NMR Data Acquisition and Processing Procedure

Dr. Jianfeng Zhu (Research Officer)

Please **DO NOT** remove from NMR lab!

Things to Avoid when Using NMR Lab

Here's a list of stuff that I have seen that you *should not* do:

- 1. Do not bring a magnetic substance near to the magnet ... after all it's a *magnet* and a very powerful one at that. Screwdrivers and wrenches are death tools around an NMR magnet ... keep them away!
- 2. Do not put little tape 'flags' with the name of your sample on your NMR tube. If the flag is left on the tube it will stick inside the magnet for sure (Murphy's Law).
- 3. Do not put your sample into a depth gauge and then try to put the whole thing, gauge and all, into the magnet.
- 4. Do not put the spinner on *upside down* and then put sample and spinner into the magnet. There *will* be problems.
- 5. Do not make the mistake of thinking that just because a sample in the autosampler carousel is past the sample injection point that it has already run. The *only* way to know if it has run is to look at the ICONNMR display.
- 6. Do **not** pull on the autosampler carousel in order to rotate it and retrieve your sample!!! Ever.
- 7. If you must take un-run samples out, PLEASE also cancel the samples in ICONNMR.
- 8. Do not be helpful and clean the NMR tube depth gauge with acetone. The gauge is plastic and will dissolve in acetone.
- 9. Do not be helpful and try to fix a broken depth gauge ... there are tiny springs in the stop mechanism that will fly out if you try to take it apart, never to be found again.
- 10. Do not put the sample into the magnet unless the lift air is turned on. Again, you risk damaging the probe if you simply drop the sample into the magnet.
- 11.Do not force the tuning/matching rods to turn further than their maximum or minimum positions ... this will cause serious internal damage to the probe and render it immediately useless until repaired.
- 12.Do not overreach when inserting or removing a sample ... you might lose your balance and injure yourself or you might break an NMR tube with sample in it.
- 13.Do not forget to shut off the lift air after you are finished with the machine.
- 14.Do not put a sample into the magnet and begin to take data when we are filling the magnets with cryogens.
- 15. *YOU* are responsible for the shimming. If you cannot shim your sample try starting from scratch by reading in the standard shim file (type 'rsh' and select 'currentshim') *before* complaining to the laboratory manager. If you still cannot shim the sample satisfactorily then contact one of the NMR facility staff.

Procedures	Commands	Notes
1. Insert sample.	<i>ej</i> → load sample → <i>ij</i>	<pre>sx # (load sample using auto-sampler).</pre>
2. Create new data set.	new or edc	
3. Read in standard parameter set.	rpar → choose	
4. Read in pulses and powers.	getprosol	gpro (Macro to shorten the command).
5. Check temperature setting.	edte \rightarrow set	
6. Lock the solvent.	lock → choose	📑 (lock display window).
7. Tune the probe.	atma	
8. Shim the magnet.	topshim	Topshim gui (open Topshim interface). 罪
9. Check acquisition parameters.	ased	
10. Adjust receiver gain.	rga	
11. Start acquisition.	zg	tr (transfer/save data to workstation).
12. Processing the data.	efp → apk (\checkmark) → absn	<i>proc</i> (Macro combining the three commands).
13. Peak picking.	рр	1 (open peak picking Interactive Bar).
14. Peak integration.	int	「 (open integration Interactive Bar).
15. Plot the spectrum.	plot	

* Refer to succeeding contents for detailed information of each step.

