

# topspi∩ User Manual

Manual for TopSpin 2.1 Version 2.1.1

**Bruker BioSpin** 

# TopSpin 2.1 Version 2.1.1

#### User Manual

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# Contents

Chapter 1	Intro	duction	. 1
-	1.1	About the User Manual	I
	1.2	Safety Regulations	II
	1.3	User Manual Conventions	II
		Font Conventions	II
		File/directory Conventions	. 111
		User Action Conventions	. 111
	1.4		. 111
		Functionality	. 111
		Available Documentation	. IV
	1.5	TOPSPIN license	. V
	1.6	TopSpin program versions	. V
•		· · · · · · · · · · · · · · · · · · ·	. V
Chapter 2	Getti	ing Started	19
	2.1	Startup TOPSPIN	.19
	2.2	Configuration	.20
	2.3	How to Display Spectra	.21
		How to Open Data from the Menu	.21
		How to Open Data from the Browser	.21
		How to Define Alias Names for Data	.22
		How to Open Data in Archive Data Directories	.22
	<b>.</b>	How to Open Data in Other Ways	.22
	2.4	How to Expand a Spectral Region.	.23
	2.5	How to Display Peaks, Integrals, together with the Spectrum.	.23
	2.6	How to Display Projections/1D Spectra with 2D Spectra	.23
	2.7	How to Superimpose Spectra in Multiple Display	.24
	2.8	How to Print or Export the Contents of a Data window	.24
		How to Print Data	.24
		How to Copy a Data Window to Clipboard	.25
	2.0	How to Store (Export) a Data window as Graphics File	.20
	2.9	How to Archive Data	.20
	2.10	How to Import NMP Data Stored in Special Formats	.21
	∠.11 2.12	How to Fit Peaks and Deconvolve Overlanning Peaks	.20 28
	2.12	How to Compute Fide by Simulating Experiments	20
	2.13	How to Add Your Own Eurocionalities	.29
	2.14	How to Create Macros	. 29 20
			.29

		How to Create AU (automation) Programs	9
		How to Create Python Programs	)
	2.15	How to Automate Data Acquisition	)
Chapter 3	The	TOPSPIN Interface	I
	3.1	The Topspin Window	1
		How to Use Multiple Data Windows	2
		How to Use the Menu bar	3
		How to Use the Upper Toolbar (1D data)	4
		How to Use the Lower Toolbar (1D data)	5
	3.2	Command Line Usage	7
		How to Put the Focus in the Command Line	7
		How to Retrieve Previously Entered Commands	7
		How to Change Previously Entered Commands	3
		How to Enter a Series of Commands	3
	3.3	Command Line History	3
	3.4	Starting TOPSPIN commands from a Command Prompt	9
	3.5	Function Keys and Control Keys40	)
	3.6	Help in Topspin	4
		How to Open Online Help documents45	5
		How to Get Tooltips45	5
		How to Get Help on Individual Commands	5
		How to Use the Command Index	5
	3.7	User Defined Functions Keys47	7
	3.8	How to Open Multiple TOPSPIN Interfaces47	7
Chapter 4	Τroι	uble Shooting	•
	4.1	General Tips and Tricks49	9
	4.2	History, Log Files, Spooler Reports, Stack Trace	9
	4.3	How to Show or Kill TOPSPIN processes	3
	4.4	What to do if TOPSPIN hangs	1
	4.5	How to Restart User Interface during Acquisition	5
Chapter 5	Data	aset Handling	7
	5.1	The Topspin Browser	7
		How to Open the Browser in a separate window	1
		How to Put the Focus in the Browser	1
		How to Select Folders in the Browser	2
		How to Expand/Collapse a Folder in the Browser	2
		How to Show/Hide Pulse program and Litle in the browser62	2
		How to Show Dataset Dates in the Browser	3
		How to change the default 1 op Level Data Directory	4
		How to Add, Remove or Interpret Alias Names	+
	5.2	Creating Data	S

		How to Create a New Dataset	.65
	5.3	Opening Data	.66
		How to Open Data Windows Cascaded	.67
		How to Open Data from the Browser	.68
		How to Automatically Select the first expno/procno of a dataset	.69
		How to Open Data from the Topspin menu	.70
		How to Open Data from the Explorer, Konqueror or Nautilus	.72
		How to Open Data from the Command Line	.73
		How to Open Special Format Data	.75
		How to Open a ZIP or JCAMP-DX file	
		from the Windows Explorer	.76
	5.4	Saving/Copying Data	.77
		How to Save or Copy Data	.77
		How to Save an Entire Dataset	.78
		How to Save Processed Data	.78
		How to Save Acquisition Data	.78
		How to Save Processed Data as Pseudo Raw Data	.78
	5.5	Deleting Data	.79
		How to Delete a Specific Dataset	.79
		How to Delete Types of Datasets	.79
	5.6	Renaming Data	.79
		How to Rename a Specific Dataset	.79
	5.7	Searching/Finding Data	.82
		How to Find Data	.82
		How to Display one of the Found Datasets	.83
	5.8	Handling Data Files	.85
		How to List/Open the Current Dataset Files	.85
		How to List/Open the current Dataset Files	
	_	in the Windows Explorer	.86
Chapter 6	Para	meter Handling	. 89
	6.1	Processing Parameters	.89
		How to Set a Processing Parameter from the Command Line	.89
		How to Set Processing Parameters from the Parameter Editor .	.90
		How to Undo the Last Processing Parameter Change	.92
		How to Display Processing Status Parameters	.92
		How to Switch to Maxent parameters	.92
		How to Change Processed Data Dimensionality	.92
	6.2	Acquisition Parameters	.93
		How to Set Acquisition Parameters	.93
		How to Set an Acquisition Parameter from the Command Line .	.93
		How to Set Acquisition Parameters from the Parameter Editor .	.94

		How to Undo the Last Acquisition Parameter Change	.96
		How to Set Pulse Program Parameters	.96
		How to Display Acquisition Status Parameters	.96
		How to Get Probehead/Solvent dependent Parameters	.96
		How to Change Acquisition Data Dimensionality	.97
		How to Set Lock Parameters	.97
		How to Set Routing Parameters	.97
Chapter 7	Data	a Processing	99
	7.1	Interactive Processing	.99
		How to Process Data with Single Commands	.99
		How to Process data with Composite Commands	100
	7.2	Semi-automatic Processing.	100
		How to Use the 1D Processing Dialog	100
		How to Use the Processing Guide in Automatic mode	101
		How to Use the Processing Guide in Interactive mode	103
	7.3	Processing Data with AU programs	103
	7.4	Serial Processing	104
Chapter 8	Prin	ting/Exporting Data1	109
	8.1	Printing/plotting Data	109
		How to Print/Plot from the Menu	109
		How to Plot Data from the Processing guide	111
		How to Plot Data with the Plot Editor	112
		How to Print the Integral list	112
		How to Print the Peak list	112
	8.2	Exporting Data	113
		How to Copy data to Other Applications	113
		How to Store (Export) a Data Window as Graphics File	114
Chapter 9	1D D	Display1	115
	9.1	The 1D Data Window	115
	9.2	Displaying one Dataset in Multiple windows	116
		How to Reopen a Dataset in a Second/Third etc. Window	116
		How to Rescale or Shift one Dataset in Multiple windows	117
	9.3	Changing the Display of a 1D Spectrum or FID	118
		How to Change the Vertical Scaling of the FID or Spectrum	118
		How to Smoothly Change the Vertical Scaling	
		of the FID/Spectrum	118
		How to Change the Horizontal Scaling of the FID or Spectrum .	119
		How to Shift a Spectral Region to the Left or to the Right	120
		How to Shift the Spectrum Up or Down	120
	9.4	Using the Tab bar	121
		How to Display the Spectrum	121

		How to Set Processing Parameters	.122
		How to Set Acquisition Parameters	.123
		How to Edit the Title	.124
		How to Edit the Pulse Program	.125
		How to Display the Peak list	.125
		How to Display the Integral list	.134
		How to view Sample Information	.142
		How to Open the Jmol Molecule Structure Viewer	.143
		How to Display the FID	.145
	9.5	1D Display Options	.145
		How to Toggle between Hertz and ppm Axis Units	.145
		How to Switch on/off the Spectrum Overview display	.145
		How to Switch Y-axis Display	.146
	9.6	Show Display Properties/Regions/Files	.146
		How to Superimpose the Cursor Information	.148
		How to Superimpose the Title on the Spectrum	.149
		How to Superimpose the main Status Parameters	
		on the Spectrum	.149
		How to Superimpose the Integral Trails/Labels	
		on the Spectrum	.149
		How to Superimpose Peak Labels on the Spectrum	.149
		How to Show Peak Annotations on the Spectrum	.150
		How to Show Individual Data Points of the Spectrum	.150
		How to Superimpose the Electronic Signature on the Spectrun	า 150
		How to Display the Main Dataset Properties	.150
		How to Display a List of Files of a Dataset	.151
	9.7	Saving Display Region	.154
	9.8	Synchronize Visible Region of all Data Windows	.155
Chapter 10	2D D	visplay	157
	10.1	The 2D Data Window	.157
	10.2	Changing the Display of a 2D spectrum	.158
		How to Change the Intensity Scaling (contour levels)	.158
		How to Smoothly Change the Vertical Scaling (contour levels)	.159
		How to Display a Contour Levels Bar in the Data Window	.159
		How to Switch on/off Square 2D layout	.160
		How to Zoom a 2D spectrum in/out	.161
		How to Shift a Spectral Region in the F2 direction (left/right)	.162
		How to Shift a Spectral Region in the F1 direction (up/down) .	.162
	10.3	Show Display Properties/Regions/Files	.162
	10.4	Using the Tab bar	.165
		How to Set Processing Parameters	.165

		Hausta Oat Association Demonstrate	405
		How to Set Acquisition Parameters	105
		How to Display the Peak list	166
		How to Display the Integral list	
		How to Display the FID	
	10.5	2D Display Options	169
		How to Switch between Hertz and ppm Axis Units	
		in F2 and F1	169
		How to Switch on/off the Spectrum Overview display	169
		How to Switch on/off the Projection display	170
		How to Switch on/off the Grid display	172
		How to Display a 2D Spectrum in Contour Mode	173
		How to Set the 2D Contour Levels	174
		How to Store interactively set Contour Levels	175
		How to Display a 2D spectrum in Pseudo Color Mode	176
		How to Display a 2D Spectrum in Oblique Mode	176
		How to Botate a 2D Spectrum in Oblique Mode	178
		How to Switch between Displaying Desitive	
		and Negative Javala	170
Chanter 11	D. F		470
Chapter 11			179
	11.1	Display Planes of 3D Data	179
		How to Switch to 2D Plane Display	180
		How to Display various Plane Orientations	180
		How to Display various Plane Positions (numbers)	181
	11.2	3D Cube Display Mode	182
		How to Display the 3D Cube	182
		How to Rotate the 3D Cube	182
		How to Scale Up/Down the 3D Cube	183
		How to Reset the Cube Size and Orientation	183
		How to Switch Depth Cueing on/off	183
		How to Display a Cube Front or Side view	183
	11.3	nD parameter display	183
	11.4	nD Fid Display.	185
	11.5	nD Peak and Integral Display	186
Chapter 12	1D Ir	nteractive Manipulation	189
•	12.1	1D Interactive Window multiplication.	189
		How to Switch to Window Multiplication Mode	189
	12.2	1D Interactive Phase Correction	191
		How to Switch to Phase Correction Mode	
		How to Perform a Typical 1D Interactive Phase Correction	192
		How to Set the Phase Pivot Point	102
		How to Perform Default Zero Order Desso Correction	102
		TIOW TO LENOTH DEIGUIL ZEID OTUELE HASE COTTECTION	

	How to Perform Interactive Zero Order Phase Correction193
	How to Perform Interactive First Order Phase Correction193
	How to Perform 90, -90 or 180° Zero Order Phase Correction . 193
	How to Reset the Phase to the Original Values
	How to Change the Mouse Sensitivity
	How to Return from Phase Correction Mode with/without Save 194
12.3	1D Interactive Integration
	How to Switch to Integration Mode
	How to Define Integral Regions
	How to Select/Deselect Integral Regions
	How to Read Integral Regions from Disk
	How to Perform Interactive Bias and Slope Correction199
	How to Set the Limit for Bias Determination
	How to Change the Mouse Sensitivity
	How to Calibrate/Normalize Integrals
	How to Scale Integrals with respect to Different Spectra201
	How to Delete Integral Regions from the Display201
	How to Scale Selected Integrals
	How to Move the Integral Trails Up/Down203
	How to Cut Integral Regions
	How to Save Integral Regions
	How to Undo the Last Region Operation
	How to Return from the Integration Mode with/without Save204
12.4	1D Interactive Calibration
	How to Switch to Calibration Mode
	How to Calibrate a Spectrum Interactively
12.5	1D Multiple Display
	How Switch to Multiple Display Mode and
	Read Multiple Spectra
	How to Select/Deselect Datasets
	How to Remove a Dataset from Multiple Display
	How to Display the Sum or Difference Spectra
	How to Save the Sum or Difference Spectra
	How to Display the Next/Previous Name/Expno
	How to Toggle between Superimposed and Stacked Display
	How to Shift and Scale Individual Spectra
	How to move the selected spectrum one place up/down 213
	How to Switch on/off the Display of Datapaths
	and Scaling Factors 214
	How to Return from Multiple Display mode 214
	How to Set the Colors of the 1 <sup>st</sup> 2 <sup>nd</sup> Dataset 214

	12.6	1D Interactive Baseline Correction	.214
		How to Switch to Baseline Correction Mode	.214
		How to Perform Polynomial Baseline Correction	.215
		How to Perform Sine Baseline Correction	.216
		How to Perform Exponential Baseline Correction	.216
		How to Preview the Baseline Corrected Spectrum	.216
		How to Reset the Baseline Correction Line	.217
		How to Change the Mouse Sensitivity	.217
		How to Save the Baseline Correction and/or Return	.217
		How to Perform Cubic Spline Baseline correction	.218
		How to Delete Spline Baseline Points from the screen	.219
		How to Return from Cubic Spline Baseline mode	
		with/without Save	.219
	12.7	1D Interactive Peak Picking	.220
		How to Switch to Peak Picking Mode	.220
		How to Define New Peak Picking Ranges	.221
		How to Change Peak Picking Ranges	.221
		How to Pick Peaks in Peak Picking Ranges only	.221
		How to Delete all Peak Picking Ranges	.222
		How to Define Peaks Manually	.222
		How to Pick Peaks Semi-Automatically	.222
		How to Delete Peaks from the Peak List	.223
		How to Return from Peak Picking Mode with/without Save	.224
Chapter 13	2D Ir	nteractive Manipulation	225
	13.1	2D Interactive Phase Correction	.225
		How to Switch to 2D Interactive Phase Correction	.225
		How to Perform a Typical 2D Interactive Phase Correction	.226
		How to Scale or Shift Individual Rows/Columns	.229
		How to Perform Smooth Phase Correction	.230
		How to Perform 90, -90 or 180° Zero Order Phase Correction	.231
		How to Reset the Phase to the Original Values	.231
		How to Change the Mouse Sensitivity	.231
		How to Show the Next/Previous Row or Column	.231
		How to Arrange Rows or Columns	.232
		How to Return from Multi-1D Phase to 2D Phase Display	.232
		How to Return from 2D Phase Mode	.232
	13.2	2D Interactive Integration	.232
		How to Move an Integral region	.237
		How to Copy an Integral region	.237
		How to Delete all Integral Regions	.237
		How to Read/Import Integral Regions	.237

		How to Save/Export Integral Regions	238
		How to Return from 2D Integration mode	238
	13.3	2D Multiple Display and Row/Column Handling	238
		How Switch to Multiple Display mode and	
		Read Multiple Spectra	238
		How to Align Multiple 2D Spectra	241
		How to Display the Next/Previous Name/Expno	241
		How to Scan Rows/Columns	242
		How to Grab a Row/Column	242
		How to Show the Next/Previous Row or Column	243
		How to Move the Selected Dataset Up/Down in Dataset List	244
		How to Extract a Row/Column	244
		How to Copy Contour Levels from First to Other Spectra	245
		How to Switch on/off 2D contour display	245
		How to Position the Baseline of the Row/Column	245
	13.4	2D Interactive Calibration	246
		How to Switch to 2D Calibration mode	246
		How to Perform 2D Calibration	247
	13.5	2D Chemical Shift Distance Measurement	247
		How to Measure a 2D Chemical Shift Distance	247
Chapter 14	Data	Window Handling	249
Chapter 14	<b>Data</b> 14.1	Window Handling           Data Windows	<b>249</b> 249
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window	<b> 249</b> 249 250
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window	<b> 249</b> 249 250 250
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window	249 249 250 250 251
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window	249 250 250 251 252
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows	249 250 250 251 252 252 252
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window	249 250 250 251 252 252 252 254
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window	249 250 250 251 252 252 252 254 255
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Maximize a Data Window	249 249 250 250 251 252 252 254 255 255
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Restore the Size and Position of a Data Window	249 249 250 250 251 252 252 255 255 255
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window	249 249 250 250 251 252 252 255 255 255 255
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window         How to Iconify all Data Window	. 249 249 250 250 251 252 252 255 255 255 255 255 255
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window         How to Iconify all Data Window         How to Maximize all Data Windows	. 249 249 250 250 251 252 252 254 255 255 255 255 256 256 256
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window         How to Iconify all Data Windows         How to Aximize all Data Windows         How to Activate the Next Data Window	. 249 . 250 . 250 . 250 . 251 . 252 . 252 . 254 . 255 . 255 . 255 . 255 . 256 . 256 . 256 . 256 . 256
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Arrange Data Windows         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window         How to Iconify all Data Window         How to Kestore the Size and Position of a Data Window         How to Close a Data Window         How to Activate the Next Data Window         Window Layouts	. 249 249 250 250 251 252 252 255 255 255 255 256 256 256 256 256 256
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Iconify (minimize) a Data Window         How to Iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window         How to Iconify all Data Window         How to Iconify all Data Window         How to Activate the Next Data Window         How to Activate the Current Window Layout         How to Save the Current Window Layout	. 249 249 250 250 251 252 252 255 255 255 255 255 256 256 256 256 256 256 256 256
Chapter 14	<b>Data</b> 14.1 14.2	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Iconify (minimize) a Data Window         How to Iconify (minimize) a Data Window         How to De-iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window         How to Iconify all Data Windows         How to Arringe all Data Windows         How to Save the Next Data Window         How to Save the Current Window Layout         How to Read a Window Layout	. 249 249 250 250 251 252 252 255 255 255 255 256 256 256 256 256 256 256 256 256 256
Chapter 14	<b>Data</b> 14.1	Window Handling         Data Windows         How to Move a Data Window         How to Resize a Data Window         How to Select (activate) a Data Window         How to Open a New empty Data Window         How to Open a New empty Data Window         How to Iconify (minimize) a Data Window         How to Iconify a Data Window         How to Restore the Size and Position of a Data Window         How to Close a Data Window         How to Iconify all Data Window         How to Arrange all Data Window         How to Activate the Next Data Window         How to Save the Current Window Layout         How to Read a Window	. 249 249 250 250 251 252 252 255 255 255 255 256 256 256 256 256 256 256 256 256 256 257

Chapter 15	Analysis	9
	15.1 Introduction	9
	15.2 Chemical Shift Distance Measurement	0
	How to Measure a Chemical Shift Distance	0
	15.3 1D Signal to Noise Calculation	0
	How to Perform Interactive S/N Calculation	0
	How to Delete the Signal Region or Noise Region	2
	How to Edit the Limits of the Signal Region or Noise Region26	2
	How to Change Width of the Signal Region or Noise Region26	2
	15.4 Relaxation Analysis	3
Chapter 16	Acquisition	1
	16.1 Acquisition Guide27	1
	16.2 Acquisition Toolbar	3
	16.3 Data window Toolbar	5
	16.4 Acquisition Status Bar	6
	16.5 Command Queuing and Scheduling	8
	16.6 Tuning and Matching the Probehead	9
	16.7 Locking	1
	16.8 BSMS Control Panel	2
	16.9 Interactive Parameter Adjustment (GS)	4
	16.10 Running an Acquisition	6
	16.11 Shape tool	0
<b>.</b>	Easy definition of Shape pulses	2
Chapter 17	Configuration/Automation	7
	17.1 NMR Superuser and NMR Administration password	7
	How to Change the NMR Administration Password	8
	17.2 Configuration	8
	How to Perform a Default Configuration on a Datastation29	9
	How to Perform a Customized Configuration on a Datastation .29	9
	17.3 Parameter set conversion	0
	17.4 Automation	0
	How to Install AU Programs	0
	How to Open the AU Program Dialog Box	0
	How to Switch to the List of User defined AU Programs	2
	How to Switch to the List of Bruker defined AU Programs30	2
	How to Define the AU Programs Source Directory	2
	How to Create an AU Program	2
	How to Edit an Existing AU Program	3
	How to Execute an AU Program	3
	How to Delete an AU Program	3
	How to Show Comments in the AU Program List	3

Chapter 18	Regulatory Compliance	05
	18.1 Audit Trails	05
	18.2 Electronic Signatures	10
	18.3 Password Controlled Login Identification	13
Chapter 19	Remote Control	19
	19.1 Remote control	19
	19.2 How to Establish a Remote Connection from your PC3	19
	19.3 How to Make a Remote Connection without a Local License 32	26
	19.4 Security of Remote Connections	26
	19.5 How to Access ICON-NMR from a Remote Web Browser	27
Chapter 20	User Preferences	29
	20.1 User Preferences	29
	How to Open the Last Used Dataset on Startup	32
	How to Define the Startup Actions	32
	How to Define Auto-Termination after Idle Time	32
	How to Define Auto-Locking after Idle Time	33
	How to Change the Preferred Editor	34
	How to Configure the Tab Bar	35
	How to Configure the Right-click Menu Function	35
	How to Change Colors of Data Objects on the Screen	36
	How to Change Colors of Data Objects on the Printer	36
	How to Change Colors of the Lock Display	37
	How to Create a New Data Window Color Scheme	37
	How to Read a Different Data Window Color Scheme	38
	How to Change Peak and Integral table Colour/Spacings	38
	How to Create Thick Lines on the Screen	40
	How to Create Thick Lines on the Printer	40
	How to Change All Fonts of the Toppplumentu	40
	How to Change the Font of the Topspin menu	41
	How to Change the Font of the Tab bar	42
	How to Change the Font of the Proweer	43
	How to Change the Fort of the Command Line	43
	How to Change the Fort of the Status Line	44
	How to Auto-Archive existing express	44
	20.2 Command Line Preferences	44
	How to Resize the Command Line	45
	How to Set the Minimum and Maximum Command Line Size 3.	46
	20.3 Disabling/Enabling Toolbar Buttons Menus and Commands 3	46
	How to Hide the Upper and Lower Toolbars	46
	How to Hide the Menubar	47
		. /

	How to Disable/Remove Toolbar Buttons	347
	How to Disable/Remove Menus or Commands	348
	How to (Re)enable a disabled Command/Menu	350
	How to (Re)enable All Commands/Menus	350
20.4	Resizing/Shifting Toolbar Icons	350
	How to Change the Toolbar Icon Size	350
	How to Shift Toolbar Icons to the Right	350
20.5	Defining Source Directory for Programs/Lists etc	351
User	Extensions	353
21.1	User Notebook	353
21.2	Macros	354
21.3	AU Programs	354
21.4	Python Programs	355
21.5	Button Panels	356
21.6	Adding User Defined Buttons to the Toolbars	359
21.7	Adding User Defined Menus to the Menubar	362
21.8	Adding User Defined Guides	364
	20.4 20.5 <b>User</b> 21.1 21.2 21.3 21.4 21.5 21.6 21.7 21.8	<ul> <li>How to Disable/Remove Toolbar Buttons</li> <li>How to Disable/Remove Menus or Commands</li> <li>How to (Re)enable a disabled Command/Menu</li> <li>How to (Re)enable All Commands/Menus</li> <li>20.4 Resizing/Shifting Toolbar Icons</li> <li>How to Change the Toolbar Icon Size</li> <li>How to Shift Toolbar Icons to the Right</li> <li>20.5 Defining Source Directory for Programs/Lists etc.</li> <li>User Extensions</li> <li>21.1 User Notebook</li> <li>21.2 Macros.</li> <li>21.3 AU Programs.</li> <li>21.4 Python Programs.</li> <li>21.5 Button Panels</li> <li>21.6 Adding User Defined Buttons to the Toolbars</li> <li>21.7 Adding User Defined Menus to the Menubar</li> <li>21.8 Adding User Defined Guides.</li> </ul>

# Chapter 1 Introduction

### 1.1 About the User Manual

#### 1. About this document

The User Manual describes the main aspects of Brukers integrated software package TopSpin. This manual enables all users who work with Bruker software to get an overview of the various functionalities of Top-Spin. The main aspects outlined in here describe the possibilities and functionaries of the TopSpin interface and elucidate working processes for data acquisition and processing.

#### 2. Target audience

The Bruker User Manual for TopSpin 2.1 and newer supports all Bruker users who already work with Bruker software products or who newly enter the software dimension of TopSpin. The main aspect of this Manual is to enable new TopSpin users and experienced TopSpin users to work with this software package.

#### 3. How to get the User Manual

The User Manual is available as a hard copy just like an electronically copy on the TopSpin DVD in the menu-section *Help*, where all other Bruker Manuals are provided, too. For detailed information about all Bruker software manuals please refer to chapter 1.4. The latest version of the User Manual is also provided on the Bruker Web Server:

http://www.bruker-biospin.com/documentation\_general.html

#### 4. How to read the User Manual

The User Manual describes especially the TopSpin interface with all its functionalities to acquire, process and interpret spectrometer data. To find information more readily you can read selected chapters, depending on your requirements, or read the User Manual in succession for general information.

# **1.2 Safety Regulations**

In order to work safely in laboratries with NMR-spectrometers all users have to follow the safety regulations for magnetic, electrical, cryogenic and chemical safety. For detailed information please refer to the safety instructions in the Beginners Guide Manual provided on the TopSpin DVD.

# **1.3 User Manual Conventions**

The User Manual utilizes different script types in order to make selected text more transparent and explicable to users. Please note that this document contains the following conventions:

#### **Font Conventions**

*abs* - commands to be entered on the command line are in *Courier bold italic* 

ProcPars - menus, buttons, icons to be clicked are in Arial bold

fid - filenames are in Courier

name - any name which is not a filename is in Arial italic

#### **File/directory Conventions**

<tshome> - the TOPSPIN installation (home) directory

#### **User Action Conventions**

- + a single user action
- 1. the first action of a sequence
- 2. the second action of a sequence
- 3. etc.
  - a) the first action of a sub-sequence
  - b) the second action of a sub-sequence
  - c) etc.

# **1.4 TOPSPIN Overview**

### Functionality

TOPSPIN is an integrated software package for:

- Displaying NMR spectra
- Printing and plotting spectra
- · Exporting displays and plots in various graphics and metafile formats
- Importing NMR data from files of various formats
- Archiving spectra in various formats such as JCAMP-DX and ZIP
- E-mailing data
- Processing 1D-6D fids and spectra: window multiplication, various transforms (Fourier, Hilbert, DOSY), phase correction, baseline correction, integration, peak picking, linear prediction, smoothing, adding spectra etc.
- Displaying multiple superimposed spectra (1D and 2D).
- Simulating 1D and multi-dimensional fids, given a pulse program and a spin system ("virtual spectrometer nmr-sim")
- Calculating T1/T2 relaxation times

- Fitting peaks with Lorentzian and Gaussian line shape models, deconvolve overlapping peaks
- Multiplet analysis
- Automatic 1D, 2D and 3D peak picking
- Automatic 1D, 2D and 3D integration
- Line shape analysis of solids spectra
- Data acquisition with Bruker Avance type spectrometers
- Supporting automated and walk-up spectrometers (ICON-NMR)
- Remote spectrometer control including web-enabled ICON-NMR
- Adding user defined functionalities to TOPSPIN (AU programs, Macros and Python programs)

#### **Available Documentation**

In TOPSPIN 2.1 and newer the  $\textbf{Help} \rightarrow \textbf{Manuals}$  submenu, contains list of available manuals for the following items:

#### General

Beginners Guides

**Acquisition - Users Guides** 

**Acquisition - Application Manuals** 

**Acquisition & Processing Reference** 

**Automation and Plotting** 

Analysis and Simulation

**Programming Manuals** 

**Technical Manuals** 

**Installation Guides** 

#### **Good Laboratory Practice**

Each document is listed with a short description of its contents.

# **1.5 TOPSPIN license**

TOPSPIN requires a license for startup. A license can be ordered online from:

```
www.bruker-biospin.de/NMR/nmrsoftw/licenses/index.html
```

If your PC controls a spectrometer, TOPSPIN will start up without a license. Furthermore, you can use TOPSPIN for developer purposes with restricted functionality. In this case you have to start it from a Windows Command prompt or Linux shell as follows;

topspin -developer

# 1.6 TopSpin program versions

The TopSpin DVD (2.1 and newer) contains the following program versions:

- TOPSPIN
- TOPSPIN Plot Editor
- ICON-NMR
- NMR-SIM
- NMR-GUIDE
- AUTOLINK

The following programs are distributed as part of the TopSpin DVD, but they must be licensed separately:

- AMIX
- AUREMOL
- PERCH NMR TOOLS (only for Windows operating system)

# Chapter 2 Getting Started

### 2.1 Startup TOPSPIN

#### **Under Windows**

IN Click the TOPSPIN icon on the desktop

or

Start TOPSPIN from a Command Prompt as follows:

- 1. Click Start  $\rightarrow$  Run, enter *cmd* and click OK
- 2. In the Command Prompt:
  - a) Enter cd <tshome>
  - b) Enter topspin

where <tshome> is the directory where TOPSPIN is installed.

#### **Under Linux**

- 1. Open a Linux Shell or Terminal Window
- 2. In the Shell/Terminal:
  - a) Enter cd <tshome>
  - b) Enter ./topspin

where <tshome> is the directory where TOPSPIN is installed.

#### Startup TOPSPIN specifying dataset

Topspin can be started with a dataset option:

1. Open a Windows Command Prompt or Linux Shell

#### 2. Enter topspin -j TOP\_DATA:<dataset path>

The specified dataset is automatically displayed after startup.

Examples:

```
topspin -j TOP_DATA:c:\bio\data\guest\nmr\exam1d_1H\1\pdata\1
```

topspin -j TOP\_DATA:c:\bio\data\guest\nmr\exam1d\_1H\1\pdata\1\1r

topspin -j TOP\_DATA:c:\jcamp.dx

topspin -j TOP\_DATA:c:\data-archive.zip

# 2.2 Configuration

After the installation of TOPSPIN, it must be configured once. TOPSPIN may be used in two different ways:

#### on a computer which controls a spectrometer

The command *cf* must be executed once, to configure the spectrometer hardware. Just type this command and follow the instructions on the screen. At the end of the dialog, further configuration commands, like *expinstall*, are offered and can be started from there.

#### on a computer which is used as datastation

The only configuration command to be executed is *expinstall*. This allows you to install pulse programs, AU programs, lists etc. Just type this command and follow the instructions on the screen, selecting **Installa-***tion for Datastation (default)*.

Note that the commands *cf* and *expinstall* can be started from the command line or from the **Options** or **Spectrometer** menu. However, the latter menu is only available after *cf* has been performed once, choosing

#### Installation for spectrometer.

After the configuration has finished, TOPSPIN is ready to be used. The configuration only needs to be repeated when you have installed a new version of TOPSPIN or if your spectrometer hardware has changed.

More details on configuration can be found in chapter 17.2 and the descriptions of *cf* and *expinstall* in the Acquisition Reference Manual.

# 2.3 How to Display Spectra

In this chapter, opening data in standard Bruker format is described. Opening other data formats is described in chapter 5.

Please note that a standard Bruker dataset is a directory tree rather than a single file:

<dir>\data\<user>\nmr\<dataset name>\<expno>\pdata\<procno>

e.g.

c:\bruker\topspin\data\guest\nmr\exam1d\_13C\1\pdata\1

#### How to Open Data from the Menu

Open the **File** menu and click **Open...** A dialog box appears. Select the first option, the Browser type **File Chooser** and click **OK**. A file browser appears. Navigate to your data directory and expand it to the level of *names*, *expnos*, or *procnos* (double-click a directory to expand it). Select the desired item and click **Display**.

The selected dataset replaces the contents of the currently selected (active) window. If no data window was displayed, a new one will be created. Alternatively, you can first create a new window by clicking **Window**  $\rightarrow$  **New Window** [Alt+w n) and then open a dataset from the file browser in that window.

The file browser can also be opened by entering *reb* on the command line.

#### How to Open Data from the Browser

TOPSPIN has data browser which, by default, displays the top level data di-

rectory (*<dir>*) with Bruker example data. You can add your own data directories, local or remote, as follows:

- 1. Move the cursor into the browser area
- 2. Right-click and choose Add New Data Dir... in the popup menu
- 3. Enter the desired data directory (< dir>) and click OK

Your data directory will now appear in the browser

In order to display data from the Browser, proceed as follows:

- 1. Expand your top level directory (*<dir>*) in the browser to the level of the data *name*, *expno* or *procno*
- 2. Select the desired item and drag it into the data area

#### How to Define Alias Names for Data

- 1. Open the dataset for which you want to define an alias name
- 2. Click the Alias tab at the top of the data browser.
- 3. Right-click in the browser and choose

#### Define alias for data in selected window

Alternatively, you can enter the command *dalias* on the command line.

#### How to Open Data in Archive Data Directories

Topspin 2.0 and newer allows opening datasets that are stored in the following directory structures:

<mydata>/<name>/<expno>/pdata/<procno>

You can do that with the TOPSPIN command *reb* or from the Operating System File Browser with **Copy & Paste** or **Drag & Drop**. Actually, the data are copied to the data directory:

<tshome>/data/<user>/nmr/<name>/<expno>/pdata/<procno>

where <tshome> is the TOPSPIN installation directory and <user> is the current (internal) TOPSPIN user.

#### How to Open Data in Other Ways

TOPSPIN provides various other ways of displaying data. You can, for example, use command line commands like *re*, *rew*, *rep* and *dir*. Details

on these features can be found in chapter 5.3 and in the Processing Reference Manual.

# 2.4 How to Expand a Spectral Region

To expand a certain spectral region:

Real Click-hold the left mouse button on one side of the region, drag the cursor to the other side and release the mouse.

If you want to cancel the expansion while dragging the mouse, just move the mouse out of the data area and release it.

An alternative way of expanding a region is clicking the button repeatedly and then shifting the spectrum to the proper position.

# 2.5 How to Display Peaks, Integrals, ... together with the Spectrum

When a spectrum is displayed, you can superimpose its title, parameters, integrals, and peaks as follows:

- 1. Move the cursor into the data window that contains the spectrum
- 2. Right-click and choose Display Properties... in the popup menu
- 3. Check the desired items and click OK

Please note that the selected items are only shown if they are available. For example, peaks and integrals are only shown if peak picking and integration have been performed, respectively (see also chapter 12). The number of displayed digits for the integral and peak labels can be set in the User Preferences (click **Options**  $\rightarrow$  **Preferences**  $\rightarrow$  **Spectrum**).

# 2.6 How to Display Projections/1D Spectra with 2D Spectra

To display projections or 1D spectra in tandem with a 2D spectrum:

1. Open a 2D spectrum

- 2. If no projections are shown, click the 💼 button in the upper toolbar or enter .pr on the command line.
- 3. Move the cursor into the F1 or F2 projection area.
- Right-click and choose one of the options. With External Projection... an existing 1D spectrum can be read. This can be a regular 1D spectrum or a 2D projection that was stored as a 1D spectrum. With Internal Projection the positive projection can be calculated and displayed.

An alternate way to calculate projections is the following:

```
\mathbb{R} Click Processing \rightarrow Display Projections...[projd]
```

or

Right-click on a 1D dataset in the browser and choose:

**Display As 2D Projection** 

# 2.7 How to Superimpose Spectra in Multiple Display

TOPSPIN allows you to compare multiple spectra in Multiple Display mode. To enter this mode, click the  $\pm$  button in the upper toolbar or enter .md on the command line. When you open a dataset now, for example drag one from the browser, it will be superimposed on the current spectrum rather than replacing it. Several multiple display functions are available now in the data window toolbar. Most importantly, you can *scale* and *shift* each spectrum individually. This allows exact alignment of corresponding peaks of different spectra.

Multiple display mode is supported for 1D and 2D spectra. In 2D, you can superimpose an arbitrary number of 1D or 2D spectra.

# 2.8 How to Print or Export the Contents of a Data Window

#### How to Print Data

A TOPSPIN data window may contain various objects like an fid, a spectrum, expansions of a spectrum, superimposed spectra, spectrum components such as parameters, peaks, integrals, cross sections etc. Whatever the content of the data window is, it can be printed as follows: type Ctrl+p or click **File**  $\rightarrow$  **Print**..., select **Print active window** in the appearing dialog box and click **OK**.

The other options in this dialog box enable you to use or create plot layouts. Details on this can be found in the Plot Editor manual to be found under **Help**  $\rightarrow$  **Manuals**  $\rightarrow$  **Plotting**.

The colors of the printed data can be chosen in the User Preferences dialog box. Just enter the command set or click **Options**  $\rightarrow$  **Preferences**... and click **Printer** in the left part of the dialog box.

#### How to Copy a Data Window to Clipboard

Under MS Windows, you can easily copy the data window contents to other applications. To do that, type copy or click **Edit**  $\rightarrow$  **Copy**. This will copy the data window contents to the clipboard. After that you can paste the clipboard contents to any Windows application.

#### How to Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TOPSPIN allows you to save the contents of a data window in a graphics file of selectable type, e.g. <code>.png</code>, <code>.jpg</code>, <code>.jpeg</code>, <code>.bmp</code>, <code>.emf</code> and <code>.wmf</code>. To do that, click **File**  $\rightarrow$  **Export**.... The resolution of such a *screen dump* equals the resolution of your screen.Note that when you import a graphics file into another program and resize it you loose information. Therefore we recommend to resample rather than resize graphics.

# 2.9 How to Process Data

Since this manual is not a general NMR text book, we assume here that you are familiar with terms like window multiplication, Fourier Transform, phase correction, etc.

Any Fid or a spectrum displayed in a TOPSPIN window can be processed by:

- typing a command on the command line, e.g. ft
- invoking a command from the **Processing** or **Analysis** menu, e.g. **Processing** → **Fourier Transform...**
- entering an interactive mode by clicking a tool button, e.g.

• entering a user defined command (usually an AU or a Python program, see Help → Manuals [Programming Manuals].

Processing and analysis commands require certain parameters to be set correctly. Most commands in the **Processing** or **Analysis** menu, like *wm* and *ftf* open a dialog box showing the available options and required parameters for that command. Other commands such as *em*, *ft*, ... start processing immediately. Before you use them, you must set their parameters from the parameter editor. To do that, enter *edp* or click the **ProcPars** Tab of the data window.

If you are a new or occasional user we recommend you to process your data with the TOPSPIN Processing Guide. This will guide you through the typical sequence of processing steps. To start the Processing Guide, click **Processing**  $\rightarrow$  **Data**  $\rightarrow$  **Processing Guide**. In **Automatic mode**, the Processing Guide will simply execute each processing command when you click the corresponding button. This requires the processing parameters to be set correctly. In interactive mode (**Automatic mode** unchecked), the Processing Guide will, at each step, open a dialog box offering you the available options and required parameters. For example, the phase correction button offers various automatic algorithms as well as an option to enter interactive phasing mode.

