Tips & Tricks

Dr. Benjamin Görling





Innovation with Integrity



General Troubleshooting

How to get support

You have a question about TopSpin?



Your question can be answered as soon as possible

Contact your local Bruker office

Send Information automatically or manually to Bruker

Get an support identification ('support token')

Execute 'savelogs'

Hot to start **savelogs**





How to use **savelogs**

Execute Savelogs				BRÚKER
This tool will collect support information about your current TOPSPIN insource you to send it via FTP to Bruker. Use this tool only if you have been inso	stallation and allows structed to do so.			
Support token		🖕 Exe	ecute Savelogs	
Additional files or directories Additional files or directories to be included in the "savelogs" file can be text field below (press "Enter" or "Add" button after each file or director	be entered in the bry) or selected	This to you to	ool will collect support information about y send it via FTP to Bruker. Use this tool o ort token	our current TOPSPIN installation and allows nly if you have been instructed to do so.
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How to use **savelogs**



🖕 Details	
All files will be saved to the file: "TopSpinSupport_dispatch-20170309_NBRHE01-3V0CQ72_Benjamin.Goerling_2017-03	3-09T14.47".
Press the "FTP" button to send this file to Bruker.	
If FTP is not possible use the "Open" button to open a file browser with the location of the file and send it for example as EMail attachment.	sult automatically to Bruker
Additional Actions	Sur automatically to Druker
Press the "FTP" button to transfer the "savelogs" file to Bruker	
Press the "Open" button to open the directory of the "savelogs" file	or manually.
Show details	
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• **TD0**

TD0







• **Temperature Calibration**

Basic Principle of Temperature Control





Effects of different/unstable temperature





How to calibrate?





Sample	Range
80% Glycol in DMSO-d6	300 – 380K
Glycol, pure	300 – 380K
4% Methanol in Methanol-d4	181.2 – 300K
Methanol, pure	180.1 – 299.9K
99.8% Methanol-d4	282 – 330K

How to calibrate?





Set correction in Temperature Control [edte]



BRUKER



• User Directories





- each user starts with a list of default directories (e.g. lists/pp and lists/pp/user)
- each user can remove one or more default directories from its list
- each user can specify one or more additional source directories
- each user can define the order of the directories which defines the search order within TopSpin









Bruker files in:

.../exp/stan/nmr/lists/pp

These files are write protected!

You can be sure that these files always contain the original Bruker library file!







User files in:

.../exp/stan/nmr/lists/pp/user

By default all user-specific files will be stored here; read- and writable

You have an easy setup to distribute user-specific files to all colleagues





Each user can define his **own source directories**

If you store them e.g. in your home directory, then they are automatically read and write protected for anybody else







These files can be easily distributed!

It is easy to use e.g. your pulse programs on different spectrometers, just define a network drive as a source directory.



Convert parameter sets [paracon]



rarameter set conversion.	Available parameter sets:
Select parameter sets for conversion of the basic frequency (BF) or the installed digitizer from the lists on the right. Directories containing parameter sets can be added via the "Preferences" dialog. Use the match field to apply wildcards to the list of parameter sets, use the checkbox below to select case sensitive (default) or case insensitive match. Execute "cf" to set a new basic frequency (BF) or a new digitizer before executing paracon! Current basic frequency: 400.13 MHz.	C:/Bruker/TopSpin3.5pl6/exp/stan/nmr/par (Bruker defined parameter sets) AL27ND ASSURE_13C ASSURE_19F ASSURE_11H ASSURE_31P B11ZG BESTPROFILE B_HNCACBGP3D Match: Select all Select none C:/Bruker/TopSpin3.5pl6/exp/stan/nmr/par/user HSQCEDETGPSISP_NUS
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Parameters of one spectrometer cannot be used at another spectrometer.

Need to be converted to spectrometer frequency and routing:

paracon

Supports user defined directories



Serial processing

Repetitive Tasks ...







SERIAL PROCESSING

Serial Processing





Serial Processing – find datasets





Serial Processing – find datasets



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Serial Processing – find datasets



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Serial Processing – commands





Serial Processing – commands example





Serial Processing – execute



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Serial Processing





Group members meet serial processing







• qumulti

Command spooler



- Any command in TopSpin can be sent to the spooler (qu <command>)
- Tasks in the spooler are executed sequentially
- It is possible to define the experiment number on which a command should be queued:



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qumulti * BRUKER 0 1 Start Process Analyse P<u>u</u>blish <u>V</u>iew Manage Create Dataset 📓 Find Dataset 🔄 Open Dataset 「 Paste Dataset Read Pars. Hz H XX *8 *2 🏹 📢 📴 💌 X \bigoplus 🖕 New job **----**Ø **T** 18 12 All expnos can Job 1 exam_DNMR_I Alias Groups be preselected Browser Last50 ure Spectrum Pro Command C:\Bruker\Top: 🕀 - 🕕 exam CMC: with option: Ė٠ exam CMC: Experiment IDs exam CMC: Ð **10 320** exam Daisy ÷ exam_DNMI Ė٠ 🔽 11 **350** 9 🖻 퉬 exam DNMI **370** V 12 🕀 🚹 10 - zg3(🗄 🐌 11 - zg3(🔽 13 **420** 5 🖶 🌗 12 - zg3(**V** 14 🗄 🌗 13 - zg3(V 15 🖶 퉬 14 - zg3(ω 🗄 퉬 15 - zg3(🔽 16 🖶 퉬 16 - zg3(**1**7 ω 🗄 🕛 17 - zg3(V 18 🕸 🐌 18 - zg30 🗄 퉬 19 - zg3(🔽 19 4 🖶 퉬 20 - zg3(20 🗄 🌗 320 - zg: 🖶 퉬 350 - zg: - N 🗄 🔒 370 - zg: <u>0</u>K Cancel 🗄 🌗 420 - zg:

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qumulti



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qumulti



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qumulti vs. Serial Processing



qumulti

For NMR data stored under one dataset name =

Using of Expnos

fast ✓

Serial Processing

For NMR data stored under several dataset names

Using of Names

powerful 🗸



Serial Integration

intser – automatic integration of a series of spectra



- User defined list of datasets
- Use integrals of first dataset in list
- Allows easy normalization of any integral
- For 1D and 2D

Define integrals in first dataset



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Advanced processing – **intser**



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intser – flowbar





intser – define list



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intser – parameters



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intser – parameters



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intser - results with global scaling