Topspin3.2 Interface



Topspin2.1 Interface



2. Create New Data Set

Topspin3.2

le New	
Prepare for a new experiment by a initializing its NMR parameters acc For multi-receiver experiments se Please define the number of rece	creating a new data set and cording to the selected experiment type. veral datasets are created. ivers in the Options.
NAME	Oct02 (folder name)
EXPNO	1 (experiment number)
PROCNO	1 (process number)
• Use current parameters (us	e the same experiment setting)
© Experiment Open experiment	riment list (<i>rpar</i>)
Options	
Set solvent:	CDCI3 -
Execute "getprosol"	
Keep parameters:	P 1, O1, PLW 1 Change
DIR DIR for dat	a → C:\Bruker\TopSpin3.2\data\jiz258 ▼
Show new dataset in new	window
Receivers (1,2,16)	1
TITLE	
	OK Cancel More Info Help

Topspin2.1

🖉 New	×				
Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the box below.					
NAME	Nov03				
EXPNO	3				
PROCNO	1				
DIR	C:\Bruker\TOPSPIN2.1pl6 DIR for data				
USER	jiz258				
Solvent	CDCI3 🗸				
Experiment Dirs.	C:/Bruker/TOPSPIN2.1pl6/exp/stan/nmr/par/user				
Experiment	Use current params. 👻				
TITLE	Experiment list				
13C zgpg Sucrose Octa-Ac 1 Receivers (1,	etate in Bezene+CDCI3 (1 drop) 2,8)				
	<u>O</u> K <u>C</u> ancel More <u>I</u> nfo <u>H</u> elp				

3. Read in Standard Parameter Set

🍐 Parameter Sets: 1	rpar			×
<u>File</u> Options	Help		Source = C:\Bruker\Top	Spin3.2\exp\stan\nmr\par\user
Find file names	<pre>enter any string, *, ? Exclude:</pre>	Clear	Go to Bruke	r default ones here
Class = Any -	Dim = Any Show Recommended			
Type = Any 🔻	SubType = Any SubTypeB = Any	Reset Filters		
13C_t1_2d_dec	13C_t1_est_1d	1d 13C	1d_13C_UDEFT	1d_170
1d_1H	1d_1H_es	1d_1H_es_nmi	1d_1H_es_nmi60	1d_1H_PE_watergate
1d_APT	1H_noe_diff	2d_COSY	2d_HMBC	2d_HMQC
2d_O17_HMQC	31P-HMQC	ktemp		
				Read Close

Existing Parameter Sets:

- Standard 1D: ¹H, ⁷Li, ¹¹B, ¹³C, ¹⁵N, ¹⁷O, ¹⁹F, ²⁷Al, ²⁹Si, ³¹P. (Format: *1d_#X*, e.g. *1d_13C*).
- Standard 2D: COSY, HMQC, HSQC, HMBC. (Format: 2d_XXXX, e.g. 2d_COSY).
- Other ¹H Expts: NOE, water suppression, T₁ estimate, homonuclear decoupling, etc.
- Other ¹³C Expts: UDEFT, DEPTq, INADEQUATE, T₁ estimate, etc.

5. Set Up Variable Temperature

Temperature Control Suite	:						
Temperature Monitorin	ng Record Correct	tion Self tune Co	nfiguration Log He	lp			
				U State:	오 On	Topsp	in3.2
Channe	el	Regulation State	Stability	Current Te	emperature	Target Temperature	Heater Power
1 5 mm CPTXI 1H-13C/ ²	15N Z-GRD Z4	Transient	Not Available	294	.3 K	295.0 K (273.0 K313.0 K) Set	2.2 % (max. 5.0 % of 90.3 W)
		State	Gas Flow	Target (Gas Flow	Standby Gas Flow	
Probe G	as	🕑 Steady	699 lph	700 S) lph iet	0 lph Set	
Accessory C	hannel	State	Current Power	Targe	t Power		
1 (Chille BCU	er)	Connected	On	s	On Set		
	T Edte						
VTU: On 😋 Probe Temp	Main display	Monitoring	Corrections S	elf-tune 🖡	≀amp Reo	cording Aux. s	C Z44866/0043
	Sample ten	nperature	298	3. D. K.	Tops	spin2.1	
	Target ter	mp.	162	3.0 K	Char	ige	
	Probe Hea	ater 🗌	On	1.4 %	Set n	nax	
	Gas flow		539	5 l/h	-	+	
	Cooling		Off		Char	nge	
					N/T0000	- First Bar	