A simple way to process 1D data is the following:

- 1. Click Processing  $\rightarrow$  Process / Plot Current data
- 2. In the appearing dialog (see Fig. 2.1):
  - a) Enable the desired processing/plotting steps
  - b) Set the parameter LB for Exponential multiplication
  - c) Select the desired LAYOUT for plotting.
  - d) Click **OK**

🥌 proc1 d						
Press OK to process / plot the selected dataset using the enabled options. The command "proc1d y" will process data without this dialog, using the last settings.						
Exponential Multiply (em)	<b>~</b>	LB [Hz] =	1			
Fourier Transform (ft)						
Auto - Phasing (apk)	✓					
Set Spectrum Reference (sref)	<b>V</b>					
Auto - Baseline Correction (abs)	<b>V</b>					
Plot (autoplot)	<b>V</b>	LAYOUT =	+/1D_H.xwp			
			OK Cancel			



#### 2.10 How to Archive Data

TOPSPIN 2.1 provides the following methods for data archiving:

- Automatic archiving of raw data after the acquisition as defined in the User preferences (click Options → Preferences → Acquisition → Configure ...)
- Copying a dataset to a desired destination directory which could for instance be located on a server. Type wrpa, click File → Save... or type Ctrl+s.
- Saving a dataset in a ZIP file. A standard Bruker dataset is a directory tree which contains several files. "Zipping" a dataset stores the entire data directory tree into a single file with the extension . bnmr.zip. To zip a dataset, type tozip, click File → Save... or type Ctrl+s. To unpack and display a zipped dataset, enter fromzip. Note that

. bnmr.zip files are fully compatible with the well known PC zip format and can be unpacked with any common unzip utility. "Zipping" can be applied to 1D, 2D, 3D and 4D data.

- Saving a dataset in JCAMP-DX format. This format is a IUPAC standard, and is available for 1D and 2D datasets. Data and parameters are stored in readable text (ASCII) format. To store data in JCAMP, type tojdx, click File → Save... or type Ctrl+s. To convert and display a JCAMP-DX file, type fromjdx.
- E-mailing data to a desired destination. Type *smail* or click File → Send To.... The mailing format is either zip or JCAMP-DX, both of which allow for data compression in order to keep the transferred data size as small as possible.

# 2.11 How to Import NMR Data Stored in Special Formats

TOPSPIN allows you to convert various data formats to standard Bruker format for display and processing. Click **File**  $\rightarrow$  **Open...** and select **Open NMR data stored in special formats**. Then follow the instructions on the screen.

# 2.12 How to Fit Peaks and Deconvolve Overlapping Peaks

Peaks of a 1D and 2D NMR spectrum can be approximated by a Lorentzian, Gaussian, or a mixture of these line shapes. Overlapping peaks may be deconvolved into a sum of such line shapes.

TOPSPIN shows the deconvolution result, i.e. peak positions, line widths and integrals on the screen and stores it in the file dconpeaks.txt. Furthermore, it switches to multiple display mode to show the original spectrum and the sum of the computed line shapes, superimposed.

To start deconvolution, expand the spectrum on the display to show the peak or peak group of interest. Then type dcon or click **Analysis**  $\rightarrow$  **Deconvolution...** 

# 2.13 How to Compute Fids by Simulating Experiments

TOPSPIN includes a "virtual spectrometer" that computes fids of any dimension. A "real" spectrometer excites a sample with high frequency pulses defined by a pulse program and measures the resulting fid. The virtual spectrometer performs this task mathematically by solving the quantum mechanical Liouville equation. The "sample" must be entered in form of a spin system description. For the computation, the same pulse program and acquisition parameters are taken as for the real experiment. The result is a time domain signal which can be processed with TOPSPIN in the same way a measured fid is processed. Techniques such a selective excitation, gradient enhanced spectroscopy, and the handling of mixtures are supported.

To start the virtual spectrometer:

IS Enter *mmrsim* on the command line or click **Analysis** → **Simulate** Fid....

### 2.14 How to Add Your Own Functionalities

The TOPSPIN functionality can be extended with various user defined commands, programs etc.

#### How to Create Macros

Writing a macro is the simplest way to create a user defined command. Just enter the command *edmac*, create a file, and enter a sequence of regular TOPSPIN commands and/or Python commands. Save the file under a name of your preference. You have created a new TOPSPIN command. Just enter its name on the command line to execute it. *edmac* shows a list of all available macros and allows you to execute one.

#### How to Create AU (automation) Programs

Writing an AU program is another way of creating a new TOPSPIN command. AU programs are more complex and more powerful then macros. They are C-language programs, which may contain C-statements, regular TOPSPIN commands, and various predefined AU macros and functions. AU programs can perform various tasks such as dataset handling, parameter handling, acquisition, processing, analysis, and printing. Note that AU programs do not support graphics related tasks.

TOPSPIN is delivered with a large set of Bruker AU programs for data processing and acquisition. Just enter *edau* to see them listed in a dialog box. The easiest way to create a new AU program is to select a Bruker AU program, save it under a new name and modify it to your needs. The chosen name is now available as a new TOPSPIN command. Alternatively, you can open a new file from the AU dialog box and write your AU program from scratch.

For details on Bruker AU programs and writing your own AU programs, click Help  $\rightarrow$  Manuals  $\rightarrow$  [Programming Manuals] AU Programming.

#### How to Create Python Programs

Writing a Python program is yet another way of creating a new TOPSPIN command. Python is a new generation scripting and object oriented programming language. Python programs are even more powerful than AU programs. They are easy to use and allow you to execute TOPSPIN commands, handle NMR data and parameters, generate graphics, and interact with the TOPSPIN user interface via dialogs, windows etc. To create a Python program, enter the command *edpy*, select a file and insert your Python statements. Graphics and interface features programmed in Python look and work the same as regular TOPSPIN features.

For details on Python programming, click **Help**  $\rightarrow$  **Manuals**  $\rightarrow$  [**Programming Manuals**] **Python Programming**. The examples mentioned there, like *pycmd1*, are delivered with TOPSPIN. Just enter their names on the command line to execute them.

The Python dialog window is also available from the TOPSPIN menu:

 $\operatorname{rss}$  Click File  $\rightarrow$  Open...and select Open other file  $\rightarrow$  Python program.

# 2.15 How to Automate Data Acquisition

TOPSPIN provides special user interfaces for automation, walk-up, biomolecular experiments, etc. To open these interfaces:

 $\texttt{IST} Type \textit{iconnmr} or click \textit{Spectrometer} \rightarrow \textbf{ICONNMR}.$ 

# Chapter 3 The TOPSPIN Interface

### 3.1 The Topspin Window

The TOPSPIN window consists of a data area, a data browser, toolbars and a menubar. Note that the browser can be inactive [hit Ctrl+d] or displayed as a separate window.

Fig. 3.1 shows the Topspin window with two data windows in the data area and the browser as an integral part.



Figure 3.1

Note that the menus and toolbars depend on the data dimensionality. The descriptions below holds for 1D data. For 2D and 3D data, the menus and toolbars are similar and will be discussed in the chapters 10, 11 and 13, respectively.

#### How to Use Multiple Data Windows

TOPSPIN allows you to use multiple data windows. Data windows can be opened from the browser or from the **Window** menu. They can contain the same of different datasets. Data windows can be arranged from the **Window** menu. One of them is the active (current) data window. The active data window:

- is the only data window receiving commands from the command line
- can be selected by clicking inside the window or hitting F6 repeatedly.
- has a highlighted title bar
- has the mouse focus

A cursor line (1D) or crosshair (2D) is displayed in all data windows at the same position. Moving the mouse affects the cursor in all data windows.

#### How to Use the Menu bar

The menu bar contains the following menus:

- File: performing data/file handling tasks
- Edit: copy & paste data and finding data
- View: display properties, browser on/off, notebook, command history
- Spectrometer: data acquisition and acquisition related tasks
- Processing: data processing
- Analysis: data analysis
- **Options**: setting various options, preferences and configurations
- Window: data window handling/arrangement
- Help: access various information, indices, manuals etc.

Experienced users will usually work with keyboard commands rather than menu commands. Note that the main keyboard commands are displayed in square brackets [] behind the corresponding menu entries. Furthermore, right-clicking any menu entry will show the corresponding command, unless right-clicking is defined otherwise.<sup>1</sup>

<sup>1.</sup> Right-click an entry part of the menubar and choose *Define Right-click Action*.

#### How to Use the Upper Toolbar (1D data)

The upper toolbar contains buttons for data handling, switching to interactive modes, display settings, and starting acquisition.

#### Buttons for data handling:



The functions of the individual buttons are:

Create a new dataset[Ctrl+n, new]

G Open a dataset [Ctrl+o, open]

Save the current dataset [Ctrl+s, sav]

Email the current dataset[smail]

Print the current dataset [Ctrl+p, print]

Copy the data path of the active data window to the clipboard [copy]

Paste the data path on the clipboard to the active data window [paste]

2d Switch to the last 2D dataset [.2d]

3d Switch to the last 3D dataset [.3d]

For more information on dataset handling, please refer to chapter 5.3.

#### **Buttons for interactive functions**

と 令 く 正 し 田 | と

The functions of the individual buttons are:

↓ Enter phase correction mode
- A Enter calibration mode
- ✓ Enter baseline correction mode
- the Enter peak picking mode
- **F** Enter integration mode
- # Enter multiple display mode
- 🔩 Enter distance measurement mode

For more information on interactive functions, refer to chapter 12 and 14.

#### Buttons for display options

№ 臥 央 🎟

The functions of the individual buttons are:

- $h_p$  Toggle between Hz and ppm axis units
- **I** Switch the y-axis display between abs/rel/off
- . ★ Switch the overview spectrum on/off
- Toggle grid between fixed/axis/off

#### How to Use the Lower Toolbar (1D data)

The lower toolbar contains buttons for display functions.

#### Buttons for vertical scaling (intensity)

\*2 /2 \*8 /8 🗢 至

- \*2 Increase the intensity by a factor of 2 [\*2]
- /2 Decrease the intensity by a factor of 2 [/2]
- \*8 Increase the intensity by a factor of 8 [\*8]

- /8 Decrease the intensity by a factor of 8 [/8]
- Change the intensity smoothly
- E Reset the intensity (baseline positions remains unchanged)

```
[.vr]
```

Note that vertical scaling can also be changed with the mouse wheel.

#### Buttons for horizontal scaling (zooming):



- Reset zooming (horizontal scaling) to full spectrum [.hr]
- Osplay the entire spectrum (baseline position and intensity scaling are adjusted if necessary) [.a11]
- Zoom in to the center (spectrum) or left edge (FID) of the displayed region, increasing the horizontal scaling. [.zi]
- Zoom in/out smoothly
- Q Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [.zo]
- Exact zoom via dialog box[.zx]
- Toggle interactive zoom mode. When switched off, interactive zooming only selects a horizontal region; baseline position and intensity scaling remain the same. When switched on, interactive zooming draws a box selecting the corresponding area.
- Undo last zoom [.z1]
- Retain horizontal and vertical scaling when modifying dataset or changing to different dataset. Global button for all data windows [.keep]

#### Buttons for horizontal shifting



- Shift to the left, half of the displayed region [.s1]
- ↔ Smoothly shift to the left or to the right
- → Shift to the right, half of the displayed region [.sr]
- ← Shift to the extreme left edge of the spectrum [.s10]
- -> Shift to the extreme right edge of the spectrum [.sr0]

#### Buttons for vertical shifting

#### **Ŧ ‡ ±**

- Shift the spectrum baseline to the middle of the data field [.su]
- Smoothly shift the spectrum baseline up or down.
- L Shift the spectrum baseline to the bottom of the data field [.sd]

For more information on display options, please refer to chapter 9.5 (1D data) and 10.5 (2D data).

# 3.2 Command Line Usage

#### How to Put the Focus in the Command Line

In order to enter a command on the command line, the focus must be there. Note that, for example, selecting a dataset from the browser, puts the focus in the browser. To put the focus on the command line:

☞ Hit the *Esc* key

or

Click inside the command line

#### How to Retrieve Previously Entered Commands

All commands that have been entered on the command line since TOPSPIN was started are stored and can be retrieved. To do that:

I Hit the ↑ (*Up-Arrow*) key on the keyboard

By hitting this key repeatedly, you can go back as far as you want in retrieving previously entered commands. After that you can go forward to more recently entered commands as follows:

 $\square$  Hit the  $\downarrow$  (*Down-Arrow*) key on the keyboard

#### How to Change Previously Entered Commands

- **1.** Hit the  $\leftarrow$  (*Left-Arrow*) or  $\rightarrow$  (*Right-Arrow*) key to move the cursor
- 2. Add characters or hit the Backspace key to remove characters
- 3. Mark characters and use *Backspace* or *Delete* to delete them, *Ctrl+c* to copy them, or *Ctrl+v* to paste them.

In combination with the arrow-up/down keys, you can edit previously entered commands.

#### How to Enter a Series of Commands

If you want to execute a series of commands on a dataset, you can enter the commands on the command line separated by semicolons, e.g.:

#### em;ft;apk

If you intend to use the series regularly, you can store it in a macro as follows:

right-click in the command line and choose Save as macro.

## 3.3 Command Line History

TOPSPIN allows you to easily view and reuse all commands, which were previously entered on the command line. To open a command history control window; click **View**  $\rightarrow$  *Command Line History*, or right-click in the command line and choose *Command Line History*, or enter the command *cmdhist* (see Fig. 3.2).

It shows all commands that have been entered on the command line since TOPSPIN was started. You can select one or more commands and apply one of the following functions:

🧟 Command History - cmdhist	×
em	
ft	
apk	
cmdhist	
l	
Execute Append Save Macro Cance	el

Figure 3.2

#### Execute

Execute the selected command(s).

#### Append

Append the (first) selected command to the command line. The appended command can be edited and executed. Useful for commands with many arguments such as *re*.

#### Save as...

The selected command(s) are stored as a macro. You will be prompted for the macro name. To edit this macro, enter *edmac* <*macro-name>*. To execute it, just enter its name on the command line.

# 3.4 Starting TOPSPIN commands from a Command Prompt

TOPSPIN commands can be executed outside of the TOPSPIN interface, from a Windows Command Prompt or Linux Shell.

#### **Under Windows**

- 1. Open a Windows Command Prompt
- 2. Enter a TOPSPIN command in the following format:

```
<tshome>\prog\bin\sendgui <topspincommand>
```

where <tshome> is the TOPSPIN installation directory.

Examples:

C:\ts2.1\prog\bin\sendgui ft

executes a 1D Fourier transform.

```
C:\ts2.1\prog\bin\sendgui re exam1d_1H 1 1 C:/bio joe reads the dataset C:/bio/joe/nmr/exam1d_1H/1/pdata/1.
```

#### **Under Linux**

- 1. Open a Linux Shell
- 2. Enter a TOPSPIN command in the following format:

```
<tshome>\prog\bin\scripts\sendgui <topspincommand>
where <tshome> is the TOPSPIN installation directory.
```

or

```
sendgui <topspincommand>
```

if the TOPSPIN home directory is in the users search path.

Examples:

```
C:\ts2.1\prog\bin\scripts\sendgui ft
```

executes a 1D Fourier transform.

sendgui re exam1d\_1H 1 1 C:/bio joe

reads the dataset C:/bio/joe/nmr/exam1d\_1H/1/pdata/1.

Note that commands are executed on the currently active TOPSPINdata window.

# 3.5 Function Keys and Control Keys

For several TOPSPIN commands or tasks, you can use a control-key or function-key short cut.

Esc	Put the focus in the command line
Shift+Esc	Display menu bar and toolbars (if hidden)
F2	Put the focus in the browser
F1	Search for string in command help or NMR
	Guide [help]
F6	Select the next window in the data area
Alt+F4	Terminate TOPSPIN [exit]
Ctrl+d	Switch the browser on/off
Ctrl+o	Open data [ <i>open</i> ]
Ctrl+f	Find data [find]
Ctrl+n	New data [new]
Ctrl+p	Print current data [print]
Ctrl+s	Save current data [ <i>sav</i> ]
Ctrl+w	Close active window [close]
Ctrl+c	Copy a text that you selected/highlighted in an
	error box, dialog box, pulse program, title etc.,
	to the clipboard
Ctrl+v	Paste text from the clipboard into any editable field.

# Focus anywhere in TOPSPIN

# Focus in the Command Line

Ctrl+Backspace	Kill current input
Ctrl+Delete	Kill current input
UpArrow	Select previous command (if available).
DownArrow	Select next command (if available).

# Focus in the Browser

Select previous dataset
Select next dataset
dir/user/name/expno selected: expand node or
collapse node, depending on the current state
procno selected: display this dataset
name/expno selected: display this dataset
multiple procnos selected: show in multiple dis-
play
one or more name/expno/procno nodes
selected: delete these datasets

# Focus anywhere in TOPSPIN

Scaling Data		
Alt+PageUp	Scale up the data by a factor of 2 [*2]	
Alt+PageDown	Scale down the data by a factor 2 [/2]	
Ctrl+Alt+PageUp	Scale up by a factor of 2, in all data windows	
Ctrl+Alt+PageDown	Scale down by a factor of 2, in all data windows	
Alt+Enter	Perform a vertical reset	
Ctrl+Alt+Enter	Perform a vertical reset in all data windows	
Zooming data		
Alt+Plus	Zoom in [.zi]	
Alt+Minus	Zoom out [.zo]	
Ctrl+Alt+Plus	Zoom in, in all data windows	
Ctrl+Alt+Minus	Zoom out, in all data windows	
Shifting Data		
Alt+UpArrow	Shift spectrum up [.su]	
Alt+DownArrow	Shift spectrum down [.sd]	
Alt+LeftArrow	Shift spectrum to the left [.s1]	
Alt+RightArrow	Shift spectrum to the right [.sr]	
Ctrl+Alt+UpArrow	Shift spectrum up, in all data windows	
Ctrl+Alt+DownArrow	Shift spectrum down, in all data windows	
Ctrl+Alt+LeftArrow	Shift spectrum to the left, in all data windows	
Ctrl+Alt+RightArrow	Shift spectrum to the right, in all data windows	

delete	Delete the selected entries
home	Select the first entry
end	Select the last entry
Shift+Home	Select the current and first entry and all in
	between
Shift+End	Select the current and last entry and all in
	between
DownArrow	Select next entry
UpArrow	Select previous entry
Ctrl+a	Select all entries
Ctrl+c	Copy the selected entries to the clipboard
Ctrl+z	Undo last action
Ctrl+y	Redo last undo action

Focus in a Table (e.g. peaks, integrals, nuclei, solvents)

Focus in a Plot Editor
------------------------

F1	Open the Plot Editor Manual
F5	Refresh
Ctrl+F6	Display next layout
ctrl+Shift+F6	Display previous layout
Ctrl+tab	Display next layout
delete	Delete the selected objects
Ctrl+a	Select all objects
Ctrl+i	Open TOPSPIN Interface
Ctrl+c	Copy the selected object from the Clipboard
Ctrl+l	Lower the selected object
Ctrl+s	Save the current layout
Ctrl+m	Unselect all objects
Ctrl+n	Open a new layout
Ctrl+o	Open an existing layout
Ctrl+p	Print the current layout
Ctrl+q	Close the Plot Editor window (Linux only)
Ctrl+r	Raise the selected object
Ctrl+t	Reset X and Y scaling of all marked objects
Ctrl+v	Paste the object from the Clipboard
Ctrl+w	Open the attributes dialog window.
Ctrl+x	Cut the selected object and place it on the Clip-
	board
Ctrl+z	Undo the last action

Note that the function of function keys can be changed as described in chapter 3.7.

# 3.6 Help in Topspin

TOPSPIN offers help in various ways like online manuals, command help and tooltips.

#### How to get a Panorama Tour

For a quick overview over TOPSPIN Interface, Acquisition, Processing, Analysis and Documentation:

#### R Click Help → Panorama Tour

#### How to Open Online Help documents

The online help manuals can be opened from the **Help**  $\rightarrow$  **Manuals** submenu. For example, to open the manual that you are reading now:

 $\texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{General}] \ \textbf{User Manual}$ 

To open the Avance Beginners Guide:

```
\texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \textbf{language} > \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Beginners Guides}] < \texttt{RS} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow (\textbf{Manuals} \rightarrow \textbf{Manuals} \rightarrow \textbf{Manuuls} \rightarrow \textbf{Manual
```

To open the Processing Reference guide:

```
IS Click Help → Manuals → [Acquisition & Processing References]
Proc. Commands and Parameters
```

Note that most manuals are stored in the directory:

<tshome>/prog/docu/english/xwinproc/pdf

The most recent versions can be downloaded from:

```
www.bruker-biospin.de
```

#### How to Get Tooltips

If you hold the cursor over a button of the toolbar, a tooltip will pop up. This is a short explanation of the buttons function. For example, if you hold the cursor over the interactive phase correction button, you will see the following:



The corresponding command line command, in this case **.***ph*, is indicated between square brackets.

Note that the tooltip also appears in the status bar at the bottom of the TOP-SPIN window.

#### How to Get Help on Individual Commands

To get help on an individual command, for example *ft*:

```
🖙 Enter £t?
```

or

r Enter help ft

In both cases, the HTML page with a description of the command will be opened.

Note that some commands open a dialog box with a **Help** button. Clicking this button will show the same description as using the help command. For example, entering re and clicking the **Help** button in the appearing dialog box

🔄 re 🛛 🔀		
Options Options Display data in same window Display data in new window		
NAME =	exam1d_13C	
EXPNO =	1	
PROCNO =	1	
DIR =	C: Voio	
USER =	guest	
OK Cancel Browse Find Help		

opens the same HTML file as entering *help re* or *re*?.

## How to Use the Command Index

To open the TOPSPIN command index:

```
Bnter cmdindex
```

or

#### $\texttt{R} Click Help \rightarrow Command Index$

From there you can search for and click any command and jump to the corresponding help page.

# 3.7 User Defined Functions Keys

The default assignment of functions keys is described in chapter 3.5 and in the document:

```
Ref Click Help \rightarrow Manuals \rightarrow [General] Control & Function Keys
```

You may assign your own commands to functions keys. Here is an example of how to do that:

- Open the file cmdtab\_user.prop, located in the subdirectory userdefined of the user properties directory (to locate this directory, enter hist and look for the entry "User properties directory="). The file cmdtab\_user.prop is initially empty and can be filled with your own command definitions.
- 2. Insert e.g. the following lines into the file:

```
_f3=$em
_f3ctrl=$ft
_f3alt=$pk
_f5=$halt
_f5ctrl=$reb
_f5alt=$popt
```

3. Restart TOPSPIN

Now, when you hit the F3 key, the command em will be executed. In the same way, Ctrl+F3, Alt+F3, F5, Ctrl+F5 and Alt+F5 will execute the commands ft, pk, halt, reb and popt, respectively. You can assign any command, macro, AU program or Python program to any function keys. Only the keys Alt+F4, F6, Ctrl+F6, and Alt+F6 are currently fixed. Their function cannot be changed.

# 3.8 How to Open Multiple TOPSPIN Interfaces

TOPSPIN allows you to open multiple User Interfaces. This is, for example,

useful to run an acquisition in one interface and process data in another. To open an addition interface, enter the command *newtop* on the command line or click **Window**  $\rightarrow$  **New Topspin**. To open yet another interface, enter *newtop* in the first or in the second interface. The display in each interface is completely independent from the others. As such, you can display different datasets or different aspects of the same dataset, e.g. raw/processed, regions, scalings etc. When the dataset is (re)processed in one interface, its display is automatically updated in all TOPSPIN interfaces.

The command *exit* closes the current Topspin interface. Interfaces that were opened from this interface remain open. Entering *exit* in the last open TOPSPIN interface, finishes the entire TOPSPIN session. The position and geometry of each TOPSPIN interface is saved and restored after restart.

# Chapter 4 Trouble Shooting

## 4.1 General Tips and Tricks

On a spectrometer, make sure the commands *cf* and *expinstall* have been executed once after installing TOPSPIN. *cf* must be executed again if your hardware configuration has changed. Sometimes, executing *cf* is useful in case of acquisition problems.

On a datastation, a default configuration is automatically done during the installation. No configuration commands are required. Only if you want to use AU programs, you must run *expinstall* once.

## 4.2 History, Log Files, Spooler Reports, Stack Trace

If you have a problem with TOPSPIN and want to contact Bruker, it is useful to have as much information as possible available. If TOPSPIN is still running, you can view log files with the commands *hist* and *ptrace*. If TOP-SPIN hangs, you can create a stack trace by hitting Ctrl+\ (Linux) or Ctrl+Break (Windows) in the TOPSPIN startup window.

## 4.2.1 TOPSPIN command-log

By default, the history (protocol) feature is switched on. This means all TOP-SPIN commands will be protocolled and can be examined by entering *hist* on the command line.

If, for some reason, history is switched off, you can switch it on as follows:

- 1. Click Options -> Preferences, click Miscellaneous
- 2. Check the entry "Record commands in protocol file"
- 3. Click OK.

## 4.2.2 TOPSPIN spooler report

TOPSPIN reports all queued, delayed and cron jobs in the so called spooler report file. The spooler report stores all jobs since TOPSPIN installation and can become very large. Therefore it should be cleaned from time to time. To do that:

- 1. Enter the command spooler
- **2.** Click Tools  $\rightarrow$  Show spooler report
- 3. Mark the entries to be deleted
- 4. Right-click in the dialog and choose Delete.
- 5. Close the Spooler report.

Note that the spooler report can also be opened from Spooler field (if enabled) in the Acquisition Status Bar by right-clicking the word **Spooler** and choosing **Show spooler report**.

## 4.2.3 TOPSPIN command, dataserver and network log

A full protocol including not only TOPSPIN commands but also dataserver and network traffic is show by the command *ptrace*. This opens the following dialog window:

ptrace -	[TopSpin Log-File]	[racer]	X
File			
Filter DF	Show all	▼ <	>
An	Time	Message	
11-20	-08:03:06.128	5200 TOPSPIN Version 2.1	
11-20	-08:03:06.128	FLEX1m license is valid until 2010-11-14	
11-20	-08:03:06.128	5200 0 cmd enter: cprserver	
11-20	-08:03:06.144	3908 proc start: cprserver (module cprserver)	
11-20	-08:03:06.580	3908 0 cmd sent: cprserver	
11-20	-08:03:07.080	5200 0 cmd enter: cprclient	
11-20	-08:03:07.080	4748 proc start: cprclient (module cprclient)	
11-20	-08:03:07.641	5304 java virtual machine	
11-20	-08:03:07.641	4748 0 cmd sent: cprclient	
11-20	-08:03:08.437	Graphical User Interface started.	
11-20	-08:03:08.484	GUI Version = 2.1 (of October 24 2007)	
11-20	-08:03:08.484	Operating system = Windows Vista	
11-20	-08:03:08.484	User properties directory=C:\Users\drud\.topspin-drudnb\prop	
11-20	-08:03:09.123	To connect to this TOPSPIN instance via Remote Connection use host=149.	. 2
11-20	-08:03:09.123	Start: opening file for local session key at 'C:\Bruker\TOPSPIN/prog/cu	ır
11-20	-08:03:09.123	Start: local session key imported successfully.	
11-20	11-20-08:03:09.123 Start: GUI session key created		
11-20	11-20-08:03:09.607 cmd=init cpr		
11-20	11-20-08:03:09.607 Start ORB: recommended port=5090.		
11-20	-08:03:10.059	Start ORB: successful on port 5090	
11-20	-08:03:10.059	cmd=cprlistener	
11-20	-08:03:10.059	Start CprListenerServer: activate.	
11-20	-08:03:10.090	Start CprListenerServer: activation successful, id = corbaloc:iiop:149.	2
11-20	11-20-08:03:10.278 Contact configuration service: URL=corbaloc:iiop:149.236.14.167:5500/Con		
11-20-08:03:10.278 Contact configuration service: local contact, using URL: corbaloc:iiop:1			1
11-20-08:03:10.293 Contact configuration service: successful.			
11-20	-08:03:10.293	Contact configuration service: local session, authentication done.	
11-20	-08:03:10.309	Datastation: true, ELCB: false, MAS2: false, VTU: true, RCU: false	
11-20	-08:03:10.340	Contact CPR: local contact, narrowing object for: corbaloc:iiop:127.0.0	1.
11-20	-08:03:10.340	Contact CPR: object is valid.	
11-20	-08:03:10.340	Contact CPR: address of CprListener is corbaloc:iiop:149.236.14.167:509	0
11-20	-08:03:10.340	Contact CPR: logon at CPR with "corbaloc:iiop:127.0.0.1:5090/%0000%00%F	°E
11-20	-08:03:10.340	<pre>1 cpr Client logon corbaloc:iiop:127.0.0.1:5090/%0000%00%FEPOA%FF</pre>	5 <b>C</b>
11-20	-08:03:10.605	Contact CPR: attempt #0 to get assigned client id	
•			•
C:\Bruker\TO	PSPIN/prog/curdir	\drud\history_j.txt	
C:\Bruker\TC	PSPIN/prog/curdir	ldrud/history	
C:\Bruker\TC	PSPIN/prog/curdir	drudistdout dataserver 3080	

Figure 4.1

Here TOPSPIN log messages from various log files are displayed time sorted.

Messages from different log files are shown in different colours. The color assignment and location of the files is shown in the lower part of the dialog window.

ptrace supports the following functions:

#### Search keywords

To search the displayed log files for a certain keyword, just enter it in the text bar at the top of the window and hit Enter.

#### Anchor specific entries

To anchor an entry:

double-click in the first column of the entry

The entry is marked with an **X**. Now you can use the < > buttons at the upper right of the window to go to the previous or next entry, respectively.

#### Add log files

By default, the procol.txt, history and dataserver log files are shown. To include additional log files to the *ptrace* list:

click File  $\rightarrow$  Add, specify the file and click Open.

Note that most log files are stored in the directory:

<tshome>/prog/curdir/<user>

#### Save the log messages

To save log messages in a text file;

click  $\textbf{File} \rightarrow \textbf{Save}$  and specify the output text file

## 4.2.4 Create a Stack Trace

If TOPSPIN hangs it can be useful to sent Bruker a stack trace about a possible cause. You can create a stack trace as follows.

- 1. Move the cursor into the TOPSPIN startup window.
- 2. Under Windows: hit *Ctrl+Break* (*=Ctrl+Pause*) Under Linux: hit *Ctrl+*\ (Control backslash)
- 3. Copy the appearing text into a text file.

## 4.2.5 Store complete log with 'savelogs'

A complete set of TOPSPIN log files can be made automatically with the command *savelogs* if the user assertively confirms.

For saving logfiles with the command savelogs do the following:

Under Windows:

- Click the *Bruker Utilities<topspin version>* icon on your desktop. An Explorer will be opened.
- Double-click Miscellaneous
- Execute the script savelogs

Under Linux:

- Open a shell.
- Type savelogs

All <tshome>/prog/curdir/<user>/\* files will be saved with *savelogs*.

The stored files can be found under following pathname:

- Under Windows XP: <userhome>\AppData\Local Settings\Temp\ TopSpinSupportFiles\_<Support-Token><operating-systemuser><year><month><day><hour><minute>.tar.gz
- Windows Vista: <userhome>\AppData\Local\Temp\ TopSpinSupportFiles\_<Support-Token><operating-systemuser><year><month><day><hour><minute>.tar.gz
- Linux: <userhome>\tmp\ TopSpinSupportFiles\_<Support-Token>\_<operating-systemuser><year><month><day><hour><minute>\.tar.gz

For detailed information about saving all possible log files and about the upload to the Bruker FTP-server please refer to the *Processing Reference Command Manual*.

# 4.3 How to Show or Kill TOPSPIN processes

To show the currently running TOPSPIN processes, enter the command *show* or *kill* on the command line. A list of processes will appear showing the process command, dataset etc.

Active commands and processes			×		
Command	Data	Status	Module	Process Id	
×fb	exam2d_HC11C	EXEC	proc2d	2228	
					-
		<u>D</u> etails	Sort modules	Kill Close	

Figure 4.2

Fig. 4.2 shows a list with one process (command **xfb**). To kill a process, select it in the list and click the button **Kill...** 

The command *show all* or *kill all* work like *show* and *kill*, except that they also show TOPSPIN system processes. Note that killing such processes may kill TOPSPIN.

## 4.4 What to do if TOPSPIN hangs

If, for some reason, TOPSPIN hangs, please do the following.

Under Linux:

- 1. Open a Shell
- 2. Enter <tshome>/prog/bin/script/killtopspin

where <tshome> is the TOPSPIN installation directory.

Under Windows:

- **1.** Click Start → Programs → Bruker TOPSPIN → TOPSPIN 2.1 → Bruker Utilities 2.1 → Miscellaneous
- 2. In the appearing window:

Click killtopspin.

Normally, this kill all TOPSPIN processes including *cpr*, *cprserver*, *dataserver* and *java*.

# 4.5 How to Restart User Interface during Acquisition

If Topspin hangs up during a data acquisition, you can restart the user interface without disturbing the acquisition. To do that:

1. Open the file:

<tshome>/prog/curdir/<user>/history

where <tshome> is the TOPSPIN home directory and <user> is the user who started TOPSPIN. Look for the term 'Java Virtual Machine' and check its PID.

- 2. Open the Task Manager (Windows) or System Monitor (Linux)
- 3. Stop the Java(w).exe process with the PID found in the history file.
- 4. Open a Windows Command Prompt or Linux Shell
- 5. Go to the TOPSPIN Installation directory
- 6. Enter topspin -client

# Chapter 5 Dataset Handling

# 5.1 The Topspin Browser

TOPSPIN offers a data browser from which you can browse, select, and open data.

The browser dialog offers the following tabs (see Fig. 5.1):

- Browser data browser showing the data directory hierarchy
- Last50 list of the 50 last open datasets
- Groups list of user defined groups of datasets
- Alias list of user defined alias name

The browser appears at the left of the TOPSPIN window and can be shown/hidden with *Ctrl+d* or by clicking the arrow buttons at the upper right of the browser.

#### The Browser tab

The browser shows data directory trees and allows you to expand/collapse their elements. Figure 5.1 shows the browser with three top level data directories and one dataset fully expanded.



Figure 5.1

The dimensionality of the data is indicated with different colors:

- black for 1D data
- blue for 2D data
- magenta for 3D data

Furthermore, the browser shows:

- the pulse program with the dataset EXPNO (e.g. 1 hxcoqf in Fig. 5.1)
- the title with the dataset PROCNO (e.g. CH-CO Cyclosporin in Fig. 5.1)

Note that the displayed pulse program is the:

- status pulse program if an acquisition has been done (raw data exist)
- setup pulse program if no acquisition has been done (raw data do not exist)

The display of title and pulse program can be switched of (see Fig. 5.2).

Display	$\rightarrow$ Display in current data window.
Display In New Window	$\rightarrow$ Display in new data window.
Display As 2D Projection	$\rightarrow$ Display 1D data as projection of active 2D data.
Scroll to active dataset	$\rightarrow$ Scroll to PROCNO of active data window.
Fully Expand Selection	$\rightarrow$ Fully expand selected node.
Show PULPROG/Title	$\rightarrow$ Switch pulsprogram/title display on/off.
Show Date	$\rightarrow$ Show acq. date (expno) or last mod. date (name)
Sort by Date	$\rightarrow$ Sort data by last modified date
Сору	$\rightarrow$ Copy dataset entry to clipboard
File Properties	$\rightarrow$ Show dataset properties.
Delete	$\rightarrow$ Delete selected entry (name,expno or procno)
Rename	$\rightarrow$ Rename dataset name, expno or procno.
Files	$\rightarrow$ Show files in selected entry (expno or procno)
Add New Data Dir	$\rightarrow$ Add new top level data directory.
Remove Selected Data Dirs	$\rightarrow$ Remove selected top level data directory



#### The Last50 tab

Clicking the **Last50** tab displays the list of the last 50 displayed datasets. Each dataset that you open, is automatically added to the current list. Fig. 5.3 shows a **Last50** list with four datasets. As in the browser, different colors are used to indicate the data dimensionality.



#### Figure 5.3

- We Hit the *Enter* key to display the highlighted dataset in the current window
- B Double-click a dataset to display it in the current window.

Remove Selected Items From List

Open Saved Last50 List...

Save Last50 List As...

- $\rightarrow$  Remove the selected dataset from the list.
- $\rightarrow$  Open a dialog to select a *Last50* list.
- $\rightarrow$  Open a dialog for saving the current *Last50* list.

## Figure 5.4

Each line displays one dataset showing its *name*, *expno*, *procno*, *top level directory* and *user*.

## The Groups tab

Clicking the **Groups** tab displays the list of user defined dataset groups. Here you can create, modify and display groups of datasets. Defining a group is useful is you work on projects where each project involves multiple datasets. It allows you to easily organizes your projects and access all data belonging to a certain project.

Display	$\rightarrow$ Display selected dataset(s) in active window			
Display In New Window	$\rightarrow$ Display selected dataset(s) in new window.			
Display Group	$\rightarrow$ Display all datasets in group in new windows.			
Add Selected Data Window	$\rightarrow$ Add selected data window to selected group.			
Add All Open Data Windows	$\rightarrow$ Add all open data windows to selected group.			
Update Window Bounds & Display Limits	$\rightarrow$ Update window bounds and dislay regions.			
Remove Selected Datasets From Group	$\rightarrow$ Remove selected datasets from group.			
Collapse All Groups	$\rightarrow$ Collapse all groups.			
Toggle Dim/Pulprog/Title	$\rightarrow$ Show/hide dimension, pulse program, title.			
Add new Dataset Group	$\rightarrow$ Add a new (empty) dataset group to the list.			
Close All Group Windows	$\rightarrow$ Close all data windows of selected group.			
Process Selected Datasets	$\rightarrow$ Process selected dataset with serial processing.			
File Properties	$\rightarrow$ Show file properties of selected dataset.			
Files	$\rightarrow$ Show file list of selected dataset.			
Сору	$\rightarrow$ Copy pathnames of selected data to clipboard.			
Figure 5.5				

Note that a group not only defines the datasets involved, but also their data window positions and dimensions and the displayed region of each spectrum.

#### The entry Update window bounds & displays regions

#### The Alias tab

Clicking the **Alias** tab displays the list of user defined alias names for datasets. Just right-click any entry to define, remove or interpret alias names.





List Selected Alias

List All Aliases

```
Remove Selected Aliases...
```

List Available Alias Commands

- $\rightarrow$  define alias for data in selected window.
- $\rightarrow$  Show selected data name, expno etc.
- $\rightarrow$  Show all data names, expnos etc.
- $\rightarrow$  Remove selected aliases from list.
- $\rightarrow$  Show available alias commands.



#### How to Open the Browser in a separate window

The browser can be opened in a separate window as follows:

Set Click Options → Preferences [set], click Window settings and check Display dataset browser in a separate window.

You must restart TOPSPIN for the change to take effect.

#### How to Put the Focus in the Browser

ire Hit the *F2* key

or

IN Click inside the browser

#### How to Select Folders in the Browser

To select a particular folder:

Reft-click the folder button

or

B Hit the arrow-up/down keys while the focus is in the browser

To select multiple folders:

IN Hold the Ctrl key and left-click multiple folders to select them

or

Hold the *Shift* key and left-click two folders to select these two and all in between.

#### How to Expand/Collapse a Folder in the Browser

To expand a collapsed folder:

- Source Click the + button to the left of the folder button
- or Double-click the folder button
- or Hit the *Right-Arrow* key while the folder is highlighted

To fully expand a collapsed folder:

IN Right-click the DIR, NAME or EXPNO node and choose Fully Expand Selection

To collapse an expanded folder:

- IF Click the button to the left of the folder button
- or Double-click the folder button
- or Hit the Left-Arrow key while the folder is highlighted

## How to Show/Hide Pulse program and Title in the browser

Right-click the data name folder button and choose

Show PULPROG /Title from the popup menu (see Fig. 5.8)

Display	
Display In New Window	
Display As 2D Projection	
Scroll to active dataset	
Fully Expand Selection	
Show PULPROG/Title	
✓ Show Date	
✓ Sort by Date	
Сору	
File Properties	
Delete	
Rename	
Files	
Add New Data Dir	
Remove Selected Data Dirs	
Figure 5.8	

#### How to Show Dataset Dates in the Browser

Right-click the data name folder button and choose Show Date

The last modified date is shown to the right of the dataset NAME, whereas the acquisition date is shown to the right of the dataset EXPNO (see Fig. 5.9).



Figure 5.9

#### How to change the default Top Level Data Directory

By default, the browser shows the TOPSPIN installation directory with the Bruker example datasets. To suppress this feature click **Options**  $\rightarrow$  **Preferences** [*set*], click **Administration** and uncheck **Show** *TOPSPIN* **data examples directory in data browser**.