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# Result of 'intser'
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# Data set list (full path) = C:\Users\BENJAM~1.GOE\AppData\Local\Ter
# Region to calibrate = 0
# Value of region to calibrate = 2.0
# Global scaling = yes # Result of 'intser'
                       # Date/time = Tue Jun 13 10:39:52 CEST 2017
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# # low field high fie # Value of region to calibrate = 2.0
  7.308494264941776 7 # Global scaling = yes
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  1.9668447801240367
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0;2.0;0.541879110289391; # # low field high field bias slope
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2;2.0174270965987207;0.5 # 1.9668447801240367 1.6014200668769478 0.0 0.0 # for region 2
3;3.0562284571461933;0.8
4;4.136608194179254;1.07 # Spectrum#; Integral 0; Integral 1;
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6;3.054762441695267;0.841;4.1420599921166925;1.0845876325140709;
7;4.218547545095421;1.122;2.0174270965987207;0.5748499797054847;
8;2.0057743467025406;0.53;3.0562284571461933;0.8323333205988354;
                        4;4.136608194179254;1.0794343635429302;
                        5;2.0072924645941086;0.5646915621179266;
                        6;3.054762441695267;0.8419335886413671;
                        7;4.218547545095421;1.129945036314264;
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intser – parameters



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	spectrum i	n the li	st	20)	1 1	10	1 1	0	- 10	[ppm]

intser – results without global scaling

```
BRUKER
```

```
# Result of 'intser'
# Date/time = Tue Jun 13 10:45:42 CEST 2017
# Data set list (full path) = C:\Users\BENJAM~1.GOE\AppData\Local\Ten
# Region to calibrate = 0
# Value of region to calibrate = 2.0
# Global scaling = no
# --- Integral info ---
# A 1.0 #regions in PPM
# # low field high field bias slope
# 7.308494264941776 7.018304051480852 0.0 0.0 # for region 1
# 1.9668447801240367 1.6014200668769478 0.0 0.0 # for region 2
# Spectrum#; Integral 0; Integral 1;
0 2.0 0.541879110289391;
1 2.0 0.5236947965883133;
2 2.0 0.5698842656318559;
3 2.0 0.544680040952201;
 2.0 0.5218934512878619;
5
 2.0 0.5626400458112735;
6 2.0 0.5512268824243687;
7 2.0 0.5357033548800292;
8 2.0 0.5705617941361856;
```

intser – parameters



	<u>F</u> ile	<u>S</u> tart <u>P</u> rocess	A <u>n</u> alyse P <u>u</u> blish	<u>V</u> iew <u>M</u> ana	age 🕜	1
1	G Bac	k	Defir	e List - Define P	a <u>r</u> ameters	
	Intser Processing				. 🛴 👬 📄 🗮	
	Options					
	Calibrate	-			De alta linta anala lo antala lo taur	
	Normalize sum of integrals	ŝ			Peaks Integrais Sample Struc	
	Required parameters					
	Number of region to calibrat	e (0, 1,) = 0				-
	Value of region to calibrate	2.0				50 -
	Normalization value	6				-
	Global scaling		no	▼		- 15 -
			OK Cance	Help		-
						-
						- -
	Normalize sets					-
211	m of all integr	al				م _ -
30	in or an incogre					-
ot (one spectrum	to				- - o
	defined value	III •	L,,, 20	10	_, <u>`ĬĹ</u> , , <u>`ŢĹ</u> , , o	

intser - results without global scaling



```
# Result of 'intser'
# Date/time = Tue Jun 13 10:56:30 CEST 2017
# Data set list (full path) = C:\Users\BENJAM~1.GOE\AppData\Local\Tem
# Normalization value = 6.0
# Global scaling = no
# --- Integral info ---
# A 1.0 #regions in PPM
# # low field high field bias slope
# 7.308494264941776 7.018304051480852 0.0 0.0 # for region 1
# 1.9668447801240367 1.6014200668769478 0.0 0.0 # for region 2
```

```
# Spectrum#; Integral 0; Integral 1;
0; 4.7209; 688051750 4;1.279 083119482496;
1; 4.7549; 313067108 7;1.245 0668693289133;
2; 4.6694 0979872927;1.330 529020127073;
3; 4.7157; 056481792;1.2842 794351820803;
4; 4.7583; 949796984;1.2416 705020301595;
5; 4.6826 091182564 95;1.31 73290881743505;
6; 4.7036; 929888285 4;1.296 3807011171453;
7; 4.7324; 476646141 5;1.267 5852335385849;
8; 4.6682 023735733 4;1.331 7597626426665;
```



Result file can be easily imported into excel → Simple graphical presentation





Write/read lists for integration

Integrate small set of spectra





Load first spectrum and integrate it





Export integral regions



<u>File Start Process Analyse Publish View Mar</u>	nage 🕜 🚺				
Λ Pro <u>c</u> . Spectrum ▼ Λ♦ Adjust Phase ▼ Ѧ Calib. A <u>x</u> is	▼ Marcel ▼ Pick Peaks ▼ ∫ Integrate ▼ Advanced ▼				
Juice_2 10 1 Z:\data\demo\nmr					
」 	\$ *X = ± ↑ \$ 8 <mark>6 3</mark> 4				
Mouse Sensitivity: 1.0 4.401 ppm / 1760.955 Hz	Save Regions To 'intrng'				
Sum = 15.8119 DEFINE REGION MODE	Save Regions To 'reg'				
Define: Drag using left mouse button Return: Left-click highlighted icon	Export integration regions				
	Export Regions To Relaxation Module and .ret.				
	Save & Show List				
	0 10 20 30				
	2.5 2.0 1.5 [ppm]				
Save region as					

Save as intrgn



	<u>F</u> ile <u>S</u> tart	Process Analyse	P <u>u</u> blish <u>V</u> iew	<u>M</u> anage 🕜			1
Miscellaneous Files: wn	nisc				grate	e ▼ A <u>d</u> vanced ▼	
File Options Help		Source	= C:\Bruker\TopSp	in3.5pl7\exp\stan\nmr\l	lists\intrng ▼		
Find file names enter a Class = Dim = Type = SubType = result_dilution.txt re t1_int te	show Recomn SubTypeB = esult_recovery.txt	Exclude: nended Reset Filters result.txt	Cleat introg introg peakr basip base_ peakl clevel reg - int2dr	- 1D integral ranges - 1D integral ranges ng - 1D peak ranges nts - baseline points for info - baseline function st - peak file for 'dcon' s - 2D contour levels reference regions for 'p ng - 2D integral ranges	r 'abs' n for 'bcm'	L	0 10 20 10 20 1 20 20 1 20 20 20 20 20 20 20 20 20 20
	4.0	3.5	3.0	2.5	2.0	1.5	[ppm]
	Save region as						

Save as intrgn





Load next spectrum and import region list



<u>File Start Process Analyse Publish View Ma</u>	anage 🕜 🚺
🔨 Proc. Spectrum 🗢 🕎 Adjust Phase 🗢 🕅 Calib. Axis	s マ M Pick Peaks マ ∫ Integrate マ Advanced マ
Juice_4 10 1 Z:\data\demo\nmr	
▋ <mark>」 </mark>	♀★×≒±↑↓ <mark>₽</mark> ₽₽↓
Mouse Sensitivity: 1.0 0.904 mmm / 361.84 Hz	Read 'intrng'
Sum = 0.0000 DEFINE REGION MODE	Read 'intrng' No Slope & Bias Corr.
Define: Drag using left mouse hutton Return: Left-click highlighted icon	Read 'intrng' Use Last Slope & Bias
	Import integration regions
	Import 'intrng' from Relaxation Experiment
	Edit 'intrng'
4.0 3.5 3.0	2.5 2.0 1.5 [ppm]
Read region	

