	Description
PULPROG	hsqcedetgp		Current pulse program
AQ_mod	DQD		Acquisition mode
FnMODE	Echo-Antiecho		Acquisition mode for 2D/3D
TD	1024	256	Size of fid
NS	2		Number of scans
DS	16		Number of dummy scans
TD0	1		Loop count for 'td0'
▼ Width			
SW [ppm]	13.3517	165.6572	Spectral width
SWH [Hz]	8012.820	25000.000	Spectral width
IN_010	0.00002000		Increment for delay D0 (F1)
ND_010	2		Number of delays in pulse program for D0 (F1)
AQ [s]	0.0639476	0.0051200	Acquisition time
FIDRES [Hz]	7.825020	97.656250	Fid resolution
FW [Hz]	125000.00		Filter width
▼ Receiver			
RG	18390.4		Receiver gain
DW [μs]	62.400		Dwell time
DW0V [μs]	0.025		Oversampling dwell time
DECIM	2496		Decimation rate of digital filter
DSPFIRM	sharp(standard)		DSP firmware filter
DIGTYP	DRU		Digitizer type
DIGMOD	digital		Digitization mode
DR	22		Digitizer resolution
DDR	10		Digital digitizer resolution
DE [μs]	6.00		Pre-scan delay
NBL	1		Number of blocks (of acquisition memory)
HPPRGN	normal		Preamplifier gain
PRGAIN	high		High power preamplifier gain



# TopSpin Customizing parameters

**used:** show parameters related to current pulse program



The screenshot shows the TopSpin software interface with the 'AcquPars' tab selected. The window title is 'exam1d\_1H 1 1 C:Bruker\ts20b4 guest'. The interface includes a menu bar (Spectrum, ProcPars, AcquPars, Title, PulseProg, Peaks, Integrals, Sample, Structure, Fid, Acqu) and a toolbar. The main area is divided into 'General' and 'Channel f1' sections.

Parameter	Value	Description
<b>General</b>		
PULPROG =	zg	Pulse program for acquisition
TD =	65536	Time domain size
NS =	16	Number of scans
DS =	4	Number of dummy scans
SWH [Hz] =	6009.62	Sweep width in Hz
AQ [s] =	5.4526453	Acquisition time
RG =	32	Receiver gain
DW [μs] =	83.200	Dwell time
DE [μs] =	6.00	Pre-scan-delay
D1 [s] =	1.00000000	Relaxation delay; 1-5 * T1
TD0 =	1	Dimension of accumulation loop
<b>Channel f1</b>		
NUC1 =	1H	Nucleus for channel 1
P1 [μs] =	9.20	F1 channel - high power pulse
PL1 [dB] =	-2.00	F1 channel - power level for pulse (default)
PL1W [W] =	20.30346489	F1 channel - power level for pulse (default)
SFO1 [MHz] =	500.1325007	Frequency of observe channel

## TopSpin Customizing parameters

### Tuning and Matching of the probe:

**wobb:** manual mode, no Automatic Tuning and Matching accessory  
(VU: w1, w2, w3 or wobb f1, wobb f2, ...)

**atma:** fully automated tuning and matching, all active channels

**atmm:** manual mode of atma

## TopSpin Customizing parameters

Typical parameters which are customized:

**ns:** number of scans  
**ds:** number of dummy scans  
**td:** time domain data points  
**sw:** spectral window [ppm]  
**swh:** spectral window [Hz]  
**o1p:** transmitter offset [ppm]  
**o1:** transmitter offset [Hz]  
**o2p:** decoupler offset [ppm]  
**rg:** receiver gain