6. Lock the Solvent

△ Solvent Description Acetic acetic acid-d4 Acetone acetone-d6 CD6 benzene-d6 CD2Cl2 dichlormethane-d2 CD3CN acetonitrile-d3 CD3CN_SPE LC-SPE Solvent (Acetonitrile) CD3O_SPE LC-SPE Solvent (Methanol-d4) CDCI3 chloroform-d CH3CN+D2O HPLC Solvent (Acetonitril/D2O) CH3CH120 HPLC Solvent (Methanol/D2O) D20 deuteriumoxide D20_salt deuteriumoxide with salt Dioxane dioxane-d8 DMF N,N-dimethylformamide-d7 DMSO dimethylsulfoxide-d6 EtOD ethanol-d6 H2O+D2O 90%H2O and 10%D2O H2O+D2O 90%H2O and 10%D2O Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Ne4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Ne4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer	🧉 Solvents table		x
Acetic acetic acid-d4 Acetone acetone-d6 C6D6 benzene-d6 CD2Cl2 dichlormethane-d2 CD3CN acetonitrile-d3 CD3CN_SPE LC-SPE Solvent (Acetonitrile) CD3OD_SPE LC-SPE Solvent (Methanol-d4) CDCI3 chloroform-d CH3CN+D20 HPLC Solvent (Acetonitril/D2O) CH3OH+D20 HPLC Solvent (Methanol/D2O) D20 deuteriumoxide D20_salt deuteriumoxide with salt Dioxane dioxane-d8 DMF N,N-dimethylformamide-d7 DMS0 dimethylsulfoxide-d6 EtOD ethanol-d6 H2O+D20 90%H2O and 10%D2O H2O+D20 90%MSO and 10%DAC Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyrdine-d6 T_H2O+D2O+Ne4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Ne4NCI col3/4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Ne4NCI col3/4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Ne4NCI col3/	△ Solvent	Description	
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C6D6 benzene-d6 CD2Cl2 dichlormethane-d2 CD3CN acetonitrile-d3 CD3CN_SPE LC-SPE Solvent (Acetonitrile) CD3OD_SPE LC-SPE Solvent (Methanol-d4) CDCl3 chloroform-d CH3CN+D2O HPLC Solvent (Methanol/D2O) D2O deuteriumoxide D2O deuteriumoxide with salt Dioxane dioxane-d8 DMF N,N-dimethylformamide-d7 DMSO dimethylsulfoxide-d6 EtOD ethanol-d6 H2C+D2C 90%H2O and 10%D2O H2C+D2C 90%H2O and 10%D2O H2C+D2C 90%DMSO and 10%D2O H2C+D2C 90%H2O and 10%D2O (CD) H2C+D2C 90%H2O and 10%D2O (CD) H2C+D2C 90%H2O and 10%D2O (CD) H2C+D2C+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2C+D2O+NaAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer	Acetone	acetone-d6	
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DMF N,N-dimethylformamide-d7 DMSO dimethylsulfoxide-d6 EtOD ethanol-d6 H2O+D2O 90%H2O and 10%D2O H2O+D2O_salt 90%H2O and 10%D2O with salt HDMSO 90%DMSO and 10%DMSO-d6 Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MEOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	Dioxane	dioxane-d8	
DMSO dimethylsulfoxide-d6 EtOD ethanol-d6 H2O+D2O 90%H2O and 10%D2O H2O+D2O salt 90%H2O and 10%D2O with salt HDMSO 90%DMSO and 10%DMSO-d6 Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+NAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MEOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	DMF	N,N-dimethylformamide-d7	
EtOD ethanol-d6 H2O+D2O 90%H2O and 10%D2O H2O+D2O salt 90%H2O and 10%D2O with salt HDMSO 90%DMSO and 10%DMSO-d6 Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Ne4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Ne4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	DMSO	dimethylsulfoxide-d6	
H2O+D2O 90%H2O and 10%D2O H2O+D2O salt 90%H2O and 10%D2O with salt HDMSO 90%DMSO and 10%DMSO-d6 Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Ne4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Ne4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	EtOD	ethanol-d6	
H2O+D2O_salt 90%H2O and 10%D2O with salt HDMSO 90%DMSO and 10%DMSO-d6 Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAcc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	H2O+D2C	90%H2O and 10%D2O	
HDMSO 90%DMSO and 10%DMSO-d6 Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MEOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	H2O+D2O_salt	90%H2O and 10%D2O with salt	
Juice fruit juice MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MEOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	HDMSO	90%DMSO and 10%DMSO-d6	
MeOD methanol-d4 Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MEOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	Juice	fruit juice	
Plasma blood plasma Pyr pyridine-d6 T_H2O+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MEOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	MeOD	methanol-d4	
Pyr pyridine-d6 T_H2O+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	Plasma	blood plasma	
T_H2O+D2O+Me4NCI (CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	Pyr	pyridine-d6	
T_H2O+D2O+NAAc sodium acetate in 90%H2O and 10%D2O, for NMR thermometer T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	T_H2O+D2O+Me4NCI	(CD3)4NCI in 90%H2O and 10%D2O, for NMR thermometer	
T_H2O+D2O+Pivalate pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	T_H2O+D2O+NaAc	sodium acetate in 90%H2O and 10%D2O, for NMR thermometer	
T_MeOD methanol-d4, for NMR thermometer TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	T_H2O+D2O+Pivalate	pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer	
TFE trifluroethanol-d3 THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine	T_MeOD	methanol-d4, for NMR thermometer	
THF tetrahydrofuran-d8 Tol toluene-d8 Urine urine QK Cancel	TFE	trifluroethanol-d3	
Tol toluene-d8 Urine urine QK <u>C</u> ancel	THF	tetrahydrofuran-d8	
Urine urine	Tol	toluene-d8	
QK Cancel	Urine	urine	
		OK Cance	