Load next spectrum and import region list



Miscellaneous Files: rmisc File Options Help Find file names I enter any Mass = I Dim = I	string, *, ?	Sou	rce = C:\Bruker	^ \TopSpin3.5r	nl7\evn\stan\nmr\list	x	grate → A <u>d</u> vanced →	J
File Options Help Find file names ▼ enter any Xass = ▼ Dim = ▼	string, *, ?	Sou	rce = C:\Bruker	r\TopSpin3.5p	nl7\evn\stan\nmr\list			
Find file names enter any lass = Dim =	string, *, ?	Exclude:			privezpistan initiati	s\intrng 🔻		
Xass = 💌 Dim = 💌 [Clea	intrng - 1D	integral ranges	•		
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ype = SubType =	SubTypeB =	Reset Filter	s				region	
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esultstabilitaet.txt t1_in	nt	test						_ 2
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							At a surgeste	<u></u> o
			Edit	Set selecte	ed item in editor	Close		-
	4.0	3.5	3.	0	2.5	2.0	1.5	[mqq]

Integrals need to be calibrated





Load next spectrum and import region list









- Can be called from command line as well
- Commands are: **wmisc** and **rmisc**

• Example: **rmisc intrng juice**

- To call specific file, the type of list and the name need to be specified (wmisc/rmisc <type> <name>)
 - intrng 1D integral ranges
 - peakrng 1D peak ranges baslpnts - baseline points for 'abs' base_info - baseline function for 'bcm' peaklist - peak file for 'dcon' clevels - 2D contour levels reg - reference regions for 'pp' int2drng - 2D integral ranges



• Useful commands

Copy parameters between datasets



	🖕 Create New Dataset - new		×				
Browser Last50 Alias Experiments	Prepare for a new experiment by initializing its NMR parameters ac For multi-receiver experiments se Please define the number of rece	creating a new data set and cording to the selected experiment type. everal datasets are created. eivers in the Options.					×
er ■ 9 - 29	NAME		e	Plot Fid A	cqu		
	NAME	~TEMP				-	[e]
🕀 🖟 12 - hmbcgpndqf - HMB(EXPNO	205				F	-
⊕ 13 - nmbcgpnaqt - HMBC ⊕ 14 - zghfigqn	PROCNO	1				-	
D - dipsi2gpphzs_psyct D - jresappraf - JRES	O Use current parameters						. e
⊕	Experiment COSYGPSW	Select				Ę	
	Ontions						
	Set solvent	DMSO				-	~
	Execute 'getprosol'					ļ	
a 203 - 2g30 □] 204 - 2g30	○ Keep parameters	P 1, PLW 1 Change				-	ω.
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⊕	Show new dataset in new	w window		••• •••••••••••••••••••••••••••••••••••		···:	• 4
⊕ 🔒 999 - zgps	Number of additional datas	sets: (1,2,16) 1				-	
Brillin 1000 - jresgppsql.bgoe Brillin 1001 - jresgppsqf.bgoe						Ē	
·						-	• 61
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Structure	TITLE					-	
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No structure available.						-	
		OK Cancel More Info	elp		0	[mqq]	
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Copy parameters between datasets





Copy parameters between datasets




















$COSY \rightarrow HSQC$



Browser Last50 Alias Experiments	2 ~TEMP 205 1 C:\NMRData\data\bgoe\nmr	
⊕ 9 - zg	Select parameters to transfer	Manual Mode Copy Parameters
er 10 - fillbegphagi - Hillbe 11 - hmbegphagi - HMB(Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Plot Fid Acc	ĮU
⊕ ↓ 12 - hmbcgpndqf - HMB(⊕ ↓ 13 - hmbcgpndqf - HMB(🤹 advanced transfer of parameters 🛛 🔀	
⊕ · Ju - zghfigqn	Select parameters to copy from reference dataset to target dataset.	
B 20 - dipsi2gpphzs_psyct D - iresappraf - JRES	Perform advanced getprosol (use hard pulses from reference expt.)	
 In the second se	Perform standard getprosol	
⊕- 🔒 105 - hmbcetgpl3nd - HN ⁼ ⊕- 🕒 106 - h2bcetgpl3 - HSO(Reference Expt.: Target Expt.:	· · ·
	~TEMP 205 1 ~TEMP 206 1 cosyappad bsacedetapsisp2.3	
⊕ ⊕ 201 - zg30 ⊕ ⊡ 202 - zg30		
⊕ _ 203 - zg30	Nucleus Parameter Value Parameter Orig. Value	-
= 204 - zg30		-4
e 205 - cosygpppqf	1H SW(F2) [ppm] 10.3672 V V> SW(F2) [ppm] 12.9895	
e-11 216 - hsgcedetapsisp2.		[
Gaution.	Additional parameters:	- w
AO will be change		
A will be change	O Use Al qPars O Use Display Region OK Edit Param List Hz/ppm Cancel	
when changing		
when enanging		
SW(F2)!		
No s veture and able.		
Should not excee	ansfer parameters to dataset: : ~TEMP 206 1 C:/NMRData/data/bgoe/nmr	Cancel
200ms for HSQC	Same POWCHK Sample POWCHK Sample Temperature Spooler	BSMS status message Time
	Current 17 Corr. 298.0 K	Δ X -2 11:45:37
	Last: 13 VI On O Reg. State: O cron: 1	Autoshim 🔮 Locked 🔮 Error 🔰 Jul 14

$\mathsf{HSQC} \to \mathsf{HMBC}$



owse	r Last50 Alias Experi	ments 2 ~TEMP 206 1 C:\NMRData\data\bgoe\nmr		
	⊕ ↓ 106 - h2bcetgpl3	HSQ(Select parameters to transfer	Manual Mode	Copy Parameters
	🖽 🌗 200 - hsqcedetgp	sisp2.3 💊 advanced transfer of parameters 🛛 🔯	u	
		Select parameters to copy from reference dataset to target dataset.		
	E 202 - 2030 E 203 - 2030	Perform advanced getprosol (use hard pulses from reference expt.)		
	🖶 🌗 204 - zg30	☑ 1H ☑ 13C		
	<u> </u> • 1			
	🖶 🎍 205 - cosygpppqf			·
		Reference Expt.: Target Expt.:		F
	■ 200 = hsqccdctgp	~TEMP 206 1 ~TEMP 208 1		
	🕂 ル 207 - zgpg30	hsqcedetgpsisp2.3 hmbcgplpndqf	•• • .	·····
	. ↓ + 1	Nucleus Darameter Value Darameter Orig Value		-
	🖶 📕 208 - hmbcgplpnd			
		EP LC		
	⊕ 1 888 - za30	1H O2 [ppm] 4.361		
	🕀 🜗 998 - zg2d	1H SW(F2) [ppm] 10.3672 V> SW(F2) [ppm] 12.9895		-
	🖶 퉬 999 - zgps	13C O1 [ppm] 75.000> O2 [ppm] 100.000		F
	1000 - jresgppsqf	bgoe 13C SW/E1) [nnm] 165 1013 X - SW/E1) [nnm] 220 0000 X		ļ ļ
	1001 - jresgppsqt			÷ E
	⊕ ∎ 9999 - 299950 ⊕ ∎ 10104 - h2bcedet	- 6/01		
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				E
uctu	re	O Use AcqPars O Use Display Region OK Edit Param List Hz/ppm Cancel	J	E
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	No structure available.	8 6 4	2	F2 [ppm]
		transfer parameters to dataset: : ~TEMP 208 1 C:/NMRData/data/bgoe/nmr		Cance
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Useful commands – expl