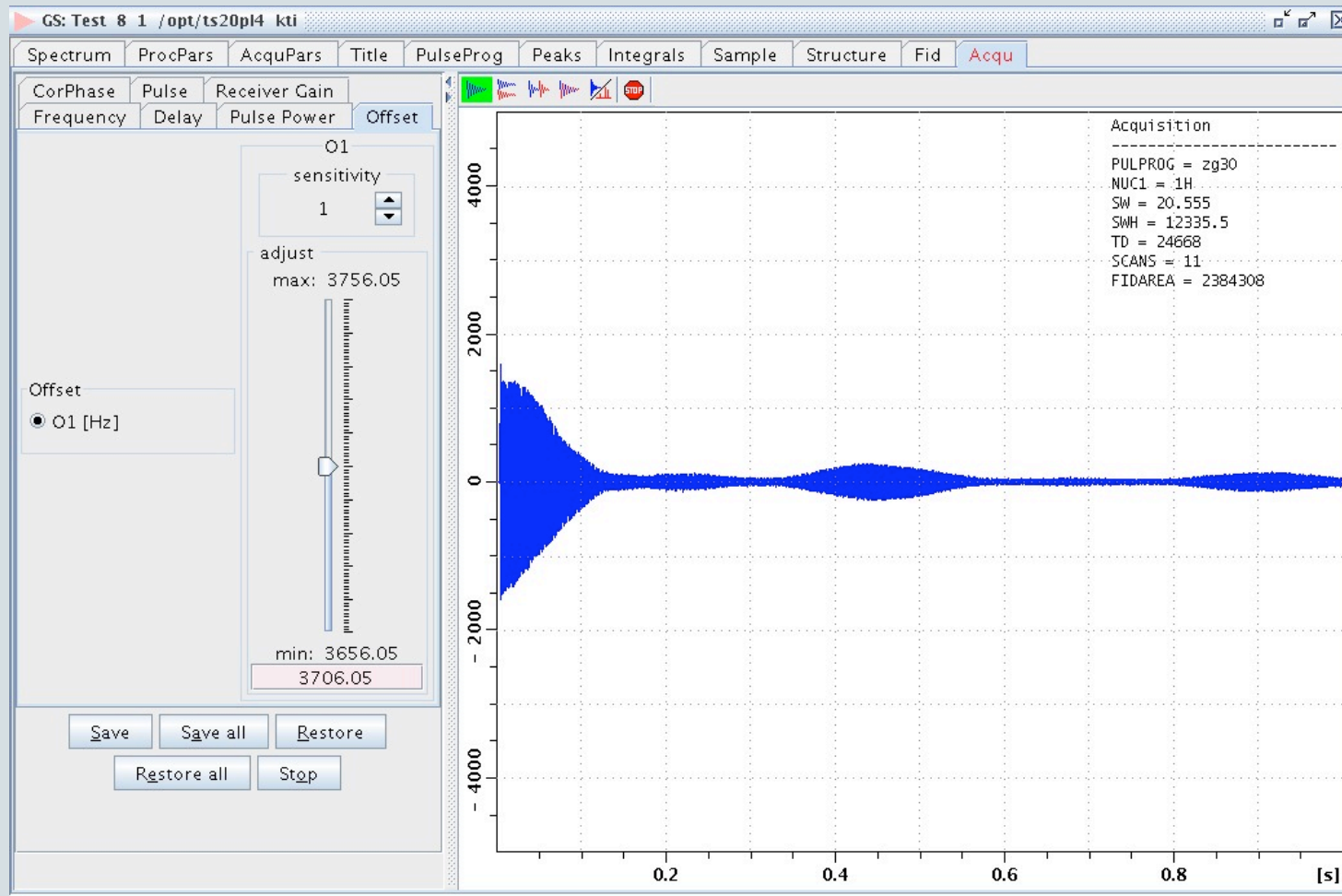


## TopSpin Optimize parameters

Parameters, which need fine tuning (transmitter offset for presaturation, power level for shaped flip-back pulses) can be optimized in the go-setup mode **gs**.

# TopSpin Optimize parameters

go-setup mode **gs**



## TopSpin Acquisition Start and Stop

### Acquisition: start and stop

#### Preparing start of acquisition:

**expt** calculate experiment time  
**rga** automatic receiver gain adjustment

#### Start acquisition:

**zg** start and overwrite existing FID  
**go** start and add to current FID (for 1D)

#### Stop acquisition:

**stop** stop immediately. For 1D, FID is lost!  
**halt** stop after current scan, FID will be saved

#### Transfer 1D-FID to disk:

**tr** required for 1D only



## TopSpin Flowchart commands for acquisition

Data set:	new, edc
Sample:	edte, lock, bsmsdisp, topshim, gradshim
Standard Parameter sets:	rpar
Probe dependent parameters:	getprosol
Customize parameters:	ased, eda
Optimize parameters:	wobb, atma, rg, rga, gs
Acquisition:	expt, zg, stop, halt, tr