Choose the solvent from the list.



Check the lock level to get a sense of shimming.

B BSMS Control Suit		3		
AUTO				^
Lock	Phase	Power	Gain	Shim
LOCK				
On-Off	Phase	Power	Gain	
SAMPLE		1		
LIFT	SPIN	Measure	Rate	Lock Lost
SHIM NonSpin: X Y Y XY X ² -Y ²	Z Z ² Z	Zª	Z4	E
	Previou	- STD BY Js Actua	al Step	
Absolute Difference			+	Reset
			Stepsize	
STDE		\bigcirc	× v	
Config				
External				-
•		ш		4
Sample: do	wn miss	ing	up Shim	coil temperature 296 K

Optimize these parameters if the lock signal is still weak after Topshim.

7. Tune the Probe

- Tuning and Matching are done automatically for most probes (atma).
- Use 'wobb' and manual tuning/matching if necessary.



8. Shim the Magnet

• Run 'topshim' alone is usually enough. If the shims are still not good, try 'topshim gui' as show below.

S TopShim
Shim Report Service
SHIM
Dimension
Optimisation solvent's default
Optimise for 1H
Use Z6 🔲 (add Z6 shim)
TUNE
Before Z-X-Y-XZ-YZ-Z
After off
Only
STATUS not running before/after Topshim.
CONTROL Start Stop Help Close

B BSMS Control Suite	x
AUTO	
Lock Phase Power Gain Shim	
LOCK	
On-Off Phase Power Gain	
SAMPLE	
LIFT SPIN Measure Rate Lock Lo	ost
SHIM NonSpin: Z Z ² Z ³ Z ⁴ X XZ Y YZ XY Manual Shimming	Ш
STD BY	
Absolute Previous Actual Step Difference - Stepsize	
Config	_
•	
Sample: down missing up Shim coil temperat	ture