Useful commands – expl top





Useful commands – expl prop

2+art

111

expl prop



<u>P</u>r expl prop: *2 /2 opens explorer (or rime konquerer) window Las in3.5 within the user est Ibru specific topspin Ibrug brup configuration directory SmartDriveNMR C:\NMRData ExamData CMC expl prop

ocess	A <u>n</u> alyse P <u>u</u> blish <u>N</u>	<u>/</u> iew <u>M</u> anage	0		1
C <u>r</u> eate					
	Eile Edit View Tools H	\.topspin-W7-400\prop			
nts	Organize 🔻 Include in lib	rary 🔻 Share with 🔻	New folder		
t50	🔶 Eavorites	📩 Name	*	Date modified	Si:
pl7\exa	E Desktop	🔒 ter	nplates	30.03.2011 14:08	- [9
	📜 Downloads	\mu us	erdefined	05.02.2015 15:54	- 1
profen	🔚 Recent Places	bro	owsedir2_Local.prop	12.06.2017 17:31	
profen		bs/	ms.prop	21.04.2017 15:24	Ā
orofen ·	🧮 Desktop	🗋 cm	ncqLayout.prop	28.05.2013 09:44	-
	🥽 Libraries	📄 da	ta_groups2.prop	08.04.2015 10:56	-
	📄 Apps	🔄 🗋 dis	able.prop	12.06.2017 17:31	
	Documents	📄 ed	itor.prop	12.06.2017 17:30	
	👌 Music	Ed:	teSettings.prop	23.03.2011 15:44	-
	📔 Pictures	🗋 glo	obals.prop	12.06.2017 17:32	-
	📄 TopSpin User Files	🗋 iio	p.prop	12.06.2017 17:31	Lo
	📄 TopSpinFiles	as 🗋 las	t50_3.prop	12.06.2017 17:31	
	📑 Videos	📄 lay	out.prop	13.06.2017 10:12	-
	🤣 Homegroup	📄 loc	:kLayout.prop	13.06.2017 14:10	-
	🥦 Applikation	🗾 ne	w-rpar-keep-list.txt	12.06.2017 17:23	Ē.o
	퉲 .diff	🔛 no	tebook.txt	25.04.2017 08:57	
	🌗 .jnati	🗋 pa	rfile-dirs.prop	19.04.2016 16:59	-
	🍌 .oracle_jre_usage	🔛 rpa	ar-keep-list.txt	12.06.2017 11:51	-
	🐌 .topspin1	set	limits_nd.prop	07.03.2017 18:13	
).topspin-W7-400	📄 sp	ooler.xml	12.06.2017 17:43	- 0
•	퉬 autoshim	📄 sp	oolerprotocol.xml	12.06.2017 21:15	ml
	🌗 cmcq	📄 tał	ole_npt.prop	03.05.2017 15:57	
	🌗 prop	tał	ole-3.0.prop	31.01.2013 11:08	
	1 1 1 1 1 1 1 1 1 1	R	1	24 04 2042 44 57	

Useful commands – expl help





Useful commands – command history





Useful commands – command line history cmdhist





How to identify parameter sets?



🍦 Parameter Sets: rpar				X
<u>File Options H</u> elp		Source =	C:\Bruker\TopSpin3.5pl7\	exp∖stan\nmr∖par ▼
Find file names 🔻 ente	r any string, *, ? E	Exclude:	Clear	
Class = Any	▼ Dim = Any ▼ ▼	Show Recommended		
Type = Any S	SubType = Any Sub	oTypeB = Any ▼ Res	et Filters	
C13CPD	C13DEPT135	C13DEPTQ135	C13UDEFT	COSYGPDFPHSW
COSYGPSW	HMBCETGPL3ND	HMBCGP	HMBCGP 15N	HSQC TOCSY
HSQC_TOCSY_ADIA	HSQCEDETGPSISP	HSQCEDETGPSISP_A	HSQCETGP_15N	HSQCETGPSISP
HSQCETGPSISP_ADIA	MLEVPHPR	MLEVPHSW	NOESYPHPR	NOESYPHSW
PROTON	ROESYPHPR	ROESYPHSW	WATERSUP	
				Read Close

How to identify parameter sets? Comments!



						V
🍦 Pa	rameter Sets: rpar					
<u>F</u> ile	Options Help			Source =	C:\Bruker\TopSpin3.5pl7	exp\stan\nmr\par 🔹
Find	Show Com	ment	Exclu	ide:	Clear	
Class	Show Date		🖊 Sh	ow Recommended		
Type	Sort by Dat	te	ihTvi		ent Filters	
Type	Edit Comm	ent	ID I Y			
C13C	Refresh Fre	om File System	C	3DEPTQ135	C13UDEFT	COSYGPDFPHSW
COSI	Manage So	ource Directories	H	/IBCGP	HMBCGP_15N	HSQC_TOCSY
HSQC	TUCST_ADIA	ROUCEDETGROIOR	H	QCEDETGPSISP_A	HSQCETGP_15N	HSQCETGPSISP
HSQC	ETGPSISP_ADIA	MLEVPHPR	M	EVPHSW	NOESYPHPR	NOESYPHSW
PROT	ON	ROESYPHPR	R	DESYPHSW	WATERSUP	

Read....