#### How to Add, Remove or Interpret Alias Names

To add an alias name:

- 1. Click the Alias tab in the browser.
- Right-click in the Alias table to open the popup menu (see Fig. 5.7). Click Define alias names for data in selected window.
- **3.** Enter an alias name in the appearing dialog box and click **OK**. Note that alias names must begin with a letter.

To remove an alias name:

- 1. Right-click the alias name
- 2. Click **Remove selected aliases...** from the popup menu (see Fig. 5.7)

Furthermore, the popup menu offers entries to display the dataset, list its properties and print the full dataset specification.

# 5.2 Creating Data

#### How to Create a New Dataset

**1.** Click File  $\rightarrow$  New [new, Ctrl+n]

or

Click the button in the upper toolbar.

- 2. Specify the dataset *name*, *expno*, *procno*, *dir*, and *user* in the appearing dialog box. If one or more datasets are open, the fields are initialized with the current dataset (see Fig. 5.10).
- **3.** Click the down-arrow of the **Solvent** box and choose a solvent from the list, or type a solvent name.
- **4.** Click the down-arrow of the **Experiment** box and choose a parameter set from the list, or type a parameter set name.
- 5. Type the dataset title in the TITLE box.
- 6. Click OK.

🆕 New			×
Prepare for a new e initializing its NMR p For multi-receiver e Please define the n	xperiment by crea arameters accord xperiments severa umber of receivers	ting a new data ing to the selec Il datasets are s in the box bel	a set and cted experiment type, created, ow,
NAME	exam1d_13C		
EXPNO	1		
PROCNO	1		
DIR	C:\Bruker\TOPSPIN		
USER	guest		
Solvent			CDCI3 -
Experiment		Use current p	arams. 👻
TITLE			
13C{1H} AV 500 Cholesterylacetate			
		ancel Mo	re <u>I</u> nfo <u>H</u> elp

#### Figure 5.10

A dataset will be created and initialized with the parameters of the chosen experiment. No fid or spectrum are available yet. They can be created by data acquisition and data processing, respectively.

# 5.3 Opening Data

TOPSPIN allows you to open data in several ways, from the browser, the menu, the Windows Explorer or the command line. Furthermore, data can be opened:

- in an existing data window replacing the current dataset.
- in a data window which is in multiple display mode, being superimposed on the current spectra.
- in a new data window which becomes the active window.

Note that if a dataset is already displayed in one window and it is opened in a second existing window, it still replaces the dataset in the latter one. As a result, the same dataset will be displayed in two windows (see also command *reopen*).

#### How to Open Data Windows Cascaded

By default, a new data window appears maximized, filling the entire data field and covering possibly existing windows. You can, however, configure TOPSPIN to open new windows cascaded. This is convenient if you want to open several data windows and then select one.

To open new windows cascaded:

- 1. Click Options → Preferences [set]
- Click Window Settings in the left part of the dialog box. The right part of the dialog box shows the window settings (see Fig. 5.11).

Window settings		
Open new internal windows "cascaded" rather than "maximized"	V	
Configure cascaded window	Change	

Figure 5.11

- 3. Check Open new internal windows 'cascaded' rather than 'max'.
- Optionally you can configure the cascaded windows by clicking the respective Change button. This will open the dialog box shown in Fig. 5.12.

🌳	×
Define the properties of cascaded windows. All numbers must be in the range 01. They are the fractions of the maximum window in the respective dimension.	s sizes
Width of window =	0.5
Height of window =	0.5
X-offset to previous window =	0.1
Y-offset to previous window =	0.1
Use standard values instead of those above =	= no 💌
<u>(</u>	<u>D</u> K <u>C</u> ancel

Figure 5.12

- **5.** Here you can specify the data window sizes and offsets as fractions of the maximum window sizes.
- 6. Click OK to close the dialog box.

## How to Open Data from the Browser

In the browser:

- Is Left-click-hold a data name, expno or procno and drag it into the data area. The data will be displayed in a new data window.
- *or* Left-click-hold a data *name*, *expno* or *procno* and drag it into an open data window. The data will replace the currently displayed data.
- or Left-click-hold a data name, expno or procno and drag it into an empty data window created with Alt+w n.
- *or* Left-click-hold a data *name*, *expno* or *procno* and drag it into a multiple display data window. The data will be superimposed on the currently displayed data.
- or Right-click a data name, expno or procno and choose **Display** from the popup menu; the data will be displayed in the current data win-

dow.

- *or* Right-click a data *name*, *expno* or *procno* and choose **Display in new window** from the popup menu; the dataset will be displayed in a new data window.
- or Hold the Ctrl key and left-click several datasets to select them or hold the Shift key and left-click two datasets to select these two and all in between. Then right-click one of the selected datasets and choose Display from the popup menu. A new window will be opened showing the selected datasets in multiple display mode. However, if the current window was already in multiple display mode, the selected spectra will be superimposed on the currently displayed spectra.

#### How to Automatically Select the first expno/procno of a dataset

If you open a dataset from the Browser by clicking a data *name*, there might be more that one *expno* and/or *procno* available. By default, TOP-SPIN then opens a dialog box from which you can select the desired *expno/procno* combination (see Fig. 5.13). Clicking **Open** will open the selected dataset, whereas clicking **Print** will print the displayed dataset list.

You can, however configure TOPSPIN to automatically open the first available *expno/procno* combination. To do that:

- 1. Click Options → Preferences [set].
- 2. Click Miscellaneous in the left part of the dialog box.
- **3.** Uncheck the item *Display EXPNO/PROCNO list when opening data.*
- 4. Click OK to close the dialog box.

🍓 exam1 d_1 3C	
This data set contains several I Open = Display the selected da Print = Print the data set list. Typ "Printer> Printer Font" in	XPNO / PROCNO pairs,corresponding to several raw/processed data files. a set. e "set" and navigate to order to change the font.
EXPNO / PROCINO - aim paispro	
171 1d zgpg30 "13	A(TH) AV 300 Automation Cholesterylacetate"
2/1 1d jmod "13C.	PT AV 300 Automation Cholesterylacetate"
3/1 1d dept135 "1	C DEPT135 AV 300 Automation Cholesterylacetate"
4/1 1d dept45 "13	DEPT45 AV 300 Automation Cholesterylacetate"
5/1 1d dept90 "13	DEPT90 AV 300 Automation Cholesterylacetate"
6/1 1d zgig30 "134	IG AV 300 Automation Cholesterylacetate"
Show dim/pulsprog/title ne	t time Open Print Save Cancel



Note that the command *rel* also opens the dialog shown in Fig. 5.13, showing the available EXPNO's under the current dataset. Similarly, *repl* shows the available PROCNO's under the current dataset EXPNO.

#### How to Open Data from the Topspin menu

1. To open a dataset:

🖙 Click the 🔄 button in the upper toolbar.

or

 $\mathbb{R}$  Click **File**  $\rightarrow$  **Open** [*open*, *Ctrl*+*o*] (see Fig. 5.14).
File	Edit	View	Processing	Analysis
N	ew (0	trl N]		
0	pen	[Ctrl O]		
R	eopen			
С	lose (C	tri W]		
С	lose A	II		
S	ave (	Ctrl S]		
Pi	rint [(	Ctrl P]		
E)				
S	end To	·		
R	un			
D	elete			

Figure 5.14

2. In the appearing dialog box (see Fig. 5.15)

🍓 Open - re	
Options Open NMR data stored in Open NMR data stored in Open other file	standard Bruker format special formats
Required parameters Browser type =	RE Dialog
ŪK	

Figure 5.15

- a) Select the option **Open NMR data stored in standard Bruker** format.
- b) Select the browser type **RE Dialog**.

- c) Click OK.
- 3. In the appearing dialog box (see Fig. 5.16).

🥌 re	
<ul> <li>Options</li> <li>Oisplay data in same windo</li> <li>O Display data in new windo</li> </ul>	w W
NAME =	exam1d_13C
EXPNO =	1
PROCNO =	1
DIR =	C: Voio
USER =	guest
QK Cancel B	rowse <u>F</u> ind <u>H</u> elp

Figure 5.16

- a) Specify the dataset name, expno etc.
- b) Click OK.

Note that the dataset specification consists of the five variable parts of the data directory tree, in this case:

#### C:\bio\data\guest\nmr\exam1d\_1H\1\pdata\1

The text boxes are initialized with the dataset in the current data window.

#### How to Open Data from the Explorer, Konqueror or Nautilus

You can open a dataset from the Windows Explorer as follows:

- 1. Open the Windows Explorer. You can do that in two different ways:
  - reference from the Windows *Start* button. Navigate to the data *name*, *expno* or *procno*.

or

by entering the command *exp1* in TOPSPIN. The Explorer shows the contents of the current dataset *procno* directory. Navigate to the desired data *name*, *expno* or *procno*. *exp1* can also be used with the argument *top* to open the TOPSPIN installation directory, *home* to open user home directory or with an absolute pathname to open that directory.

The command *expl spect* opens the Explorer in <*tshome>/conf/instr/ current instrument>* The command *expl prop* opens the Explorer in the user's properties directory *User-HOME/topspin<name\_of\_PC>/prop* 

By entering *expl <illegal argument>* all available options are shown.

- 2. Now you can open a dataset with:
  - drag & drop: click-hold a dataset name or any of its sub-folders or files and drag it into the TOPSPIN data area or data window.

#### or

IS copy & paste: right-click a dataset and choose copy from the popup menu. In TOPSPIN, click Edit → Paste [paste] (see Fig. 5.17).

Edit	⊻iew	Spectromete			
<u>C</u> 0	ру				
<u>P</u> aste					
Find data [Ctrl F]					

Figure 5.17

Likewise, a dataset can be opened from the Windows window or Internet Browser.

#### How to Open Data from the Command Line

To open a dataset from the command line:

- 1. Enter re
- 2. Specify a dataset in the appearing dialog box (see Fig. 5.16).

3. Click OK

To open a new procno of the current dataset:

- 1. Enter rep
- 2. Specify a procno in the appearing dialog box.
- 3. Click OK

To open a dataset in a new window:

- 1. Enter rew
- 2. Specify a dataset in the appearing dialog box.
- 3. Click OK

To open a new *procno* of the current dataset in a new window:

- 1. Enter repw
- 2. Specify a procno in the appearing dialog box.
- 3. Click OK

To open a data browser and read a dataset from there:

- 1. Enter reb
- 2. Select a dataset from the appearing dialog box.
- 3. Click Display

Note that *re*, *rep* and *reb*:

- Replace the data in the currently selected data window.
- Open the data in a new window when they are used after typing *Alt+w n*
- Add the data in the currently selected window if this is in multiple display mode.

whereas *rew* and *repw*:

• Always open the dataset in a new window.

Topspin 2.0 and newer allows opening datasets stored in the following directories structures:

```
<mydata>/<dataname>/<expno>/pdata/<procno>
```

To do that

- Enter *reb* on the command line, browse to the desired dataset and click the **Display** button
- or
- Is Open the Operating System File Browser, browse to the desired dataset and open it in Topspin with Copy & Paste or Drag & Drop.

Note that this will create a copy of the dataset in the standard Topspin datapath:

```
<tshome>/data/<user>/nmr/<dataname>/<expno>/pdata/<procno>
```

where <user> is the current internal Topspin user. This copy can be processed, deleted or overwritten, even if the original dataset is write protected. The original data set is left unchanged.

#### How to Open Special Format Data

Apart from the standard Bruker data format, TOPSPIN is able to read and display various other formats. To do this:

```
\mathbb{R} Click File \rightarrow Open [open, Ctrl+o]
```

select the option **Open NMR data stored in special formats**, select the desired file type (see Fig. 5.18) and click *or*.

A dialog will appear which depends on the chosen file type. Just follow the instructions on the screen.

The following file types are supported:

- JCAMP-DX Bruker TOPSPIN<sup>1</sup> data stored in JCAMP-DX format
- Zipped TOPSPIN Bruker TOPSPIN data stored in ZIP format
- WINNMR Bruker WINNMR data
- A3000 Bruker Aspect 3000 data
- VNMR data acquired on a Varian spectrometer
- JNMR data acquired on a Jeol spectrometer
- Felix 1D data, FID or spectrum, which are stored in FELIX format.

<sup>1.</sup> Note that the TOPSPIN data format is identical to the XWIN-NMR data format.

Note that in all cases, the data are stored in a single data file which is unpacked/converted to standard Bruker format, i.e. to a data directory tree.

💐 Open - fromjdx						
Options Open NMR data stored in standard Bruker format Open NMR data stored in special formats Open other file						
Required parameters	JCAMP-DX					
<u>o</u> k	Cancel Help					

Figure 5.18

# How to Open a ZIP or JCAMP-DX file from the Windows Explorer

Data stored in ZIP or JCAMP-DX format can also be opened directly from the Windows Explorer. You can do that in one of the tree following ways:

#### Drag & drop

IN Click-hold a file with the extension .dx or .zip and drag it into the TOPSPIN data area or data window.

#### Copy & paste

- 1. Right-click a file with the extension .dx or .zip and choose **copy** from the popup menu.
- **2.** In TOPSPIN, click **Edit**  $\rightarrow$  **Paste** [**paste**]

#### Associate JCAMP-DX files with a script

- 1. Create a file with the extension .cmd (e.g. jcamp.cmd) with a text editor.
- 2. Enter the following line:

```
<tshome>\prog\bin\sendgui.cmd fromjdx %1
```

and store the file.

- 3. Open the Explorer and find the JCAMP-DX file.
- 4. Right-click the filename and choose Open with  $\rightarrow$  Choose program  $\rightarrow$  Browse
- 5. Find and select the script and click OK.

Now, every file with the extension  $.\,\mathrm{dx}$  will automatically be opened in TOPSPIN when double clicked.

# 5.4 Saving/Copying Data

#### How to Save or Copy Data

You can save the current dataset as follows:

**1.** Click File  $\rightarrow$  Save [Ctrl+s].

This will open a dialog box (see Fig. 5.19).

🖕 wrpa	🖕 wrpa 📃 🔀				
Please spe	Please specify destination data set				
NAME	exam1d_13C				
EXPNO	1				
PROCNO	1				
DIR	C:\Bruker\TOPSPIN				
USER	guest				
OK <u>C</u> ancel <u>H</u> elp					
	E'				

Figure 5.19

- 2. Select an option and, if applicable, a file type.
- 3. Click OK to execute the option.

The options correspond to the following command line commands:

• wrpa - copies the current data to a new data name or expno

- toccpn convert experiment information to ccpn format<sup>1</sup>
- tozip convert a dataset of any dimension to ZIP format
- tojdx convert a 1D or 2D dataset to JCAMP-DX format
- totxt convert a 1D or 2D dataset text format
- wpar write parameter set
- convdta save digitally filtered data as analog filtered data
- wrp, wra, genfid, wmisc write various files

#### How to Save an Entire Dataset

- **1.** Click File  $\rightarrow$  Save [*Ctrl+s*].
- 2. Select the option Copy dataset to a new destination [*wrpa*] and click OK
- 3. Specify the dataset variables and click OK

#### How to Save Processed Data

- **1.** Click File  $\rightarrow$  Save [*Ctrl+s*].
- 2. Select the option Save other file
- 3. Select File type Processed data as new procno [wrp] and click OK
- 4. Enter a processing number (procno) and click OK

#### How to Save Acquisition Data

- **1.** Click File  $\rightarrow$  Save [Ctrl+s].
- 2. Select the option Save other file
- 3. Select File type Acqu. data as new expno [wra] and click OK
- 4. Enter a experiment number (expno) and click OK

#### How to Save Processed Data as Pseudo Raw Data

- **1.** Click File  $\rightarrow$  Save [Ctrl+s]
- 2. Select the option Save other file
- 1. For detailed information about the ccpn format please refer to www.ccpn.ac.uk

- 3. Select File type 1r/1i as fid [genfid] or 2rr/2ii as ser [genser]
- 4. Click OK
- 5. Enter a destination expno.

(optionally, you can specify further data path specifications)

6. Click OK

# 5.5 Deleting Data

#### How to Delete a Specific Dataset

Right-click the data *name*, *expno* or *procno* in the browser, then click **Delete...** 

A confirmation dialog will appear. Just click **OK**, if you are sure you want to delete. Note that TOPSPIN does not allow you to delete the last available dataset, e.g. the last *procno* under an *expno*, the last *expno* under a *name* or the last *name* under a *user*.

#### How to Delete Types of Datasets

To delete certain types of data like 1D raw data, 2D processed data etc.:

```
\mathbb{R} Click \ File \rightarrow Delete...
```

or

Sector **delete** on the command line.

The dialog window shown in Fig. 5.20 will appear. Here you can select the data type and selection criteria.

# 5.6 Renaming Data

#### How to Rename a Specific Dataset

- 1. Right-click the data *name*, *expno* or *procno* in the browser, then click **Rename...**
- **2.** In the appearing dialog: Enter the new *name*, *expno* or *procno*

#### 3. Click OK

💐 dela 🛛 🔀
Browse Options
◯ An entire data set with all EXPNOs/PROCNOs
<ul> <li>Acquisition data</li> </ul>
O Processed data
◯ Data acquired at certain dates
◯ 1D raw data ("fid")
◯ 1D processed data ("1r/1i")
◯ 2D/3D raw data ("ser")
◯ 2D processed data ("2rr/2ii")
O Imaginary processed data ("1i")
OMacro
O AU program
O Python program
O Pulse program
O Parameter list
O 'Miscellaneous' file
Required parameters
Name = *
Data directory = C: /bio
User = guest
<u>O</u> K <u>C</u> ancel <u>H</u> elp

Figure 5.20

1. Select a data type option

For each option, the corresponding command appears in the title of the dialog box. These commands can also be used to delete data from the command line.

2. Specify the Required parameters

Note that you can use the wildcards:

- Asterix (\*) for any character and any number of characters.
- Question mark (?) for any single character.
- 3. Click OK

A dialog box will appear showing the matching datasets. For example, if you select the option **An entire dataset ...**:

1. Select dataset entries for deletion (selected entries are highlighted).

To select multiple entries: click them holding the *Shift* or *Ctrl* key.

2. Click **OK** to delete the entire data directory.

If you select the option **Acquisition data** or **Processed data**, you can choose between deleting the data files only and deleting the entire *expno* or *procno* directory, respectively (see Fig. 5.21).

🔤 dela			<u></u>	<
Data directory = C: <i>I</i> bio User = guest Name = *13*				
Options O Delete the selected EXPNOs with all t Delete the raw data files of the select	heir PROCNOs ted EXPNOs			
NAME	EXPNO	ACQU. DATA	SIZE	
exam1D 13C fid exam1d 13C exam1d 13C exam1d 13C exam1d 13C exam1d 13C	1 1 2 3 4		fid 64 K fid 64 K fid 64 K fid 64 K fid 64 K	
		<u>o</u> k (	ancel <u>H</u> elp	)

Figure 5.21

# 5.7 Searching/Finding Data

#### How to Find Data

You can find TOPSPIN data according to various criteria. To start searching, do the following:

1. Click Edit  $\rightarrow$  Find data [Ctrl+f | find] to open the Find data window (see Fig. 5.22).

🍓 Find data			×		
Searching will be performed in all data directories marked in the data directories list below! The checkboxes at the right will enforce exact matching if enabl					
NAME					
EXPNO					
PROCNO					
USER					
Title					
Pulse Prog.					
Dimension		Any 💊	•		
Data type		Any 💊	•		
Date, from: mm/dd/yy					
Date, till: mm/dd/yy					
Data directories					
C:\Bio					
C:\bio1					
C:\ts2.0					
<u> </u>					
<u>o</u> k (	<u>R</u> eset mask	<u>C</u> ancel	Help		

Figure 5.22

- 2. Enter the search items in the upper part of the dialog. Note that:
  - There will be searched for items containing the specified string
  - Exact matching is performed for dataset variables, NAME, EXPNO, PROCNO and USER, if the checkboxes at the right are enabled.
  - The search is restricted to data created between the specified dates. Note that this refers to the acquisition date.
  - The Reset mask button allows you to reset the default criteria.
- **3.** Select the **Data directories** to be searched in the lower part of the dialog. If no directories are selected, all will be searched.
- 4. Click OK

to start the search. A list of data that fulfil the defined criteria will appear (see Fig. 5.23).

🥌 Search result						
Found: 6 Data Sets. Please right-click in a list for more options!						
exam1d_13C 1 1 C:\bio guest	1	zgpg30	2004-03-30 10:43:33			
exam1d_13C 2 1 C:\bio guest	1	jmod	2004-03-30 11:01:05			
exam1d_13C 3 1 C:\bio guest	1	dept135	2004-03-30 11:18:36			
exam1d_13C 4 1 C:\bio guest	1	dept45	2004-03-30 11:53:06			
exam1d_13C 5 1 C:\bio guest	1	dept90	2004-03-30 12:27:39			
exam1d_13C 6 1 C:\bio guest	1	zgig30	2004-03-30 13:35:54			
			Display Close			

Figure 5.23

Note that on exiting TOPSPIN, the search criteria will be rest to default.

#### How to Display one of the Found Datasets

In the search result window (see Fig. 5.23):

1. Click one or more datasets to select them.

2. Click Display

to display the selected dataset(s) in the current data window. If multiple datasets are selected they are displayed in a new data window in multiple display mode.

The search result window offers a right-click context menu with various options (see Fig. 5.24).



#### Display

Display the selected dataset(s) in the current data window. If multiple datasets are selected they are displayed in the same data window in multiple display mode. Equivalent to clicking the **Display** button or pressing *Enter*.

#### **Display In New Window**

Display the selected dataset(s) in a new window. If multiple datasets are selected they are displayed in the one new data window in multiple display mode.

#### **Display As 2D Projection**

Display the selected dataset as a projection of the current 2D dataset. A dialog will appear allowing you to choose F1-projection, F2-projection or both. If multiple datasets are selected, only the first one is considered. If the current dataset is not a 2D dataset, nothing happens.

#### Sort This Column

Sort the selected column in ascending order.

#### Sort + Reverse

Sort the selected column in descending order.

#### Save Selection in file...

Save the list of selected datasets in a text file. First opens a file dialog where you can select or specify a filename. The saved dataset list can, for example, be used for serial processing (command *serial*, see also *Process Selected Datasets* below).

#### Add selection to dataset group...

Selected datasets can be defined as dataset group.

#### **File properties**

Show main dataset parameters like *Dimension*, *Pulse program*, *Acquisition Date*, *Nuclei*, *Spectrometer frequency* and *Solvent*.

#### Files

Show the files in the processed data directory of the selected dataset.

#### **Process Selected Datasets**

Perform serial processing on the selected datasets. Opens a dialog where you can change or edit the dataset list and specify the command, macro or Python program to be executed (starts the command *serial*).

The **Close** button allows you to close the search result dialog.

# 5.8 Handling Data Files

#### How to List/Open the Current Dataset Files

A Bruker dataset is represented by a directory tree which contains files in the *expno* and *procno* subdirectories. These files contain the actual data, parameters, lists etc.

Right-click inside the data window and choose Files from the popup

menu.

Display Properties... Save Display Region To... Restore Display Region From Params. F1/2 Set plot height for current position File Properties... Files

If the spectrum is displayed, the files in the *procno* subdirectory are shown. If the **Fid** is displayed, the files in the *expno* subdirectory are shown.

Select a file and click **Open** to view its contents.

Note that this only makes sense for ascii files.

# How to List/Open the current Dataset Files in the Windows Explorer

To list the current dataset files in the Windows Explorer:

- **1.** Click File  $\rightarrow$  Run...
- Select Open file explorer [exp1] in the appearing dialog box (see Fig. 5.25)
- 3. Click OK

Alternatively, you can enter the command *exp1* on the command line. The Windows Explorer will be opened showing the processed data files (the files in the *procno* directory) of the current dataset. Under Linux a Web browser like KDE Konqueror or Gnome Mozilla will be opened.

To open a file:

Bouble-click the file or right-click the folder icon and choose Open



Figure 5.25

If TOPSPIN data area contains no datasets, the *exp1* command opens the Explorer showing the users home directory. When entered on the command line, *exp1* can also be used with the argument *top* to open the TOP-SPIN installation directory, *home* to open user home directory or with an absolute pathname to open that directory.

# Chapter 6 Parameter Handling

## **6.1 Processing Parameters**

Processing parameters can be set/changed in three different ways:

- from the parameter editor: click the ProcPars tab or enter edp
- from the command line: e.g. enter si
- from a command dialog box: e.g. wm

#### How to Set a Processing Parameter from the Command Line

Enter the parameter name on the command line. For example to set the size:

1. Enter *si* 

for 1D data, the following dialog box will appear:



for 2D data, the following dialog box will appear:

🂩 SI			×
Size of real sp	ectrum		
SI =	1024	1024	
		<u>0</u> K	<u>C</u> ancel

- 2. Specify the desired value(s), e.g. 32768 or 32k
- 3. Click OK

#### How to Set Processing Parameters from the Parameter Editor

To open the processing parameter editor:

IF Click the **ProcPars** tab in the Tab bar of the data window.

or

Sector **edp** on the command line.

exam1d_1H 1	1 C:\bio guest							×
Spectrum ProcPars	AcquPars Title	PulseProg	Peaks	Integrals	Sample	Structure	Fid Acq	łu
🗠 M S 1,2,	▼ #							
Reference Window	▼ Reference	32768	_	_		Size of	real spec	^
Phase Baseline	SF [MHz] =	500.13	00000			Spectro	ometer fre	
Fourier	OFFSET [ppm] =	11.008				Low fie	eld limit of	
Integration	SR [Hz] =	0.00				Spectr	um referei	
Peak Automation Miscellaneous User	HZpPT [Hz] = ► Window function ▼ Phase correction	0.1833	99			Spectra	al resolutic	
	PHC0 [degree] =	-111.45	56			Oth ord	er correct	~



At the left of the parameter editor window you will see a list of parameter sections.

The processing parameter editor supports the following functions:

- Is Collapse/expand a parameter section by clicking the ▼ button. Note that the section Window function in Fig. 6.1 is collapsed.
- Solution of the data window toolbar.
- $\mathbb{R}$  Enter (part of) a parameter name in the search field and click M.
- Click a parameter section, e.g. Phase at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.
- Solution of the set of
- Click the .... button to the right of parameters like AUNMP to open a list of the corresponding programs/lists.

- Right-click the E button to the right of parameters like AUN-MP to open the current program/list with an editor.
- Hit the Tab key to jump to the next parameter field.
- Hit **Shift+Tab** to jump to the previous parameter field.
- Is Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

#### How to Undo the Last Processing Parameter Change

- Real Click the following button:
  - Undo last parameter change.

#### How to Display Processing Status Parameters

Source Click the following button:

s Show processing status parameters.

Note that the command *dpp* opens the parameter editor and automatically shows the status parameters.

#### How to Switch to Maxent parameters

Real Click the following button:

M Switch to Maxent parameters.

#### How to Change Processed Data Dimensionality

Real Click the following button:

1,2... Change data dimensionality.

This changes the number of parameter columns and value of the processing parameter PPARMOD. TOPSPIN 2.1 and newer support data dimensionalities up to 8D.

The parameter editor does not allow you to modify status parameters. Processing status parameters reflect the status of the processed data and are used for further processing, display or plotting. Changing them can make the dataset inconsistent. In rare cases, however, it can be useful to change a status parameter and TOPSPIN allows you to do that from the command line. If, for instance, you want to change the F1 status parameter MC2 of a 2D dataset, you have to enter:

s mc2

Note that the command *s* is used for 1D, 2D and 3D dataset. TOPSPIN automatically recognizes the dimensionality of the data and displays the parameter in all relevant dimensions. Note that, for example, the parameter MC2 only exists in F1.

## **6.2 Acquisition Parameters**

#### How to Set Acquisition Parameters

Acquisition parameters can be set/changed as follows:

- from the parameter editor: click the AcquPars tab or enter eda
- from the command line: e.g. enter td
- from the interactive parameter adjustment window (enter gs)

#### How to Set an Acquisition Parameter from the Command Line

Enter the parameter name on the command line. For example to set the time domain size:

1. Enter td

for 1D data, the following dialog box will appear:



for 2D data, the following dialog box will appear:

🢩 TD		×
Size of fid (F2, F1)		
TD =	1024	256
		<u>O</u> K <u>C</u> ancel

- 2. Specify the desired value(s), e.g. 65536 or 64k
- 3. Click OK

### How to Set Acquisition Parameters from the Parameter Editor

To open the acquisition parameter editor:

Real Click the AcquPars tab in the Tab bar of the data window.

or

🖙 Enter *eda* on the command line.

Fig. 6.2 shows an example of the acquisition parameter editor with the Experiment parameters displayed.

exam1d_13	IC 1 1 C:\Bio g	uest				[		
Spectrum Proc	Pars AcquPars	Title Puls	eProg Peaks	Integrals	Sample	Structure F	id Acqu	
ωЛS	🔰 📰 1,2,	V #						
Experiment Width	▼ Experimer	t					^	
Receiver	PULPROG =		zgpg30			Current pulse pr		
Nucleus	AQ_mod =	C	)QD	*		Acquisition mode		
Durations	TD =		65536		Size of fid			
Power	NS =		256			Number of scan:		
Program	DS =		4			Number o	of dumm	
Probe	TD0 =		1			Loop cou	nt for "t	
Lists Wobble	► Width		·				_	
Lock	▼ Receiver							
Automation	RG =		32768			Receiver	gain	

Figure 6.2

The processing parameter editor supports the following functions:

- Real Collapse/expand a parameter section by clicking the **v** button. Note that the section Width in Fig. 6.2 is collapsed.
- Collapse/expand all parameter sections by clicking the large **T** button of the data window toolbar.
- 🖙 Enter (part of) a parameter name in the search field and click 🙀 .
- Real Click a parameter section, e.g. Experiment at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.
- R Click in a parameter field, e.g. TD, to set the parameter value.
- Click the . button to the right of parameters like PULPROG to open a list of the corresponding programs/lists.

- Right-click the E button to the right of parameters like PUL-PROG to open the current program/list with an editor.
- IF Hit the Tab key to jump to the next parameter field.
- Hit **Shift+Tab** to jump to the previous parameter field.
- IN Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

#### How to Undo the Last Acquisition Parameter Change

- Real Click the following button:
  - Undo last acquisition parameter change.

#### How to Set Pulse Program Parameters

- Source Click the following button:
  - **I** Show pulse program parameters [*ased*]
- The button will change to A . To make this the default setting:
  - Click **Options**  $\rightarrow$  **Preferences**, click **Miscellaneous**, check the entry "Show ased parameter selection with eda" and click **OK**.

#### How to Display Acquisition Status Parameters

Real Click the following button:

s Show acquisition status parameters.

Note that the command *dpa* opens the acquisition parameter editor and automatically shows the status parameters.

#### How to Get Probehead/Solvent dependent Parameters

Real Click the following button:

Set probehead/solvent dependant parameters [getproso1].

Probehead and solvent dependant parameters can be set up with the command *edprosol*.

#### How to Change Acquisition Data Dimensionality

Ref Click the following button:

123 Change data dimensionality.

This changes the number of parameter columns and value of the acquisition parameter PARMODE.

#### How to Set Lock Parameters

Enter the command *edlock* and set the lock parameters in the appearing dialog box. For a detailed description of *edlock*, please refer to the Acquisition Reference manual or enter *edlock*? on the command line.

#### How to Set Routing Parameters

Enter the command *edasp* and set the routing parameters in the appearing dialog box. For a detailed description of *edasp*, please refer to the Acquisition Reference manual or enter *edasp*? on the command line.

# Chapter 7 Data Processing

### 7.1 Interactive Processing

Interactive processing allows full control over the processing sequence. However, it requires detailed knowledge about the required parameters (see chapter 6.1) and commands. Therefore, it is only suitable for the advanced user. New or intermediate users are recommended to use the Processing Guide for semi-automatic processing (see chapter 7.2).

#### How to Process Data with Single Commands

Data can be processed by entering single commands on the command line. A typical 1D processing sequence would be:

- em : exponential window multiplication
- ft : Fourier transform
- apk : automatic phase correction
- sref : automatic calibration (referencing)
- abs : automatic baseline correction

This allows you full control over each individual processing step.

#### How to Process data with Composite Commands

Data can also be processed with so called composite commands. These are combinations of single processing commands. The following composite commands are available.

- ef : Exponential multiplication + Fourier transform
- *efp* : Exponential multiplication + Fourier transform + phase correction
- fmc : Fourier transform + magnitude calculation
- *fp* : Fourier transform +phase correction
- gf : Gaussian multiplication + Fourier transform
- *gfp* : Gaussian multiplication + Fourier transform + phase correction

They can be entered on the command line or clicked from the menu. For the latter option:

```
\texttt{ISP} Click Processing \rightarrow More transforms \rightarrow Shortcuts
```

Just like single commands, composite commands can be used in Macros, AU programs and Python programs.

## 7.2 Semi-automatic Processing

#### How to Use the 1D Processing Dialog

1D data processing often involves the same sequence of steps, which can easily be performed as follows:

- 1. Click Processing -> Process / Plot Current data
- 2. In the appearing dialog (see Fig. 2.1):
  - a) Enable the desired processing/plotting steps
  - b) Set the parameter LB for exponential multiplication
  - c) Select the desired LAYOUT for plotting.
  - d) Click OK

🔄 proc1 d			2	<
Press OK to process / plot the sele using the enabled options. The command "proc1d y" will proce using the last settings.	cted di ess dai	ataset ta without this	s dialog,	
Exponential Multiply (em)	✓	LB [Hz] =	1	
Fourier Transform (ft)				
Auto - Phasing (apk)	✓			
Set Spectrum Reference (sref)	✓			
Auto - Baseline Correction (abs)	<b>V</b>			
Plot (autoplot)		LAYOUT =	+/1D_H.xwp	
			<u>O</u> K <u>C</u> ancel	]

Figure 7.1

#### How to Use the Processing Guide in Automatic mode

The Processing Guide in automatic mode guides you through the entire processing sequence of data selection, processing, printing and archiving with minimum user interaction.

#### 1. Click Processing $\rightarrow$ Data $\rightarrow$ Processing Guide

The Processing Guide window will appear as an integral part of the current data window (see Fig. 7.2).





- 2. In the Processing Guide window:
  - a) Check Automatic mode
  - b) Click **Open data set** and click **OK** to open a dataset manually, e.g. from the browser or click **Browse** to open the File Chooser.

#### c) Click Window function $\rightarrow$ Fourier Transform $\rightarrow$ etc.

Each processing step will be executed without user interaction.

#### How to Use the Processing Guide in Interactive mode

The Processing Guide in interactive mode guides you through the entire processing sequence of data selection, processing, printing and archiving requiring some user interaction.

#### 1. Click Processing → Data → Processing Guide

The Processing Guide window will appear as an integral part of the current data window.

- 2. In the Processing Guide window:
  - a) Uncheck Automatic mode
  - b) Click **Open data set** and click **OK** to open a dataset manually, e.g. from the browser or click **Browse** to open the File Chooser.
  - c) Click Window function  $\rightarrow$  Fourier Transform  $\rightarrow$  etc.

For each step a dialog box will appear where you can enter options, parameters etc. For details on these items, please refer to the corresponding commands in the Processing Reference Guide.

# 7.3 Processing Data with AU programs

Data processing can be performed by using AU programs. An AU program is actually a C-program which contains TOPSPIN commands (macros) and/or C-language statements. Various standard AU programs are delivered with TOPSPIN. A typical 1D processing AU program is *proc\_1d*. A simplified version of this AU program is:

EF APK SREF ABS AUTOPLOT QUIT

It executes the commands ef, apk, sref, abs and autoplot. To run this

AU program, just enter *proc\_1d* on the command line <sup>1</sup>. You can create your own AU programs with the command *edau*. Note that an AU program must end with QUIT or QUITMSG("your message"), and that all statements must be specified in capital letters. For more information on AU programs, please refer to the AU programming manual:

# $\operatorname{I\!S\!P}$ Click Help $\rightarrow$ Manuals $\rightarrow$ [Programming Manuals] AU Programming

As an alternative to AU programs, you can also write Python programs, which allow you to use TOPSPIN commands, User Interface functions and Graphic functions. For more information:

# $\operatorname{I\!S\!P}$ Click Help $\rightarrow$ Manuals $\rightarrow$ [Programming Manuals] Python Programming

# 7.4 Serial Processing

TOPSPIN allows you to process a series of datasets using serial scripts. The dataset list and command(s) to be used can be easily setup from the TOP-SPIN interface as follows. Enter the command *serial* on the command line. This will open the dialog window shown in Fig. 7.3.

Serial Processing - Define Datasets
Please define the full path name of the dataset list to be processed.
Click on:
> Browse For List = locate an existing dataset list
> Find Datasets = search for datasets and use the selected ones as the list
> Edit List = edit the current or a new dataset list
> Next = continue with command definition
Browse For List     Eind Datasets     Edit List     Next >     Cancel
Figure 7.3

<sup>1.</sup> Before you can use any Bruker AU program, *expinstall* must have been executed once.

The same dialog window will be shown by using the menu bar Processing Serial Processing.

The dialog offers you the following options:

#### **Browse for list**

This buttons opens an Explorer in which you can locate an existing datset list.

#### **Find Datasets**

You can for Datasets in all data directories marked in the appearing dialog window list (see Abbildung 7.4).

🥌 Find data		norde und diere weiten er der diese die se				
Searching will be perform marked in the data direct The checkboxes at the ri	ned in all data tories list belo ght will enford	a directories w! ce exact matching if er	abled.			
NAME	13					
EXPNO						
PROCNO						
USER	T					
Title	-					
Pulse Prog.		Search result				
Dimension		Found: 9 Data Sets. Please right-click in a list for	more options!			
Data type		ekamito 130 I 1 F \Bruik	enloospin guest	1	zgop30	2004 03 30 11 43 33
Data from: mm/dd/av		exam1d_13C 1 2 F:\Bruk	en'TopSpin guest	1	zgpg30	2004-03-30 11:48:33
Date, nom. minvou/yy		exam1d_13C 1 8 F:\Bruk	enTopSpin guest	1	zgpg30	2004-03-30 11:45:35
Date, till: mm/dd/yy		examite_13C 11 1 F1Bru	kentopspin gues adTopSpin quast		zgpg30	2004-03-30 11:43:33
		examinu_13C_2_1_F.VBruk	entopapin guesi. entopapin quest	1	dent135	2004-03-30 12:18:36
Data directories		exam1d 19C 4 1 F:\Bruk	enTopSpin guest enTopSpin quest	1	dept45	2004-03-30 12:53:06
		exam1d_13C 5 1 F:\Bruk	enTopSpin guest	1	dept90	2004-03-30 13:27:39
C:\NMR data		exam1d_13C 6 1 F:\Bruk	enTopSpin guest	1	zgig3D	2004-03-30 14:35:54
F:\Bruker\TopSpin						
F:\Bruker\topspin1.3pl	5					
E \Bruker\tonsnin1 3nl	3					
<u>o</u> k	<u>R</u> eset ma					

Figure 7.4

#### Edit List

This button will open a texteditor in which you can edit the current or

a new dataset list.

Next

After having defined the full datasetpath and clicking next the following dialog will appear:

Serial Processing - Define Command						
Please define the command to be executed on the datasets.						
Examples:						
1) efp						
2) Ib 0.8;em;ft;pk						
3) c:\mymacros\mac-efp (a full path indicates a macro)						
<ol><li>c:\mypys\py-efp.py (a full path with '.py' indicates a Python script)</li></ol>						
Click on:						
> Browse For Macro = locate a TopSpin macro						
> Browse For Python = locate a TopSpin Python program						
> Execute = start processing the dataset list						
> Back = return to list definition						
> Show = show datsets while processing						
Show Browse For Macro Browse For Python Execute $< Back$ Cancel						

Figure 7.5

Continue with command definition, for example for Macros or Python programs. You can even Browse for Macros or Python programs. The
following dialog will appear, dependent from your selection:

🔄 Python Programs						X
<u>File</u> Options <u>H</u> elp	Source =	PSPIN2.1-alpha\exp\stan\nmr\py	*			
Search in names [*?]	Search					
Cursor2d.py	exam-em-ft-apk.py	exam-multi-efp.py	exam-pulsp	rog.py	exam-splitser.py	
exam-sum-real.py	inadph.py	inadph2.py	ineptrdsp.p	У	py-test-suite.py	
					<u> </u>	el

Figure 7.6

After having chosen a Python program or a Macro, push the button execute for finishing serial processing command. In Figure

Abbildung 7.7 you can see the look of the actual dialog.