9. Acquisition Parameters

🖕 Bruker TopSpin 3.2 on SSSC-EVO as jiz258					
Start <u>Acquire</u> Process A <u>n</u> alyse	P <u>u</u> blish <u>V</u> i	iew <u>M</u> anage	2		1
Sample - 🗰 Loo	k V Tune ▼	📕 Spin 👻 🖙 Sh	nim 👻 💕 Prosol s	🔻 🚾 Gain 👻 🍉 Go 👻 Options	~
	→\v)↑ ∰ →\v)↓ [_]		·····································		
Browser Last50 Groups	ruker\TopSpin3.2\data\iiz	258			
C:\Bruker\TopSpin3 2\data\iiz258	Pars AcquPars Titl	e PulseProg Peaks	Integrals Sample Str	ucture Plot Fid Acqu	
		Droh			/0042
	: C V 86	Plob	e. 5 mm CPTX	1 1H-13C/15N Z-GRD Z44000	/0043
General B	General				
⊕- ↓ 4 - zgig	PULPROG	zg30	E	Pulse program for acquisition	
B - B - 2gpg30 B - B - B - 2g	TD	65536		Time domain size (number of data po	oints in FID)
	SWH [Hz, ppm]	12019.23	20.0263	Sweep width (spectrum width)	
	AQ [sec]	2.7262976		Acquisition time (length of FID, in se	econds)
	RG	203		Receiver gain	
	DW [µsec]	41.600		Dwell time (time interval betw	ween two data points in FID)
	DE [µsec]	6.50		Pre-scan-delay	
	D1 [sec]	1.0000000		Relaxation delay; 1-5 * T1	(at+d1: relaxation delay)
	DS	0		Number of dummy scans	
	NS	64		1 * n, total number of scans: NS * TD0	
	TD0	1		Dimension of accumulation loop	
	Channel f1				
	SFO1 [MHz]	600.1737063		Frequency of ch. 1	
	O1 [Hz, ppm]	3706.30	6.175	Frequency of ch. 1	(middle of the spectrum)
	NUC1	1H Edit		Nucleus for channel 1	
	P1 [µsec]	12.50		F1 channel - 90 degree high power pulse	(nulse and nower)
	PLW1 [W, -dBW]	15	-11.76	F1 channel - power level for pulse (default)	(pulse and power)
			Amplifier Control	Acquisition information	Lock Sample Probe Temperature
				no acquisition running	294.9 K