Close

Comments



Parameter Sets: rp	ar X	
File Options Help	Source = C:\Bruker\TopSpin3.5pl7\exp\stan\nmr\par	
Find file names ven	ter any string, *, ? Exclude: Clear	
Class = Any	▼ Dim = Any ▼ Show Recommended	
Type = Any	SubType = Any SubTypeB = Any Reset Filters	
C13CPD	13C with 1H decoupling, 1024 scans, 235 ppm	
C13DEPT135	DEPT 135 experiment, CH3/CH positive, CH2 negative, 256 scans, 160 ppm	
C13DEPTQ135	DEPTQ 135 experiment, CH3/CH positive, CH2/C negative, 256 scans, 220 ppm	
C13UDEFT	UDEFT experiment, faster 13C acquisition, but improved S/N, 384 scans, 220 ppm	
COSYGPDFPHSW	Gradient selected double quantum filtered phase sensitive COSY	
COSYGPSW	Gradient selected COSY	
HMBCETGPL3ND	1H-13C HMBC with gradient selection using 3-fold low pass filter for better 1J suppression	
HMBCGP	1H-13C HMBC with gradient selection	
HMBCGP_15N	1H-15N HMBC with gradient selection	
HSQC_TOCSY	1H-13C HSQC-TOCSY with gradient selection 600 MHz >= BF1	
HSQC_TOCSY_ADIA	1H-13C HSQC-TOCSY with gradient selection BF1 >= 700 MHz	
HSQCEDETGPSISP	1H-13C multiplicity edited HSQC with gradient selection 600 MHz >= BF1	
HSQCEDETGPSISP	1H-13C multiplicity edited HSQC with gradient selection BF1 >= 700 MHz	
HSQCETGP_15N	1H-15N HSQC with gradient selection	
HSQCETGPSISP	1H-13C HSQC with gradient selection 600 MHz >= BF1	
HSQCETGPSISP_A	1H-13C HSQC with gradient selection BF1 >= 700 MHz	
MLEVPHPR	Phase sensitive TOCSY with solvent supression	
	Read Close	



Archiving & Accounting



Apply

Reset...

• Accounting in TopSpin has to be activated manually once

<u>F</u> ile	<u>S</u> tart	<u>A</u> cquire	<u>P</u> rocess	A <u>n</u> alyse	P <u>u</u> blish	<u>V</u> iew	Mana	age 🕜			1 L B
			Pr <u>e</u> fer	ences Spe	ctr <u>o</u> meter ▼	Security	∠ ▼ <u>C</u> α	ommands v	<u>R</u> emote		
	*	8 *2 🏹 🥰	T		🤹 User prefe	erences					—
		8 *2 *** 8 /2 ·** 7 ***			User prefet Administra Window se Processing Text edito Regulated Miscellane Remote co Directories Acquisition More prefet	erences ation items ettings g preferer rs I Environn eous onnection s n erences	s nces nents	Directories Dir. of struc Global sear Manage sou Acquisition Show "ased Overwrite e Display digi Auto open a Configure a Automatical More prefere Spectra Dis Spectra Dis Spectra Prin Browser Pre Status Bar I Lock Displa	ture files for structure view ch path for plot layouts urce directories for edpul, o parameter selection with xisting FID without inquiry (tal resolution in FID display acquisition window after 'zg uccounting & data archiving ly perform getprosol during ences play Preferences nting Preferences eferences Preferences y Preferences	er edau, etc. "eda" ZG safety off) / window ' g after 'zg' g rpar/edc/new	Change Change Change Change Change Change Change
								BSMS Displ	ay Preferences		Change 💂
							Search			Apply Close	Reset

Archiving configuration



Like archive option in ICON-NMR

will archive each acquisition which has been started from within TopSpin GUI

(for AU programs: use '**XCMD("sendgui zg")**'

🤤 Setup Auto-Archiving & Accounting		—			
When acquisition ('zg') is finished, TopSpin allows you to - write accounting info to be evaluated by the command 'account' - to copy the acquired dataset to a desired archiving directory.					
When 'zg' is executed multiple times on the same dataset, TopSpin will increment the EXPNO while archiving so as to never override already archived data. You may specify an additional EXPNO offset for this case.					
The accounting info is stored in the fi " <topspin homedir="">/prog/curdir/acqh</topspin>	ollowing directo history"	ory, one file per day:			
The archiving directory may contain the following tags: \$USERHOME or \$USER. They are replaced by the login user's home directory or name, respectively, at archiving time.					
Auto-archive after 'zg' =		no 🗸			
Archiving directory =	C:\Users\demo				
EXPNO offset =	1000				
Write accounting info after 'zg' =		yes 🔹			
	Browse	<u>O</u> K <u>C</u> ancel			

Archiving configuration



If an experiment is executed a second time, the dataset is added to the archive as a new expno

Increment is user-specific.

Setup Auto-Archiving & Accounting		×			
hen acquisition ('zg') is finished, TopSpin allows you to write accounting info to be evaluated by the command 'account' to copy the acquired dataset to a desired archiving directory.					
Vhen 'zg' is executed multiple times (on the same da	taset, TopSpin will			
ncrement the EXPNO while archiving	so as to never	override already			
rchived data. You may specify an ac	dditional EXPNC	O offset for this case.			
he accounting info is stored in the following directory, one file per day: <topspin homedir="">/prog/curdir/acqhistory" he archiving directory may contain the following tags: SUSERHOME or \$USER. They are replaced by the login user's ome directory or name, respectively, at archiving time.</topspin>					
Auto-archive after 'zg' =		no 👻			
Archiving directory =	C:\Users\demo				
EXPNO offset =	1000				
Write accounting info after 'zg' =		yes 🔻			
	Browse	<u>O</u> K <u>C</u> ancel			

Archiving configuration



A new accounting possibility is implemented.

🖕 Setup Auto-Archiving & Accounting X When acquisition ('zg') is finished, TopSpin allows you to - write accounting info to be evaluated by the command 'account' - to copy the acquired dataset to a desired archiving directory. When 'zg' is executed multiple times on the same dataset, TopSpin will increment the EXPNO while archiving so as to never override already archived data. You may specify an additional EXPNO offset for this case. The accounting info is stored in the following directory, one file per day: "<topspin homedir>/prog/curdir/acqhistory" The archiving directory may contain the following tags: \$USERHOME or \$USER. They are replaced by the login user's home directory or name, respectively, at archiving time. Auto-archive after 'zg' = no C:\Users\demo Archiving directory = EXPNO offset = 1000 Write accounting info after 'zg' = yes OK Browse Cancel



- The accounting file (a file per day; XML format) will be stored in: <topspinhome>/prog/curdir/acqhistory
- The accounting file can be opened via
 Manage → Spectrometer → Spectrometer Usage (account)



or the TopSpin command account









🍓 Select Acquisit	tion History Files	The subscription in the local difference in the local	×
Look in:) acqhistory	•	🏂 📂 🛄 -
Recent Items	acq2013-10 acq2013-10 acq2013-11	0 <mark>-31.xml</mark> I-01.xml	
Desktop			
My Documents			
Computer			
Network			
	File name:	acq2013-10-31.xml	The
	Files of type:	History files	Cal



🖕 A	counting Proto	ocol			×
File	Edit Sea	rch			
1	Accounting	g Protoc	ol		^
2	Created: 2	2013-11-	01 17:46:14 C	ET	
3	TopSpin: 🕻	3.2			
4					
5	User: nmr:	su / Sve	n		
6	#Datasets	Dim	Exp.Time	Failed	
7	4	1	3.30 min	0	
8	0	2	0.00 sec	0	
9	0	>2	0.00 sec	0	E
10	Sum =				
11	4	Any	3.30 min	0	
12					
13					
14	Period				
15	From: 2013	3-11-01	17:29:51 CET		
16	To: 2013	3-11-01	17:36:36 CET		
17					-
18					1:1