Serial Processing - Define Command 🛛 🛛 🔀							
Please define the command to be executed on the datasets.							
Examples:							
1) efp							
2) Ib 0.8;em;ft;pk							
3) c:\mymacros\mac-efp (a full path indicates a macro)							
<ol><li>c:\mypys\py-efp.py (a full path with '.py' indicates a Python script)</li></ol>							
Click on:							
> Browse For Macro = locate a TopSpin macro							
> Browse For Python = locate a TopSpin Python program							
> Execute = start processing the dataset list							
> Back = return to list definition							
> Show = show datsets while processing							
em;ft;abs;apk							
Show Browse For Macro Browse For Python Execute < Back Cancel							

Figure 7.7

After executing the serial processing, TopSpin 2.1 and newer displays following feedback-dialog:



Figure 7.8

## Cancel

Leave this dialog.

# Chapter 8 Printing/Exporting Data

# 8.1 Printing/plotting Data

# How to Print/Plot from the Menu

The current data window can be printed as follows:

- **1.** From the TOPSPIN menu:
  - 🖙 Click the button 🎒 in the upper toolbar
  - or Click File → Print
  - or Enter print or Ctrl+p

All these actions are equivalent; they open the Print dialog box (see Fig. 8.1).

🤤 Print [Ctrl+P] 🕘 p	olot 🔀
Options Print active window [pi Print with layout - start Print with layout - plot of	rnt] Plot Editor [plot] directly [autoplot]
Required parameters	D_H.xwp
Use plot limits <ul> <li>from screen / CY</li> <li>from Plot Editor Reset /</li> <li>as saved in Plot Editor</li> <li>Dverride plotter saved</li> </ul>	Fill data set list Actions O from your default portfolio O from portfolio saved in data set in Plot Editor:
CURPLOT =	Dell Photo AIO Printer 922

Figure 8.1

- 2. In the Print dialog box:
  - a) Select Print active window [prnt]
  - b) Click OK

Before printing starts, the operating system print dialog box will appear. Here you can, for example, select the printer name and the printer properties.

The Print dialog box (see Fig. 8.1) contains two further options:

- Print with layout start Plot Editor [plot] If you select this option and click OK, the Plot Editor will be started. This option is equivalent to entering plot on the TOPSPIN command line.
- **Print with layout plot directly** [*autoplot*] Selecting this option activates the Plot Editor layout list box. Select

the desired layout and click **OK** to print. Standard layouts are delivered with TOPSPIN. They use the Windows default printer. User defined layouts use the printer defined in the Plot Editor. On a 1D dataset, only 1D layouts are listed, on a 2D dataset only 2D layouts are listed etc.

For the last two options, the following Required Parameters are available:

#### **Use plot limits**

• from screen/ CY

The plot limits and maximum intensity are used as they are on the screen (processing parameter F1P, F2P and CY, respectively).

## • from Plot Editor Reset Actions

The plot limits and maximum intensity are set according to the Plot Editor Reset Actions (right-click inside the Plot Editor data field and choose **Automation** to set the Reset Actions).

## • as saved in Plot Editor

The plot limits and maximum intensity are set in the specified layout

# Fill dataset list

# • from your default portfolio

The portfolio contains the current TOPSPIN dataset plus the data from the default Plot Editor portfolio.

#### from port folio saved in dataset

The portfolio contains the current TOPSPIN dataset plus the data from the portfolio stored in this dataset.

# **Override Plotter saved in Plot Editor**

If enabled, the plotter defined in the Plot Editor layout will be overridden by de plotter defined by the processing parameter CURPLOT.

# How to Plot Data from the Processing guide

Printing/plotting data can be done from the Processing guide by clicking the **Plot/Print** button. If **Automatic mode** is checked, the active data window will be printed as it appears in the screen. If **Automatic mode** is unchecked, you will get the dialog box as displayed in Fig. 8.1.

# How to Plot Data with the Plot Editor

The Plot Editor can be started from the Print dialog or from the command line (command *plot*). The Plot Editor allows you to create layouts and plot data. The complete functionality is described in the online manual, which can be opened as follows:

 $\texttt{ISP} \ Click \ \textbf{Help} \rightarrow \textbf{Manuals} \rightarrow [\textbf{Automation and Plotting}] \ \textbf{Plotting}$ 

# How to Print the Integral list

1. Click the Integrals tab of the data window (see Fig. 8.2).

exam1d_1H	l 1 1 C:\bio gue	st			<u>_ 8 ×</u>
Spectrum Pr	ocPars AcquPa	rs   Title   Pul:	sProg   F	Peaks Integrals	Sample 💽
△ Object	Integral (abs)	Integral [rel]	Peaks	Range (F1) from	Range (F1) to
-Integral 1	21786348.44	1.6650	0	7.872	8.603
-Integral 2	20849330.78	1.5934	0	7.410	7.870
⊕–Integral 3	45796921.97	3.5000	1	7.056	7.408
-Integral 4	131363188.00	10.0393	0	4.491	6.158
Integral 5	20473381.47	1.5647	0	3.979	4.489
±−Integral 6	1068216295.19	81.6376	32	0.304	3.977

2. Enter print or Ctrl+p to print it.

Figure 8.2

# How to Print the Peak list

- 1. Click the **Peaks** tab of the data window (see Fig. 8.3).
- 2. Enter print or Ctrl+p

exam1d_1H 1 1 C:\bio guest									
Spectrum	ProcPars	AcquPars	Title	PulseProg	Peaks	Integrals	Sample	Struct	
Peak	V v(F1)	) [ppm]	Intens	sity H	Half widt	h [ppm]			
1		8.6147		0.10		0.0092	i.	^	
2	!	8.5986	0.11		0.0044				
3	E.	8.5561		0.01		0.0007		_	
4		8.5421 0.00		0.00	0.0007				
5	5 8.5279		0.00 0.00		0.0015	015			
6	1	8.5059		0.00		0.0000			
7	3	8.4974		0.01		0.0018			

Figure 8.3

# 8.2 Exporting Data

# How to Copy data to Other Applications

Under MS Windows, you can easily copy the data window contents to other applications. To do that:

Reference Click Edit  $\rightarrow$  Copy [copy].

This will copy the data window contents to:

• the clipboard. After that you can paste the clipboard contents to any Windows application.

On Windows systems the command **Edit**  $\rightarrow$  **Copy** [*copy*] saves bmp-format, whereas the command *copy wmf* stores the old wmf-format.

On Linux systems the command *copy* stores png-files into a temporary file. The pathname of this file is copied to clipboard.

Please note:

Some programs, when importing spectra from the clipboard or metafile, do not display the contained information correctly. Particularly when you resize the imported graphics, sections of the text, the spectrum, or the axis sometimes have disappeared. Usually this is only a display problem. When you print the respective page, the representation is correct.

# How to Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TOPSPIN allows you to save the contents of a data window in a graphics file of selectable type. Supported formats are .png, .jpg, .jpeg, .bmp, .emf, .wmf and .pdf. To do that:

- **1.** Click File  $\rightarrow$  Export.... [exportfile].
- 2. Navigate to the storage folder.
- 3. Enter the destination filename and extension.
- 4. Click Export

The resolution of such a *screen dump* equals the resolution of your screen. When you import a graphics file into an other program, you may loose information when resizing the graphics.

Note that exporting a data window to PDF-format is only supported in TOPSPIN 2.1 and newer.

# Chapter 9 1D Display

# 9.1 The 1D Data Window

The 1D data window consists of a data field, a title bar, a Tab bar and buttons. Fig. 9.1 shows a data window with a 1D spectrum.



Figure 9.1

# 9.2 Displaying one Dataset in Multiple windows

TOPSPIN allows you to display one dataset in multiple data windows. This is, for example, convenient to view various regions or various objects (spectrum, fid, parameters etc.) of the same dataset.

# How to Reopen a Dataset in a Second/Third etc. Window

- 1. Select (activate) the desired dataset.
- **2.** Click File  $\rightarrow$  Reopen [reopen].

Multiple data windows with the same dataset are indicated with a number in square brackets, e.g. [1], in the title bar (see Fig. 9.2).

exam1d_1H 1 ·	1 C:\bio_guest[1]	_O×
Spectrum ProcP:	ars AcquPars Title PulsProg Pe	aks Integ 💶 🛌
2 [*1e6]		
exam1d_1H 1 ·	1 C:\bio_guest[2]	_O×
Spectrum ProcP:	ars AcquPars Title PulsProg Pe	aks Integ 💶 🕨
2 [*1e6]		
exam1d_1H 1	1 C:\bio guest [3]	
Spectrum ProcPa	ars AcquPars Title PulsProg Pe	aks 🛛 Integ
က S 🔛 🌺		
Reference	Window function	<u> </u>
Window	LB [Hz] = 0.30	<u> </u>
		•

Figure 9.2

# How to Rescale or Shift one Dataset in Multiple windows

Display buttons like \*2 and **T** only work on the active data window. The same counts for the keys **Alt+PageUP** and **Alt+PageDown**. However, when used with the control key, they work on all windows, for example:

```
☞ Hit Ctrl+ *2, Ctrl+Alt+PageUp Of Ctrl+Alt+PageDown
```

# 9.3 Changing the Display of a 1D Spectrum or FID

TOPSPIN offers buttons to scale or shift the spectrum vertically and horizontally.

# How to Change the Vertical Scaling of the FID or Spectrum

Hit one of the following the keys:

- Alt+PageUp: Increase the intensity by a factor of 2.
- Alt+PageDown: Decrease the intensity by a factor of 2.
- *Alt+Enter*: Reset the intensity.

or

- Real Click one of the following buttons:
  - \*2 Increase the intensity by a factor of 2 [\*2].
  - \*8 Increase the intensity by a factor of 8 [\*8].
  - /2 Decrease the intensity by a factor of 2 [/2].
  - /8 Decrease the intensity by a factor of 8 [/8].
  - EReset the intensity [.vr].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all data windows, press the *Ctrl* key while clicking one of the above buttons.

#### How to Smoothly Change the Vertical Scaling of the FID/Spectrum

```
Solution and move the mouse
```

or

IN Turn the mouse wheel while the cursor is in the data window.

# How to Change the Horizontal Scaling of the FID or Spectrum

IF Click-hold the button and move the mouse:

Q Zoom in/out smoothly.

or

Real Click one of the following buttons:

- Zoom in to the center (spectrum) or left edge (FID) of the displayed region, increasing the horizontal scaling. [.zi]
- Q Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [.zo]
- E Perform an exact zoom via a dialog box [.zx].
  - a) Enter the coordinates of the desired region in the dialog box:



- b) Click OK
- Undo last zoom [.z1].
- Reset horizontal scaling to show the full spectrum [.hr].
- Osplay the entire spectrum (baseline position and intensity scaling are adjusted if necessary) [.a11]
- Toggle interactive zoom mode. When switched off, interactive zooming only selects a horizontal region; baseline position and intensity scaling remain the same. When switched on, interactive zooming draws a box selecting the corresponding area.
- L Retain horizontal and vertical scaling when modifying dataset or

changing to different dataset [.keep]. Effects all data windows.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

# How to Shift a Spectral Region to the Left or to the Right

R Click-hold the following button and move the mouse:

- ↔ Smoothly shift to left or right.
- or

Solution of the following buttons:

- ← Shift to the left, half of the displayed region [.s1].
- → Shift to the right, half of the displayed region [.sr].
- ← Shift to the extreme left edge of the spectrum [.s10].
- $\rightarrow$  Shift to the extreme right edge of the spectrum [.sr0].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

# How to Shift the Spectrum Up or Down

To shift the FID or spectrum display up or down:

Solution Click-hold the button and move the mouse:

- Smoothly shift the spectrum baseline up/down.
- or

Real Click one of the following buttons:

- Shift the spectrum baseline to the middle of the data field [.su].
- L Shift the spectrum baseline to the bottom of the data field [.sd].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

# 9.4 Using the Tab bar

Tabs of the data window can be activated by clicking them or by entering the corresponding commands, as specified between square brackets, on the command line. Note that command line commands always work on the currently selected (active) data window.

The Tab bar can be configured from the User Preference box (command *set*).

# How to Display the Spectrum



Section Click the Spectrum tab [spec]

This displays the processed data. If these do not exist, the text '*No processed data available*' appears.

#### How to Set Processing Parameters

Second Click the **ProcPars** tab [edp]

exam1d_1H 1 1 C:\bio guest								
Spectrum Pr	ocPars	AcquPars Title	PulseProg	Peaks	Integrals	Sample	Structure	Fid Acqu
Reference Window Phase Baseline Fourier		SF [MHz] = OFFSET [ppm] = SR [Hz] = HZpPT [Hz] = ▼ Window functior	500.13 11.008 0.00 0.1833	99			Spectro Low file Spectro Spectro	ometer fre eld limit of um referei al resolutic
Peak Automation	~	WDW =	EM		~	)	Windov	v functior 🔽

This opens the processing parameter editor (see also chapter 6.1). The following extra buttons are available:

- Jundo last value change. Can be used to undo multiple changes.
- M Switch to Maxent parameters.
- S Status parameter display. The button turns green when activated [dpp].
- 123 Change processed dataset dimensionality (parameter PPARMOD).

Collapse/expand all parameter sections.

A Search for specified parameter.

Changed parameters are automatically saved.

#### How to Set Acquisition Parameters

Second Click the AcquPars tab [eda]

📕 exam1d_1H 1 1 C:\bio guest 🛛 📃 🗖 🔀								
Spectrum ProcP	ars AcquPars Title P	ulseProg Peaks Integra	s Sample Structure Fid Acqu					
юЛS	📙 🔣 1,2, 🔻 🏘							
Experiment	▼ Experiment							
Receiver	PULPROG =	zg	E Current pulse pr					
Nucleus	AQ_mod =	DQD 💉	Acquisition mode					
Durations	TD =	65536	Size of fid					
Power	NS =	16	Number of scan:					
Program	DS =	4	Number of dumn					
Probe	TD0 =	1	Loop count for "t					
Lists	▼ Width							
Lock	SVV [ppm] =	12.0160	Spectral width 🛛 👽					
Automation 👻	<	10	>					

This opens the acquisition parameter editor (see also chapter 6.1)). The following extra buttons are available:

- Indo last value change. Can be used to undo multiple changes.
- Show pulse program parameters [ased].

S Status parameter display. The button turns green when activated [*dpa*].

Set probehead/solvent dependant parameters [getprosol].

Set nuclei and routing [edasp]

12. Change raw dataset dimensionality (parameter PARMODE).



Search for specified parameter.

Changed parameters are automatically saved.

Note that the ... and E button to the right of the PULPROG parameter allow

you to show the pulse program list or edit the current pulse program, respectively.

# How to Edit the Title

Click the **Title** tab [edti]

🔜 exam1	exam1d_13C 1 1 C:\Bio guest									
Spectrum	ProcPars	AcquPars	Title	PulseProg	Peaks	Integrals	Sample	Structure	Fid	Acqu
	νE									
13C{1H}	AV 300 A	utomation (	Choles	terylacetate						

This allows you to edit the title that appears in the data window and on the plot.

- Save the title file under its current name.
- Save the title file under a new name.
- Reload the title file. Undo modifications since the last save.

E Open the title file with the external editor (defined in User Preferences).

# How to Edit the Pulse Program

See Click the PulsProg tab]

exam1d_13C	1 1	C:\Bio gu	iest							
Spectrum ProcPa	rs	AcquPars	Title	PulseProg	Peaks	Integrals	Sample	Structure	Fid	Acqu
<b>S</b> Л Е (	)									
Pulse program: zgpg	130									
l ze										~
dll p112:f2										_
2 30m do:f2										
10u p113:f2										<u>a</u>
dll cpd2:f2										
DELTA										
4u do:f2										~

This allows you to edit the current pulse program. The following extra buttons are available here:

- **s** Toggle status pulse program.
- **T** Start the graphical pulse program display [*edcpu1*].
- E Show the pulse program in an external editor [nmrsim].
- (i) Search for more info in the knowledge base

#### How to Display the Peak list

Click the Peaks tab

<b>1</b> exam	1d_1H 1 1 (	C:\bio guest			
Spectrum	ProcPars	AcquPars Tit	tle PulseProg	Peaks Integrals	Sample Structur
Peak	Index (F1)	v(F1) [ppm]	Intensity [abs]	Intensity [rel]	Half width [ppm]
1	19569.9	3.8319	11472303.78	11.04	0.0044
2	20929.9	3.3332	12495443.09	11.95	0.0037
3	21320.4	3.1900	13371661.03	12.67	0.0037
4	21603.7	3.0861	12663022.38	12.03	0.0040
5	21707.1	3.0482	13159654.59	12.36	0.0037
6	21947.3	2.9601	13733719.44	12.93	0.0033
7	22658.2	2.6994	13251895.75	12.48	0.0040
8	26579.7	1.2614	15909845.88	15.00	0.0059
9	26615.4	1.2483	13804594.47	12.98	0.0077

#### Figure 9.3

This displays the peak list. By default, the peak list shows the following entries:

Peak: the peak number

v(F1) [ppm]: the chemical shift

Intensity [abs]: the absolute peak intensity

Intensity [rel]: the relative peak intensity

Half width [ppm]: the peak width at half-height

#### Display the spectral region around a peak

Right-click the desired peak

this will open the popup menu shown in Fig. 9.4.

Show spectrum	
Expand spectrum 🔷 🕨	In current window
Delete	In correlated window
Edit annotation	
Remove 🕨	
Define as reference	
Annotate by reference	
Shift peaks	
Show detailed information	
Сору	
Export	
Import	
Print	
Print preview	
Table properties	

Figure 9.4

Here you can choose from the following options:

```
Show spectrum \rightarrow In correlated window
```

to open a new data window showing the full correlated spectrum

Is Expand spectrum → In current window

to change the current data window to spectrum display, showing the region around the selected peak

- INST Expand spectrum → In correlated window to open a new data window showing the region around the selected peak
- Edit Annotation Edit the annotation of the current peak.
- Define as reference  $\rightarrow$  Complete table Define the entire peak table as a reference for annotation.
- Define as reference  $\rightarrow$  Selection Define the selected peaks as a reference for annotation.

#### IN Annotate by reference...

Create annotations according to the peaklist of the reference dataset. You will be prompted for the allowed variation in chemical shift.

#### Shift peaks...

Shift all peaks. You will be prompted for the number of ppm to be shifted.

#### Show detailed information

Show peak information, dataset information and peak picking parameters.

#### Export entries of the peak list

Entries of the peak list can easily be exported to Excel or any other program as follows:

**1.** For multiple peaks:

Select the desired entries while pressing the *Ctrl* or *Shift* key

- 2. Right-click a peak entry to open the popup menu (see Fig. 9.4).
- 3. Click **Export...** to export the selected peaks.
- **4.** This opens a dialog box where you can specify the filename and file type. For the latter you can choose from:
  - Auremol peaklist (.ml)
  - Comma Separated Values (.cvs)
  - Mixed Shape deconvolution peak list (peaklist)
  - TOPSPIN peak list (.xml)
  - XEASY peak list (.peaks)
  - XWIN-NMR peak list (.txt)

**Important**: Check the box in the lower-left corner to export the selected peaks only or uncheck it to export the entire list. Then click **Export**.

#### Delete/remove peaks from the peak list

To delete one peak:

Right-click the peak and choose **Delete** from the popup menu

To delete multiple peaks:

- 1. Select the peaks while pressing the Ctrl or Shift key
- 2. Right-click one of the peaks and choose **Delete** from the popup menu
- To remove possible duplicate peaks:
  - RS Right-click any entry and choose  $\textbf{Remove} \rightarrow \textbf{Duplicate peaks}$
- To remove possible peaks outside of the spectrum:
  - R Right-click any entry and choose  $\textbf{Remove} \rightarrow \textbf{Peaks positioned}$  outside of the spectrum

To remove solvent peaks:

rs Right-click any entry and choose  $\textbf{Remove} \rightarrow \textbf{Solvent Peaks}$ 

#### Copy the peak List

Instead of exporting entries of the peak list, they can also be copied to the Clipboard and pasted to another application like Excel. To do that:

1. For multiple peaks:

Select the desired entries while pressing the *Ctrl* or *Shift* key

- 2. Right-click a peak entry to open the popup menu (see Fig. 9.4).
- 3. Click Copy... to copy the selected peaks to the Clipboard.

#### Print the peak List

To print the peaklist:

Right-click a peak entry and choose Print...

or

Sector **print** on the command line

or

🖙 Press Ctrl-p

All actions will print the entire peaklist.

To preview a print:

Right-click a peak entry and choose Print preview...

#### Import a peak List

A peak list from a different dataset or program can be imported as follows:

- 1. Right-click an entry to open the popup menu (see Fig. 9.4).
- 2. Click Import...
- **3.** In the appearing dialog box, navigate to the directory where the list resides and select the peak list, choosing from:
  - Auremol peaklist (.ml)
  - MULABEL peak list (labels)
  - TOPSPIN peak list (.xml)
  - XEASY peak list (.peaks)
  - XWIN-NMR peak list (.txt)

As such you can import a peak list from a different dataset or program or a previously exported list from the current dataset. Note that peak picking commands store the peak list in the processed data directory under the name peak.xml (TOPSPIN 2.1 or newer) or peak.txt (XWIN-NMR and TOPSPIN 2.0 or older).

#### Shortcuts

Double-click a peak: zoom into spectrum, i.e. show region around that peak.

*Enter* key: zoom into spectrum, i.e. show region around selected peak(s).

Delete key: delete the selected peak(s) from the peak list.

*Ctrl+c*: copy selected peaks to the Clipboard.

Ctrl+a: select all peaks.

Home: select the first peak.

End: select the last peak.

Shift+Home: select current and first peak and all in between.

Shift+End: select current and last peak and all in between.

Note that these keys only work when the cursor focus is in the data window.

#### Table properties:

Various properties of the peak table can be configured. To do that:

- 1. Right-click an entry to open the popup menu (see Fig. 9.4).
- 2. Click Table properties...
- **3.** In the appearing dialog box, with 3 tabs:
  - Column

Allows you to select the columns to be displayed, set the column width and the number of fraction digits. Furthermore, you can switch on/off scientific notation of values for each column individually.

Colours

Allows you to set various colours of the table.

• Spacings

Allows you to set various spacings of the table

🕌 Table properties	$\mathbf{\times}$
Column Colours Spacings	
🗹 Peak	^
Region	
🔲 Туре	_
🗹 Index (F1)	=
🗹 v(F1) [ppm]	
V(F1) [Hz]	
🗹 Intensity [abs]	
Intensity [rel]	~
Column properties	
Column width 15 🗘	
Fraction digits 0 🗘	
Scientific notation 🗹	
<u>O</u> K <u>C</u> ancel <u>App</u>	ly

Figure 9.5

When you move the cursor over the peak list, the active peak will, by default, be highlighted in <u>blue</u> (see peak 3 in Fig. 9.6). If the correlated spectrum is also displayed, a vertical line moves along, showing corresponding position in the spectrum (see Fig. 9.6)





As soon as you click a peak, it is selected and, by default, displayed in red (see peak 1 in Fig. 9.6). Note that this peak remains selected, i.e. is used by *Enter* and *Delete*, until a different peak is selected.

To extend the peak list, for example with *Regions*, *Type* and *Index* entries, right-click any part of the header bar.

To sort the peaks according to peak number, ppm value or intensity, click the header of the respective entry.

Peaks are only available if peak picking has been done (command *pp*). The peak list can be printed with *print* [*Ctrl+p*]. List items can be selected with the mouse, copied with *Ctrl+c* and pasted to other applications, e.g. a text editor.

# How to Display the Integral list

Real Click the Integrals tab [11, 1ipp, 1ippf]

exam1d_1H	I 1 1 C:\bio gue	st [1]			
Spectrum Pr	ocPars AcquPa	rs   Title   Puls	sProg Peaks	Integrals   e	Sample) 💶 🕨
△ Object	Integral (abs)	Integral [rel]	Peaks Rang	e (F1) from R	ange (F1) to
-Integral 1	21807940.16	1.6664	0	8.603	7.872
—Integral 2	20864697.28	1.5943	0	7.870	7.410
—Integral 3	45809321.78	3.5003	0	7.408	7.056
—Integral 4	131427635.19	10.0425	0	6.158	4.491
—Integral 5	20492465.62	1.5658	0	4.489	3.979
Integral 6	1068317028.12	81.6307	0	3.977	0.304
exam1d_1H	l 1 1 C:\bio gues	st [2]			<u> </u>
exam1d_1H	l 1 1 C:\bio gues ocPars AcquPa	st [2] rs   Title   Puls	sProg Peaks	s Integrals S	ample I
exam1d_1H	l 1 1 C:bio gues ocPars AcquPar	st [2] rs   Title   Puls	sProg Peaks	s   Integrals   S	ample)
exam1d_1H	l 1 1 C:\bio gues ocPars AcquPa	st [2] rs   Title   Puls	sProg Peaks	s   Integrals   S	Sample A
exam1d_1H	l 1 1 C:bio gue: ocPars AcquPar	st [2] rs   Title   Puls	sProg Peaks	s   Integrals   S	ample)
exam1d_1H Spectrum Pr	l 1 1 C:bio gue: ocPars AcquPa	st [2] rs Title Puls	sProg Peaks	s   Integrals   S	ample I
exam1d_1H Spectrum Pr	I 1 1 C:bio gues	st [2] rs Title Puls	sProg Peaks	s   Integrals   S	ample)
exam1d_1H	ocPars AcquPar	st [2] rs Title Puls	Prog Peaks	s   Integrals   S	Cample I

Figure 9.7

This displays the integral list (upper part of Fig. 9.7). By default, this shows the following items:

Object: the integral number

Integral [abs]: the absolute integral value

Integral [rel]: the relative integral value

Peaks: the number of peaks within the integral range

Range (F1) from: the left edge of the integral range

Range (F1) to: the right edge of the integral range

Please note the difference between the following items:

- selected integral: the entry that has been clicked last (Integral 3 in Fig. 9.7). If you right-click an entry, it is selected and you can execute one of the commands from the popup menu (see Fig. 9.8) The keys Enter and Delete work on the selected entry.
- active integral: the entry on which the cursor resides (Integral 1 in Fig. 9.7). The active integral is also marked in the correlated spectrum by a black vertical line (see lower part of Fig. 9.7 and description below). When you move the cursor over the integral list, the vertical line in the correlated spectrum moves along with it and vice versa.

Note that the colours of the selected and active integral can be set in the table properties (see below).

## Display the spectral region around an integral

To display the spectral region around a particular integral:

Right-click the desired integral

This will open the popup menu shown in Fig. 9.8.

Expand	
Expand all	
Show spectrum	
Expand spectrum 🔸	In current window
Delete	In correlated window
Define as reference	
Calibrate by reference	
Сору	
Export	
Import	
Print	
Print preview	
Table properties	

Figure 9.8

Here you can choose from the following options:

Show spectrum → In correlated spectrum to open a new data window showing the full correlated spectrum

#### $\bowtie$ Expand spectrum $\rightarrow$ In current window

to change the current data window to spectrum display, showing the region around the selected integral

IS Expand spectrum → In correlated window to open a new data window showing the region around the selected integral (lower part of Fig. 9.7)

Note that clicking the marked entry in the right-click popup menu is equivalent to pressing the *Enter* key.

#### **Export/Import Entries of the Integral List**

Entries of the integral list can easily be exported to Excel or any other program as follows:

1. For multiple integrals:

Select the desired entries while pressing the Ctrl or Shift key

- 2. Right-click an entry to open the popup menu (see Fig. 9.8)
- 3. Click one of the following menu items:
  - Copy

Copy the selected integral(s) entry to the Clipboard. Equivalent to clicking **Edit**  $\rightarrow$  **Copy** or hitting *Ctrl+c*. Copied integrals can easily be pasted in any other application such as Excel.

• Export...

Export selected integrals. Check the box in the lower-left corner to export the selected integrals only or uncheck it to export the entire list. Then click **Export**.

#### **Calibrate Integrals to Compare Spectra**

Integrals from the current and other spectra can be calibrated with respect to a reference integral. To do that:

- **1.** Right-click the reference integral and choose **Define as reference** from the popup menu. This will determine the calibration constant.
- **2.** Right-click any integral and choose **Calibrate by reference** This will divide all integrals by the calibration constant, setting the reference integral to 1.0.

Now you can read any other spectrum, and calibrate its integrals with respect to the reference integral defined above. To do that:

- 1. Read the spectrum
- 2. Enter *int* to define the integral ranges (if this has not been done yet)
- 3. Click the Integrals tab
- **4.** Right-click any integral in the list and choose **Calibrate by refer-ence** from the popup menu.

Note that the calibration constant is lost when TOPSPIN is restarted.

#### Display the integral list with peaks

The integral list in Fig. 9.7 shows only integrals. However, if peak picking has been done, the integral list also shows the peaks within each integral range (see Fig. 9.9).





Note that the integral entries can be collapsed, (hiding the peaks) or expanded (showing the peaks). As soon as one or more integrals entries are expanded, two extra columns appear showing:

v(F1) [ppm]: the chemical shift of the peak

Intensity: the peak intensity

Depending on whether or not integrals are expanded, the right-click popup menu contains the following extra items:

• Expand

Expand the current integral showing all peaks within it.

• Expand all

Expand all integrals showing all peaks within them.

Collapse all

Collapse all integrals hiding all peaks within them.

In addition to the integral entry, an individual peak within an integral can be activated (by placing the cursor on it) or selected (by clicking it). In Fig. 9.9, peak 7 is selected and the correlated spectrum is displayed. Peak 5 is active which is also shown by the vertical line in the correlated spectrum.

# Delete an Integral from the Integral List

To delete one integral:

Right-click the integral and choose Delete from the popup menu

To delete multiple integrals:

- 1. Select the integrals while pressing the Ctrl or Shift key
- 2. Right-click one of the integrals and choose **Delete** from the popup menu

Note that these keys only work when the cursor focus is in the data window.

# Table properties:

Various properties of the integral table can be configured. To do that:

- 1. Right-click an entry to open the popup menu (see Fig. 9.10).
- 2. Click Table properties...
- 3. In the appearing dialog box, with 3 tabs:

#### 4. Columns

Allows you to select the columns to be displayed, set the column

- width and the number of fraction digits. Furthermore, you can switch on/off scientific notation of values for each individual column.
- Colours

Allows you to set various colours of the table.

# • Spacings

Allows you to set various spacings of the table

5.

📓 Table properties 🛛 🔀
Column Colours Spacings
Object
✓ Integral [abs]
✓ Integral [rel]
Peaks     Range (E1) from
Range (F1) to
✓ v(F1) [ppm]
Intensity [abs]
Column properties
Column width 126 🤤
Fraction digits 2 💭
Scientific notation
OK Cancel Apply

Figure 9.10

# Shortcuts

**Enter** key: zoom into spectrum, i.e. show region around selected integral(s))

Delete key: delete the selected integral(s) from the integral list

Ctrl+c: copy selected integrals to the Clipboard.

Ctrl+a: select all integrals.

Home: select the first integral

*End*: select the last integral

Shift+Home: select current and first integral and all in between

Shift+End: select current and last integral and all in between

Double-clicking an integral will show the peaks within the integral region if they exist. It they do not exist, it will zoom into spectrum showing the integral region.

Note that these keys only work when the cursor focus is in the data window.

## How to view Sample Information

Source Click the Sample tab [edsam]

exam1d_1H 1 1 C:\Bio guest								
Spectrum ProcPa	ars AcquPa	ars Tit	e PulseProg	Peaks	Integrals	Sample	Structure Fid	Acqu
🖪 🖳 🗠 🕇	· -   †	+						
Sample Description								
Sample ID								
Origin								
Concentration								
Buffer								
Contact								
Comment								

Figure 9.11

This table can be used to fill out any sample information you want to store with the dataset. The table can easily be modified or extended with the following functions:

To select an item: double-click it!

- Save the sample information table with the dataset.
- Save the sample information table as default.
- Reload the original table discarding any changes
- + Add a new item to the table. You will be prompted for an identification name and the desired number of lines
- Remove the selected item from the table
- ↑ Move the selected item one place up in the table
↓ Move the selected item one place down in the table

### How to Open the Jmol Molecule Structure Viewer

Second Click the **Structure** tab [jmol]:



Figure 9.12

opens the *Jmol* molecule structure viewer. TOPSPIN 2.1 contains Jmol version 10. This has the following features:

- The viewer displays the structure file that resides in the *expno* of the current dataset. If this does not exist, the structure file defined by the acquisition parameter CHEMSTR is displayed. CHEMSTR can define a full pathname or a filename. In the latter case, the file is searched for in the directory defined in the User Preferences. To set this directory, click Options → Preferences, select Directory path names, enter a directory and click OK. If no structure file is found, you can open one by clicking File → Open in the Molecule Viewer
- The following structure file types are supported: .xyz, .mol, .pdb, .cml, .out, .mmlgp, .res, .cif, .gpr, .hin, .nwo.

- Secondary structure elements of proteins (backbone, cartoons, ribbons, ...) can be displayed in selectable sizes and colors.
- Mouse button effects:

Rotate a molecule around the x- and y-axis by pressing the left mouse button, and moving the mouse left/right or up/down, respectively.

Rotate a molecule around the z-axis by pressing the middle mouse button and moving the mouse left/right.

Zoom in or out a molecule by pressing the middle mouse button, and moving the mouse up or down.

RASmol command scripts are supported. To send a RASmol command to the currently displayed molecule enter:

isjmol <RASmol command>

Here are some example:

☞jmol zoom 400 ☞jmol ribbon 200 ☞jmol color ribbon yellow

You may create TOPSPIN macros containing RASmol commands. Just enter *edmac* on the TOPSPIN command line and insert the RASmol commands in the appearing editor. Here is an example:

jmol load /mystructures/alphahelix.pdb # load a structure jmol backbone 0.7 # display its backbone with 0.7 Angstrom size jmol color backbone yellow # change backbone color jmol background green # change background color jmol zoom 200 # zoom structure

The available RASmol commands are described in the Jmol Help menu.

• Multiple molecules (or multiple aspects of one molecule) can be displayed simultaneously. To do that just open multiple data sets or open the same dataset in multiple data windows and click on the **Structure** Tab in each window.

### How to Display the FID

Source Click the Fid tab [fid]



displays the raw data. If these do not exist, the text '*No raw data available*' appears. The following additional buttons appear at the right of the lower toolbar:

- Show FID in shuffled mode
- www Show FID in unshuffled mode

If you open a new dataset, the **Spectrum** tab is activated, no matter which tab was selected before. If you enter any interactive mode, for example phase correction mode, the Tab bar is replaced by a toolbar for that mode.

### 9.5 1D Display Options

### How to Toggle between Hertz and ppm Axis Units

Click the following toggle button in the upper toolbar:

h/p Toggle between Hz and ppm axis units [.hz]

### How to Switch on/off the Spectrum Overview display

The spectrum overview shows the entire spectrum at the top of the data window. It is useful when only a certain region of the spectrum is dis-

played. In the overview, the displayed region is marked as a green area. To switch on the spectrum overview, click the following toggle button in the upper toolbar:

Switch the spectrum overview display on/off [.ov]

To shift the displayed region, simply click-hold the green area in the overview spectrum and move the mouse (see Fig. 9.13).

### How to Switch Y-axis Display

Click the following toggle button in the upper toolbar:

**EX** Switch the y-axis display between abs/rel/off [.y]

Fig. 9.13 shows a data window with the spectrum overview on, ppm axis units, and absolute y-axis display.



Figure 9.13

### 9.6 Show Display Properties/Regions/Files

If you right-click inside the data window, the following popup menu will

appear:

Display Properties... Save Display Region To... Restore Display Region From Params. F1/2 File Properties... Files...

If you choose **Display Properties...**, a dialog box (see Fig. 9.14) will appear.

💩 . dopt				
Please select the components to be displayed together with the spectrum (if available):				
Cursor information				
Title				
Status parameters				
Acquisition parameters				
Integrals				
Integral labels				
Peak labels				
Peak annotations				
Multiplets				
Show data points				
Electronic Signature				
Molecular Structure				
<u>O</u> K <u>C</u> ancel				

Figure 9.14

Here you can check or uncheck the spectrum components that you want to be displayed in the data window.

Note that the **Display Properties...** dialog box can also be opened from the **View** menu.

### How to Superimpose the Cursor Information

To superimpose the cursor information on the spectrum:

- 1. Right-click in the data window and choose **Display Properties** [.dopt]
- 2. Check Cursor information in the appearing dialog box and click OK

### How to Superimpose the Title on the Spectrum

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check Title in the appearing dialog box and click OK

## How to Superimpose the main Status Parameters on the Spectrum $^{\rm 1}$

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check Status parameters in the appearing dialog box and click OK

### How to Superimpose the Integral Trails/Labels on the Spectrum

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check Integrals and, if desired, Integral labels in the appearing dialog box
- 3. Click OK

If no integrals appear, the integral regions have not been determined yet. This can be done with the *int* command.

### How to Superimpose Peak Labels on the Spectrum

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check Peak labels in the appearing dialog box and click OK

If no peak labels appear, peak picking has not been done yet. This can be done with the pp command.

<sup>1.</sup> These are the status parameters that also appear on the plot.

### How to Show Peak Annotations on the Spectrum

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check **Peak labels** and **Peak Annotations** in the appearing dialog box and click **OK**

Peak annotations appear, on peaks for which annotations have been defined, instead of regular peak labels showing chemical shift values. If no peak labels or annotations appear, peak picking has not been done yet. This can be done with the pp command.

### How to Show Individual Data Points of the Spectrum

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check Show data points in the appearing dialog box and click OK
- 3. Expand the spectral region where you want to see individual points.

### How to Superimpose the Electronic Signature on the Spectrum

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check Electronic Signature in the appearing dialog box and click OK

The electronic signature, entered with *esign*, will appear below the title.

### How to Display the Main Dataset Properties

Right-click inside the data window and choose File Properties

An information box as displayed in Fig. 9.15 will appear.

Properties	
exam1d_1H 1 1 C:\Bio gu	iest
Dimension (Proc/Acqu)	1D / 1D
Pulse program	zg
Acquisition date	30 Mar 2004 15:00:44
Nuclei	F1: 1s AXNUC = 1H.
SFO1[MHz]	500.13250065
Solvent	CDCI3
Acquired data available	Yes
Processed data available	Yes
TITLE	
1H Cyclosporin	
	Close

Figure 9.15

Note that this is status information which cannot be changed.

### How to Display a List of Files of a Dataset

Right-click inside the data window choose Files

Fig. 9.16 shows the file list when the **Fid** tab is active, i.e. when the raw data are displayed. It is the contents of the *expno* directory.

🔄 File list 🛛 🔀
Directory =
C: Bioldata guest (nmr/exam1d_1H)
pdata [Dir]
acqu
acqus
audita.txt
cyclosporina.pdb
fid
format.temp
prosol_History
pulseprogram
sample_info.prop
scon
uxnmr.par
Open Cancel

Figure 9.16

Fig. 9.17 shows the file list that appears when the **Spectrum** tab is active, i.e. when the processed data are displayed. It is the contents of the *procno* directory.

🛃 File list 🛛 🔀
Directory = C:\Bio\data\guest\nmr\exam1d_1H\1\pdata\1
1i
1r
auditp.txt
curdat2
dumy.xwp
email_exam1d_1H_1_1.pdf
intrng
last_plot.xwp
layout.xwp
outd
parm.txt
peak.txt
peaks
portf
portfolio.por
proc
procs
title

Figure 9.17

The contents of any file in the list can be displayed as follows:

- 1. Select a filename (it will be highlighted)
- 2. Click Open

Note that this only makes sense for ascii files, e.g.  $acqu^*$ ,  $proc^*$  or files with the extension .txt.