## TopSpin Flowchart commands for acquisition

Data set:	new, edc
Sample:	edte, lock, bsmsdisp, topshim, gradshim
Standard Parameter sets:	<b>rpar</b>
Probe dependent parameters:	getprosol
Customize parameters:	eda, ased
Optimize parameters:	wobb, atma, rg, rga, gs
Acquisition:	expt, zg, stop, halt, tr



# Selected list of parameter sets

**CBCACONHGPWG3D**

**CBCACONHGP3D**

**CCANHGP3D**

**CCACONHGP3D.2**

**CCACONHGP3D**

**CBCANHGPWG3D**

**CBCANHGP3D**

**CCCONHGP3D3**

**CCCONHGP3D2**

**CCCONHGP3D1**

**CCCONHGP3D**

**CCANHGP3D.2**

**CCCONHGPWG3D3**

**CCCONHGPWG3D2**

**DIPSIHSQCF3GPSI3D**

**HCACOGPJC3D**

**HCACOGP3D**

**HBHANHGPWG3D**

**HBHANHGP3D**

**HBHACONHGPWG3D**

**HBHACONHGP3D**

**HACAHCOSYGP3D**

**HCCCONHGPWG3D3**

**HCCCONHGPWG3D2**

**HCCCONHGP3D3**

**HCCCONHGP3D2**

**HCCCONHGP3D1**

**HCANNHGP3D**

**HCAHCOSYGP3D**

**HCCHECOSGP3D**

**HCCHDIGP3D2**

**HCCHDIGP3D** *HCCH-TOCSY*

**HCCHCOSYGP3D**

**HCCHCOGP3D**

**HNCACBGPJC3D**

**HNCACBGP3D**

**HNCACOSYGP3D**

**HNCACOGPWG3D**

**HNCACOGP3D**

**HNCACBGPWG3D**

**HNCAH3D**

**HNCAGPWG3D** *watergate*

**HNCAGP3D**

**HNCAECOSGP3D2**

**HNCAECOSGP3D**

**HNCADQZQGP3D**

**HNCOCACGP3D**

**HNCOCACBGPWG3D**

**HNCOCACBGP3D**

**HNCOCACAGP3D**

**HNCAJCGP3D**

**HNCAHAGP3D**

**HNCOECOSGP3D**

**HNCOCOGP3D**

**HNCOCGP3D**

**HNCOCAGPWG3D**

**HNCOCAGP3D**

**HNHBECOSGP3D**

**HNHAGP3D**

**HNCOGPWG3D**

**HNCOGPHB3D2**

**HNCOGPHB3D**

**HNCOGP3D**

**HNNHDIGP3D**

**HNHBGP3D**

**MLEVHSQCETGP3D**

**MLEVHSQCETF3GP3D**

**NA = Nucleic Acid**

**NA\_HCCHFWDIECGP3D**

**NA\_HCCHECGP3D**

**NA\_GHCCHFWDIGP3D**

**NA\_HCPDIETGPSI3D**

**NA\_HCNETGPSISP3D**

**NA\_HCNETGPSI3D**

**NA\_HCCNHDIGPWG3D**

**NA\_HCCHFWDIGP3D**

**NA\_HCPETGPSI3D**

**NOESYHSQCF3GP193D**

**NOESYHSQCETGP3D**

**NOESYHSQCETF3GP3D**

**NOESYHSQCGPSM3D**

**NOESYHSQCGPSISM3D**

**NOESYHSQCFPF3GPSI3D**

**NOESYHSQCF3GPSI3D**

**TR = TROSY**

**TRHNCACOGP3D**

**TRHNCACBGP3D**

**TRCBCANHGP3D**

**TRCBCACONHGP3D**

**TRHNCAGP3D2.2**

**TRHNCAGP3D.2**

**TRHNCAGP3D2** *latest version*

**TRHNCAGP3D**

**TRHNCOGP3D**

**TRHNCOCAGP3D**

**CCACONHGP2H3D**

**CCCONHGP2H3D**

**CCANHGP2H3D**

**HNCACOGP2H3D**

**HNCACBGP2H3D**

**HNCACOGP2H3D.2**

**HNCAGP2H3D** *<sup>2</sup>H-decoupled*

**HNCOCAGP2H3D**

**HNCOCACBGP2H3D**

**HNCOGP2H3D**

**TRHNCACBGP2H3D**

**TRHNCAGP2H3D2**

**TRHNCAGP2H3D**

**TRHNCACOGP2H3D**

**TRHNCOGP2H3D**

**TRHNCOCAGP2H3D**

**TRHNCOCACBGP3D**

**TRHNCOCACBGP2H3D**

## TopSpin Standard Parameter files

How do I interpret the meaning of the parameter file name?:  
*example: rpar HNCOGP3D all*

### edpul Pulprog.info

;Pulprog.info

;The two-character codes used are the following:

ar	experiment for aromatic residues
at	adiabatic TOCSY
bi	with bird pulse for homonuclear J-decoupling
bp	using bipolar gradients
cc	cross correlation experiment
cp	with composite pulse
ct	constant time
cw	decoupling using cw command
cx	using CLEANEX_PM
dc	decoupling using cpd

.....