• User-specific accounting with TopSpin-internal users



🤤 User preferences		×
Administration items	Administration items	-
Window settings	Auto-open last used dataset when restarting TopSpin	V
Processing preferences	Show TopSpin data examples directory in data browser	
Text editors	Setup users for TopSpin-internal login/logoff and esign	Change
Regulated Environments	Automatic termination of TopSpin when idle time exceeded	Chan
Remote connection	Automatic locking of TopSpin when idle time exceeded	Change
Directories	Enable automatic command spooling	V
Acquisition	Window settings	
More preferences	File menu: Show "File" text rather than icon (restart!)	
	Fonts and colors	Change
	Size of tool bar icons [pixels]	24
	Make TopSpin main toolbar detachable	
	Open new internal windows "cascaded" rather than "maximiz	zed"

TopSpin-internal users



User ID	User Name	Allowed Signature Meanings
Robin	Robin	Operator
sven	sven	Operator
Add User	Change Mea	nings Remove User Passwd Length



 Switching the user can be executed with the commands login / logoff

🖕 Bruker TopSpin 3.2 on AVIII300Z420W7 as nmrsu / Sven				- O X
<u>Start A</u> cquire <u>P</u> rocess A	nalyse P <u>u</u> blish	<u>V</u> iew <u>M</u> anage 🕢		1 <mark>B</mark>
Pr <u>e</u> ferences Spectr <u>o</u> meter → Security → Commands → <u>R</u> emote				
Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state Image: Second state	Image: Acquisition finished: N Spectrum ProcPars	Lock TopSpin for Other Users (lockgui) Logoff From Internal User (logoff) Login As Internal User (login)	Sample Structure Plot Fid Acqu	
 Interview Content Interview Content	Institute OC Project-No ABC12 Project 8	Change Internal User Password (chpwd) E-Sign Data Set (esign) Show/Verify Audit Trails (audit)		- - - -

۵	X
Please iden	tify yourself
User ID =	Sven 🗸
Password =	
	OK Cancel

User-specific accounting in TopSpin







Save/Convert Data Sets

Save data as...





Copy data set to new destination



<u>F</u> ile <u>S</u> tart <u>P</u> rocess A <u>n</u> alyse P <u>u</u> blish <u>V</u> iew <u>M</u> anage	1
📄 C <u>r</u> eate Dataset) 🅃 F <u>i</u> nd Dataset) 🖄 Open <u>D</u> ataset 📭 Pas <u>t</u> e Dataset) 🔡 R <u>e</u> t	ad Pars.
1 exam1d_1H 1 1 C:\Bruker\TopSi Spectrum ProcPars AcquPars Title	
Options Options Options Options	
 Save data set in a ZIP file Save data set in a JCAMP-DX file 	- - .
 Save data set as experiment to CCPN project Save data of currently displayed region in a text file 	
 Save parameters as a new experiment Save digital as analog filtered data 	- - - -
Save other file	
File type = processed data as new PROCNO V	- - -
<u>OK</u> <u>Cancel</u> <u>H</u> elp	
8 6 4 2	0 [ppm]

Save data set as ZIP file



<u>Fi</u> le <u>S</u> tart <u>P</u> rocess A <u>n</u> alyse P <u>u</u> blish <u>V</u> iew <u>M</u> anage 🕢	1
📄 C <u>r</u> eate Dataset) 🖼 F <u>i</u> nd Dataset) 🧐 Open <u>D</u> ataset) 🌓 Pas <u>t</u> e Dataset) 🔡 R <u>e</u> a	id Pars.
1 exam1d_1H 1 1 C:\Bruker\TopSt tozip	
1H Cyclosporin Options Options Options	[*1 eG]
Save data set in a ZIP file Save data set in a JCAMP-DX file	- -
Save data set as experiment to CCPN project	-
Save parameters as a new experiment	- - - - - -
Save other file	
Required parameters File type = acqu. data as new EXPNO	- - - 55
<u>OK</u> <u>Cancel</u> <u>H</u> elp	
LI II II II II II II III III III IIII IIII	₩' <u>\</u>
	0 [mpm]

Save data set as ZIP file



<u>F</u> ile <u>S</u> tart	Process Analyse Publish View Manage	• 🕜	1
	🗋 C <u>r</u> eate Dataset [😹 F <u>i</u> nd Dataset 🌍 Open <u>D</u> atas	set 🔽 Pas <u>t</u> e Dataset 🗟 R <u>e</u> ad Pars.	
Image: Second	$\begin{array}{c} *2 & \textcircled{\begin{tabular}{c} *2 \\ /2 & \fbox{\begin{tabular}{c} 2 \\ \hline 2 \hline 2 \\ \hline 2 \\ \hline 2 \hline 2 \hline 2 \hline 2 \\ \hline 2 $		
1 exam1d_1H 1 1	C:\Bruker\TopSpin3.5pl7\examdata		
Spectrum ProcPars	AcquPars Title PulseProg Peaks Integrals Sample Structure	Plot Fid	
1H Cyclosporin	🖕 tozip	X	- 1 e
	Please specify destination		ר ה - -
	Name of archive file =	exam1d_1H.topspin.zip	-
	Directory of archive file =	C:\Users\benjamin.goerling	-
	Type of archive file =	ZIP-compress	-
	Include these data types =	FID+RSPEC+ISPEC	- 6:
	Zip current EXPNO/PROCNO only, or all of	fexam1d_1IFID+RSPEC+ISPEC	-
		FID+RSPEC	-
		FID	-
		RSPEC+ISPEC	0.5
		RSPEC	-
		PARAMS	
ļ~	, Lite Martine Manuel Martine M	Mr. Marina Marina Marina M	
	8 6	4 2	0 [ppm]

Save data set in a JCAMP-DX file



Create Dataset Image: Paste Dataset Read Pars. Image: Paste Dataset Image: Paste Dataset Image: Paste Dataset Image	<u>F</u> ile <u>S</u> tart <u>P</u> rocess A <u>n</u> alyse P <u>u</u> blish <u>V</u> iew <u>M</u> anage 🕢	1
Image: Second	📄 C <u>r</u> eate Dataset) [Find Dataset) 🧐 Open <u>D</u> ataset) 📭 Pas <u>t</u> e Dataset) 🔡 R <u>e</u> a	ad Pars.
1 examid_1H 1 1 CkBruker\TopS Spectrum ProcPars AcquPars IH Cyclosponin Options © Copy data set to a new destination Save data set in a ZIP file © Save data set in a JCAMP-DX file © Save data set as experiment to CCPN project © Save data set as a new experiment © Save data set as analog filtered data © Save other file Required parameters File type = Cup Lotter QK QK QK QK QK QK QK QF		
IH Cyclosporin Options Copy data set to a new destination Save data set in a ZIP file Save data set in a JCAMP-DX file Save data set as experiment to CCPN project Save data of currently displayed region in a text file Save digital as analog filtered data Save other file Required parameters File type = acqu. data as new EXPNO	1 exam1d_1H 1 1 C:\Bruker\TopSi Spectrum ProcPars AcquPars Title	
Required parameters File type = QK QK <	1H Cyclosporin Options Copy data set to a new destination Save data set in a ZIP file Save data set in a JCAMP-DX file Save data set as experiment to CCPN project Save data of currently displayed region in a text file Save data as a new experiment Save digital as analog filtered data Save other file	1.0 1.0 1.5 1.6
	Required parameters File type = acqu. data as new EXPNO QK Cancel Help Multiplication 8 6	







JCAMP is a IUPAC standard format! It is an ASCII file that contains all necessary information of the spectrum/FID.