Dataset files can also be displayed/opened with the command *exp1*. This opens the Windows Explorer, or under Linux, the Konqueror or Mozilla, showing the contents of the *procno* directory.

### 9.7 Saving Display Region

The currently displayed spectral region can be stored as follows:

Right-click in the data window and choose **Save Display Region To...** This will open the dialog box shown in Fig. 9.18.

🔄 Save display region to 🛛 🔀
Options <ul> <li>Parameters F1/2 (e.g. used by 'restore display',) [dpl]</li> <li>Parameters ABSF1/2 (e.g. used by 'absf, apkf')</li> <li>Parameters STSR/STSI (used by strip ft)</li> <li>Parameters SIGF1,2 (signal region) (used by 'sino')</li> <li>Parameters NOISF1,2 (noise region) (used by 'sino')</li> </ul>
O A text file for use with other programs

Figure 9.18

Here the following options are available:

• Parameters F1/2 [dp1]

to save the displayed region for restoring the display later. The region is stored in the parameters F1P and F2P.

To restore the saved region, right-click in the data window and choose:

**Restore Display Region from Params F1/2** 

• Parameters ABSF1/2

to save the displayed region for baseline correction (command *absf*) or phase correction (command *apkf*). The region is stored in the processing parameters ABSF1 and ABSF2.

• Parameters STSR/STSI

to save the displayed region for Strip FT (commands like *ft* and *trf*).

The region is stored in the processing parameters STSR and STSI.

#### • Parameters NOISF1/2

to save the displayed region as the signal region for Signal to Noise calculation (command *sino*). The region is stored in the processing parameters SIGF1 and SIGF2.

#### • Parameters SIGF1/2

to save the displayed region as the noise region for Signal to Noise calculation (command *sino*). The region is stored in the processing parameters NOISF1 and NOISF2.

#### • A text file for use with other programs

to save the displayed region in a text file. This file can be viewed with any editor or used by external programs.

### 9.8 Synchronize Visible Region of all Data Windows

The visible region of all data windows can be synchronizes as follows.

Soom in or out one dataset while holding the Ctrl key

or

Soom in or out one dataset and then enter the .sync command

# Chapter 10 2D Display

### 10.1 The 2D Data Window

The 2D data window consists of a data field, a title bar, a Tab bar and buttons.

Fig. 10.1 shows a data window with a 2D spectrum.



Figure 10.1

### 10.2 Changing the Display of a 2D spectrum

TOPSPIN offers various buttons to scale or shift a 2D spectrum both vertically and horizontally.

### How to Change the Intensity Scaling (contour levels)

Click the button:

\_ Change the intensity scaling (contour levels) [edlev]

or

IN Hit one of the keys:

- Alt+PageUp: Increase the intensity by a factor of 2.
- Alt+PageDown: Decrease the intensity by a factor of 2.
- Alt+Enter: Reset the intensity.

or

- Regional Click one of the following buttons:
  - \*2 Increase the intensity (decrease the levels) by 2 [\*2].
  - \*8 Increase the intensity (decrease the levels) by 8 [\*8].
  - /2 Decrease the intensity (increase the levels) by 2 [/2].
  - /8 Decrease the intensity (increase the levels) by 8 [/8].
  - Reset the intensity to the last saved intensity (contour levels)

[**.**vr].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all data windows, press the *Ctrl* key while clicking one of the above buttons.

### How to Smoothly Change the Vertical Scaling (contour levels)

To change levels, multiplying all levels with the same factor:

I Click-hold the 🖕 button and move the mouse.

or

rear Turn the mouse wheel while the cursor is in the data window.

To change the level distance (increment), leaving the base level the same:

 $\mathbb{R}$  Click-hold the  $\mathbb{R}$  button and move the mouse.

### How to Display a Contour Levels Bar in the Data Window

- 1. Right-click in the data window and choose **Display Properties...** [.dopt]
- 2. Check Contour Levels Bar in the appearing dialog box and click OK (see Fig. 10.2).



Figure 10.2

### How to Switch on/off Square 2D layout

Right-click inside the data field and click Square Layout On/Off





The F2 scaling will be adjusted to reach a square display.

### How to Zoom a 2D spectrum in/out

Real Click one of the following buttons:

- E Zoom in to the center (spectrum) or left edge (FID) of the displayed region, increasing the horizontal scaling. [.zi]
- Q Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [.zo]
- ( Perform an exact zoom via a dialog box [.zx].

ie exa	ictzoom		×			
Please enter the exact coordinates of the desired expansion.						
	F2 [ppm] F1 [s]					
From	9.5699		0.0000			
То	-0.5081		0.0246			
<u>O</u> K <u>C</u> ancel						



- a) Enter the coordinates of the desired region in the dialog box.
- b) Click OK
- 🔊 Undo last zoom [.z1].
- Show full spectral width in F2 [.f2r].
- Show full spectral width in F1 [.f1r].
- (A) Show full spectrum [.a11].
- **II.** Retain horizontal and vertical scaling when modifying dataset or changing to different dataset. Effects all data windows [.keep].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

### How to Shift a Spectral Region in the F2 direction (left/right)

Real Click one of the following buttons:

- ← Shift to the left, half of the displayed region [.s1].
- → Shift to the right, half of the displayed region [.sr].

or

IF Click-hold the button and move the mouse:

Smoothly shift in any direction.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

### How to Shift a Spectral Region in the F1 direction (up/down)

Real Click one of the following buttons:

- ↑ Shift the spectrum up, half of the displayed region [.su].
- Shift the spectrum down, half of the displayed region [.sd].

### or

Real Click-hold the button and move the mouse:

Smoothly shift up/down and left/right.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

### **10.3 Show Display Properties/Regions/Files**

If you right-click inside the data window, the popup menu shown in Fig.

10.5 will appear.

Display Properties
Edit Contour Levels
Save Display Region To
Restore Display Region From Params, F1/2
File Properties
Square Layout On/Off
Files

### Figure 10.5

Here you can select various display properties, region setting and file properties. If you choose **Display Properties...**, a dialog box (see Fig. 10.6) will appear.

🛃 . dopt 🛛 🔀					
Please select the components to be displayed together with the spectrum (if available):					
Cursor information					
Title					
Status parameters					
Acquisition parameters					
Integrals					
Integral labels					
Peak labels					
Contour levels bar					
Show projections					
Electronic Signature					
Molecular Structure					
Visible projections					
○F1 ○F2 ⊙	F1 + F2				
<u>ok</u>	<u>C</u> ancel				

#### Figure 10.6

Here you can set various display options including parameter, integrals, peaks, contours, projections and electronic signature. The number of displayed digits for the integral and peak labels can be set in the User Preferences (click **Options**  $\rightarrow$  **Preferences**  $\rightarrow$  **Spectrum**).

### 10.4 Using the Tab bar

The 2D data window is a tabbed pane. This means its contents depends on the currently active tab in the Tab bar. The individual tabs are basically the same as for 1D display (see chapter 9.4). There are, however, some differences, which are discussed below.

### How to Set Processing Parameters

#### Source Click the ProcPars tab [edp]

The 2D processing parameter editor contains a column for each of the two dimensions F2 and F1 (see Fig. 10.7). Note that not all parameters exist in both dimensions.

exam2d_HC	1 1 C:\bio guest			
Spectrum ProcPa	ars AcquPars Title Pu	ulseProg Peaks	Integrals Sample St	ructure Fid Acqu
C M D S	1,2, <b>V</b> 🏔	F2	F1	Frequency axis
Phase Baseline	▼ Reference SI =	4096	4096	Size of real spe Spectrometer fr Low field limit o Spectrum refer
Peak Automation	OFFSET [ppm] =	9.570	157.823	
Miscellaneous User	HZpPT [Hz] =	1.230548	5.086263	Spectral resolut
	VVDVV =	QSINE		Window functic

Figure 10.7

### How to Set Acquisition Parameters

Second Click the AcquPars tab [eda]

The 2D acquisition parameter editor contains a column for each of the two dimensions F2 and F1 (see Fig. 10.8). Note that not all parameters

exist in both dimensions.

📑 exam2d_HC 1 1 C:\bio guest 📃 🗖 🔀							
Spectrum ProcPar	s AcquPars Title	PulseProg	Peaks	Integrals	Sample	Structure	Fid Acqu
ю Л S 🔰	1,2, 🔻 🕯	M					
Experiment  Vidth Receiver	▼ Experiment		F2		F1	Frequ	ency axis 🐴
Nucleus	PULPROG =	hmqcg	pqf			E Currei	nt pulse p
Durations	AQ_mod =	DQD		*		Acqui	sition moc
Power	FnMODE =			QF		🔽 Acqui	sition moc
Program	TD =	1024		128		Size o	f fid
Probe	NS =	4				Numb	er of scar
Lists	DS =	16				Numb	er of dumi
Lock	TD0 =	1				Loop	count for 🖌
Automation 👱	<	1111					>

Figure 10.8

### How to Display the Peak list

R Click the Peaks tab

exam2d	_HC 1 1 C:\bio g	uest		
Spectrum	ProcPars Acqui	Pars   Title   Pu	ılsProg <b>∫ Peak</b>	S Integral 💽
△ Peak	v(F2) [ppm]	v(F1) [ppm]	Intensity	Annotation
1	7.2485	128.2981	-32061761.86	pk1 📃
2	4.2892	74.4625	-9039344.24	pk2 💻
3	5.7988	59.4354	-9582402.76	pk3
4	5.3677	58.3070	-8589930.29	pk4 👻
•				

### Figure 10.9

This displays list of peaks if these have been calculated (command pp).

The list is basically the same as for 1D spectra. The only difference is that there are two columns for the two dimensions:

v(F2) [ppm]: the chemical shift in the F2 direction

v(F1) [ppm]: the chemical shift in the F1 direction

To specify or edit an annotation, click inside the *Annotation* field and enter a character string. The peak annotations are shown in the correlated spectrum (see Fig. 10.10)



Figure 10.10

### How to Display the Integral list

See Click the Integrals tab

exam2d_HC	1 1 C:\bio gu	est					×
Spectrum Pro	cPars AcquP	ars   Title   Pul	sProg	Peaks   Inte	grals   Samp	ole Strud	•
△ Object	Integral [abs]	Integral [rel]	Peaks	v(F2) [ppm]	v(F1) [ppm]	Intensity	
t ⊞–Integral 1	0.00	0.0000	1				
🛨 Integral 2	0.00	0.0000	1				
🗄 🕂 Integral 3	0.00	0.0000	1				
🛨 Integral 4	19711450.50	1.0000	1				
🗄 🕂 Integral 5	0.00	0.0000	1				
Hintegral 6	0.00	0.0000	2				
Peak 6				5.5751	126.2371	-3446703.37	
Peak 7				5.6386	126.2227	-4532891.75	
🕂 🕂 Integral 7	0.00	0.0000	1				-

### Figure 10.11

This displays list of integrals if these have been calculated (command *int*). The list is basically the same as for 1D spectra. The only difference is that, when peaks are shown, there are two columns for the chemical shift:

v(F2) [ppm]: the chemical shift in the F2 direction

v(F1) [ppm]: the chemical shift in the F1 direction

Furthermore, a stored or exported 2D integral list can be imported as follows:

- 1. Right-click an entry to open the popup menu
- 2. Click Import...
- **3.** In the appearing dialog box, navigate to the directory where the list resides and select the integral list.

As such you can import an integral list from a different dataset or a previously exported list from the current dataset. Note that integration commands store the integral list in the processed data directory under the name integrals.txt. Exported integrals are stored in the files <name>.txt and <name>.reg, where <name> is the name specified by the user.

### How to Display the FID

Source Click the Fid tab [fid]

2D raw data consist of a series of FIDs which are displayed in a row. Individual FIDs can be displayed by zooming in. To do that, click  $\textcircled$  repeatedly. Now you can shift and zoom in/out the data to display different FIDs (see Fig. 10.12)



Figure 10.12

### 10.5 2D Display Options

### How to Switch between Hertz and ppm Axis Units in F2 and F1

Real Click the following multi-state button in the upper toolbar:

 $h_{p}$  Switch between Hz and ppm axis units in F2 and F1 [.hz]

### How to Switch on/off the Spectrum Overview display

IS Click the following toggle button in the upper toolbar:

Switch the spectrum overview display on/off [.ov]

With the spectrum overview on, the data window will, for example, look like

this:

pectrum	ProcPars	AcquPars	Title	PulseProg	Peaks	Integrals	Sample	Structure	Fid Acc
1.05	- marine								Ē
							CE.	-	Ē
									E i
	4.100							5.27	E.
	~10		<b>1</b>					2>	
	~		- 		2		œ	27	1

### How to Switch on/off the Projection display

IS Click the following toggle button in the upper toolbar:

Bwitch the projection display on/off [.pr]



With the projections displayed, a 2D dataset looks like this:

In this example, the F1 projection is selected as indicated by the filled blue square whereas the F2 projection is not selected. A selected projection can be rescaled using the toolbar rescale buttons of function keys. If you right-click inside the projection area of the data window, the following popup menu appears:

External Projection	
Internal Projection	
Baseline At Center	
Baseline At Bottom	

Clicking **External Projection** opens the a dialog box where you can specify or search for a 1D dataset and display this as a projection of the current 2D dataset.

Clicking **Internal Projection** calculates and displays the positive projection and displays it along with the 2D spectrum.

Clicking **Baseline at Bottom** or **Baseline at Center** allows you to put the projection baseline at the respective positions.

Alternative ways to calculate/display projections are:

Right-click on a 1D dataset in the browser and choose:

#### **Display As 2D Projection**

or

IS Click Processing → Calculate projections [proj]

This will open the dialog box shown in Fig. 10.13.

🥌 f2projp					
Options					
<ul> <li>Calculate positive projection</li> </ul>					
<ul> <li>Calculate negative projection</li> </ul>					
◯ Calculate sum					
◯ Calculate disco sum					
◯ Read positive projection					
Read negative projection					
O Update rows/cols from display					
Required parameters					
Projection (sum) of =	rows 🔽				
Display projection =	on 2D 🛛 🔽				
First row/col =	1				
Last row/col =	1024				
Destination PROCNO =	999				
Disco reference col/row =	1				
OK <u>C</u> ancel <u>H</u> elp					

### Figure 10.13

From here, you can calculate positive, negative, sum and disco projections and either show them with the 2D spectrum or display them in separate data window as a 1D data. For more details on the corresponding commands (as shown in the header of the dialog box), please refer to the Processing Reference Manual.

### How to Switch on/off the Grid display

Real Click the following multi-state button in the upper toolbar:

Switch between 'no grid', 'axis aligned grid' and 'fixed grid' [.gr]

Fig. 10.14 shows an example of axis aligned grid display.



Figure 10.14 Axis aligned grid display

### How to Display a 2D Spectrum in Contour Mode

Real Click the following button in the upper toolbar:

Switch to contour display mode [.co]





### How to Set the 2D Contour Levels

IF Click the following button in the lower toolbar

★ Edit contour levels [edlev, .1v]

This will open the following dialog box shown in Fig. 10.15. Contour levels can be entered manually or they can be calculated.

#### Manual setup

This allows you to create an arbitrary sequence of levels

- 1. Enter the level values in the fields 1, 2, ... at the top of the dialog box.
- 2. Click **Apply** to update the display or **OK** to store the levels, update the display and close the dialog box.

### Calculation

This allows you to easily create a geometric or equidistant sequence of levels.

- 1. Click one of the following items:
  - Multiply with increment to create a geometric sequence of levels.
  - Add increment

to create a equidistant sequence of levels.

- 2. Enter the desired Base level, Level increment and Number of levels.
- 3. Click Fill to display and activate the sequence.
- **4.** Click **Apply** to update the display or **OK** to store the levels, update the display and close the dialog box.

The Contour level sign allows you to select positive levels, negative levels or both.

🥘 exam 2 d_HC	1 1 C:\bio guest		×				
1 9	9990701.0	-9990701.0	^				
2	17983261.9	-17983261.9					
3	32369871.4	-32369871.4					
4 .	58265768.4	-58265768.4					
5 1	104878383.2	-104878383.2					
6 1	188781089.7	-188781089.7					
7	339805961.5	-339805961.5					
8 6	611650730.7	-611650730.7					
9 (	0.0	0.0					
10 0	0.0	0.0	~				
Calculation meth  Multiply with  Add increme  Contour level sig  Positive & Ne  Positive Negative	od increment nt gative						
	Positive	Negative	_				
Base level	5669127.1	-5669127.1	_				
Level increment	1.800	1.800					
Number of levels		8					
Fill Clear Apply							
			1				

Figure 10.15

### How to Store interactively set Contour Levels

To store contour levels that were set interactively, for example by clicking

\*2 or pressing Alt+PageUp:

Real Click the following button in the lower toolbar:

Store contour levels [.1s]

The levels are stored in the file:

/<dir>/data/<user>/nmr/<name>/<expno>/pdata/<procno>/clevels

### How to Display a 2D spectrum in Pseudo Color Mode

IF Click the following button in the upper toolbar:

Switch to image color display mode [.im]

In pseudo color mode, a spectral region looks like this:



Note that in pseudo color mode, the contours are superimposed, in black, when you zoom in on a small region of the spectrum.

### How to Display a 2D Spectrum in Oblique Mode

IF Click the following button in the upper toolbar

Switch to oblique display mode [.st]

In oblique mode, a spectral region looks like in Fig. 10.16.



Figure 10.16

In this mode you can manipulate the display in various ways. Just rightclick inside the data window and choose one of the options from the appearing popup menu (see Fig. 10.17)



Figure 10.17

### How to Rotate a 2D Spectrum in Oblique Mode

Click-hold one of the following button and move the mouse up/down:

- Kotate around x-axis.
- **Gy** Rotate around y-axis.

### How to Switch between Displaying Positive and Negative levels

Click the following multi-state button in the lower toolbar:

+/\_ Switch between *positive*, *negative* and *both* contours [.1t].
# Chapter 11 nD Display

# 11.1 Display Planes of 3D Data

3D data can be displayed as 2D planes or as a 3D cube. By default, the first F3-F1 plane is displayed (see Fig. 11.1) The plane orientation and number is shown. The cube in the lower left corner graphically indicates which plane is displayed. The full 2D display functionality is available (see chapter 10).



Figure 11.1

#### How to Switch to 2D Plane Display

If the 3D cube is displayed you can switch to 2D plane display by clicking one of the following buttons:

- Switch to 2D contour display.
- Switch to 2D image display.
- <sup>∧</sup> Switch to 2D oblique display.

#### How to Display various Plane Orientations

Click one of the following buttons:

12 Show F1-F2 planes.

- 23 Show F2-F3 planes.
- 31 Show F3-F1 planes.

#### How to Display various Plane Positions (numbers)

Click one of the following buttons:

- + Show the next plane.
- Show the previous plane.
- Scan planes smoothly.
- E Enter the exact plane number. This will open the dialog shown in Fig. 11.2. Here, you can specify the desired plane number as well as switch to a different plane orientation.

<u>é</u>	
Valid plane indexes F3=[12048] 1H [5.12,0.11] ppm F2=[1128] 13C [56.91,17.09] ppm F1=[1256] 1H [5.12,0.11] ppm ⊡Select the visible plane	
<ul> <li>○ F2-F3</li> <li>● F1-F3</li> <li>○ F1-F2</li> </ul>	F1 1 F2 1 F3 1
Use ppm for plane selection	
	<u>O</u> K <u>C</u> ancel Apply

Figure 11.2

# 11.2 3D Cube Display Mode

#### How to Display the 3D Cube

Click the following button:

Show 3d cube (see Fig. 11.3).



Figure 11.3

#### How to Rotate the 3D Cube

Click-hold one the following buttons and move the mouse up/down:

Kotate cube around x-axis.

- (y Rotate cube around y-axis.
- z5 Rotate cube around z-axis.

#### How to Scale Up/Down the 3D Cube

- **1.** Right-click inside the data window.
- 2. Choose Larger or Smaller from the popup menu (see Fig. 11.4).

#### How to Reset the Cube Size and Orientation

Click the following button:

R Reset to default size and orientation.

# How to Switch Depth Cueing on/off

- 1. Right-click inside the data window
- 2. Choose Depth Cueing On/off (see Fig. 11.4)

Depth cueing makes data points which are closer to the viewer appear brighter and those that are further away appear dimmer. This increases the depth effect of the 3D image.

Larger		
Smaller		
Default View		
Depth Cueing On/Off		
Figure 11.4		

# How to Display a Cube Front or Side view

Click one the following buttons:

- 12 Show F1-F2 plane.
- 23 Show F2-F3 plane.
- 31 Show F3-F1 plane.

# 11.3 nD parameter display

TOPSPIN 2.1 and newer support parameter display of up to 8D data. To show processing parameters:

Is click the ProcPars tab of the data window

or

IN enter *edp* on the command line

Parameters of each direction are shown in a separate column. Fig. 11.5

2 exam3d 1 1 C:\bio guest					
Spectrum ProcPars	s AcquPars Title	PulseProg Peaks	Integrals Sample	Structure Fi	
∞ M S tź. ▼	<i>2</i> 4				
Reference		F3	F2	F1	
Window	Reference				
Phase Receline	SI	2048	128	256	
Fourier	SF [MHz]	600.1300000	150.9027490	600.1300000	
Peak	OFFSET [ppm]	5.11956	56.91221	5.11956	
Automation	SR [Hz]	-0.00	0.00	0.00	
Miscellaneous	HZpPT [Hz]	1.467191	46.950119	11.737530	
User	AQORDER	3-2-1	*		
	Window function				

Figure 11.5

shows the processing parameter display of a 3D dataset.

To show acquisition parameters:

IF click the AcquPars tab of the data window

or

IS enter eda on the command line

2 exam3d 1 1 C:\bio guest									
Spectrum Proc	Pars	s AcquPars	Title	PulseProg	Peaks	Integrals	Sample	Structure	e Fi
ю Л S 🔰	:	1.2. V M			Ins	talled prob	e: not de	fined	
Experiment	^				F3		F2		F1
Width		Experim	ient						
Receiver				la a la ali ava O	al.				
Nucleus		PULPRUG		ncchaigp3	a	_			
Durations		AQ_mod		DQD	1	×			
Power		FnMODE				States-	TPPI	State:	s-TPPI
Program		TD		1024		64		128	
Probe		NS		8					
Lists		DS		256					
Wobble		тра		1					
Lock	_			·					
Automation	_	▼ Width							

Parameters of each direction are shown in a separate column. Fig. 11.5



shows the acquisition parameter display of a 3D dataset.

# 11.4 nD Fid Display

nD raw data can be displayed as a series of 1D FIDs. To do that:

 $\mathbb{R}$  click the **FID** tab of the data window

or

reason enter fid on the command line

# 11.5 nD Peak and Integral Display

TOPSPIN 2.1 and newer support peak and integral display of up to 8D data.

To show the nD peak list:

Is click the Peaks tab of the data window

or

real enter peaks on the command line

Fig. 11.7 shows the peak list of a 3D dataset.

2 exam3	id 1 1 C:\bio gue	est			
Spectrum	ProcPars Acqu	Pars Title Puls	eProg Peaks	Integrals Sample	Structu
Peak	✓ v(F3) [ppm]	v(F2) [ppm]	v(F1) [ppm]	Intensity [abs]	
195	4.7638	50.5341	4.7577	1173060.00	
189	4.5952	46.8005	4.5817	1165831.00	
27	4.5927	37.4667	2.7041	939474.50	
82	4.5927	37.4667	2.3521	996713.50	
367	4.5194	51.7786	4.5035	1739381.50	
11	4.4998	19.4212	1.0025	921312.75	
186	4.4998	34.3554	1.9022	1163831.25	
426	4.4998	21.9103	1.0025	2310150.75	
591	4.4998	29.9996	1.1590	10377060.25	
<					>

Figure 11.7

The chemical shift in each of the three dimensions is shown in a separate column.

To show the nD integral list:

Is click the Integrals tab of the data window

or

register ints on the command line

Fig. 11.7 shows the integral list of a 3D dataset.

1 exam3d 1 1 C:\Bruker\TOPSPIN guest						
Spectrum Proc	Pars AcquPars Title	PulseProg Peak	5 Integrals	Sample Str		
△ Object	Integral [abs]	Integral [rel]	Peaks	v(F3) (ppm		
	re-Integral 1 502432597.00		2	1.87(		
	Integral 2 266808232.25		1	4.470		
⊡ntegral 3	1433384326.00	0.2884	3	0.86		
Integral 4	533366464.00	0.1073	1	0.989		
Integral 5 328194187.25		0.0660	1	4.390		
Integral 6 116979144.00		0.0235	1	3.14:		
⊡integral 7	Integral 7 124751045.00		1	2.92		
⊕ Integral 8	204916237.50	0.0412	1	0.723		
	FIG	ure 11.8				

The chemical shift in each of the three dimensions is shown in a separate column.

Peaks and integrals only appear if they have been calculated (commands *pp* and *int*, respectively).

# Chapter 12 1D Interactive Manipulation

The upper toolbar of the 1D menu offers various buttons for interactive manipulation. If you click such a button, the active data window will switch to the corresponding mode. An interactive manipulation mode is data window specific, i.e. it only applies to the active window.

# **12.1 1D Interactive Window multiplication**

TOPSPIN 2.0 and newer supports 1D interactive window multiplication.

#### 12.1.1 1D Interactive Window Multiplication Procedure

#### How to Switch to Window Multiplication Mode

Reference Click the *Processing*  $\rightarrow$  *Window Multiplication* [wm], enable **Manual window adjustment** in the appearing dialog and click *OK*.

or

Sector **.winf** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 12.2) and the data window itself will be divided into three parts:

• a parameter part at the left

- a spectrum part at the upper right
- a FID part at the lower right.



Figure 12.1

- Show both spectrum and FID.
- Show FID only.
- L. Show spectrum only.
- i Switch cursor information on/off (toggle)
- $\square$  Save windows settings to source 2D dataset<sup>1</sup> and return.
- 1. 2D data from which current 1D dataset was extracted, e.g. with *rser*.

- Save window settings and return
- Return without save.

You can perform interactive window manipulation as follow:

- 1. Select the window function (parameter WDW)
- 2. Set the corresponding parameter(s), e.g.
  - LB for exponential
  - LB and GB for Gaussian
  - SSB for sine bell and squared sine

The displayed spectrum and/or FID will be automatically adjusted as you change the window function and parameters.

3. Click I to store the window settings and return.

Now you can perform further processing steps like Fourier transform, phase correction etc.

# **12.2 1D Interactive Phase Correction**

Manually acquired spectra can be phased corrected automatically, with commands like *apk* or *apks* or, interactively, in phase correction mode.

#### 12.2.1 1D Interactive Phase Correction Procedure

#### How to Switch to Phase Correction Mode

Click the indicated button in the upper toolbar:

or enter .ph on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 12.2)



Figure 12.2 Data window in phase correction mode

A The yellow button indicates that you are in phase correction mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

#### How to Perform a Typical 1D Interactive Phase Correction

For a typical 1D phase correction, take the following steps:

- **1.** Click-hold the button **0** and move the mouse until the until the reference peak is exactly in absorption mode.
- **2.** Click-hold the button **1** and move the mouse until the entire spectrum is exactly in absorption mode.
- **3.** Click the button is to save and execute the phase correction and return.

#### 12.2.2 1D Interactive Phase Correction Details

#### How to Set the Phase Pivot Point

By default, the phase pivot point is set to the biggest magnitude intensity of the displayed region of the spectrum. To change the pivot point:

- 1. Right-click on the desired pivot point position
- 2. Choose Set pivot point from the popup menu (see Fig. 12.2)

#### How to Perform Default Zero Order Phase Correction

- **1.** Right-click in the data window
- 2. Choose Calculate ph0 in the popup menu (see Fig. 12.2)

The spectrum will automatically be corrected according to the calculated value.

#### How to Perform Interactive Zero Order Phase Correction

- 1. Click-hold the following button (button turns green):
  - **1** Zero order phase correction (parameter PHC0).
- 2. Move the mouse until the reference peak is exactly in absorption mode.
- 3. Release the mouse (button turns grey).

#### How to Perform Interactive First Order Phase Correction

- 1. Click-hold the following button (button turns green):
  - 1 First order phase correction (parameter PHC1).
- **2.** Move the mouse until the entire spectrum is exactly in absorption mode.
- 3. Release the mouse (button turns grey).

#### How to Perform 90, -90 or 180° Zero Order Phase Correction

- Real Click one of the following buttons:
  - 90 Perform 90 zero order phase correction [.ph90].
  - -90 Perform -90° zero order phase correction [.phm90].
  - 180 Perform 180° zero order phase correction [.ph180].

#### How to Reset the Phase to the Original Values

- Source Click the following button:
  - **R** Reset zero and first order phase values [.phr].

#### How to Change the Mouse Sensitivity

Real Click one of the following buttons:

- ⊿ Increase (double) the mouse sensitivity [.inc].
- ▶ Decrease (halve) the mouse sensitivity [.dec].
- II Reset the mouse sensitivity.

#### How to Return from Phase Correction Mode with/without Save

To return while saving the phase correction to the current dataset:

Real Click the following button:

[] Save, execute and return [.sret].

This will perform the following tasks:

- Execute phase correction (command *pk*).
- Save the current phase correction values.
- Leave the phase correction mode.

To return without save:

Source Click the following button:

Return, discarding any changes [.ret].

To return while saving the phase correction to the source 2D dataset:

Real Click the following button:

Gave to 2D [.s2d].

This is only applicable on rows or columns extracted from 2D data. The phase values will be saved to the 2D dataset from which the current 1D dataset was extracted.

# 12.3 1D Interactive Integration

Integration of 1D data can be done automatically, with the commands abs

and *li* or, interactively, as described in this paragraph.

#### How to Switch to Integration Mode

Is Click the indicated button in the upper toolbar:



or enter .int on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 12.3). The first button (define integrals) is automatically activated (is green).



Figure 12.3 Data window in integration mode

The yellow button indicates that the data window is in integration mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

If integral regions have already been determined, for example with *abs* or with a previous interactive integration, these regions are displayed in the

data window, along with the integral values. You can remove them, change them or add to them, as described below.

#### How to Define Integral Regions

To define integral regions interactively:

- 1. Click the following button (button turns green):
  - Define integral region interactively.

Note that the define integrals button is automatically activated on entering the integrals mode.

- 2. Put the red cursor line at one edge of a peak or multiplet.
- **3.** Left-click-hold and drag the cursor line to the other edge of the peak or multiplet.
- 4. Do step 2 and 3 for all regions to be defined.
- 5. Click the green button to leave the "define region" mode (button turns grey).

To define integral regions via a dialog box:

1. Click the following button:

d Define region via dialog.

2. In the appearing dialog box:



Enter the exact values for the region limits.

3. Click *OK* to define the selected region.

#### How to Select/Deselect Integral Regions

To select/deselect all displayed integral regions:

🖙 Click the button: 🖵 button

To select a single integral region:

- **1.** Right-click in the integral region.
- 2. Choose *Select/Deselect* from the popup menu.

To select the next integral region:

🖙 Click the 📑 button

To select the previous integral region:

🖙 Click the: ≒ button.

To select multiple integral regions:

- 1. Click the button: button to select all integrals
- 2. Deselect the integral that are not to be selected.

Selected integral regions are indicated by a color filled integral label. In the Fig. 12.4, the five left most regions are selected, the region around 6 ppm is currently being deselected.



Figure 12.4

Note that:

- If no integral is selected, the next and previous integral button select the first or last integral respectively.
- the select all integrals button remains green while all or multiple integrals are selected. This indicated a selection mode.

#### How to Read Integral Regions from Disk

You can read integrals regions from disk which have been stored by automatic integration (command *abs*) or by a previous interactive integration.

To read integrals:

1. Click the following button:

Read integral regions.

The following popup menu will appear:

Read 'intrng'

Read 'intrng' No Slope & Bias Corr.

Read 'intrng' Use Last Slope & Bias

Import 'intrng' from Relaxation Experiment

Edit 'intrng'

Figure 12.5

- 2. From the popup menu, choose one of the following entries:
  - Read 'intrng'

to read the last saved integral regions and apply the saved slope and bias correction values.

- *Read 'intrng' no slope & bias corr.* to read the last saved integral regions but do not apply the saved slope and bias correction values.
- *Read 'intrng' use last slope & bias* to read the last saved integral regions applying the last slope and bias correction values.
- *Read 'intrng' from Relaxation Experiment* to read the last stored integral regions of the T1/T2 relaxation experiment.
- Edit 'intrng'

to edit the file (intrng) that contains the integral regions and slope and bias correction values. Changes in this file are automatically shown on the screen.

#### How to Perform Interactive Bias and Slope Correction

To perform interactive bias correction:

**1.** Select the integral(s) that you want to correct (right-click in the region).

If no integral is selected, bias correction will work on <u>all</u> integrals.

2. Click-hold the following button (it turns green) and move the mouse,

/ Integral bias correction.

until the integral bias is correct.

**3.** Release the mouse (button turns grey).

To perform interactive slope correction:

**1.** Select the integral(s) that you want to correct (right-click in the region).

If no integral is selected, slope correction will work on all integrals.

2. Click-hold the following button (it turns green) and move the mouse,

√s Integral slope correction.

until the integral slope is correct.

3. Release the mouse (button turns grey).

#### How to Set the Limit for Bias Determination

- Source Click the following button:
  - # Limit for bias determination.

#### How to Change the Mouse Sensitivity

- Solution Click one of the following buttons:
  - ⊿ Increase (double) the mouse sensitivity [.inc].
  - ▶ Decrease (halve) the mouse sensitivity [.dec].
  - II Reset the mouse sensitivity.

#### How to Calibrate/Normalize Integrals

Calibrating integrals means setting the value of a reference integral and adjusting all other integrals accordingly. To do that:

- 1. Right-click in the reference integral region.
- 2. Choose Calibrate from the popup menu (see Fig. 12.6).
- 3. Enter the desired value for the reference integral and click OK

Normalizing integrals means setting the sum of all integrals and adjusting individual integral values accordingly. To do that:

- 1. Right-click in the reference integral region.
- 2. Choose Normalize from the popup menu (see Fig. 12.6).
- 3. Enter the desired sum of all integrals and click OK

Select / Deselect
Calibrate
Normalize
Lastscal
Delete

Figure 12.6

Calibrating and normalizing only effects the current dataset. To scale integrals with respect to a reference dataset, choose *lastscal* from the right/click popup menu (see below).

#### How to Scale Integrals with respect to Different Spectra

Integrals can be scaled with respect to the last spectrum that was integrated interactively. To do that:

- 1. Right-click in the reference integral region.
- 2. Choose *Lastscal* from the popup menu (see Fig. 12.6).

As such, you can compare integrals of different spectra. Note that this only make sense for spectra which have been acquired under the same experimental conditions. The scaling factor is stored in the file:

<tshome>/prog/curdir/<user>/intscale

#### How to Delete Integral Regions from the Display

To delete the selected integral regions from the display:

Source Click the following button:

 $\mathbf{\mathfrak{R}}$  Delete selected integral regions from the display.

To delete a single integral region from the display:

- **1.** Right-click in the integral region.
- 2. Choose Delete from the popup menu (see Fig. 12.6)

To delete all integral regions from the display:

IN Click the following buttons:

- Select all integral regions.
- $\swarrow$  Delete selected integral regions from the display.

Note that regions are only deleted from the screen. Regions which are saved on disk (in the intrng file) are not affected.

#### How to Scale Selected Integrals

Integral scaling only manipulates selected integrals. However, if no integrals are selected, it works on all integrals.

Real Click one of the following buttons:

- \*2 Scale up selected integrals by a factor of 2.
- /2 Scale down selected integrals by a factor of 2.
- Scale selected integrals up/down smoothly.

To scale up/down integrals by a factor entered via a dialog:

- 1. Click the following button:
  - \*X Scale integrals via a dialog.
- 2. Enter a scaling factor, e.g. 2.5. in the appearing dialog.

🔄 calib 🛛 🔀		
Calibrate selected integrals		
New value 2.6634		
<u>Q</u> K <u>C</u> ancel		

3. Click OK to apply this factor.

To scale all integrals to the same height:

Source Click the following button:

**=** Scale/unscale all integrals to the same height.

The individual scaling factor for each region is displayed above the integral. Clicking this button again rescales all integrals to their original height.

#### How to Move the Integral Trails Up/Down

To move the integrals (selected and unselected) up or down:

Real Click one of the following buttons:

- ↓ The left edge of the selected integral is put just above the baseline. If no integral is selected, the lowest integral is used.
- The right edge of the selected integral is put at 3/4 of the window height. If no integral is selected, the highest integral is used.
- Shift all integral trails up/down smoothly.

#### How to Cut Integral Regions

1. Click the following button (button turns green):

LUC Ut integral region.

- **2.** Move the red cursor line into an integral region to the position where it must be cut and click the left mouse button.
- 3. Do step 2 for each integral region that must be cut.
- **4.** Click the (green) button to leave the *cut integral* mode (button turns grey).

In case of overlapping integrals, you must select the integral to be cut before you actually cut it.

#### How to Save Integral Regions

1. Click the following button:

Save integral regions.

The following popup menu will appear:

Save Regions To 'intrng' Save Regions To 'reg' Export Regions To Relaxation Module and .ret. Save & Show List



- 2. Choose one of the following entries:
  - Save regions to 'intrng' Save the currently displayed integral regions including the slope and bias correction values.
  - Save Regions to 'reg' Save the integral regions to the file reg.
  - *Export Regions To Relaxation Module and .sret* Used on relaxation data only. Exports the integral regions for T1/T2 relaxation analysis and exits from integration mode.
  - Save & show list Save the currently displayed integral regions including the slope and bias correction values and show the integrals on the screen.

#### How to Undo the Last Region Operation

- Real Click the following button:
  - Undo the last region operation.

#### How to Return from the Integration Mode with/without Save

To return and save the integrals to the current dataset:

Ref Click the following button:

Save integrals and return [.sret].

As such, you will:

• save the integral regions and corresponding slope and bias corrections to the file intrng.

- save the integral regions, slope and bias corrections and integral values to the file integrals.txt. This file is displayed when you click the *Integrals* Tab.
- leave the integration mode.

To return without save:

Ref Click the following button:

Return, discarding any changes [.ret].

# **12.4 1D Interactive Calibration**

A 1D spectrum can be calibrated (referenced), automatically, with the command *sref* or, interactively, as described below.

#### How to Switch to Calibration Mode

IF Click the indicated button in the upper toolbar

or enter **.***ca1* on the command line. The Tab bar of the active data window will be replaced by a toolbar.



Figure 12.8 Data window in calibration mode

The yellow button indicates that the data window is in calibration mode.

#### How to Calibrate a Spectrum Interactively

In calibration mode:

- 1. Position the red cursor line at the reference peak.
- 2. Left-click at that position.

The following dialog box will appear:

🔄 calibrate 🛛 🔀
Spectrum calibration frequency
Cursor frequency in ppm: -0.0050
<u>O</u> K <u>C</u> ancel

Note that the units (Hz or ppm) correspond to the axis units of the display.

3. Enter the frequency you want to assign to the reference peak.

#### 4. Click OK

The spectrum will be calibrated and re-displayed. TOPSPIN will automatically leave calibration mode.

# 12.5 1D Multiple Display

The multiple display mode allows you to display multiple superimposed spectra. The spectra will be ppm aligned or Hz aligned, according to the selected axis unit. Each spectrum can be individually shifted and scaled allowing exact alignment of corresponding peaks in different spectra. The number of superimposed spectra is unlimited.

Although multiple display is normally used for spectra with matching nuclei, it allows you to superimposed spectra with non-matching nuclei. You will get a warning that the nuclei do not match. Just just click OK to continue.

#### How Switch to Multiple Display Mode and Read Multiple Spectra

One way to superimpose data in multiple display is to read one dataset, switch to multiple display mode and add other datasets:

- 1. Read a 1D dataset.
- 2. Click the putton in the upper toolbar or type .md on the command line.

The data window will switch to multiple display mode.