## Example: rpar HNCA\*

**HNCAGP3D**      gradient selected

**HNCAGPWG3D**    **watergate version**

**HNCAGP2H3D**     $^2\text{H}$ -decoupled /  $^1\text{H}$ -suppression by  $180^\circ$ -pulses

**TRHNCAGP3D2**    **TROSY** /  $^1\text{H}$ -suppression by  $180^\circ$ -pulses

**TRHNCAETGP3D**    **TROSY** / echo-antiecho /  $^1\text{H}$ -suppression by  $180^\circ$ -pulses  
(JMR 144 (2000) 123)

**TRHNCAGP2H3D**    **TROSY** /  $^2\text{H}$ -decoupled / for 100% deuterated proteins

**TRHNCAGP2H3D2**    **TROSY** /  $^2\text{H}$ -decoupled / for partially deuterated proteins  
/  $^1\text{H}$ -suppression by  $180^\circ$ -pulses

## Other triple resonance parameter sets

**HNCOCAGP3D**  
**HNCOCAGPWGD**  
**HNCOCAGP2H3D**  
**TRHNCOCAGP3D**  
**TRHNCOCAGP2H3D**

**HNCOCACBGP3D** „transfer“  
**HNCOCACBGPWG3D**  
**HNCOCACBGP2H3D**  
**TRHNCOCACBGP3D**  
**TRHNCOCACBETGP3D** echo-antiecho  
**TRHNCOCACBGP2H3D** <sup>2</sup>H-decoupled

**HNCACBGP3D** „out&back“ / for larger proteins  
**HNCACBGPWG3D**  
**HNCACBIGPWG3D** intra-residue only  
**HNCACBGP2H3D**  
**TRHNCACBGP3D**  
**TRHNCACBIGP3D** intra-residue only  
**TRHNCACBGP2H3D**

**HAHBCONHGP3D**  
**HAHBCONHGPWG3D**  
**TRHAHBCONHGP3D**

**HAHBNHGP3D**  
**HAHBNHGPWG3D**  
**TRHAHBNHGP3D**

**HNCOGP3D**  
**HNCOGPWG3D** watergate  
**TRHNCOGP3D** TROSY

**HNCACOGP3D**  
**HNCACOGPWGD**  
**HNCACOGP2H3D** <sup>2</sup>H-decoupled  
**TRHNCACOGP3D**  
**TRHNCACOGP2H3D**

**CBCACONHGP3D** „transfer“ / for smaller proteins  
**CBCACONHGPWG3D**  
**TRBCACONHGP3D**

**CBCANHGP3D** „transfer“ / for smaller proteins  
**CBCANHGPWG3D**  
**TRBCANHGP3D**  
**TRBCANHETGP3D**  
**SEQTRBCANHGP3D** sequential TROSY

**HCCCONHGP3D2** H(CCCO)NH  
**HCCCONHGPWG3D2**

**HCCCONHGP3D3** (H)CC(CO)NH  
**HCCCONHGPWG3D3**  
**CCCONHGP2H3D** <sup>13</sup>C-start

## Other useful parameter sets

### <sup>13</sup>C-correlated experiments

HCCHDIGP3D

HCCH-TOCSY

HCCHDIGP3D2

(H)CCH-TOCSY

HCCHCOGP3D

HCCH-COSY

NOESYHSQCETGP3D

3D-NOESY-HSQC

### <sup>15</sup>N-correlated experiments

NOESYHSQCF3GPSI3D

15N-NOESY-HSQC sensitivity enhanced

NOESYHSQCF3GP193D

15N-NOESY-HSQC with 3919 watergate

NOESYTZGP3D

15N-NOESY-ZQ-TROSY for large proteins

## Other useful parameter sets

### 2D Homonuclear-correlated experiments

<b>NOESYPHPR</b>	<b>NOESY, phase sensitive, presat</b>
<b>NOESYGPPH19SW</b>	<b>NOESY, phase sensitive, 3919 WATERGATE</b>
<b>MLEVPHPR</b>	<b>TOCSY, phase sensitive, presat</b>
<b>MLEVGPPH19SW</b>	<b>TOCSY, phase sensitive, 3919 WATERGATE</b>
<b>DIPSI2GPPH19</b>	<b>TOCSY, phase sensitive, 3919 WATERGATE, DIPSY2 spin lock</b>