Save data set in a JCAMP-DX file



<u>File Start Process Analyse Publish View M</u> anage 🕜	1
📄 C <u>r</u> eate Dataset) 🖼 F <u>i</u> nd Dataset) 🜍 Open <u>D</u> ataset 🌓 Pas <u>t</u> e Dataset 🔡 R <u>e</u> ad Pars.	
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pI7\examdata	
Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Plot Fid	
1H Cyclosporin	- - - - -
🖕 tojdx	- - 6 - 6
Please specify destination	-
Name of archive file = exam1d_1H.dx	-
Directory of archive file = C:\Users\benjamin.goerling	- C
Type of archive file = JCAMP DIFF/DUP -	-
Include these data types = FID+RSPEC+ISPEC -	
JCAMP version = 6.0	-
<u>Browse</u> <u>OK</u> <u>Cancel</u> <u>H</u> elp	- - - -
I A the share the the the the	
	o [ppm]


For JCAMP format, you can choose between the following compression mode:

- FIX (=0) : table format
- PACKED (=1) : no spaces between the intensity values
- SQUEEZED (=2) : the sign of the intensity values is encoded in the first digit
- DIFF/DUP (=3) : the difference between successive values is encoded, suppressing repetition of successive equal values (default = DIFF/DUP)



For the included data types, you have the following choices:

- FID: raw data
- RSPEC+ISPEC: real and imaginary processed data
- RSPEC: real processed data
- PARAMS: parameter files
- FID+RSPEC+ISPEC: raw data, real and imaginary processed data
- FID+ALL_PROCNOS: raw data and all processed data
- ALL_EXPNOS_DIM_1_2: all EXPNOS of the dimensions 1D and 2D under this <NAME>

📕 exam1d_1H.dx - Editor

Datei Bearbeiten Format Ansicht ?

<u>-</u>0×

##TITLE=1H Cyclosporin ##JCAMPDX= 6.0 \$\$ Bruker NMR JCAMP-DX V2.0 ##DATA TYPE= NMR FID ##DATA CLASS= NTUPLES ##ORIGIN= UXNMR, Bruker Analytische Messtechnik GmbH ##OWNER= root \$\$ TOPSPIN Version 1.2 \$\$ 2004-09-21 23:17:47.879 +0200 gaty@SVEN \$\$ Compression mode = diff/dup ##.OBSERVE FREQUENCY= 500.13250065 ##.OBSERVE NUCLEUS= /1H ##.DELAY= (6, 6) ##.ACQUISITION MODE= SIMULTANEOUS (DQD) ##.ACQUISITION SCHEME= undefined ##.AVERAGES= 16 ##.DIGITISER RES= 18 ##SPECTROMETER/DATA SYSTEM= spect ##.PULSE SEQUENCE= zq ##.SOLVENT NAME= CDC13 ##.SHIFT REFERENCE= (INTERNAL. CDC]3. 0. 11.008) ##AUDIT TRAIL= \$\$ (NUMBER, WHEN, WHO, WHERE, WHAT) version 1.2.b.15 \$\$ ##TITLE= Audit trail. TOPSPIN \$\$ ##JCAMPDX= 5.01 \$\$ ##ORIGIN= Bruker BioSpin GmbH \$\$ ##OWNER= nmrsu \$\$ \$\$ d:/data/nmrsu/nmr/exam1d_1H/1/audita.txt \$\$ ##AUDIT TRAIL= \$\$ (NUMBER, WHEN, WHO, WHERE, WHAT) 1,<2004-03-30 16:00:49.843 +0200>,<nmrsu>,<KASTOR>, <created by zg, POWCHK disabled, PULCHK disabled configuration hash MD5: 91 84 CA F9 28 91 F3 2D B7 D4 7D 96 EC CF 24 FE data hash MD5: 64K 92 8A 14 05 B3 09 B1 4C 6C 7A AD 10 96 4D A5 B8>) \$\$ ##END= \$\$ **\$\$ \$\$** hash MD5 \$\$ \$\$ 75 DB OB AO EF AG 51 CA 3C 5D 36 1B OA 21 AE EB ##\$RELAX= ##\$BRUKER FILE EXP=format.temp \$\$ EDIT_PAR COMMAND FILE \$\$ \$\$ DI_MODE LONG \$\$ ED_ENTRY ACQU \$\$ ORDER FILE \$\$ \$\$ \$\$ HEADER "F2 - Acquisition Parameters T_NAME Date_ TYPE R64 CLASS ACQU SUBRANGE 0.0 50000000 "Date_=itodate(DATE)" REL INV_REL "DATE=datetoi(Date_,DATE)"

Some examples about the content of JCAMP:

Parameters

Acquisition audit trail

Parameter on the plot

📕 exam1d_1H. dx - Editor

\$\$

Datei Bearbeiten Format Ansicht ?

\$\$;\$Id: Avance2.incl,v 1.10 2003/02/25 14:46:08 ber Exp \$
\$\$ # 6 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zq" 2

Some examples about the

\$\$ \$\$ content of JCAMP: \$\$ # 1 "mc_line 9 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg expanding def |\$\$ define delay M⊂WRK \$\$ define delay MCREST \$\$ "MCWRK = 0.500000*30m" \$\$ "MCREST = 30m - 30m" \$\$ # 9 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zq" **\$\$** 1 ze \$\$ # 1 "mc_line 9 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zq expanding definition of mc command after ze" \$\$ # 10 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg \$\$ # 1 "mc_line 10 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zq expanding start label for mc command" \$\$ 2 MCWRK * 2 |\$\$ LBLF0, MCREST "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zq" \$\$ # 11 \$\$ d1 \$\$ p1 ph1 \$\$ _go=2 ph31 \$\$ # 1 "mc_line 14 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg expanding mc command in line" \$\$ MCWRK wr #0 \$\$ MCWRK zd \$\$ lo to LBLFO times td0 \$\$ \$\$ # 15 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg" \$\$ exit \$\$ \$\$ \$\$ ph1=0 2 2 0 1 3 3 1 \$\$ ph31=0 2 2 0 1 3 3 1 \$\$ \$\$ \$;pl1 : f1 channel - power level for pulse (default) |\$\$;p1 : f1 channel – high power pulse \$\$;d1 : relaxation delay; 1-5 * T1 |\$\$;NS: 1 * n, total number of scans: NS * TDO \$\$ \$\$ |\$\$;\$Id: zg,v 1.7 2002/06/12 09:05:19 ber Exp \$ ##\$RFLAX= ##\$BRUKER FILE EXP=uxnmr.par version 1.2.b.15 \$\$ ##TITLE= Parameter file. TOPSPIN \$\$ ##JCAMPDX= 5.0 Spectrometer \$\$ ##DATATYPE= Parameter Values \$\$ ##ORIGIN= Bruker BioSpin GmbH \$\$ ##OWNER= nmrsu configuration \$\$ \$\$ 2004-03-24 09:47:27.794 +0100 nmrsu@KASTOR \$\$ \$\$ D:/Bruker/ts12b15/conf/instr/spect/uxnmr.par \$\$ ##\$A⊂B= 0 **\$\$** ##\$ACBTAT= (0..15)