- 3. Add a dataset as follows:
  - Left-click-hold the dataset in the browser and drag it into the data window.

or

Right-click the dataset in the browser and choose *Display* from the popup menu.

or

Enter *re* and specify the additional dataset in the appearing dialog box.

Another way to superimpose data in multiple display is to read multiple

datasets simultaneously:

1. In the browser:

```
Be Hold down the Ctrl key and click multiple datasets to select them.
```

or

- Hold down the *Shift* key and click two datasets to select these two and all datasets in between.
- 2. Right-click any of the selected data:
  - Choose *Display* from the popup menu. This will show the data in the active data window if that is in multiple display mode or, otherwise, show the data in a new window.

or

Schoose *Display in new window* from the popup menu. This will show the data in a new window.

In multiple display mode, the Tab bar of the active data window is replaced by a toolbar. Fig. 12.9 shows three comparable 1D spectra and the sum of all three.



Figure 12.9 Data window in multiple display mode

The yellow button indicates that the data window is in multiple display mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

Furthermore, the browser is split in two parts as shown in Fig. 12.10.



The additional lower part shows:

- which datasets are displayed in the active data window.
- which datasets are selected (these are highlighted).

#### How to Select/Deselect Datasets

To select a dataset:

- Real Click in the corresponding area in the data window.
- or Click the small square at the upper right of the spectrum.
- or Click the corresponding entry in the lower part of the browser.
- In the lower part of the browser, you can:
  - Real Click one dataset to select it.
  - or Hold down the Ctrl key and click multiple datasets to select them.
  - or Hold down the *Shift* key and click two datasets to select these two and all datasets in between.

When you select a dataset, the corresponding small square is filled (see Fig. 12.9) and its entry in the lower part of the browser is highlighted (see Fig. 12.10).

Note that:

- no spectrum selected = all spectra selected
- scale/shift buttons of the data window toolbar only work on selected spectra

To deselect a dataset:

Select a different dataset.

To deselect all datasets:

Real Click the following button:

🖖 Deselect all datasets.

#### How to Remove a Dataset from Multiple Display

- 1. Select the dataset(s) you want to remove.
- 2. Click the following button:

Kemove selected data from the screen.

Note that the data on disk are not affected. Furthermore, the first spectrum cannot be removed from the screen.

#### How to Display the Sum or Difference Spectra

Source Click one of the following button (button turns green):

 $\triangle$  Show the difference between the first and the sum of the other datasets.

 $\Sigma$  Show the sum of all datasets in the multiple display window.

#### How to Save the Sum or Difference Spectra

- 1. Click the following button:
  - Save the displayed sum or difference spectrum.
- 2. In the appearing dialog box, specify the destination procno.

#### How to Display the Next/Previous Name/Expno

To compare a series of spectra you can interactively increment or decrement the dataset name or expno. A dataset name is incremented according to the ICON-NMR naming convention of increasing extensions, e.g. name.001, name.002 etc.

Real Click one of the following button (button turns green):

- E- Show the previous name/expno/procno of the last dataset
- E+ Show the previous name/expno/procno of the last dataset
- E<sub>i</sub> Set the increment options. Clicking this button will open the following dialog:

4	
Data set increment options	
Expno increment Preserve individual scaling	1
	<u>OK</u> <u>C</u> ancel

Figure 12.11

Here you can choose to increment the procno, expno or name, set the expno increment and switch individual scaling on/off.

#### How to Toggle between Superimposed and Stacked Display

Real Click the following button:

#### How to Shift and Scale Individual Spectra

To compare the intensity and chemical shift of corresponding peaks, you can shift and scale individual spectra. To do this:

- 1. Display the spectra in multiple display mode as described above.
- 2. Expand the spectra to display the desired region or peak.
- **3.** Select one of the spectra (e.g. by clicking it in the lower part of the browser).
- **4.** Click-hold the  $\blacklozenge_S$  button and move the mouse to align the intensities.
- 5. Click-hold the 🏤 button and move the mouse to align the peak positions.

The alignment can be facilitated by showing the difference spectrum (  $\triangle$  button) and minimize that. Note that you can also scale the selected spectra up/down with the buttons **\*2**<sub>s</sub> and **/2**<sub>s</sub>. The **‡**<sub>s</sub> button allows you to move the selected spectra vertically. Clicking the **R** button resets individual scaling and shifting.

The performed scaling and shifting are displayed in the data window (see Fig. 12.12 and 12.13).



Figure 12.12



Figure 12.13

#### How to move the selected spectrum one place up/down

Real Click the following button:

↑ Move the selected spectrum one place up in the list.

Source Click the following button:

↓ Move the selected spectrum one place down in the list.

Note that the first spectrum and calculated spectra (sum of difference) cannot be moved up/down.

# How to Switch on/off the Display of Datapaths and Scaling Factors

Real Click the following button:

L Switch on/off display of datapaths and scaling factors.

#### How to Return from Multiple Display mode

Real Click the following button:

Return from multiple display mode [.ret].

# How to Set the Colors of the 1<sup>st</sup>, 2<sup>nd</sup>, .. Dataset

The colors of the different datasets in the multiple display mode can be set in the *User preferences* dialog box. To set, for example, the color of the second spectrum:

References and click the *Change* button for the item *Color of 2nd 1D spectrum*.

TOPSPIN 2.0 and newer allows you to set 8 different colors for different spectra in multiple display.

# 12.6 1D Interactive Baseline Correction

Baseline correction can be performed with commands like *abs* or *absd* or, interactively, as described below.

#### How to Switch to Baseline Correction Mode

Source Click the indicated button in the upper toolbar:
or enter .bas1 on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 12.14).



Figure 12.14 Data window in baseline correction mode

The yellow button indicates that the data window is in baseline correction mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

## How to Perform Polynomial Baseline Correction

1. Click the following button (button turns green):

Perform polynomial baseline correction.

In the data window, a red horizontal line will appear as well as the equation that describes the polynomial function:



- **2.** Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
- **3.** Repeat step 2 with the buttons **B**, **C**, **D** and **E** until the red line coincides with the entire baseline of the spectrum.

## How to Perform Sine Baseline Correction

1. Click the following button (button turns green):

Perform sine baseline correction.

A red horizontal line will appear as well as the equation describing the sine function:

```
f(x) = A + B*sin(C*x + D)
```

- **2.** Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
- **3.** Repeat step 2 with the buttons **B**, **C** and **D** until the red line coincides with the entire baseline of the spectrum.

## How to Perform Exponential Baseline Correction

1. Click the following button (button turns green):

Perform exponential baseline correction.

A red horizontal line will appear as well as the equation describing the exponential function:

f(x) = A + B\*exp(C\*x)

- **2.** Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
- **3.** Repeat step 2 with the buttons **B** and **C** until the red line coincides with the entire baseline of the spectrum.

## How to Preview the Baseline Corrected Spectrum

Before actually performing the baseline correction, you can preview the result by displaying the difference between the uncorrected spectrum and the red correction line.

To do that:

- 1. Click the following button (button turns green):
  - $\triangle$  Preview corrected spectrum (show difference).

The corrected spectrum will be displayed in red.

If the baseline is correct, click the I button to save the correction. If further correction is needed, click the button to show the original spectrum and the red correction line.

## How to Reset the Baseline Correction Line

- 1. Click the following button:
  - **0** Reset the red correction line to zero.

If the difference spectrum is displayed (the  $\triangle$  button is active), clicking the reset button will restore the original spectrum.

## How to Change the Mouse Sensitivity

Real Click one of the following buttons:

- Increase (double) the Mouse Sensitivity [.inc].
- ▶ Decrease (halve) the Mouse Sensitivity [.dec].
- II Reset the Mouse Sensitivity.

## How to Save the Baseline Correction and/or Return

To return while saving the baseline correction:

IN Click the following button:

[] Save baseline correction and Return [.sret]

This will perform the following tasks:

- Execute the baseline correction [bcm].
- Save the baseline correction values A, B, C, D and E.
- Leave the baseline correction mode.

To return while discarding any changes:

Click the following button:

Return, Discarding any changes [.ret].

## How to Perform Cubic Spline Baseline correction

Real Click the following button:

Ht Define points for cubic spline baseline correction.

The toolbar of the data window will change as shown in Fig. 12.15.



Figure 12.15 Data window in spline baseline correction mode

The cursor line in the data window turns red. If a list of baseline points already exists, you are prompted to overwrite or append to these points. If you choose *Append*, the labels of the existing points are displayed on the screen. If you choose *Overwrite*, no labels are displayed. Nevertheless, the existing points are only overwritten when you define and save new points.

To define new baseline points:

- 1. Move the cursor line to a baseline point and left-click at that position.
- 2. Do this for at least five baseline points.

Fig. 12.15 shows a spectrum with five defined baseline points. Note that here the points have been chosen at the right part of the spectrum for dis-

play reasons only.

## How to Delete Spline Baseline Points from the screen

To delete one baseline point:

- 1. Right-click the baseline point position in the data window.
- 2. Choose *Delete Current* from the popup menu (see Fig. 12.16).

Quit					
Save & Quit					
List `baslpnts`					
Delete All					
Delete Current					
Enter zoom					

Figure 12.16

To delete all baseline points:

- 1. Right-click any position in the data window.
- 2. Choose Delete All from the popup menu (see Fig. 12.16).

## How to Return from Cubic Spline Baseline mode with/without Save

To return while saving the baseline points:

Real Click the following button:

[] Save baseline points and Return [.retsab].

To return while discarding any changes:

Source Click the following button:

Return, Discarding any changes [.ret].

Alternatively, you can right-click in the data window and choose *Save & Quit* or *Quit*, respectively.

## 12.7 1D Interactive Peak Picking

Peak picking can be performed, automatically, with the commands *pps* or, interactively, in the peak picking mode.

## How to Switch to Peak Picking Mode

Solution in the upper toolbar:



or enter .pp on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 12.17).



Figure 12.17 Data window in peak picking mode

The yellow button indicates that you are in peak picking mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

щ.

Note that the up button is automatically activated, i.e. you are in *Define* peak picking range mode

## How to Define New Peak Picking Ranges

- **1.** Put the cursor at the upper-left corner of a peak picking range.
- **2.** Left-click-hold and drag the mouse to the lower-right corner of the range.

The peak picking range will be marked green. The minimum and maximum intensity are set and the peaks in the range are picked and displayed.

- 3. Repeat step 1 and 2 for each peak picking range to be defined.
- 4. Click the green button to leave the "Define peak picking range" mode.

Note that the parameters MI and MAXI are set to the lowest minimum and the highest maximum intensity, respectively, of all ranges.

## How to Change Peak Picking Ranges

1. Click the following button (button turns green):

n Change peak picking ranges.

2. Put the cursor on one of the edges of the peak picking range.

The cursor turns into a double-headed arrow.

- **3.** Left-click-hold and drag the peak range edge to its new position.
- **4.** Optionally: repeat step 2 and 3 for the other edge and for other peak ranges.
- 5. Click the green button to leave the "Change peak picking range" mode.

## How to Pick Peaks in Peak Picking Ranges only

Peaks in a peak range are automatically picked when the range is defined. If peaks have been deleted from a rang, they can be picked again as follows:

- **1.** Right-click in the data field.
- 2. Choose Pick Peaks On Ranges from the popup menu.

Alternatively, you can enter *pp1* on the command line. This command can be entered in Interactive peak picking mode or in the normal display mode.

## How to Delete all Peak Picking Ranges

or

Right-click in the data field and click *Delete All Ranges* in the popup menu.

## How to Define Peaks Manually

1. Click the following button (button turns green):

1. Define peaks manually.

A red vertical line will appear in the data window.

**2.** Put the red cursor line at the desired peak and click the left mouse button.

The peak label will appear at the top of the data window.

- 3. Repeat step 2 for each peak to be defined.
- 4. Click the green button to leave the "Define peaks" mode.

## How to Pick Peaks Semi-Automatically

1. Click the following button (button turns green):

1. Define peaks semi-automatically.

- 2. Move the cursor into the data window.
- 3. Put the cursor line near the desired peak.
- 4. Left-click to pick forward

or

Right-click to pick backward (see Fig. 12.18).

A red cursor line will appear at the nearest peak whose intensity is between MI and MAXI.

5. Right-click to add the selected peak to the peak list (see Fig. 12.18).

Add Peak To List

Pick Backward

Figure 12.18

The peak label will appear at the top of the data window.

6. Click the green button to leave the "define peaks semi-automatically" mode.

## How to Delete Peaks from the Peak List

To delete a specific peak:

- 1. Right-click on a defined peak.
- **2.** Choose *Delete peak under cursor* from the popup menu (see Fig. 12.19).



Figure 12.19

To delete all peaks:

 $\mathbb{R}$  Click the 🐹 button in the data window toolbar.

or

Right-click in the data field and click *Delete All Peaks* in the popup menu.

#### How to Return from Peak Picking Mode with/without Save

To return while saving the peak list and peak ranges:

IN Click the following button:

[] Save the Peak Region and Peak List and Return [.sret].

This will:

- Save the peak list to the file peak.xml and the peak ranges to the file peakrng.
- Leave the peak picking mode.

To return while discarding any changes:

Source Click the following button:

Return, discarding any changes [.ret].

# Chapter 13 2D Interactive Manipulation

The upper toolbar of the 2D menu offers various buttons for interactive manipulation. If you click such a button, the active data window will switch to the corresponding mode. An interactive manipulation mode is data window specific, i.e. it only applies to the active window.

## **13.1 2D Interactive Phase Correction**

2D spectra can be phase corrected interactively in both the F2 and F1 direction by selecting certain rows and/or columns and phase correct them.

## 13.1.1 2D Interactive Phase Correction Procedure

## How to Switch to 2D Interactive Phase Correction

Click the corresponding button in the upper toolbar as indicated below:



or enter .ph on the command line.

The Tab bar of the active data window will be replaced by a toolbar. Fig.

13.1 shows an example of an unphased 2D inverse spectrum.



Figure 13.1 Data window in phase correction mode

- The yellow button indicates that you are in phase correction mode.
- Toggle the contour display on/off.
- **R** Switch to *phase row* mode to display rows of selected peaks.
- Switch to *phase columns* mode to display columns of selected peaks.
- Save the phase values to the 3D data from which this 2D was extracted.
- ↓ Return.

## How to Perform a Typical 2D Interactive Phase Correction

In this example we will perform F1 phase correction (columns) only. Take the following steps:

1. Select two or more peaks in different parts of the spectrum. To do

that:

- a) Zoom in on a peak by drawing a box around it. To do that, clickhold the left mouse button and move the mouse (see Fig. 13.2).
- b) Right-click at the peak position and choose *Add* from the popup menu.



Figure 13.2

- c) Click the 🕘 button to display the full spectrum.
- d) Zoom in on the next peak and add in the same way as the first one.
- e) Zoom in on the next peak etc.
- Fig. 13.3 shows an example of three selected peaks.



Figure 13.3

**2.** Click the button C<sup>1</sup> to phase correct the columns (F1).

A new data window called *Phase 2D* will appear showing the columns of the selected peaks (see Fig. 13.4).

	Phase	2D :	exa	m2d	_HC	1.1	C:\bi	o gu	est											L
$\mathcal{A}_{r}$	붛	0	1	R	90	-90	180	⊿	⊾	Ш	+	-	III	≡	#:	<b>P</b>	Ļ		•	
p	ivot	= 12	28.4	14 pp	m	Phas	e in	crem	ient	= 0	.20	ph	= 0	0.00	0 p)	hl =	0.0	00		
	olur	nn 4	17 /	7.2	569	ppm	1													
				r							-									
			Ì																	
	:olur	nn Ģ	44.	4.2	983	ppn	L			<u> </u>			~~~~							
										$-\gamma$										- 11
										V										
	olur	nn 8	99 /	.97	48 p	pm														
						· .											Υ.			- 11
																	5	V		

Note that the toolbar and the right-click popup menu offer the full 1D phase correction functions.

By default, all columns are selected as indicated by the filled blue squares ■. The red vertical line indicates the default pivot point in the upper column.

- 3. A typical way to perform phase correction is:
  - Click-hold the **0** button for zero order correction and move the mouse until the reference peak of the first column is exactly in absorption mode.
  - Click-hold the **1** button for first order correction and move the mouse until the reference peak in other column is exactly in absorption mode.
  - Click the 🗐 button to execute, save and return (see Fig. 13.5).

Phase 2D : exam2d_HC 1 1 C:\bio guest	
<mark>小 告 0 1 R</mark> 90 -90 180 ⊿ ⊾ II + − III ≡ # 🖳 →	<b>▲ →</b>
pivot = 128.44 ppm Phase increment = 0.20 ph0 = 83.36 ph1 = -180.80	
Column 417 / 7.2569 ppm	
Γ	
Column 644 4.2983 ppm	
	1
Column 899 / .9748 ppm	

Figure 13.5

## 13.1.2 2D Interactive Phase Correction Details

## How to Scale or Shift Individual Rows/Columns

To select one row or column:

Real Click in the corresponding part of the data window.

The selected row/column will be marked with a filled blue square  $\blacksquare$  whereas unselected rows/columns will be marked with an unfilled blue square  $\Box$ . Selecting a single row /column allows you to shift and scale it separately from the other rows/columns as shown in Fig. 13.6.

Phase 2D : exam2d_HC 1 1 C:\bio guest	
<mark>小 告 0 1 R</mark> 90 -90 180 ⊿ ⊾ II + − III ≡ # 🖳 →	<b>∢ →</b>
pivot = 128.44 ppm Phase increment = 0.20 ph0 = 83.36 ph1 = -180.80	
Column 417 / 7.2569 ppm	
Γ μ	
Column 644 / 4.2983 ppm	
Υ V	
Column 200 / 0749 mm	[ <sup>1</sup>
Column 8997.9748 ppm	<u> </u>
V V	

Figure 13.6

To select all rows or columns,

IN Click the following button:

⅓ Select all rows or columns.

## How to Perform Smooth Phase Correction

To perform zero order phase correction:

- 1. Click-hold the following button (it turns green) and move the mouse:
  - **0** Zero order phase correction.

until the reference peak of the first row/column is exactly in absorption mode.

2. Release the mouse (button turns grey).

The parameter PHC0 will be set accordingly.

To perform first order phase correction:

- 1. Click-hold the following button (it turns green) and move the mouse:
  - 1 First order phase correction.

until the reference peak of the second and further rows/columns is exactly in absorption mode.

2. Release the mouse (button turns grey).

The parameter PHC1 will be set accordingly.

## How to Perform 90, -90 or 180° Zero Order Phase Correction

Click one of the following buttons:

- 90 90° zero order phase correction.
- -90 -90° zero order phase correction.
- 180 180° zero order phase correction.

## How to Reset the Phase to the Original Values

Click the following button:

**R** Reset zero and first order phase.

## How to Change the Mouse Sensitivity

Click one of the following buttons:

- ⊿ Increase (double) the mouse sensitivity [.inc].
- ▶ Decrease (halve) the mouse sensitivity [.dec].
- **II** Reset the mouse sensitivity to 1.0.

## How to Show the Next/Previous Row or Column

To show the next row/column, click the following button:

+ Show next row/column.

Note that only the selected row/column is increased. If all rows/columns

are selected, only the first one is increased.

To show the previous row/column, click the following button:

- Show previous row/column.

Note that only the selected row/column is decreased. If all rows/columns are selected, only the first one is decreased.

## How to Arrange Rows or Columns

Click one of the following buttons:

- III Arrange rows/columns horizontally.
- $\equiv$  Arrange rows/columns vertically (see Fig. 13.6).
- **#** Arrange rows/columns vertically in a split window.

## How to Return from Multi-1D Phase to 2D Phase Display

Click the following button:

[] to save, execute and return.

This will perform the following tasks:

- Execute phase correction.
- Save the current phase correction values.
- Leave the multi-1D phase mode.

Click the following button:

J to return to the 2D phase display without save.

## How to Return from 2D Phase Mode

Click the following button:

J Return.

## 13.2 2D Interactive Integration

TOPSPIN 2.1 and newer supports interactive 2D integration.

## 13.2.1 How to Switch to 2D Interactive Integration

Click the corresponding button in the upper toolbar as indicated below



or enter .int on the command line.

The Tab bar of the active data window will be replaced by a toolbar. Fig. 13.7 shows an example of a 2D inverse spectrum.



Figure 13.7 Data window in interactive integration mode

**I** The yellow button indicates that you are in integration mode.

- "Define integral region" mode (active when green)
- Move integral region (green when active).
- Copy a region.

÷

Delete all integral regions.

Read/import integral regions.

- Save/Export integral regions.
- Integrate current regions/define reference.
- Save integral regions and return.
  - Return without save.

#### 13.2.2 2D Interactive Integration Procedure

When you switch to 2D integration mode, the "Define integral region" mode is active by default. This means you can immediately start defining the integral regions. To do that:

- 1. Click and hold the left mouse button at any corner of a region to be defined, move the mouse to draw a box around that region and release the mouse.
- 2. Choose one of the following options from the appearing popup menu:

*Integrate: a* : to add up all intensities in the region

Integrate: +: to add up all positive intensities in the region

Integrate: - : to add up all negative intensities in the region

*Integrate: a* + - : to add up all intensities in the region and store separate entries for *all*, *positive* and *negative* intensities.

*Integrate: a* + : to add up all intensities in the region and store separate entries for *all* and *positive* intensities.

*Integrate: a* - : to add up all intensities in the region and store separate entries for *all* and *negative* intensities

*Integrate:* + - : to add up all intensities in the region and store separate entries for *positive* and *negative* intensities.

The integral regions will be displayed along with their storage num-

bers and modes (see Fig. 13.8).



Figure 13.8

- **3.** Click the **I** button and choose *Integrate current regions* from the pulldown menu to integrate the defined regions.
- **4.** Click the **I** button again and choose *List integral values* from the pulldown menu to show the list of integrals.

Table 13.1 shows the list of integrals based on the regions defined in Fig. 13.8.

#	SI_F	row1	row2	row1	row2	Abs. Int.	Inte- gral	
	SI_F 2	col1	col2	col1 ppm	col2 ppm		grai	
1	1024	666	689	50.1458 3	46.4313 2	9.2529e+00 8	882.42	а
	1024	510	522	6.04420	5.89291			
2	1024	597	632	61.2893 4	55.7175 9	1.1135e+00 9	1062	+
	1024	520	533	5.91452	5.74162			
3	1024	652	692	52.4673 9	45.9670 1	- 3.7699e+00 7	- 35.953	-
	1024	566	579	5.31659	5.15089			
4	1024	683	721	47.3599 5	41.3238 8	1.0072e+00 9	960.57	а
	1024	589	605	5.02122	4.81230			
5	1024	683	721	47.3599 5	41.3238 8	1.064e+009	1014.7	+
	1024	589	605	5.02122	4.81230			
6	1024	683	721	47.3599 5	41.3238 8	- 5.6725e+00 7	- 54.097	-
	1024	589	605	5.02122	4.81230			
7	1024	502	543	76.6116 8	70.11130	1.2637e+00 9	1205.2	а
	1024	637	649	4.38726	4.23598			
8	1024	502	543	76.6116 8	70.11130	1.2911e+00 9	1231.3	+
	1024	637	649	4.38726	4.23598			

Table 13.1

Alternatively, you can define a reference integral and integrate the defined regions of the same or of a different dataset, relative to this integral. For this purpose the **1** button offers the following menu items:

- *Integrate current regions rel. to reference* You will be prompted for the reference integral number and value.
- *List integral values* The output list will now show an additional column with the normalized integral values.
- *Define current dataset as reference* You will be prompted for the reference integral number and value.
- *Integrate and use ref. dataset for calibration* The integral value defined on the reference dataset is used for calibration.

## How to Move an Integral region

- **1.** Click the button <u>m</u> (it turns green).
- 2. Move the mouse into the region to be moved.
- 3. Left-click-hold and move the mouse to move the region.
- 4. Release the mouse at the desired position.

## How to Copy an Integral region

- 1. Click the button 🔢 (it turns green)
- 2. Move the mouse into the region to be moved
- 3. Left-click-hold and move the mouse to the desired position
- 4. Release the mouse to copy the region.

## How to Delete all Integral Regions

- **1.** Click the button  $\mathbf{\mathcal{H}}$ .
- 2. Click OK to confirm deletion.

## How to Read/Import Integral Regions

- 1. Click the button 🦳.
- 2. Click *Read intrng* to read the last stored integral ranges

or

Click *Import Integration Regions* to import an exported integral region file (see below)

## How to Save/Export Integral Regions

- 1. Click the button
- 2. Click *Save Regions to* intrng to save the regions to the current dataset PROCNO (file int2drng)

or

Click *Export Integration Regions* to export the integration region file for general usage; i.e. usage with other datasets.

## How to Return from 2D Integration mode

Click the following button:

[] to save the current integral regions and return.

Click the following button:

J to return to the 2D integration mode without save.

## 13.3 2D Multiple Display and Row/Column Handling

2D multiple display shows a 2D spectrum with an arbitrary number of 1D and/or 2D spectra superimposed.

Spectra are ppm aligned or Hz aligned, according to the selected axis unit.

A superimposed 1D spectrum is automatically displayed in the direction of the matching nucleus (for a hetero-nuclear 2D) or in the F2 direction (for a homo-nuclear 2D).

Although multiple display is normally used for spectra with matching nuclei, it allows you to superimposed spectra with non-matching nuclei. You will get a warning that the nuclei do not match. Just just click *OK* to continue.

## How Switch to Multiple Display mode and Read Multiple Spectra

Switching to multiple display and reading multiple spectra can be done in

two different ways:

 Read a 2D dataset and click to switch to multiple display mode. Then add 1D and/or 2D spectra, e.g. from the browser or with *re*.

or

• Select multiple spectra in the browser, right-click one of them and click *Display*.

For a more detailed description of reading multiple data in multiple display mode, see chapter 12.5.

In multiple display mode, the Tab bar of the active data window is replaced by a toolbar (see Fig. 13.9).



Figure 13.9 Multiple display with two 2D spectra superimposed



Figure 13.10 Multiple display with a 1D spectrum superimposed on a 2D spectrum

The yellow button indicates that the data window is in multiple display mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

The browser in multiple display is split in two parts (see Fig. 13.11). The additional lower part shows:

- which datasets are displayed in the active data window
- which datasets are selected (they are highlighted)



Figure 13.11

## How to Align Multiple 2D Spectra

2D spectra in multiple display can be individually shifted. To do that:

- 1. Select one of the spectra in the lower part of the browser.
- 2. Click-hold the 🕂 button and move the mouse.

Fig. 13.12 shows a region of two comparable 1H/13C inverse 2D datasets which are shifted relative to each other.

Clicking the **R** button resets individual scaling and shifting.



Figure 13.12

## How to Display the Next/Previous Name/Expno

To compare a series of spectra you can interactively increment or decrement the dataset name or expno. A dataset name is incremented according to the ICON-NMR naming convention of increasing extensions, e.g. name.001, name.002 etc.

Real Click one of the following button (button turns green):

E- Show the previous name/expno/procno of the last dataset

- E+ Show the previous name/expno/procno of the last dataset
- E<sub>i</sub> Set the increment options. Clicking this button will open the following dialog where you can choose to increment the procno, expno or name, set the expno increment and switch individual scaling on/off.

#### How to Scan Rows/Columns

Click the following button (it turns green) and move the mouse in the data field:

⊥⊥1 to scan rows in the 2D spectrum.

Click the following button (it turns green) and move the mouse in the data field:

 $\pm$  to scan columns in the 2D spectrum.

Click the following button (it turns green) and move the mouse in the data field:

ht to scan rows and columns in the 2D spectrum.

To scale up the displayed row/column:

R Click the left mouse button or turn the mouse wheel up.

To scale down the displayed row/column:

Real Click the middle mouse button or turn the mouse wheel down.

#### How to Grab a Row/Column

You can grab a row or column, i.e. keep it displayed in the data window as follows:

- 1. Scan rows or columns as described above and hold at the desired position.
- 2. Right-click in the data window.
- 3. Choose Grab Row/Column from the popup menu (see Fig. 13.13).

Note that a grabbed row/column appears in the lower apart of the browser. It can be selected there and individually scaled or shifted.

Toggle Rows/Colu	imns
Extract Row/Colun	nn
Grab Row/Columr	1
Baseline At Cente	r
Baseline At Botton	n

Figure 13.13





Fig. 13.14 shows row 619 with the 1D baseline at the center of the data window.

## How to Show the Next/Previous Row or Column

To show the next row/column, click the following button:

+ Show next row/column.

To show the previous row/column, click the following button:

- Show previous row/column.

Alternatively, you can turn the mouse wheel, while pressing the Shift key to show the next/previous rows/columns.

## How to Move the Selected Dataset Up/Down in the Dataset List

To move the selected dataset up, click the following button:

↑ Move the selected dataset up.

To move the selected dataset down, click the following button:

↓ Move the selected dataset down.

## How to Extract a Row/Column

- 1. Scan rows or columns as described above and hold at the desired position.
- 2. Right-click in the data window and choose *Extract Row/Column* from the popup menu (see Fig. 13.13).
- **3.** Specify the row/column number and output *procno* in the dialog box. Note that the ROW/COLUMN field is initialized with the grabbed row/column or, if no grabbing was done, with the current row/column.
- 4. Click OK

The extracted row or column is stored as a 1D dataset under the specified PROCNO and displayed in a new data window. In the upper left part is this, the row number and source 2D dataset is specified (see Fig. 13.15).



Figure 13.15

## How to Copy Contour Levels from First to Other Spectra

Click the following button:

斉 Copy contour levels from the first to the other spectra.

Note that the contour levels are only changed on screen, not on disk.

## How to Switch on/off 2D contour display

Click the following button:

Switch on/off 2D contour display.

## How to Position the Baseline of the Row/Column

To put the baseline at the center of the data window:

- **1.** Right-click in the data window.
- 2. Choose in *Baseline At Center* from the popup menu (see Fig. 13.13).

To put the baseline at the bottom of the data window:

- **1.** Right-click in the data window.
- 2. Choose in *Baseline At Bottom* from the popup menu (see Fig. 13.13).

This works both in the scan submode or on a grabbed row/column.

## **13.4 2D Interactive Calibration**

A 2D spectrum can be calibrated, automatically with the command *sref* or, interactively as described below.

## How to Switch to 2D Calibration mode

Solution of the corresponding button in the upper toolbar:.



or enter .cal on the command line. The Tab bar of the active data window will be replaced by a toolbar (see Fig. 13.16).



Figure 13.16 Data window in calibration mode



The yellow button indicates that the data window is in calibration mode.

## How to Perform 2D Calibration

In calibration mode:

1. Left-click in the data window at the reference peak.

The following dialog box will appear:

💼 calibrate 🛛 🗶									
Spectrum calibration frequency									
F2 [ppm] -0.1621	F1 [ppm]								
<u>о</u> к	Cancel								

Note that the units for F2 and F1 (Hz or ppm) correspond to the axis units of the display.

- **2.** Enter the F2 and F1 frequency you want to assign to the reference peak.
- 3. Click OK.

The spectrum will be calibrated and re-displayed. The calibration button will turn grey again.

## **13.5 2D Chemical Shift Distance Measurement**

## How to Measure a 2D Chemical Shift Distance

- 1. Click the following button (button turns green):
  - Sector Chemical shift distance measurement.
- **2.** Click-hold the left mouse button at one peak position and drag the mouse to another peak position.

The distance in ppm, will be displayed.

**3.** Right-click in the data window to quit distance mode (button turns grey).



Figure 13.17 Data window in distance measurement mode

## Chapter 14 Data Window Handling

## 14.1 Data Windows

The TOPSPIN window has a data area that may contain multiple data windows. The size of the data area depends on the overall size of the TOPSPIN window and on presence of the Browser and/or Processing Guide. Fig. 14.1 shows the TOPSPIN window with the Browser and three data windows.



Figure 14.1

Note that the three data windows show different data objects: 1D processing parameters, a 1D spectrum and a 2D spectrum.

## How to Move a Data Window

Solution of the title bar and move the mouse.

## How to Resize a Data Window

- 1. Move the cursor to the window edge until it becomes a doubleheaded arrow.
- 2. Left-click-hold that position and move the mouse.

Depending on the position of the double-headed arrow, you can change the window height, width or both (see Fig. 14.2)


Figure 14.2

### How to Select (activate) a Data Window

The active data window is the window of which the title bar is highlighted. The TOPSPIN menu, tool bars and command line commands correspond to and act on that window. Only one data window is active at a time.

To activate a different data window:

Real Click in the desired data window or click its title bar.

or

Click one of the colored radio buttons above the data area. The pressed radio button (the green one in the example below) corresponds to the current dataset.



If you hold the cursor over one of the buttons without clicking it and wait a few seconds, the corresponding dataset specification will be shown.

Is Click Window  $\rightarrow \underline{x}$  dataname expno procno dir user

where <u>x</u> is the number of the desired window and *dataname*, *expno*, *procno*, *dir* and *user* refer to the dataset displayed in that window.

or

Hit the *F6* key to activate the next window. Repeat that until the desired window is the active window.

#### How to Open a New empty Data Window

```
\mathbb{R} Click Window \rightarrow New window [Alt+w-n]
```

The new data window will become the active window and will, by default, cover the entire data area, hiding possible existing data windows. To open a dataset in the new window, drag a dataset from the browser or from the Windows Explorer into the new window or click  $File \rightarrow Open$  (see also chapter 5.3).

## How to Arrange Data Windows

If the data area contains multiple data windows, you can arrange them in various ways. All the arrange commands arrange the windows left to right and/or top to bottom in the order in which the windows have been active. The currently active data window will therefore be positioned at the top and/or left of the data area.

To arrange the data windows as a grid:

```
\square Click Window \rightarrow Arrange as a Grid
```

Depending on the number of windows, they will be arranged vertically and/or horizontally (see Fig. 14.3).



Figure 14.3

To arrange data windows in stack (see Fig. 14.4):

Real Click Window  $\rightarrow$  Arrange in Stack



Figure 14.4

To arrange data windows side by side (see Fig. 14.5):

 $\square$  Click Window  $\rightarrow$  Arrange Side-by-Side



Figure 14.5

To cascade data windows (see Fig. 14.6):

 $\square \bigcirc Click Window \rightarrow Cascade$ 



Figure 14.6

Note that you can instruct TOPSPIN to open new data windows cascaded rather than maximized as well configure cascaded windows (command  $set \rightarrow Window \ settings$ , see also chapter 5.3)

# How to Iconify (minimize) a Data Window

Real Click the Lotton in the windows title bar

or

IF Click *Window*  $\rightarrow$  *Iconify all* to iconify all windows.

## How to De-iconify a Data Window

IS Click the 
∎ button or double-click the title bar.

## How to Maximize a Data Window

In Click the Dutton or double-click the title bar.

The window will cover the entire data area. Note that a maximized window cannot be moved of resized but can be restored (in size and position), iconified or closed.

## How to Restore the Size and Position of a Data Window

IN Click the <a>Image button</a> or double-click the title bar.

Note that this is only possible if the title bar contains the  $\blacksquare$  button. This is only the case after the window has been maximized or iconified.

## How to Close a Data Window

To close the active data window:

```
\mathbb{R} Click \ File \rightarrow Close \ [Crt1-w]
```

or

 $\mathbb{R}$  Click the  $\mathbb{X}$  button in the windows title bar.

To close any data window:

IN Click the IN button in the data windows title bar

or

 $\mathbb{R}$  Click the title bar and then click  $File \rightarrow Close [Crtl-w]$ .

To close all data windows:

 $\mathbb{R}$  Click *File*  $\rightarrow$  *Closeall* [*closeall*]

## How to Iconify all Data Windows

 $\square Click \textit{Window} \rightarrow \textit{Iconify all}$ 

## How to Maximize all Data Windows

 $\square \ \ \, \mathbb{Click} \textit{ Window} \rightarrow \textit{Maximize all}$ 

The active window will be displayed on top, all other windows are hidden.

## How to Activate the Next Data Window

IS Click Window  $\rightarrow$  Next window [F6].

The windows title bar will become highlighted.

# 14.2 Window Layouts

A data window layout defines the position, geometry and window type of one or more TOPSPIN windows. The following windows types are available:

- data windows
- lock display window
- acquisition display window
- BSMS display window
- temperature unit window

## How to Save the Current Window Layout

- **1.** Click Window → Save layout
- 2. In the appearing dialog box: Specify the layout File name (extension .prop) and click *Save Layout*

## How to Read a Window Layout

- **1.** Click Window → Read layout
- 2. In the appearing dialog box: Specify or click the layout File name and click *Read Layout*

Windows are arranged according to the following rules:

- Each currently displayed window type gets the position and geometry to the corresponding definition in the layout.
- If a window type is displayed but not defined in the layout, it keeps its current position and geometry.
- If a window type is defined in the layout but not displayed, the layout definition is ignored.
- Multiple *data* windows are, arbitrarily, assigned to the available data window definitions.

## How to Swap Data Windows

Within a certain layout, you can easily swap two TOPSPIN windows with the command *swin*. If the data area contains exactly two windows, *swin* simple swaps their position and geometry. If it contains more than two data windows, *swin* opens a list from which you can select any window to be swapped with the currently selected (active) window. Swapping windows can also be executed from the *Window* menu.

## How to Toggle Window Decoration

By clicking *Window ' Window Layout ' Toggle Window Decoration* easy toggling of window decoration is available. Especially users who work with many different windows will get more space on their monitor by using this function that hides - respectively shows - the title of the current window and reduces the used font.

# Chapter 15 Analysis

## **15.1 Introduction**

TOPSPIN offers various data analysis methods including chemical shift measurement, signal to noise calculation and T1/T2 relaxation analysis as described in this chapter. Furthermore, it offers the following structure analysis tools:

• Multiplet Analysis

This allows you to easily define multiplets and deduce chemical shifts, coupling constants, multiplicities and connections.

- Daisy (TOPSPIN 2.0 and newer) This allows you to simulate spectra based on chemical shifts and coupling constants.
- Solids Line Shape Analysis This allows you to simulate and fit calculated spectra to various experimental 1D solid NMR spectra.
- Jmol

A 3D Structure Viewer for displaying chemical structures.

- 2D molecule structure editor A program for drawing chemical structures., offering a large number of drawing tools.
- DNMR (Dynamic NMR) Lineshape Analysis
   A program to simulate temperature dependent NMR spectra, interactively set up and iteratively refine the model parameters to get the best fit of the measured and simulated 1D NMR spectra.

Structure analysis tools can be started from the *Analysis* menu. They are all described in the following manuals:

Reference Click Help  $\rightarrow$  Manuals  $\rightarrow$  [Analysis and Simulation] Structure Analysis Tools

except for Daisy, which is described in the separate manual:

 $\texttt{IS} Click \textit{Help} \rightarrow \textit{Manuals} \rightarrow [\texttt{Analysis and Simulation}] \textit{ Daisy}$ 

# **15.2 Chemical Shift Distance Measurement**

## How to Measure a Chemical Shift Distance

- 1. Click the following button (button turns green):
  - Sector Chemical shift distance measurement.
- **2.** Left-click-hold at one peak position and drag the mouse to another peak position.

The distance in ppm, will be displayed.

**3.** Right-click in the data window or move the cursor out of the data window to leave distance measurement mode (button turns grey).

# 15.3 1D Signal to Noise Calculation

## How to Perform Interactive S/N Calculation

1. Click Analysis → Signal/Noise Calculation [.sino].

The current signal region (parameters SIGF1-SIGF2) and noise region (parameters NOISF1-NOISF2) are displayed.



Figure 15.1 Data window in S/N measurement mode

- 2. Move the mouse into the data window.
- **3.** Left-click-hold and drag the mouse from one edge of the *signal* region to the other edge.

A horizontal double-headed arrow will indicate the signal region.

**4.** Left-click-hold and drag the mouse from one edge of the *noise* region to the other edge.

A horizontal double-headed arrow will indicate the noise region.

**5.** Right-click any position in the data window. The popup menu as shown in Fig. 15.2 will appear.



Figure 15.2

#### Choose Start S/N calculation

The other entries allow you to redefine or clear the regions. After the noise calculation has finished, the result will appear on the screen.

### How to Delete the Signal Region or Noise Region

To delete the current signal region:

- 1. Right-click in the data window.
- 2. Choose *Clear SIGREG* from the popup menu (see Fig. 15.2).