12. Processing the Data (1)

Bruker TopSpin 3.2 on SSSC-EVO as jiz258					
<u>Start</u> <u>A</u> cquire <u>P</u> roces	s A <u>n</u> alyse	P <u>u</u> blish <u>V</u> iev	w <u>M</u> anage 🌘	9	<u>1</u>
A Pro	o <u>c</u> . Spectrum ▼	Adjust Phase	≂ ∫ 👌 Calib. A <u>x</u> is ⊲	✓ M Pick Peaks → ∫ Integrate → Ad	Ivanced ~
	ਸ਼ © ⊮⊉⊧ <mark>⊥</mark> ⊥	₩ŵ Ŧ ▶₩ ₩ ₽₩			
Browser Last50 Groups	1 Oct02 1 1 C:\Bru	ker\TopSpin3.2\data\jiz258			
C:\Bruker\TopSpin3.2\data\jiz258	Spectrum Proce	Pars AcquPars Title	PulseProg Peaks Inte	grals Sample Structure Plot Fid Acqu	
	5 12. ME	V #			
	Reference				
terrie 3 - zg ⊕ 4 - zgia	Window	Reference			Topspin2.1
₽- 1 5 - zgpg30	Phase	SI	65536	Size of real spectrum	
⊕	Fourier	SF [MHZ]	600.1700000	Spectrometer frequency	E.
	Integration	SR [Hz]	0	Spectrum reference frequency	4
	Peak	HZpPT [Hz]	0.183399	Spectral resolution	,
	Miscellaneous	SPECTYP	UNDEFINED	 Type of spectrum e.g. COSY, 	HMQC,
	User	Window function	n		
		WDW	EM 🔹	Window functions for trf_xfb	
			0.30	Line broadening for em	
		GB	0	Gaussian max. position for gm	n, 0 <gb<1< td=""></gb<1<>
		SSB	0	Sine bell shift SSB (0,1,2,)	
		TM1	0	Left limit for tm 0 <tm1<1< td=""><td></td></tm1<1<>	
		TM2	0	Right limit for tm 0 <tm2<1< td=""><td></td></tm2<1<>	
		Phase correction	on		
		PHC0 [degrees]	169.157	0th order correction for pk	
		PHC1 [degrees]	-19.462	1st order correction for pk	
		PH_mod	no 👻	Phasing modes for trf, xfb,	
		Baseline corre	ction		
		ABSG	5	Degree of polynomial for abs	(05)
		ABSF1 [ppm]	10.00000	Left limit for absf	.
				Amplifier Control Acquisition information	Lock Sample Probe Temperature
				no acquisition running	1 294.9 K
					📕 📕 🔰 🗸 On 📀 🛛 Reg. State: 📀

12. Processing the Data (2)



15. Plot the Spectrum (1)



15. Plot the Spectrum (2)



Bruker Pulse Program (1)



1	ze (Reset sca	n counter and enable the execution of dummy scans.)
2	30m	(Set up a label for loop.)
	d1	(Apply a delay of 'd1'.)
	p1*0.33 ph1	(Apply a 30° pulse on f1 with phase list 'ph1'.)
	go=2 ph31	(Execute one scan and then loop to line '2' (NS-1) times.)
	30m mc #0 to	2 F0 (zd) (mc macro to write data, including a disk writer
		(<i>wr</i>), a file increment (<i>if</i>) and memory initialization (<i>zd</i>).)
exit	t	(The end of the pulse sequence.)



Bruker Pulse Program (2)



C:\Bruker\TopSpin3.2\exp\stan\nmr\lists\pp\zgpg30
File Graphical assistant Edit text Options Help
<> -><- <> ▲11 Last zoom
🛛 Expression 🗹 Names 🗌 Values 🔽 Loops 🔽 Grid 🗌 Blocks
H 1
PLW 12 PLW 13 PLW 12 PLW 13
C 13 ZE P1*0.33 pm = [0,2] ZD
1 2
D110 30m 10u D11 DELTA 4u 10u 100m 1 30m
Go loop
MC loop
4 III III
📥 Bruker TopSpin (Student License) — 🗆 🗙
Elle Edit View Breeseeing Analysis Ontions Window Holn
□ 🔄 🗉 🗃 🗃 🖪 🖪 20 30 🔨 券 🤨 並 🔳 並 ↘ % 臥 央 ▦ ∥
*2 /2 *8 /8 ♦ 🛬 🕅 🙆 🕀 🖵 🎯 🗉 👦 🛄 ← ↔ → 🔶 → 🗡
Browser
B:\WRdata\SS: File: zgpg (C:\Bruker\TopSpin3 2)evp\stap\pmr\lists\pp)
Description of Parameters
:pl1: f2 channel - power level for CPD/BB decoupling
:pl13: f2 channel - power level for second CPD/BB decoupling
<pre>;pl:: fl channel - high power pulse</pre>
;d1 : relaxation delay; 1-5 * T1
;d11: delay for disk I/O [30 msec]
;ns: 1 * n, total number of scans: NS * TDO
;cpd2: decoupling according to sequence defined by cpdprg2
<pre>;pcpd2: f2 channel - 90 degree pulse for decoupling sequence</pre>