### Where is the parameter file for a NOESY with Excitation Sculpting?

Not all versions of an experiment are covered by parameter files

Start from a related experiment and:

- change the pulse program: **pulprog noesyegpph** instead **noesyphpr**
- check corresponding parameters with **ased**

## Other useful parameter sets

### 2D Heteronuclear-correlated experiments

<b>13C:</b>	<b>HSQCETGP</b>	<b>HSQC, echo-antiecho</b>
	<b>HSQCETGPSISP</b>	<b>HSQC, echo-antiecho, sensitivity improved, adiabatic <sup>13</sup>C inversion</b>
	<b>HSQCETGPSISP.2</b>	<b>HSQC, echo-antiecho, sensitivity improved, adiabatic <sup>13</sup>C inversion and refocussing</b>
<b>15N;</b>	<b>HSQCETF3GP</b>	<b>HSQC, echo-antiecho</b>
	<b>HSQCETF3GPSI</b>	<b>HSQC, echo-antiecho, sensitivity improved</b>

## Quick Guide

### Let's run a 3D CBCACONH with WATERGATE

**edc**  
**rpar CBCACONHGPGW3D all**  
**lock**  
**atma f1**  
**topshim**  
**pulsecal**  
**getprosol 1H x us y db**

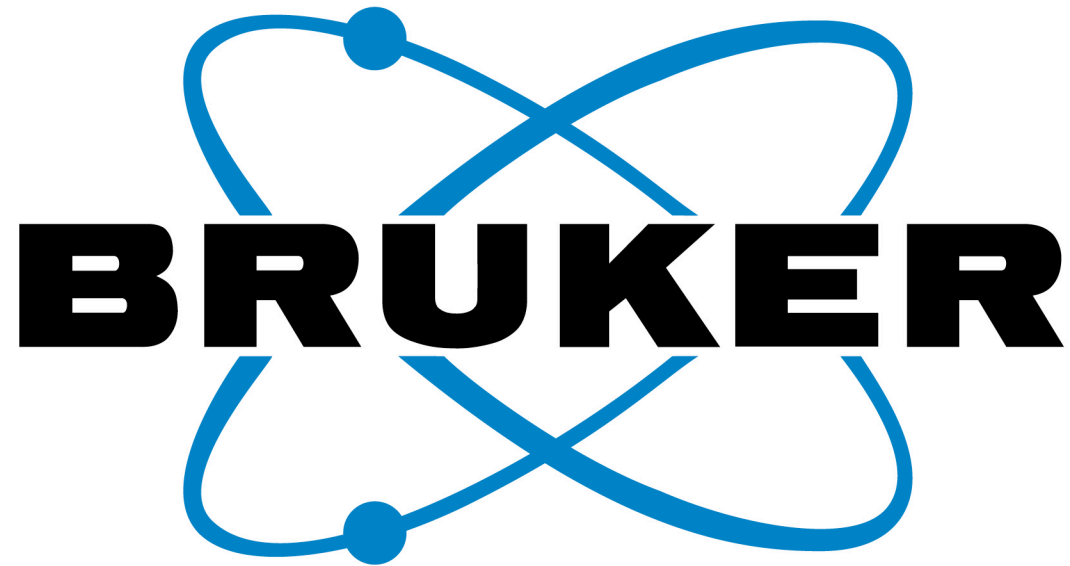
**ased**  
**eda**

**rg**  
**expt**  
**zg**

new data set  
read parameter file  
lock on solvent  
tune and match 1H channel automatically  
gradient shimming  
determine 1H pulse automatically  
set all pulses, recalculate all 1H pulses

all pulse parameters and delay correct?  
check NS, spectral windows and number of increments  
typically = 200  
check total experiment time  
start the acquisition





[www.bruker-biospin.com](http://www.bruker-biospin.com)