📕 exam1d_1H.dx - Editor

##\$SREGLST= <1H.CDCl3>

##\$sw_p= 6009.6153846154

Bruker specific parameters

##\$SI= 32768 ##\$SIGF1= 0

##\$SIGF2= 0 ##\$SINO= 400

##\$SSB= 0 ##\$STSI= 0 ##\$STSR= 0

##\$SYMM= 0 ##\$S_DEV= 0 ##\$TDeff= 0 ##\$TDoff= 0

##\$TI= <>
##\$TILT= no
##\$TM1= 0
##\$TM2= 0
##\$TOPLEV= 0
##\$USERP1= <user>
##\$USERP3= <user>
##\$USERP4= <user>
##\$USERP4= <user>
##\$USERP5= <user>

##\$WDW= 1 ##\$XDIM= 8192 ##\$YMAX_p= 0

##VAR_NAME=

##VAR_TYPE=

##SYMBOL=

##VAR_DIM=

##UNITS=

##FIRST=

##FACTOR=

##NTUPLES= NMR FID

##VAR_FORM= AFFN,

TIME,

32768,

SECONDS,

0.0001664,

INDEPENDENT,

×,

Ο,

\$\$

##\$SIOLD= 32768

Datei Bearbeiten Format Ansicht ?

_ 7 🛛

Some examples about the content of JCAMP:

Parameters

Spektrum/FID

##LAST= 5.4524288, ##MIN= -1582073, Ο. ##MAX= 5.4524288. 1314760, \$\$ Real data points ##PAGE= N=1 ##DATA TABLE= (X++(R..R)), XYDATA 40A91799M48n12N83o60P40q26Ř21j029j140j256j388j535j691j853K027k220Ķ425 58A264k637K868l103L334l557L743l850L786l356K129J032r650L8944k54830j358190 73a582073j854586M11558j302000j226544L6290j273191P96721j73042q89244 82e47767085271J45978j133348M44279M72009o35168M01170M84267o82213j71544 92c37066M33522i38221i43080j49054K9818l61o3958k5415K47905m7122l02574 103a97498M2830Ĵ5182L7174L23007j95939k51125L66947j45751k03962N14158 113C05023]20019m99378040266j11166n52803080611R8671n48724M78064J4400

FID/REAL,

DEPENDENT,

R,

1,

Ο,

ASDF,

32768,

FID/IMAG

DEPENDENT

Ι

ARBITRARY UNITS, ARBITRARY UNITS

1

ASDE

32768

Datasets as text file



The command **tojdx** converts NMR dataset into JCAMP format. It contains also peak information, audit trail, pulse program etc. Works on 1D and 2D data, raw/real/imaginary data.

The command **totxt** has been implemented to store the data of the displayed region in text format. Works on 1D and 2D data.

A new AU program **convbin2asc** has been implemented. It writes a 1D spectrum, with or without imaginary data points, into a file in ASCII table format.

Datasets as text file		
	File Edit Format View Help	
totxt	<pre>##TITLE=1H Cyclosporin ##JCAMPDX= 6.0 \$\$ Bruker NMR JCAMP-DX V2.0 ##DATA TYPE= NMR SPECTRUM ##DATA CLASS= NTUPLES ##ORIGIN= UXNMR, Bruker Analytische Messtechnik GmbH ##OWNER= root \$\$ XWIN-NMR Version 3.5 \$\$ Tue Sep 21 02:15:35 2004 w. Europe Daylight Time (UT+2h) BRUKER\svcu@XENIA ##.OBSERVE FREQUENCY= 500.13250065 ##.OBSERVE NUCLEUS= ^1H ##.ACQUISITION MODE= SIMULTANEOUS (DQD)</pre>	
🗉 exam1d_1H.txt - WordPad	$\square \square \boxtimes = 16$ = 16 RES= 18	
<u>File E</u> dit <u>V</u> iew Insert F <u>o</u> rmat <u>H</u> elp	TER/DATA SYSTEM= spect	
🗅 🚅 🖬 🎒 🔃 👭 🐰 階 🋍 い 🖳	NAME= $CDCl_3$ FERENCE= (INTERNAL, CDCl_3, 0, 11,008)	
<pre># File created = Saturday, April 16, 2005 6:27:36 AM CEST # Data set = a-009 # Spectral Region: # LEFT = 11.008049964904785 ppm. RIGHT = -1.0080566166148195 p</pre>	IL= \$\$ (NUMBER, WHEN, WHO, WHERE, WHAT) Audit trail, TOPSPIN Version 1.3.b.7 X= 5.01 = Bruker BioSpin GmbH svcu r/topspin1.3/data/guest/nmr/exam1d_1H/1/pdata/1/auditp.txt	
#	📱 ascii-spec.txt - WordPad	
# SIZE = 32768 (= number of points) #	File Edit View Insert Format Help	
" # In the following ordering is from the 'left' to the 'right' # Lines beginning with '#' must be considered as comment lines		
# _156545_52125	1, -5009457, 5505.364, 11.0079	^
-156179.59375	2, -4997747, 5505.181, 11.0075 3 -4993183 5504 998 11 0071	
-156036.96875	4, -4982248, 5504.814, 11.0068	
-155695.25	5, -4960490, 5504.631, 11.0064	
	6, -4943883, 5504.447, 11.0060	
-154347 34375	7, -4939115, 5504.264, 11.0057	
-153882.15625	8, -4924229, 5504.081, 11.0053	
-153178.4375	10, -4885418, 5503.714, 11.0046	
-152669.3125	11, -4876791, 5503.530, 11.0042	
-152399.71875	12, -4871369, 5503.347, 11.0038	
For Help, press F1	13, -4856147, 5503.164, 11.0035	
	14, -4842060, 5502.980, 11.0031	
	15, -4031020, 5502.797, 11.0027	
convhin 2pcc	17, -4807014, 5502.430, 11.0020	
CONVDITZASC	18, -4791021, 5502.247, 11.0016	
	19, -4780020, 5502.063, 11.0013	
	20, -4765746, 5501.880, 11.0009	
	21, -4/50/65, 5501.696, 11.0005	~
	For Help, press F1	

NMR meets Excel





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