To delete the current noise region:

- 1. Right-click in the data window.
- 2. Choose *Clear NOISEREG* from the popup menu (see Fig. 15.2).

#### How to Edit the Limits of the Signal Region or Noise Region

- **1.** Right-click in the data window.
- 2. Choose *Edit regions...* from the popup menu (see Fig. 15.2).
- 3. Enter new limit values in the appearing dialog box.

🤹 sino		×		
Define sino para	ameters:			
	From [ppm]	To [ppm]		
SIGREG	8.6355	0.4351		
NOISEREG	10.7777	9.2045		
<u>O</u> K <u>C</u> ancel				

#### 4. Click OK

The S/N value is automatically recalculated and displayed.

#### How to Change the Width of the Signal Region or Noise Region

- 1. Right-click in the data window.
- 2. Choose Change region width... from the popup menu (see Fig. 15.2).

3. Enter new width values in the appearing dialog box.

🤹 sino					
Define sino parameters:					
	Width	Unit			
SIGREG	8.2004	ppm			
NOISEREG	1.5731	ppm			
<u>O</u> K <u>C</u> ancel					

4. Click OK

Note that as you change the width, the right limit is modified correspondingly. The left limit is kept. The S/N value is automatically recalculated and displayed.

# **15.4 Relaxation Analysis**

Typically, relaxation data consist of a series of 1D FIDs measured with varying delays and stored as pseudo 2D data. To analyze these data, Topspin offers an easy to use T1/T2 Relaxation Guide. Relaxation curves of various experiment types with up to six components can be fitted.

To start the Relaxation Guide:

 $\square$  Click Analysis  $\rightarrow$  T1/T2 Relaxation [t1guide].

This will open the dialog box as shown in Fig. 15.3.





Just click the successive icons and follow the instructions on the screen. Note that holding the cursor over an icon shows the command line command that is executed when the icon is clicked. If you prefer to execute these commands from the command line, just click the *Close* button to close the Relaxation Guide.

#### Extract Slice

Prompts you for the FID or spectrum to be extracted for peak determination (see Fig. 15.4). Click *FID* to extract an FID or *Spectrum* to extract a spectrum. Note that the latter only works if the pseudo 2D data have been processed. If you click FID, the extracted FID is automatically processed. We recommend to enter the FID or spectrum number which was meas-

🥌 Ext	ract a row from 2d data 🛛 🛛
?	Fid or Spectrum must be extracted From the 2d relaxation data. This row should correspond to an experiment with the maximum or minimum delay time. All further data preparation will be done in respect to this row.
	FID Spectrum Cancel

Figure 15.4

ured with the longest delay. It can be found in the *vdlist* file in the EXPNO data directory. Then you can choose between:

- *Manual Integration*. This will switch to Interactive integration mode The highest peak in each region will be used for relaxation analysis.
- *Manual Peak Picking*. The selected peaks will be used for relaxation analysis.



Figure 15.5

#### Peaks/Ranges

Switches to interactive integration or peak picking mode as chosen

above. Here you can define the ranges or peaks to be included in the relaxation analysis. Then use is button to export regions/peaks to Relaxation Module and quit the interactive mode.

#### **Relaxation Window**

Switches the 1D data window to relaxation analysis mode (see Fig. 15.6)



Figure 15.6

and performs a default fitting. By default, this is one-component, T1-intensity fitting (Function type *uxnmrt1*) for peak 1. If the dataset was already fitted, the previous type of fitting is performed. The fitting curve is displayed in the data section and a *Brief Report* is shown in the parameter section. If this default fitting is appropriate, you can view, interpret and print the results as described below. If not, you can perform the desired fitting as described below.

#### Perform Fitting and Calculate the Relaxation Time

Depending on the experiment, you can perform the appropriate fitting as follows:

- 1. Select a *Fitting type*: *Intensity* or *Area*. Either every point reflects the intensity of the biggest peak in the defined integral range or the integral itself. Both of them can be used but, depending on the experiment, one of them usually give a better fitting curve.
- 2. Click the button to open the parameter dialog box. Select a *Function Type* and set the required parameters (see below).
- 3. Click OK.
- 4. Perform fitting and calculate the relaxation time:

Fit the relaxation curve for the current peak.



Fit the relaxation curve for all peaks.

Fit data according to the ASCII file t1ascii.

View and interpret the results as described below.

## **Function Types and Parameters**

The TOPSPIN relaxation routine offers functions for various relaxation experiments with up to 6 components:

**uxnmrt1** for one-component T1 experiments. Set the parameter *List file name* to the list type used during the acquisition. Set *Pick data points* to PD or PD0 (see below). The T1 fitting function is defined by the function:

$$I(t) = I(0) + P \times \exp\left(\frac{t}{T_1}\right)$$

where I is Intensity or Area according to the Fitting Type. The best fit is calculated by varying I(0), P and T1 in an iterative process accord-

ing to the Levenberg-Marquardt algorithm. Clicking (>) and (>) executes the commands *ct1* (current peak) and *dat1* (all peaks), respectively.

**uxnmrt2** for one-component T2 experiments. Set the parameter *List file name* to the list type used during the acquisition. Set *Pick data points* to PD or PD0 (see below). A T2 fitting function is defined by the function:

$$I(t) = P \times \exp\left(\frac{t}{T2}\right)$$

where *I* is Intensity or Area according to the Fitting Type. The best fit is calculated by varying P and T2 in an iterative process according to the Levenberg-Marquardt algorithm. Clicking  $\bigcirc$  and  $\bigotimes$  executes the commands *ct2* (current peak) and *dat2* (all peaks), respectively.

invrec, satrec, cpt1rho, expdec, gaussdec, lorgauss linear, varbigdel, varlitdel, vargrad, vardamp: these functions can be used for various experiments with up to 6 components, except for cpt1rho and lorgauss which allow only 4 and 3 components, respectively. They all use the simplex algorithm and require some parameters to be set:

- Enter the Number of components
- Click the Setup button to set the Iteration Control parameters. For each component, the initial guess (G) and step rate (S) can be set. The initial guess for I[0] must be selected such that the sum of all components does not exceed 1. If there is only one component, I[0] is usually set to 1. The step rate is usually set to about one tenth of the initial guess. If the step rate of a variable is set to zero, then this variable is not changed during the iterations. Note that the initial guesses can also be set with the set to olbar button. Clicking and simfit all (all peaks), respectively.

The Fitting Function to pick data points can be:

- *pd* pick data points for relaxation analysis (Drift value interpreted)
- *pd0* pick data points for relaxation analysis at constant peak positions (drift value ignored)
- *pft2* pick data points for T2 calculation of 1D raw data.

#### View the Fitting Results

When the fitting procedure has finished, the fitting curve is displayed in the data section and a *Brief Report* appears in the parameter section (see Fig. 15.6). The latter consists of:

- the calculated relaxation value
- the fitted parameters
- the standard deviation SD

For further examination of the result, click one of the following buttons:

- Show the fitting result of the previous peak/area.
- + Show the fitting result of the next peak/area.
- Switch x-axis to linear scaling.
- Switch x-axis to logarithmic scaling.
- Switch x-axis to square root scaling.
- Switch y-axis to logarithmic scaling. Note that this only works for curves with positive intensities/areas only.
- Import integrals from dataset ~TEMP.
- Export integrals to dataset ~TEMP
- L Toggle button to hide/show information in the curve field, including algorithm, peak number and relaxation value.
- (i) Show an extended report, including the fitted intensity or area

distribution. This consists of the same information as the brief report plus a table with the intensity or area distribution. Example:

```
Dataset : C:/bio/data/guest/nmr/tltest/1/pdata/1
INTENSITY fit :
I[t]=I[0]+P*exp(-t/T1)
12 points for Peak 1, Cursor Point = 7.221 ppm
Results
           Comp. 1
I[0] =
       1.215e+000
Ρ
        -2.211e+000
     =
Τ1
     =
            19.449s
SD
    = 3.685e-003
   tau
       ppm integral intensity
       7.221 2.5811e+009 1.9737e+008
30.000s
10.000s
         7.221 -3.2898e+008 -2.9056e+007
8.000s
          7.221 -7.8525e+008 -6.4616e+007
          7.221 -1.6289e+009 -1.3101e+008
5.000s
```

• • •

#### Print, Export of Copy the Fitting Results

To print the fitting curve:

 $\mathbb{R}$  Click *File*  $\rightarrow$  *Print* 

To export the fitting curve as a graphics file:

Real Click *File*  $\rightarrow$  *Export* 

To copy the fitting curve to the Windows Clipboard:

 $\square$  Click *Edit*  $\rightarrow$  *Copy* 

# Chapter 16 Acquisition

This chapter describes TOPSPIN acquisition as far as the interface is concerned. Individual acquisition command are described in the Acquisition Reference manual.

# **16.1 Acquisition Guide**

If you are a new or occasional user, we recommend you to acquire your data with the TOPSPIN Acquisition Guide. This will guide you through the typical sequence of acquisition steps. To start the Acquisition Guide, click *Spectrometer*  $\rightarrow$  *Acquisition Guide*.



#### Figure 16.1

In *Automatic mode*, the Acquisition Guide will simply execute each command when you click the respective button. This requires the acquisition parameters to be set correctly. In interactive mode (*Automatic mode* unchecked), the Acquisition Guide will, at each step, open a dialog box offering you the available options and required parameters. Note that the last button *To processing* will open the processing equivalent of the Acquisition Guide, the Processing Guide.

# **16.2 Acquisition Toolbar**

Acquisition can be prepared, started and controlled from *Spectrometer* menu. Clicking this menu opens the pulldown menu shown in Fig. 16.2 :

Spectrometer	Processing	Analysis	Opt			
Interactive A	Interactive Acquistion Guide [topguide]					
Data Acquis	ition Flowchar	t				
Basic/Select	tive Experimer	nts				
ICON-NMR			•			
Adjustments	3		•			
Acquisition			•			
Setup			•			
Sample			•			
Shim contro	I		•			
Accessories			•			
Shape Tool	[stdisp]					
Excitation Profile [exprof]						
Acquisition Status Bar On/Off						

Figure 16.2

Here you find several cathegories of acquisition related commands. Each entry give access to a submenu with various commands. Fig. 16.3, for example, shows the *Setup* submenu.

Hardware Configuration [cf] Ethernet addresses of hardware [ha] Experiment Installation [expinstall] Parameter set conversion [paracon] Probe table setup [edhead] Solvent dependent parameter setup [edprosol] Lock parameter setup [edlock] Nuclei table setup [ednuc] Solvent table setup [edsolv] Amplifier linearization setup [cortab] Convert gradient field maps [convfieldmaps]

#### Figure 16.3

For most entries, the command line command, for example *expinstall*, is specified in square brackets. Furthermore, Topspin can be configured such that right-clicking any menu entry will display the corresponding command line command. To do that right-click in an empty part of the menubar and choose *Define Right-click Action*.

For convenience, common acquisition commands can also be started from the TOPSPIN toolbar. The right part of the upper toolbar shows the following buttons:



Start the acquisition. Acquires NS scans in the current dataset, overwriting

possibly existing data. Equivalent to the command zg.

- Halt the acquisition. This stops the acquisition after the current scan has finished. All data acquired so far are saved. Equivalent to the command *halt*.
- Stop the acquisition. This stops the acquisition immediately. Data acquired after the last disk write (if any) are lost. Equivalent to the command *stop*.

W- Open the online FID display window. Shows the currently acquired

FID. Only works during acquisition. Equivalent to the command *acqu*.

- Open the Lock display window. Shows the lock signal. Equivalent to the command *lockdisp*.
- Calculate the experiment time. Shows the total experiment time and file size of the raw data. Equivalent to the command *expt*.
- Set SFO1, O1, O2 and O3 interactively. Puts a red cursor line in the data window. A left-click at the desired frequency opens a dialog box where you can set O1, O2 and/or O3.
- Set the sweep width to the current region and the spectrometer frequency to the center of the current region. Update the parameters SW and SFO1, respectively.
- Ht Setup a frequency list interactively.

# 16.3 Data window Toolbar

TOPSPIN 2.0 and newer support dataset specific acquisition the display. It is activated by clicking the Acqu tab of the data window toolbar.



Figure 16.4

From here, you can start various acquisition commands like:

- Start acquisition [zg]
- Halt the acquisition [halt]
- Stop the acquisition [*stop*].
- Probe matching and tuning [wobb].
- Interactive Parameter Adjustment [gs].

Data specific acquisition display allows you to open multiple acquisition display windows, one for each dataset.

Note that the *Acqu* tab is automatically activated when the acquisition is started from the TOPSPIN menu, toolbar or command line

# 16.4 Acquisition Status Bar

The acquisition can be followed and controlled from the acquisition status bar. Before you use the acquisition status bar, it must be configured from the User Preferences window. To do that:

- **1.** Click Options  $\rightarrow$  Preferences [set].
- **2.** Click *Acquisition status bar* in the left part of the *User preferences* box. This will show the status bar items (see Fig. 16.5).

1	Acquisition status bar	
	Auto open acquisition status bar	
	Include spooler	~
	Include time	<b>~</b>
	Include sample temperature	
	Include acquisition status	<b>~</b>
	Include acquisition indicator	<b>~</b>
	Include lock signal	
	Include MAS spinning rate	
	Include peak power check (POWCHK) indicator	
	Include sample state	

#### Figure 16.5

**3.** Check the desired entries.

To switch the acquisition status bar on:

```
IS Click Spectrometer → Acquisition Status Bar On/Off
```

or

Right-click in the status line at the bottom of the TOPSPIN window and choose the popup menu *Acquisition Status Bar On/Off* 

With the entries selected above, the right part of the status bar will look like this.

Acquisition information	Fid Flash	Sample	Time	Spooler
scan: 2 / 16 residual time:1m27s experiments: 1 / 1	-		10:49 Jul 15	running: 0 queued: 0 delaved: 0

The acquisition status bar not only displays information, it also allows you to perform various actions, e.g.:

- Double-click the Time field to view detailed time and date information.
- Double-click the Lock field to open the lock display.
- Double-click the Fid Flash field to open the wobble display.

- Right-click the Fid Flash field to switch on/off FID flashing.
- Right-click the **Acquisition information** field to open the following popup menu:

Show acquisition display
Start rga
Start acquisition
Start wobble
Start gs
Stop acquisition

from this menu, you can start various acquisition commands.

• Right-click the VTU field to open the following popup menu:



Clicking Options will open the following dialog box:

🎍 🔀				
Temperature monitor options				
Scale = Kelvin 🔽				
Update rate [s] = 30				
<u>O</u> K <u>C</u> ancel				

Figure 16.6

# 16.5 Command Queuing and Scheduling

TOPSPIN 2.0 and newer support command queuing (spooling) and scheduling. Acquisition commands like *zg*, *go*, *rga* and *atma* are automatically queued, if this feature is *on* (default *off*). This allows you, for example, to enter multiple *zg* commands on different datasets. Automatic queuing can be switched on as follows:

- 1. Click Options → Preferences
- 2. In the User Preferences dialog:

re Enable Auto-Spooling under Administration Items

Processing commands can be queued with the command qu. For example, the command sequence zg; qu xfb on a 2D dataset, will start an acquisition and, when this has finished, process the data.

Acquisition and processing commands can be scheduled with the command *at*. Enter *help qu* or *help at*, fo more details on the respective commands.

Queued commands can be viewed in the Spooling field of the acquisition status bar. Note that the spooling field must be activated in the User Preferences window (command *set*).

# 16.6 Tuning and Matching the Probehead

Tuning and matching of conventional probeheads, (non ATM), is performed with the wobble procedure. To start this:

1. Enter wobb on the command line.

The data window toolbar switches to the *Acqu* tab and the wobble window is opened (see Fig. 16.7).



Figure 16.7

The buttons of the wobble toolbar have the following functions:

- Change the number of wobble steps [wbst].
- Change the wobble sweep width [wbsw].
  - Change the wobble frequency.
- Switch to the next channel/nucleus (if available).
- Stop the wobble procedure.
- 2. Turn the tuning and matching knobs on the probehead until the wobble curve is exactly in the middle and its minimum reaches the zero line.

Automatic tuning and matching of ATM probeheads can be performed with the command *atma*.

# 16.7 Locking

The lock display can be opened by clicking the # button in the toolbar or entering *lockdisp* on the command line. The lock display window will appear (see Fig. 16.8).

Lock Displa	ay			
E\$ 🖀 🖬	🖬 🖩 🛱	ل 🏟		

Figure 16.8

Here, you can view the lock signal, either during the lock-in procedure or, as shown above, after lock-in has been successful. At the top of the lock window the following buttons are available:

- Open the user preferences window [set].
- Toggle lock monitor mode.
- Lock the magnetic field [lock].
- Toggle lock display mode between *single* and *dual* color. Colors can be set in the User preferences (command *set*).

Switch grid mode between *both*, *vertical*, *horizontal* and *off*.

- Hake the lock display external.
- Put focus into TOPSPIN window.

Close the lock display window.

Note that an external lock display window is independent from the TOPSPIN window. You can for example, minimizes TOPSPIN while keeping the lock display open.

The lock display can also be opened by double-clicking the lock field in the acquisition status bar (see par. 16.4)

The lock process can be started by entering *lock* on the command line. This command is described in the Acquisition Reference manual.

# 16.8 BSMS Control Panel

The BSMS control panel allows shimming, locking, sample handling and helium level measurement. To open this panel:

Sector **bsmsdisp** on the command line

The BSMS Control Suite window will appear (see Fig. 16.9)

BSMS Con	trol Suite					
Main Lock	Main Lock Sample & Level Shim Autoshim Service					
-AUTO						
Phase	Power	Gain Lock				
1.00%						
LOCK	Dhaca	Downer Coin				
LUCK	Priase	Power Gain				
SAMPLE						
LIFT	SPIN					
-SHIM						
Z	x	Y				
 Z <sup>2</sup>	XZ	YZ				
<u>Z</u> <sup>3</sup>	XY	χ²-Υ²				
VALUE	Previous	Actual				
Absolute		Step +				
Difference		Step -				
		J				
Stepsize	1 1	( ' '   ' '   ' '   0 100 1e3 1e4				
Sample:	down	missing up				
		O Ö				
	~					

Figure 16.9

The individual functions BSMS control panel are described in detail in the Acquisition Reference manual.

# 16.9 Interactive Parameter Adjustment (GS)

Several parameters can be adjusted interactively, while observing the acquired FID. To start this:

🖙 Enter gs on the command line.

A split window will appear showing:

- the FID display (see Fig. 16.10)
- the GS parameter adjustment dialog (see Fig. 16.11)



**Figure 16.10** 

The buttons of the FID display are the same as for the acquisition command zg (see paragraph Fig. 16.10).

The GS parameter adjustment dialog offers tabs at the top of the window to select power, frequency, delay etc. The selected parameter is shown in the middle of the window. The slider at the right of the window allows you to change the selected parameter. The current value can be viewed and modified in the field below the slider. The sensitivity of the slider can be set in



Figure 16.11

the field *Sensitivity* above the slider. The effect of the change can be viewed in the FID display, the right part of the window. This can be manipulated with the FID display buttons as described in chapter 16.10.

At the bottom of the window you find the following buttons:

• Save : Save the value of the current parameter.

- Save all : Save the values of all changed parameters.
- *Restore* : Restore the value of the current parameter.
- *Restore all* : Restore the value of all changed parameters.
- *Stop* : Stop the acquisition and quit the GS window.

# 16.10 Running an Acquisition

A typical acquisition is performed as follows:

- 1. Create a new dataset.
  - a) Click  $File \rightarrow New$  [new, Ctrl+n].

🦉 New 🔀						
Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type.						
NAME	protona					
EXPNO	1					
PROCNO	1					
DIR	C:\bio					
USER	guest					
Solvent			CDCI3	*		
Experimen	t	Use current par	ams.	~		
TITLE	TITLE					
1H Cyclosporin						
	<u>o</u> k	<u>C</u> ancel M	lore <u>I</u> nfo <u>H</u> el	p		

Figure 16.12

b) Specify the datapath variables *name*, *expno*, *procno*, *dir* and *user*, select the desired *Solvent* and *Experiment*, enter the *Title* and click *OK*.
The dataset will appear in the data field with no raw and no processed data available.

📕 protona 1 1 C:/Bio guest 📃 🗖 🔀					
Spectrum ProcPars	s AcquPars Title Pu	IseProg Peaks Inte	egrals Sample Structure Fid Acqu		
ю Л S 🔰	123 🔻 🎮				
Experiment Width	Experiment	n	<u>^</u>		
Receiver	PULPROG =	zg	E Current pulse pr		
Nucleus	AQ_mod =	DQD 🛛 🔽	Acquisition mode		
Durations	TD =	65536	Size of fid		
Power	NS =	16	Number of scan:		
Program	DS =	4	Number of dumm		
Probe	TDO =	1	Loop count for "t		
Lists Wobble	► Width				
Lock	▼ Receiver				
Automation	RG =	32	Receiver gain		
Miscellaneous	DW [µs] =	83.200	Dwell time		
User Routing	DIAMOV/ fue1 -	2 600	Oversemina du 🎽		

2. Click the AcquPars tab to display the acquisition parameters.



- a) Optionally: click  $\Pi$  to show the pulse program parameters only.
- b) Click the H button to read the prosol parameters

or

Set the relevant parameters manually.

As an alternative to step 2, you can set the acquisition parameters interactively in the GS window (see par. 16.9).

- 3. To start the acquisition:
  - Click **b** in the upper toolbar or enter **z**g on the command line.

The data window toolbar will automatically switch to the Acqu tab and

the FID display window will appear:



Figure 16.14

The buttons in the toolbar have the following functions:

- Show FID in shuffled mode.
- We Show FID in unshuffled mode, horizontally arranged.
- Show FID in unshuffled mode, vertically arranged.
- Show FID in unshuffled mode, interleaved.
- Switch between FID and spectrum.
- Stop the acquisition [stop].
- Halt the acquisition [halt].

Clicking the 🖌 button to switch to real time FT, turns the button

green and opens two extra buttons:

Switch between FID and spectrum.

- Real time FT settings.
- ▲ Toggle calculation of peak with at 50%, 5.5% and 1.1% height (Shown as status parameters).

Clicking the solution opens the following dialog window:

🍓 Configure realtime ft		
Set options for realtime ft.		
Window function:	em 🗾	
Phase correction mode:	mc 🔽	
Baseline correction mode:	quad 🔽	
<u>0</u> K	<u>C</u> ancel	

The acquisition information will appear in the acquisition status bar at the bottom of the TOPSPIN window, for example:

Acquisition information	Fid Flash	Sample	Time	Spooler
scan: 2 / 16 residual time:1m27s experiments: 1 / 1	-		10:49 Jul 15	running: 0 queued: 0 delaved: 0

4. When the acquisition has finished:

IS Enter *efp* to process the FID.

The processed spectrum will be displayed in the data window that was opened upon creating the dataset (see Fig. 16.15).



Figure 16.15

From here, the processed data can be analysed, printed and/or archived.

# 16.11 Shape tool

The Shape tool interface allows you to create/manipulate RF shapes and waveformat.

To start the Shape Tool interface:

IS Click Spectrometer → Shape Tool

or enter *stdisp* on the command line.

The Shape Tool window will appear (see Fig. 16.16.). This consists of a toolbar, a command line and a split pane with a data section at the right and a parameter section at the left.

If Shape Tool is opened with a dataset the current dataset will be displayed (see Fig. 16.17).

ShapeTool [1]	
🗟 🖳 🗛 🔨 m 🔹 端 🍾	1d ∰ <b>∛</b> \
Gauss Parameters 1000 Size of Shape 1.0 Truncation Level [%]	Amplitude 9 02 00 Phase 9 02 09 9 02 09 9 03 0 05 0 10 0 1

Figure 16.16

By default, a 1000 point Gauss shape is displayed with Truncation level 1.0.

The TOPSPIN menu is changed showing the additional *Shapes* and *Manipulate* menus and the adjusted *File*, *Analysis* and *Options* menus.

File Edit View Shapes Analysis Manipulate Options Window Help

Note that all functions of the interactive Shape Tool can also be performed non-interactively with the TOPSPIN command *st*. This command must entered with the appropriate arguments on the command line while the associated dataset is displayed and selected.

A full description of the interactive and non-interactive Shapetool can be found under:

Reference Click  $Help \rightarrow Manuals \rightarrow$  [Acquisition Application Manuals] Shape-tool

#### Easy definition of Shape pulses

The usage of shaped pulses for the selective excitation is a nontrivial task that couples together all parameters such as the power level, pulse length and the excited region.

TopSpin 2.1 and newer offers easy setup of selective experiments.

For usage Shape tool is typically started by the command *stdisp* on a finished 1D preparation experiment.

- **1.** Define the excitation regions (also see Fig. 16.7)
  - a) creates a new region on the display.
     The region is put in the middle of the currently visible area. By using the mouse position and width can be changed.
  - b) 🚧 deletes defined regions.

This command removes all regions. Single region can be removed using the region pop up menu.



Figure 16.17

- 2. Edit the excitation parameters
  - a) **E** opens a region editor. The region extent, the excitation type and the waveform assigned to

the region can be edited. Selection "Use same shape for all regions" button assigns the same rotation type and waveform to all regions.

<u>.</u>			
Use same Shape	e for all Regions		
Left Limit (ppm)	Right Limit (ppm)	Type of rotation	Shape
5.4886	5.2586	Excitation (lz->ly)	✓ E-Burp2 ✓
2.4758	2.1678		
			QK Apply Cancel

Figure 16.18

The setting of available waveforms depends on the selected rotation type. The following itemization explains the rotation types:

- Excitation Used for selective excitation, the magnetization rotates from Iz to horizontal plane
- Inversion Inverts the magnetization vector in the vertical plane (Iz to -Iz)
- Refocusing Inverts the magnetization in the transversal plane (ly to -ly)
- 3. Calculate the pulse and display the excitation profile (see Fig. 16.19)
  - A The resulting waveform is generated and the excitation profile is calculated.



Figure 16.19

- 4. Store the results
  - Pressing the *save* button writes the waveform on the disk an saves the necessary parameters (pulse length, power level) to the target data set. Used parameters are set in *Options 'Define Parameter Table*. The target dataset may differ from the current data (e.g. the spectrum on which Shape Tool started).

All regions and corresponding parameters (rotation type, waveform name) are stored on the disk in the directory where the acquisition parameters reside.

Following simple text format is used by the file "Region File":

```
#Topspin excitation region list
#Mon Apr 30 08:59:43 CEST 2007
#Used format:
# Left (ppm) Rigth (ppm) RotationType Waveform RotationAngle
#Field RotationAngle is not mandatory
5.4886 5.2586 0 EBurp2 93.6
2.4758 2.1678 0 EBurp2 93.6
```

This region definition is stored automatically after each change. The definition is also read automatically when starting Shape Tool.

For further information about Shape Tool and its functionalities please refer to the Shapetool Manual.

# Chapter 17 Configuration/Automation

### 17.1 NMR Superuser and NMR Administration password

During TOPSPIN installation, you are prompted to define:

 the username for the so called NMR Superuser. Under Windows this must be the name of an existing user. Under Linux it can also be a non-existing user, which is then automatically created by the installation program. After the installation, the NMR Superuser is the owner of all TOPSPIN program files. Logging in as this user allows you to remove these files, change file permissions etc. The name of the NMRSUPERUSER will be stored in the file:

```
<tshome>/conf/nmrsuperuser
```

 the NMR Administration password to be used for TOPSPIN configuration commands. This password can be freely chosen and is not connected to any user. It is asked for by TOPSPIN commands like *cf*, *expinstall* etc. The encrypted NMR Administration password is stored in the file:

```
<tshome>/conf/nmradminpassword
```

Note that the NMR Superuser login password and the NMR Administration password have different purposes and are totally independent. Changing one of them does not affect the other.

#### How to Change the NMR Administration Password

The NMR Administration password can be changed as follows

#### **Under Windows**

- 1. Login as NMR Superuser or Administrator.
- 2. Open a Command Prompt.
- 3. Enter:

<x>\perl\bin\perl <x>\prog\bin\installnmr <x> <NMRSUPERUS-ER>

where <x> in the TOPSPIN installation directory.

4. Enter the old password and new password as requested.

#### Under Linux

- 1. Login as NMR Superuser or root.
- 2. Open a Shell.
- 3. Enter:

```
<x>/prog/bin/installnmr <x> <NMRSUPERUSER>
```

where <x> in the TOPSPIN installation directory.

4. Enter the old password and new password as requested.

If you don't know the old NMR Administration password, you can still define a new one. In that case, you have to delete the file:

```
<x>\conf\nmradminpassword
```

before you run the *installnmr* script.

# **17.2 Configuration**

The main configuration steps are performed by the commands *cf* and *expinstall*. They can be started from the:

- Command line
- Options → Spectrometer tools menu

• Spectrometer  $\rightarrow$  Setup menu

However, the *Spectrometer* menu is only available after *cf* has been performed once, choosing *Installation for spectrometer*.

#### How to Perform a Default Configuration on a Datastation

A default configuration can be used on a datastation. It is <u>automatically</u> performed (no *cf* required) during the installation of TOPSPIN on a new computer, a new disk or in a new TOPSPIN installation directory. The default configuration name is *Bruker\_default\_av500* and corresponds to a Avance 500 MHz spectrometer.

For manual or interactive data processing, the automatic default configuration is sufficient. If, however, you want to use AU programs, you must execute *expinstall* once, selecting *Installation for Datastation (Default)*.

#### How to Perform a Customized Configuration on a Datastation

If you want to configure your datastation according to a spectrometer other than default, you must first copy the configuration directory:

<tshome>/conf/instr/<instrum>

from that spectrometer to the datastation. Here:

<tshome> is TOPSPIN home, the directory where TOPSPIN is installed. Note that this can be different on the spectrometer than on the datastation.

<instrum> is the configuration name.

After copying the configuration directory, you have to perform *expin-stall* as follows:

• Click Spectrometer → Setup → Experiment installation or enter expinstall on the command line

Follow the instructions on the screen. In successive dialog boxes check/select the options below and click *Next* to continue:

- Installation for Datastation (Customize)
- High Resolution Systems
- The configuration name as it was copied from your spectrometer

- The items you want to install
- Select the desired printer and paper format for the parameter sets
- The spectrometer frequency, acquisition mode and pre-scan-delay

In the last dialog box, click *Finish*. The installation of the selected items, will start now. Wait until this process has finished.

For more details on *expinstall*, please refer to the description of this command in the Acquisition Reference manual.

# 17.3 Parameter set conversion

The command *paracon* changes the basic frequency in parameter sets. This allows you to use parameter sets which were created on a spectrometer with a different frequency. It opens dialog box shown in Fig. 17.1

Here you can setup a list of available parameter sets. You can select Bruker and/or User defined parameter sets and use a match string. The matching parameter sets appear in the right part of the dialog box. To start the conversion, select one or more parameter sets and click OK.

# 17.4 Automation

#### How to Install AU Programs

To install AU programs, you have to run the command *expinstall* (see chapter 17.2).

#### How to Open the AU Program Dialog Box

To get a list of all AU programs, enter edau or:

- **1.** Click *File*  $\rightarrow$  *Run*...
- 2. Click *Execute an AU program* in the appearing dialog box.
- 3. Click OK

A dialog box showing either the Bruker defined or User defined AU programs. Fig. 17.2 shows a dialog box with two User defined AU programs.

Parameter set conversion	🔀
Deremeter set conversion	Available naramater ceto
Faranieter set conversion.	
Select parameter sets for conversion of the	PROTON
basic frequency (BF) from the list on the right.	PROTON128
Use the checkboxes to select bruker or	PROTON256
user definedparameter sets.	PROTONCONLF
Use the match field to apply wildcards	PROTONEXP
to the list of parameter sets.	PROTONLF
	PROTONLFEXP
Use of to set the basic frequency (BF).	PROTONNR
Current basic frequency: 300.15 MHz.	PROTONNREXP
Bruker defined parameter sets	PROTONNRLF
	PROTONT1
_	PROTONinfo
User defined parameter sets	
Match: PROT*	
Case insensitive match	
Select all	Select <u>n</u> one <u>C</u> ancel <u>O</u> K

Figure 17.1

🎑 AI	J Program	ns				×
<u>F</u> ile	<u>O</u> ptions	<u>H</u> elp				
my_au	1	my_au2				
(	Edit	Compile Execut	e More	ļnfo D	elete	<u>C</u> ancel

Figure 17.2 List with two User defined AU programs

Note that Bruker AU programs are only shown if the command *expin-stall* has been executed once, after the installation of TOPSPIN.

#### How to Switch to the List of User defined AU Programs

 $\mathbb{R}$  Click *Options*  $\rightarrow$  *User defined* in the AU program dialog box

#### How to Switch to the List of Bruker defined AU Programs

 $\mathbb{R}$  Click *Options*  $\rightarrow$  *Bruker defined* in the AU program dialog box

#### How to Define the AU Programs Source Directory

- 1. Click *Options* → *Manage Source Directories* in the AU program dialog box
- 2. In the field AU Programs: Add or modify AU program source directories

#### How to Create an AU Program

- **1.** Click  $File \rightarrow New$  in the AU program dialog box.
- **2.** Enter the AU program lines in the edit field of the appearing dialog box.
- 3. Click Save as...to store the AU program under a new name.
- 4. You will be prompted to compile the AU program: click OK.

Alternatively, you can enter edau <name> on the command line to create

the AU program <name>.

#### How to Edit an Existing AU Program

1. Double-click the AU program name in the AU program dialog box

or

Click the *Edit* button to edit the highlighted AU program.

- 2. Modify the AU program according to you wishes.
- **3.** Click *Save* to store the AU program under the name shown in the title bar.
- 4. You will be prompted to compile the AU program: click OK.

Alternatively, you can enter *edau* <*name>* on the command line to edit the AU program <*name>*.

#### How to Execute an AU Program

- 1. Select the AU program in the AU program dialog box.
- 2. Click the *Execute* button.

Alternatively, you can enter *<name>* or *xau <name>* on the command line to execute the AU program *<*name>.

If the AU program has not been compiled, compilation is automatically performed before the execution starts.

#### How to Delete an AU Program

- 1. Select the AU program in the AU program dialog box.
- **2.** Click *File*  $\rightarrow$  *Delete* or click the *Delete* button.

# How to Show Comments (short descriptions) in the AU Program List

To switch on/off the comments in the AU program list:

Is Click *Options*  $\rightarrow$  *Comment on/off* in the AU program dialog box.

A comment is a short description of the AU program which is also part of the AU program header.

# Chapter 18 Regulatory Compliance

TopSpin complies with the FDA 21 CFR Part 11 regulations. Please read the , accessible under  $Help \rightarrow Manuals \rightarrow$  [Good Laboratory Practice] 21 *CFR Part 11 compliance*. This chapter describes the respective functionalities provided by TOPSPIN in detail.

#### **18.1 Audit Trails**

A TOPSPIN data set consists of acquisition (= raw) data and processed data. These are stored in a directory tree with the following structure:

<dir>\data\<user>\nmr\<name>\<expno>\pdata\<procno>

The acquisition data are stored in the *expno* sub-directory and the processed data are stored in the *procno* subdirectory.

#### 18.1.1 The raw data audit trail

Each *expno* sub-directory contains a text file *audita.txt*, the audit trail of the raw data. This reflects the acquisition state of the raw data, and contains a checksum for the file itself (*audita.txt*) and one for the raw data file (*fid* or *ser*). The latter links the audit file with the raw data. By means of the checksums, any illegal manipulation of the audit file or the raw data file can be detected, using the TOPSPIN commands *audit* or *auditcheck*. Whenever

an acquisition is started, the possibly existing audit file is overwritten by a new one, belonging to the new raw data file. By default, the user is warned when the current dataset already contains raw data, thus preventing accidental overwriting (The option "Override existing fid without inquiry" is, by default, off (see *Options*  $\rightarrow$  *Preferences*  $\rightarrow$  *Acquisition*).

#### 18.1.2 The processed data audit trail

Each *procno* sub-directory contains a text file auditp.txt, the audit trail of the processed data. It reflects the processing state of the processed data and contains a checksum for the file itself (auditp.txt), and a checksum for the real processed data files (1r, 2rr, 3rrr, ...). The latter links the audit file with the processed data. By means of the checksums, any illegal manipulation of the audit file or the processed data file can be detected, using the TOPSPIN commands *audit* or *auditcheck*. Whenever a processing command is performed, the current audit file is updated with this command and its associated parameters. When processing starts from scratch (from a raw data file), the existing audit file is overwritten. As such, the processed data can always be regenerated from raw data by applying the commands and parameters listed in the audit trail.

If the laboratory management does not allow data files or audit trails to be deleted, a respective saving procedure must be established. For this purpose, TOPSPIN provides data copying commands, which may be called in a user defined macro or AU program, before a new acquisition or processing starts.

#### 18.1.3 Viewing audit trails

Since audit trails are regular ASCII text files, they can be viewed or printed with any text editor, outside of TOPSPIN. Within TOPSPIN, you can use the command *audit* for this purpose. This opens the dialog box show in Fig. 18.1.



Figure 18.1

The first two entries allow you to view the audit trail files. The third entry performs an audit trail check, i.e. a data consistency check. If both raw and processed data are consistent, you will get the message shown in Fig. 18.2.



Figure 18.2

If the data have been manipulated outside of TOPSPIN, e.g. with third party software, the checksum will be inconsistent. Fig. 18.3 shows the message

for inconsistent processed data.

auditcheck 🖉		×
Ĩ	audit file for acquisition: OK processing: OK raw data: checksum OK proc data: Invalid data checksum	
	<u>C</u> lose <u>D</u> etails	

Figure 18.3

The fourth and fifth entry in Fig. 18.1 allow you to add a comment to the raw or processed audit trail files, respectively.

#### 18.1.4 Audit trail contents

The contents of an audit file is grouped in the following way:

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

These entries have the following meaning:

#### NUMBER

Running number of an entry, starting with 1.

#### WHEN

Date of the entry, e.g. <2004-03-30 10:55:36.171 +0200>, where the last value represents the offset in hours to Universal Time (UTC).

#### WHO

The user logged in, at the time the entry was generated. It has one of the two forms: <user1> or <user1/user2>. <user1> is always the user who is logged into the operating system (Windows or Linux user), and who started TOPSPIN. <user2> only appears, if the NMR administrator has setup an internal TOPSPIN user administration, and the op-

tion *Enforce "login" for working with* TOPSPIN in the User Administration dialog is enabled (see below, command *uadmin*). In this case <user2> is the current internal TOPSPIN user.

#### WHERE

The network name of the current computer, e.g. <EOS2>.

#### PROCESS

The TOPSPIN process (module) which performed the acquisition or processing.

#### WHAT

The type of acquisition or data manipulation performed.

Note that if only the entries NUMBER, WHEN, WHO, WHERE, WHAT be present, then the audit trail was created by TOPSPIN 1.3 or older.

### 18.1.5 Adding a comment to an audit trail

Audit trail entries are normally generated automatically by a respective acquisition or processing command. However, a user can also add a comment manually, using the *audit* command. This will generate a regular entry, the comment will appear under the WHAT section and is preceded by the tag "*user comment.*".

You may also add a comment to the raw data or processed data audit trail from an AU program, using the macros AUDITCOMMENTA(comment) or AUDITCOMMENTP(comment), respectively. Alternatively, you can store the comment in a file auditc.txt in the *expno* or *procno* directory, and use the macros GDCHECK\_RAW or GDCHECK

## 18.1.6 Auditing user-defined data manipulations

When manipulating a data file with a user-defined algorithm, e.g. by means of an AU program or external program, the data file and the respective audit trail become inconsistent (detectable with the command *auditch-eck*), and the data set is no longer compatible with regulations. In order to solve this problem, TOPSPIN provides a function *CheckSumFile*, which adds the correct data checksum to the audit trails, and a function *AuditAppend* for additional text (an alternative to the comment function described above). These functions are described in the AU manual which can be opened by clicking  $Help \rightarrow Manuals \rightarrow$  [Programming Manuals] AU programming.

#### 18.1.7 Audit Trails in JCAMP-DX and ZIP archives

The TOPSPIN commands *tojdx* and *tozip* allow you to store a data set into a single file in the internationally standardized ASCII-type JCAMP-DX format or in the well-known ZIP format, respectively. Both storage formats retain the audit trails. When unpacking such files with *fromjdx* or *fromzip*, respectively, the original data set in standard Bruker format is restored. The command *auditcheck* may be used to check whether the data are still consistent. If, for example, JCAMP-DX or ZIP file have been manipulated, the data might not be consistent.

## **18.2 Electronic Signatures**

#### 18.2.1 Signing a data set

The command *esign* adds an electronic signature to the raw data or to the processed data of a data set. It opens a dialog where you can select the data component to be signed, the signature meaning and, optionally, add a comment. *esign* requires that the NMR administrator has set up a list of users who are allowed to sign a data set, along with definitions of signature *meanings* (e.g. review, approval). See below for details, command *uad-min*.

실 esign	$\overline{\mathbf{X}}$		
Add Electronic Signature To Data Set: exam1d_13C 1 1 C:\bio guest			
Data component to be signed =	Raw & Processed Data 🛛 👻		
Select Signature Meaning =	all 💌		
Comment =	Your comment		
	Sign now Cancel		

Figure 18.4

#### 18.2.2 Structure of a signature

In TOPSPIN, an electronic signature is realized as a special entry appended to the audit trail of the raw or processed data. It is therefore linked with the data and protected against manipulations just like any other audit trail entry. Signatures can be viewed with the command *audit*. An electronic signature consists of the following items:

#### USER ID

The ID of the user logged in at the time *esign* was executed. This is either the user who was logged into the operating system (Windows or Linux user), and who started TOPSPIN, or the TOPSPIN internal user. Which of these two modes is applied depends on how the NMR administrator configured TOPSPIN: If the option *Enforce "login" for working with* TOPSPIN is disabled (see below, command *uadmin*), the first mode is active, otherwise the second.

What is the difference between the modes?

 In the first case, the System User (= Windows or Linux user) who started TOPSPIN signs the data set. Prior to signing, *esign* requests this user's password, which is administrated by the operating system (OS). No internal TOPSPIN user management plays a role. *Advantage:* This mode is entirely OS compliant. *Disadvantages:* a) TOPSPIN termination/restart is required when a different user wants to sign data (alternatively several licenses would admit simultaneous TOPSPIN sessions). b) All TOPSPIN users must have an OS login.

 In the second case, any TOPSPIN internal user who is enabled by the NMR administrator (with uadmin) may sign. Advantage: Convenient and easy usage. Disadvantage: TOPSPIN internal user management is required (internal users and their passwords).

#### **USER NAME**

The complete name of the signer as specified by the NMR administrator during user administration (command *uadmin*).

#### SIGNATURE MEANING

The meaning of a signature, e.g. *Review* or *Approval*. A user may only select meanings that were assigned to him by the NMR administrator during user administration.

#### SIGNATURE COMMENT

Any text.

#### 18.2.3 Displaying the electronic signature in the data window

The electronic signature can be displayed in the data window by setting the corresponding display component. To do that:

- 1. Right-click in the data window and choose *Display Properties*... [.dopt].
- 2. Check *Electronic Signature* in the appearing dialog box and click OK.

The electronic signature will appear, at the upper left corner, below the title.

#### 18.2.4 Plotting the electronic signature

When plotting a dataset using TOPSPIN's plot editor (commands *plot* and *autoplot*), an electronic signature is automatically plotted (unless this feature is disabled), if the last entry of the audit trail of the data to be plot-

ted is an electronic signature. This ensures that after signing no more data manipulations have been performed.

#### 18.2.5 Multiple signatures

The command *esign* may be applied several times to a data set, for instance if two persons (say an operator and an administrator) must sign in accordance with company regulations.

#### 18.2.6 Validity and security of signatures

TOPSPIN electronic signatures of data sets must not be confused with digital signatures as defined in applicable law. Digital signature laws are usually country dependent. They require the administration of passwords (more general: electronic keys which authenticate the owner of the document) to be performed by authorized trust centers. In contrast, TOPSPIN uses OS-encrypted passwords or internal user passwords encrypted by TOPSPIN itself.

For this reason, a Standard Operating Procedure (SOP) of the company or institution that wishes to apply TOPSPIN signatures must exist defining the role of TOPSPIN signatures.

For this reason, companies and institutions that want to apply TOPSPIN signatures must have a Standard Operating Procedure (SOP), which defines the role of these signatures.

Note that digital signatures complying with respective laws requires special software, and the involvement of trust centers. Bruker refers to the respective commercial software for this purpose.

# **18.3 Password Controlled Login Identification**

#### 18.3.1 Definition of an internal user

In TOPSPIN, the NMR administrator may set up a list of *internal* TOPSPIN *users*. An internal user need not have a user account for the operating system and is only known to TOPSPIN. Such a user is characterized by the following items:

USER ID

A short unique string of characters identifying a user (e.g. guest)

#### USER NAME

A long string of characters, usually the full name of a user (e.g. Franz J. Maier)

#### SIGNATURE MEANINGS

A list of items separated by comma (e.g. Approval, Review), an empty string or the special string "-NONE-". In the latter two cases, this user cannot electronically sign data. In all other cases, the user is allowed to sign. The *esign* dialog allows the user to select one of the items to specify the meaning of the signature.

#### PASSWORD

A password for this user, required for using TOPSPIN and for applying an electronic signature.

#### 18.3.2 How to set up internal users

In order to define or modify the list of internal users:

enter the command uadmin

or

#### $\texttt{IS} Click Options \rightarrow Preferences \rightarrow Administration items$

Click the *Change* button to the right of the object *Setup users for Top-Spin-internal login/logoff and esign.* 

You will be prompted for the NMR administrator password. A dialog will appear.

🦥 User Administration - uadmin 🛛 🔀				
Enforce "I	ogin" for working with	TopSpin		
User ID	User Name	Allowed Signature Meanings		
carol	Carol Smith	-NONE-		
diane	Diane Lopez	all		
james	James Evans	review		
larry	Larry Hill	approval		
Add User Change Meanings <u>R</u> emove User Passwd Length				
Save Save+Close Help Cancel				



where you can add, remove and/or modify users

#### 18.3.3 How to change the internal user password

To change the password of the internal user:

real enter *chpwd* on the command line

or

 $\texttt{IS} Click \textit{Options} \rightarrow \textit{Administration} \rightarrow \textit{Change internal user password}$ 

and enter the new password twice, as requested.

#### 18.3.4 Login/Logoff

The *uadmin* command allows the administrator to make a TOPSPIN internal user mandatory. To do that, enable *Enforce "login" for working with Top-Spin* at the top of the dialog, click *Save+Close* and restart TOPSPIN. After the restart, a login prompt will be displayed and TOPSPIN cannot be used with-

out entering an internal user and his password.

To log off the internal user:

real enter logoff on the command line

or

 $\square Click Options \rightarrow Administration \rightarrow Log off$ 

and enter the user name and password as requested.

If TOPSPIN internal user is not mandatory, i.e. the entry *Enforce "login" for working with TopSpin* is disabled, you are not prompted to login after TOP-SPIN startup. You can, however, still login as internal user with the command *login*.

#### 18.3.5 Locking TOPSPIN's Graphical User Interface

TOPSPIN can be blocked, such that it does no longer accept user input via mouse or keyboard. To do that:

regional enter lockgui on the command line

or

 $\mathbb{R}$  Click Options  $\rightarrow$  Administration  $\rightarrow$  Lock TopSpin user interface

A window will appear (see Fig. 18.6) indicating the locked status and offer-

ing buttons to unlock.

TopSpin locked by user: carol at Wed Jul 13 16:53:52 BST 2005. Please press a button to unlock.
'carol' to unlock
NMR administrator to unlock

Figure 18.6

Only the current user or the NMR Administrator can unlock the user interface. While TOPSPIN is locked, all background activity such as data acquisition and processing continue.

For safety reasons TOPSPIN can be forced to execute *lockgui* automatically when no commands from the command line, menus or tool buttons have been entered for a certain period of time (for instance because the current user has left). In order to enable automatic locking

- **1.** Click Options  $\rightarrow$  Preferences [set]
- 2. Click Administration Items in the left part of the dialog box.
- **3.** Click the *Change* button to the right of the object *Automatic locking* of *TopSpin when idle time exceeded*.
- **4.** Enter the maximum allowed idle time (in minutes) in the dialog and click *OK*.

# Chapter 19 Remote Control

#### **19.1 Remote control**

TOPSPIN supports remote control. This means, for example, that you can control your spectrometer from any PC in the laboratory network or, over the internet, from your PC at home. Using your local TOPSPIN interface, you have access to the remote data directories and remotely running TOPSPIN commands. Furthermore, in TOPSPIN 1.3 and newer, ICON-NMR is web-enabled which means it can be controlled from any web browser which is networked to the spectrometer. Note that remote access is operating system independent.

# 19.2 How to Establish a Remote Connection from your PC

In order to establish a remote connection, you have to perform a few steps, both on the local and on the remote system. Note that the <u>local system</u> is the computer you are sitting at, and the <u>remote system</u> is the computer you are connecting to. Up to 5 local systems can connect to TOPSPIN on a remote system.

#### 19.2.1 Setup the remote system

The remote system must be enabled for remote access and, furthermore, individual data directories must be exported.

#### Enable the system for network access

- 1. Log in on the remote system
- 2. Start TOPSPIN
- **3.** Click *Options*  $\rightarrow$  *Preferences* [set]
- 4. Click *Miscellaneous* in the left part of the dialog box.
- **5.** Click the *Change* button to the right of the object *Configure remote access*.
- 6. Enter the Administration password as requested
- 7. In the appearing dialog box (see Fig. 19.1):
  - a) Click Remote Access Enable
  - b) Click *Add* and enter the data directories that you want to export for remote access, e.g.: C:\bio and click *OK*.
  - c) Click OK to close the dialog.

Configure remote access				
Enable or disable remote access to TopSpin.				
Select "Remote access enabled" to allow remote access to this TopSpin installation, select "Remote access disabled" to prevent remote access (default).				
Warning: You must restart TopSpin to activate the modification! Any previous modifications in the file omniorb.conf will be lost!				
Directories must be exported in order to enable remote access to these Use \$INSTDIR for the data directory in the TopSpin home directory.	directories.			
Remote access				
Remote access enabled				
◯ Remote access disabled				
Exported directories				
\$INSTDIR	Add			
C: Voio	Edit			
	Delete			
<u>ok</u> (	<u>C</u> ancel			



- 8. Click *OK* to save and close the preferences dialog.
- 9. Restart TOPSPIN.

A list of exported directories is stored the file:

<tshome>/prog/server/export.conf

Now a running TOPSPIN on this system can be accessed from any computer in the network.

#### Identify the port number

To identify the TCP/IP port number used by TOPSPIN:

- 1. Start TOPSPIN
- 2. Enter hist
- 3. Look for the line

To connect to this TOPSPIN .... use host=<xxxx>., port=<yyyy>

in the upper part of the dialog window. The number at the end of this line (<yyyy) is the desired port number, which must be used to set up the local system (see chapter 19.2.2). By default, this is port number 5500. Only if this port is already used by a program other than TOPSPIN, a different port is used.

#### **Export data directories**

- 1. Log in on the remote system as Administrator (windows) or root (Linux).
- 2. Edit the file <tshome>/prog/server/export.conf

By default, this file contains the lines:

EXPORTMODE=ALL \$XWINNMRHOME

This first entry should be left as it is. The second entry exports the data directory <tshome>/data for remote access. By default, that this is the directory that contains the Bruker example datasets.

**3.** Add the data directories that you want to export for remote access, e.g.:

```
C:\bio
D:\nmr
```

for the directories C:\bio\data and D:\nmr\data, respectively. Please use a separate line for each entry!

4. Save the file export.conf and close the editor.

#### 19.2.2 Setup the local system

#### Define the remote system

- 1. Log in on the local system
- 2. Start TOPSPIN
- **3.** Click Options  $\rightarrow$  Preferences [set].
- 4. Click *Miscellaneous* in the left part of the dialog box.
- 5. Click the *Change* button at the entry *Setup remote systems*. In the appearing dialog (see Fig. 19.2),

Server ID	leda
Host name or address	leda software.bruker.de
TCP/IP port number	5500
Ad	d <u>C</u> ancel <u>R</u> emove

Figure 19.2

enter the following information:

- Server ID: an arbitrary name for the remote system
- Hostname or address: the hostname or IP address of the remote host
- TCP/IP port number of the remote TOPSPIN as identified in chapter 19.2.1.
- 6. Click *Add* to add the remote host.
- 7. Click *OK* to save the changes and close the dialog.

Note that you can define multiple remote systems, for example different spectrometers in your laboratory.

#### Connect to the remote system

- 1. Click Options → Remote connection...
- 2. Select the desired *Remote system* from the appearing dialog box and click *OK*.



Figure 19.3

Now you are prompted for a user and password (**both case sensitive**) on the remote computer.

🍓 Remote I	ogin X	
Please enter the name and password for the TOPSPIN session on the remote computer:		
(This connection is secure.)		
User:	guest	
Password:	*****	
	<u>O</u> K <u>C</u> ancel	

Figure 19.4

The TOPSPIN browser will show the exported data directory trees of the remote system. You are now ready to acquire, process or analyse remote data.

#### 19.2.3 Setup the firewall

A remote system in a network can be protected by a firewall. Any firewall between the local and remote TOPSPIN must be configured for TOPSPIN remote access.

If the remote PC is running under Windows XP with Service Pack 2, the Windows Firewall is, by default, installed and running. Consider the following possibilities:

#### Firewall on PC with Windows XP-SP2, Topspin installed

If TOPSPIN is installed, the firewall is probably configured for TOPSPIN remote access <sup>1</sup>. If it is not or you are not sure, you can configure it as follows:

- **1.** Click Start  $\rightarrow$  Programs  $\rightarrow$  Bruker TOPSPIN  $\rightarrow$  TOPSPIN 2.0  $\rightarrow$  Bruker Utilities
- 2. Click Miscellaneous
- 3. Double click Command Prompt
- 4. In the Command Prompt window, enter:

cd prog\bin\utilities\Miscellaneous setfirewall.cmd auto

#### Firewall on PC with Windows XP-SP2, no Topspin installed

Configure the firewall as described in the Installation Guide for Windows XP.

On all other systems, the firewall must be configured manually by the network administrator. To do that view the file:

<tshome>/prog/server/corba.conf

and open the ports specified here, incremented by 50.

For more information, please refer to the installation guides for Windows or Linux or inspect the contents of the file corba.conf.

Note that the firewall must be configured for TOPSPIN:

- spectrometer control
- remote access

<sup>1.</sup> During TOPSPIN installation, you can choose to automatically configure the firewall or not. PC's delivered by Bruker Germany, always have the firewall configured for TOP-SPIN.

TOPSPIN can be used for processing/analysis on a local datastation, even if it is not registered on the firewall. However, you will get a few Security Alert messages during startup.

## 19.3 How to Make a Remote Connection without a Local License

TOPSPIN requires a license to operate on your local computer. However, you can make a remote connection without a local license.

To do this, you have to start TOPSPIN as follows:

- 1. Open a Windows Command Prompt or Linux Shell.
- 2. Go to the TOPSPIN installation directory.
- 3. Enter topspin -client
- **4.** TOPSPIN will start up and show an empty data field but no browser. Before startup you will get the error message: "*The program failed to communicate with local* ....". Just click *or* to continue.
- 5. Click *Options*  $\rightarrow$  *Remote connection...* and establish a remote connection as described in chapter 19.2.

Note that without a local license:

- TOPSPIN on the remote system must run with a licence.
- Local data cannot be accessed.

## **19.4 Security of Remote Connections**

All data transferred during a remote control session is, by default, encrypted. This ensures that nobody can see data or commands by observing and recording your network traffic. TOPSPIN uses the Secure Socket Layer (SSL) technology for encryption, which is also used for secure web sites. SSL needs digital certificates on both sides of a connection to achieve a valid authentication. After a TOPSPIN installation, default certificate files are provided to secured connections. There is a chance, however small, such connections are attacked by a malicious person who also has the same default certificate files. If, for this reason, you want to create your own set of certificate files, you can do this by executing a script that is installed in <tshome>/prog/server/make\_new\_certificates and follow the instructions given there. To start a remote connection, the new certificate files must be installed on BOTH machines.

## 19.5 How to Access ICON-NMR from a Remote Web Browser

In TOPSPIN 1.3 and newer, ICON-NMR is web-enabled. The standard Bruker Automation Software now provides a built-in website which can be activated to allow remote access to ICON-NMR from any web browser which is networked to the spectrometer workstation. Experiments may be cancelled/submitted, the run may be paused or halted and spectra in PDF format are available from the browser window. No added software apart from ICON-NMR is required and configuration is performed via the standard ICON-NMR Configuration window. For security a SSL/HTTPS connection is supported. Pocket PC Internet Explorer is also supported for full spectrometer control via Windows Mobile 2003 (TM) or equivalent. PDF files of spectra may also be viewed on this platform making the mobile pocket spectrometer a reality.

The configuration of ICON-NMR web interface is described in the ICON-NMR manual, accessible  $Help \rightarrow Manuals \rightarrow$  [Automation and Plotting] *Icon-Nmr Automation Interface*. Note that ICON-NMR remote control does not require and is fully independent of TOPSPIN remote control.

# Chapter 20 User Preferences

## **20.1 User Preferences**

TOPSPIN can be tailored to your preference in many respects. This ranges from startup options to spectrum objects, menu settings, remote connections etc. Every standard user can create his/her own set of preferences.

To set user preferences:

• Click Options → Preferences [set]

A dialog box will appear with, at the left side, the categories that can be tai-

#### lored (see Fig. 20.1)

🔄 User preferences		
Administration items	Administration items	<b>^</b>
Spectrum	Auto-open last used dataset when restarting TopSpin	
Contour plot	Show TopSpin data examples directory in data browser	
Spectrum title Spectrum cursor	Setup users for TopSpin-internal login/logoff and esign	Change
Spectrum parameters	Automatic termination of TopSpin when idle time exceeded	Change
Printer Fonts / Dialogs / Icons	Automatic locking of TopSpin when idle time exceeded	Change
Window settings	Auto-spooling	
Miscellaneous	Spectrum	
Directory path names	Tabbed pane layout	Change
Acquisition status bar	Change spectral window color scheme	Change
BSMS display	Save spectral window colors as a new color scheme	Save as
Lock display	Background color	Change
	Color of 1st 1D spectrum	Change



Click the cathegory of which you want to view/change certain objects. It will become highlighted and the corresponding objects will be displayed at the right part of the dialog box. For example, if you click *Spectrum*, the spectrum objects will appear at the top of the dialog box. The rest of this paragraph will describe some examples of setting various user preferences.

#### 20.1.1 Define User Preferences Location for all Users

User Preferences are, by default, stored in the current users home directory:

<userhome>/.topspin-<hostname>

During the first TOPSPIN session, files with default settings are created there. They can then be modified with the *set* command and used in later sessions.

You can, however, also store user preferences at one central location,

which are then used by all users. This location can even be a remote drive allowing you to use the same preferences on all computers in the network.

To do that:

- 1. Make a backup copy of the file <tshome>/javaenv.cmd.
- 2. Open the file <tshome>/javaenv.cmd using a text editor.
- Locate the line "set SYSTEM\_PROPS=-DXWIN-NMRHOME="%XWINNMRHOME%" -DCOMPUTERNAME=%COM-PUTE......." near the beginning of the file.
- Append a white space character and then:
   -DPROPDIR=<dir>
   to the end of this line, where <dir> is the definition of the storage directory, consisting of one or more parts (see below)
- **5.** Close the editor.

The definition of the storage directory for User Preferences can take three forms:

-DPROPDIR=<mydir>

Stores the user properties in <mydir>/prop

```
Example: -DPROPDIR="/x y z"<sup>1</sup>
```

```
-DPROPDIR=<mydir> USER<sup>2</sup>
```

Stores the user properties in <mydir>/<login id>/prop, where <login id> is the id under which the user is logged into the operating system

Example: -DPROPDIR="/x y z USER" 1

-DPROPDIR=CURDIR

Stores the user properties in <tshome>/prog/curdir/<login id>/prop, where <login id> is the id under which the user logged into the operating system

Please note that the specified directory must writable for all TOPSPIN users.

<sup>1.</sup> The double quotes are only required if the directory contains white spaces

<sup>2.</sup> Specify exactly 1 space between the pathname and the string USER

#### 20.1.2 TOPSPIN Startup Actions

## How to Open the Last Used Dataset on Startup

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Check, under Administration items, the option :

Auto-open last used data set

#### How to Define the Startup Actions

TOPSPIN allows you to define any commands to be executed automatically after startup. To do that:

- **1.** Click *Options* → *Administration* → *Edit Startup File*.
- 2. Enter the desired startup command(s), in the appearing editor, for example:

re exam1d\_13C 1 1 c:\\bio guest efp apk abs

The above lines would cause TOPSPIN to display the dataset:

```
C:/bio/data/guest/nmr/exam1d_13C/1/pdata/1
```

and execute the command efp, apk and abs on it.

Note that you can use a single forward slash (/) or a double backslash (\\) as path separator.

Note that in TOPSPIN 2.1 and newer, the file <code>autostart.mac</code> is a regular Topspin macro. In older versions, however, the file <code>autostart.prop</code> was used with a different format.

## How to Define Auto-Termination after Idle Time

TOPSPIN can be configured to be terminated after a user specified idle time. To do that:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click the Change button to the right of the object

Automatic termination of TOPSPIN when idle time has exceeded

enter the NMR Administration password as requested and enter the number of minutes of allowed idle time.

- 3. Click *OK* to close the dialog, click *OK* to close the Preferences dialog.
- 4. Restart TOPSPIN to activate the change.

If the user does not execute any commands (from the command line, menu or tool buttons), a dialog will appear with an *OK* button (to terminate immediately) and/or *Cancel* button (to continue).

Automatic termination frees the license used by this TOPSPIN instance for other users. This solves the problem of users leaving TOPSPIN open and blocking a floating license although they do not currently use it.

## How to Define Auto-Locking after Idle Time

TOPSPIN can be configured to lock the interface after a user specified idle time. To do that:

- 1. Click Options  $\rightarrow$  Preferences [set].
- 2. Click the Change button to the right of the object

Automatic locking of TOPSPIN when idle time has exceeded

enter the NMR Administration password as requested and enter the number of minutes of allowed idle time.

3. Click *OK* to close the dialog, click *OK* to close the Preferences dialog.

If the user does not any commands (from the command line, menu or tool

buttons), the TOPSPIN interface will be locked (see Fig. 20.2).

TopSpin locked by user: carol at Wed Jul 13 16:53:52 BST 2005. Please press a button to unlock.
'carol' to unlock
NMR administrator to unlock

Figure 20.2

## How to Change the Preferred Editor

You can choose your preferred editor as it is used by commands like *edau*, *edpu1*, *edcpd* etc. To do that:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click *Miscellaneous* in the left part of the dialog box.
- **3.** Click the *Change* button to the right of the object *Preferred text editor*

enter the desired Editor and its path. For example for Wordpad under Windows 2000/XP, this would look like:

🔄 Editor definition	$\sim$
Please specify an ID name and the editor's path (The ID is an arbitray name).	
Editor ID =	Wordpad
Full path =	C:\Program Files\Windows NT\Accessories\word¢
	<u>R</u> emove <u>S</u> ave <u>C</u> ancel

4. Click *Save* to save the changes.

If no editor is specified here, the TOPSPIN internal editor is used. It the file being edited is read-only, the TOPSPIN internal viewer is used.

## How to Configure the Tab Bar

The default Tab bar at the top of the data window consist of Tabs to switch between various dataset objects like *Spectrum*, *Parameters*, *Title*, etc. You can, however, configure the Tab bar to contain Tabs for interactive data manipulation like *phase correction*, *integration* etc. These Tabs have the same function as the corresponding buttons in the upper tool bar (see chapter 2 and 14) but are easier to access. You can configure the Tab bar as follows:

- **1.** Click *Options*  $\rightarrow$  *Preferences*
- 2. Click Spectrum in the left part of the User preferences box.
- 3. Click the *Change* button to the right of the object *Tabbed pane layout*.
- 4. Check the desired Tabs, uncheck the others.
- 5. Click OK

#### How to Configure the Right-click Menu Function

Right-clicking a pull-down or popup menu, can perform various actions. This can be configured as follows:

1. Right-click an empty part of the menubar and choose Define Right-

Click Action from the popup menu.

Marka 🛛 🔛
Define right-click action on a menu item No action when right button clicked Display help (if available) Execute menu item Display command assigned to menu item

Figure 20.3

- 2. In the appearing dialog (see Fig. 20.3), select the desired action.
- 3. Click OK

## 20.1.3 Changing Colors

## How to Change Colors of Data Objects on the Screen

The color of various objects in a data window on the screen, like 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> spectrum, axis, parameters etc. can be changed. To set these colors:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Spectrum in the left part of the User preferences box.
- **3.** Click the *Change* button to the right of the object you want to change e.g.:



- 4. Select the desired color in the appearing dialog box and click OK
- 5. Click Apply

## How to Change Colors of Data Objects on the Printer

The color of data objects on the printer is independent from the color of the

corresponding object on the screen. To set print colors:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click *Printer* in the left part of the *User Preferences* box.
- **3.** Click the *Change* button to the right of the object you want to change, e.g.:



- 4. Select the desired color in the appearing dialog box and click OK
- 5. Click Apply

## How to Change Colors of the Lock Display

The colors of lock display objects can be changed as follows:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Lock display in the left part of the User preferences box.
- **3.** Click the *Change* button to the right of the object you want to change, e.g.:



- 4. Select the desired color in the appearing dialog box and click OK
- 5. Click Apply

#### How to Create a New Data Window Color Scheme

To create a new data window color scheme:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- **2.** Change any color of the objects *Spectrum*, *Spectrum title*, *Spectrum cursor or Spectrum parameters*.
- 3. Click Apply
- 4. Click Spectrum in the left part of the User preferences box.
- 5. Click the button Save as... to the right of the object:

Save spectral window colors as a new color scheme

and enter a new name in the appearing dialog box.

6. Click OK

#### How to Read a Different Data Window Color Scheme

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Spectrum in the left part of the User preferences box.
- 3. Click in the list box to the right of the object:

Change spectral window color scheme

and select an element from the appearing list.

4. Click OK

TOPSPIN is delivered wit two colors schemes:

- *light* (default): a white background with black axes
- *dark*: a dark blue background with a white axes

## How to Change Peak and Integral table Colour/Spacings

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click *Miscellaneous* in the left part of the *User preferences* box.
- 3. Click in the list box to the right of the object:

Table colors (see Fig. 20.4)

for simple tables like peaks, solvents, nuclei tables

Tree table colors

for nested lists like the integral table.

🛃 Table properties 🛛 🔀		
Colours Spacings		
▼ Table header		
Column header foreground		
Column header background		
▶ Foreground		
▶ Background		
► Selection		
Restore defaults		
OK <u>C</u> ancel <u>Apply</u>		

Figure 20.4

Set the desired colours and spacings.

4. Click OK

Note that table colours and spacings can also be change from a table. To do that, right-click any table entry and choose *Table properties*...

## 20.1.4 Changing Lines

## How to Create Thick Lines on the Screen

To create thick (double width) lines for high resolution display or screendumps:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click *Spectrum* in the left part of the dialog box.
- 3. Enable the entry Use thick lines
- 4. Click OK

## How to Create Thick Lines on the Printer

To create thick (double width) lines for high resolution display or screendumps:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click *Printer* in the left part of the dialog box.
- 3. Enable the entry Use thick lines
- 4. Click OK

## 20.1.5 Changing Fonts

## How to Change All Fonts of the Topspin Interface

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- **3.** Set the entry *Change size fonts listed above by .... points* You can enter a positive or negative number.

Fig. 20.5 shows an example of increasing the font sizes by 4 points.

Fonts / Dialogs / Icons		
Menu font	Dialog.plain / Plain / 16	Change
Dialog window font	Dialog.plain / Plain / 12	Change
Command line font	Dialog.plain / Plain / 16	Change
Status line font	Dialog.plain / Plain / 16	Change
Printer font	DialogInput.plain / Plain / 10	Change
Change size of fonts listed above by points		4

#### Figure 20.5

4. Click OK to store the new value.

Fonts / Dialogs / Icons		
Menu font	Dialog.plain / Plain / 20	Change
Dialog window font	Dialog.plain / Plain / 16	Change
Command line font	Dialog.plain / Plain / 20	Change
Status line font	Dialog.plain / Plain / 20	Change
Printer font	DialogInput.plain / Plain / 10	Change
Change size of fonts listed above by	points	0

#### Figure 20.6

Fig. 20.6 shows the same part of the Preferences dialog box dialog box after the change of fonts. Note that:

- The value all four font entries has been increased by 4.
- The font of the dialog box itself is larger.
- The change size has been reset to 0.

#### How to Change the Font of the TOPSPIN menu

To change the font of the TOPSPIN menu:

**1.** Click *Options*  $\rightarrow$  *Preferences* [set].

- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- 3. Click the *Change* button to the right of the *Menu font* object:

Menu font dialog / Plain / 18 Change

- 4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
- 5. Click OK to store the new font.
- 6. Click Apply

The default menu font is *Dialog/Plain/18* and looks like this:

## File Edit View Spectrometer Processing

After changing the font to, for instance, to *Serif/Italic/18*, the menu looks like this:

<u>F</u>ile <u>E</u>dit <u>V</u>iew <u>S</u>pectrometer <u>P</u>rocessing

A change in menu font also affects all sub-menus and popup menus.

#### How to Change the Font of the Tab bar

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- 3. Click the *Change* button to the right of the *Dialog window font* object.
- 4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
- 5. Click OK to store the new font.
- 6. Click Apply

Fig. 20.7 and Fig. 20.8 shows a Tab bar with font size 10 and 14 respectively.

Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Fid Figure 20.7 Tab bar with font size 10 Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Struct Figure 20.8 Tab bar with font size 14

#### How to Change the Font of Dialog Boxes

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- 3. Click the *Change* button to the right of the *Dialog window font* object.
- 4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
- 5. Click OK to store the new font.
- 6. Click Apply

Fig. 20.9 shows an example of a dialog box with the font *Times New Roman Italic* 

🥌 re	
Options ⊙ Display data in same windo ◯ Display data in new windo	w W
NAME =	exam1d_1H
EXPNO =	1
PROCNO =	1
DIR =	C: Voio
USER =	guest
QK Cancel Browse Find Help	

Figure 20.9

## How to Change the Font of the Browser

To change the font of the browser:

**1.** Click *Options*  $\rightarrow$  *Preferences* [set].

- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- 3. Click the *Change* button to the right of the *Dialog window font* object.
- 4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
- 5. Click OK to store the new font.
- 6. Click Apply

TOPSPIN must be restarted for this change to become effective. Note that this change will affect all dialog boxes.

## How to Change the Font of the Command Line

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- 3. Click the *Change* button to the right of the *Command line font* object.
- 4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
- 5. Click OK to store the new font.
- 6. Click Apply

## How to Change the Font of the Status Line

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- 3. Click the *Change* button to the right of the *Status line font* object.
- 4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
- 5. Click OK to store the new font.
- 6. Click Apply

## 20.1.6 Changing Acquisition settings

## How to Auto-Archive existing expnos

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click Acquisition in the left part of the dialog box.
- **3.** Click the Change button to the right of the item *Configure Accounting & Data Archiving after 'zg'* (see Fig. 20.10).
- **4.** In the appearing dialog (see Fig. 20.11), configure archiving as

described in the dialog.

5. Click OK.

Acquisition	
Overwrite existing FID without inquiry (ZG safety off)	
Auto open acquisition window after 'zg'	<b>V</b>
Configure accounting & data archiving after 'zg'	Change



🔄 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 following directory, one file per day: " <topspin homedir="">/prog/curdir/acqhistory"</topspin>		
Auto-archive after 'zg' =	no 🗸	
Archiving directory =	C:\Documents and Settings\Jos v	
EXPNO offset =	1000	
Write accounting info after 'zg' =	no 💌	
Browse OK Cancel		

Figure 20.11

## 20.2 Command Line Preferences

## How to Resize the Command Line

By default, the TOPSPIN command line shows one command, the com-

mand that is currently entered, e.g.:

apk

However, you can resize the command line to show the currently entered command plus the last and second last command, e.g.:



You can toggle between the two different command line sizes as follows:

or

• Right-click in the command line and click Resize command line

#### How to Set the Minimum and Maximum Command Line Size

By default, the size of the command line can be toggled between 1 and 3. You can, however, change this minimum and maximum value, respectively. To do that:

- **1.** Click *Options*  $\rightarrow$  *Preferences* [set].
- 2. Click *Fonts/Dialogs/Icons* in the left part of the dialog box.
- **3.** Specify the *Minimum visible command lines* (> 0).
- **4.** Specify the *Maximum visible command lines* ( $\geq$  *Minimum visible*).
- 5. Click Apply

## 20.3 Disabling/Enabling Toolbar Buttons, Menus and Commands

#### How to Hide the Upper and Lower Toolbars

Right-click in an empty area of one of the toolbars and choose:

Hide the toolbars

from the appearing popup menu (see Fig. 20.12).

To restore the toolbars:

IS press the keys SHIFT+ESC

Make Button Invisible... Make Button Inactive Reactivate All Invisible/Inactive Buttons Add User-Defined Button... Remove This User-Defined Button... Change Icon Size... Change Toolbar Offset... Hide Toolbars (type SHIFT ESC to reset) Print Associated Command

Figure 20.12

## How to Hide the Menubar

Right-click in an empty area of the Menubar and choose:

#### Hide the menubar

from the appearing popup menu.

To restore the menubar:

press the keys SHIFT+ESC

#### How to Disable/Remove Toolbar Buttons

Buttons of the upper or lower toolbar can be disabled or removed as follows:

- 1. Right-click a toolbar button.
- 2. Choose one of the entries:

Make this button invisible to remove the button from the toolbar

Make this button inactive to disable the button (it will appear greyed)

To restore the complete toolbars, click:

Reactivate all invisible or inactive buttons to restore the default toolbar

#### How to Disable/Remove Menus or Commands

By default, all existing TOPSPIN commands can entered from the menu and/or from the command line. You can, however, selectively disable/remove commands or menus. This is typically done by system administrators who want to disable certain functions for standard users.

Open the Menu Configuration table as follows:

- **1.** Click Options  $\rightarrow$  Preferences [set].
- 2. Click Fonts/Dialogs/Icons in the left part of the dialog box.
- **3.** Click the *Change* button of the entry *Disable/Enable menus and commands*.

The table consists of the following columns:

Command	Description	Menu	Status
---------	-------------	------	--------

You can disable/remove:

• Menus, e.g. Options

to be found in the column Menu

- Sub-menus, e.g. Options → Administration tools to be found in the column Menu
- *Menu entries*, e.g. *Options* → *Preferences* to be found in the column **Description**
- Commands, e.g. set

to be found in the column Command

Note that in this configuration table, each *menu entry* corresponds to a certain *command*. In the TOPSPIN menu, most commands are indicated in square brackets behind the corresponding menu entries, e.g.:

IS Processing → Fourier transform [ftf]

Menu entries which are not used very often appear without the corre-

sponding command indicated, e.g.:

 $\square$  Options  $\rightarrow$  Preferences

However, if you want, you can look up the corresponding command, in this case *set*, in the configuration table and use it.

As an example, we will describe how you can disable/remove the *menu entry Remote connection..* in the *Options* menu:

- **1.** Open the configuration table as described above.
- 2. Scroll to the Description Remote connection
- 3. Set the *Status* to disabled.
- 4. Click Apply

Clicking the TOPSPIN *Options* menu, will now show the following popup menu:

Options	Window	Help	
Preferences			
Remote Connection			
Spectrometer Tools 🔹 🕨			Þ
Administration Tools		ools	Þ

The entry *Remote connection..* is greyed and can no longer be used.

Go back to the Configuration table, change the *Status* of *Remote connection...* to invisible and click *Apply*.

Clicking the TOPSPIN Options menu, will now show following popup menu:

Options	Window	Help	)
Preferences			
Spectrometer Tools			Þ
Administration Tools		Þ	

The entry *Remote connection.*. has disappeared.

Note that if you disable or remove a *menu entry*, the corresponding *command* is automatically disabled. For example, if you disable:

 $\square$  Analysis  $\rightarrow$  Deconvolution [dcon]

entering *dcon* on the command line will lead to an error message.

## How to (Re)enable a disabled Command/Menu

- 1. Open the Menu Configuration table as described above.
- 2. Set the Status of a disabled or removed (invisible) entry to enabled.
- 3. Click *OK* to close the Configuration table.

## How to (Re)enable All Commands/Menus

- 1. Open the Menu Configuration table as described above.
- 2. Click the *Reset* button to <u>enable</u> all menus and commands.
- 3. Click OK to confirm the appearing message.
- 4. Click the *OK* button to close the Configuration table.

## 20.4 Resizing/Shifting Toolbar Icons

## How to Change the Toolbar Icon Size

- 1. Right-click of the toolbar,
- 2. In the appearing popup menu (see Fig. 20.13), click:

🖙 Change Icon Size...



Figure 20.13

3. Enter the icon size in the appearing dialog and click OK.

## How to Shift Toolbar Icons to the Right

1. Right-click at an empty area of the toolbar.

2. In the appearing popup menu (see Fig. 20.13), click:

Stange Toolbar Offset...

3. Enter the toolbar offset in the appearing dialog and click OK.

4.

## 20.5 Defining Source Directory for Programs/Lists etc.

TOPSPIN 2.1 and newer allow you to defined the source directories for pulse programs, AU programs, integral ranges, various lists etc. In TOPSPIN 2.0 and older, the source directory for these items was fixed: <tshome>/exp/stan/nmr. Now you can define a individual source directories for each item. To do that:

- 1. Open the dialog of any of the items, e.g. with the command *edau*, *edlist* or *edmisc*.
- 2. Click Options → Manage Source Directories

A dialog will appear showing a list of items with the current source di-

Pulse Programs =	C:\ts21\exp\stan\nmr\lists\pp\user C:\ts21\exp\stan\nmr\lists\pp 
CPD Programs =	C:\ts21\exp\stan\nmr\lists\cpd\user C:\ts21\exp\stan\nmr\lists\cpd

Figure 20.14

rectories. By default, two source directories are present, one for user defined items and one for Bruker items. This list can be modified or extended with your preferred source directories, e.g.:

C:\my-pulse-programs\ C:\ts21\exp\stan\nmr\lists\pp\user C:\ts21\exp\stan\nmr\lists\pp

You can do this for each item separately. Items will be searched for in the order of the directories specified.

# Chapter 21 User Extensions

TOPSPIN offers various ways to extend the standard commands, buttons, programs etc.

## 21.1 User Notebook

You can create your own user specific notebook with the command:

```
\mathbb{R} View \rightarrow Notebook [nbook]
```



Figure 21.1

This can be used to store and retrieve any personal notes, information etc.

## 21.2 Macros

A macro contains a sequence of TOPSPIN commands. It can be created with the command *edmac*. A simple macro for processing and plotting the current dataset is:

```
em
ft
apk
sref
autoplot
```

All entries in a macro file must be written in lower case letters.

In TOPSPIN 1.3 and newer, a macro may contain Python commands. Any line in a macro that starts with:

py>

executes a Python command. An example of such a macro is:

```
re examld_13C 1 1 C:\bio guest
efp
py>NEWWIN() # open new window
re examld_1H 1 1 C:\bio guest
efp
py>x = INPUT_DIALOG()
py>if x == None: EXIT()
py>y = 2* int(x[0])
py>MSG("done: y=" + str(y))
```

Note that commands like NEWWIN(),  $\texttt{INPUT_DIALOG}()$ , MSG() and EXIT() are Bruker defined whereas "x=" and "if" are original Python commands.

Once created, a macro can be executed by entering its name on the command line.

## 21.3 AU Programs

An AU program may contain TOPSPIN commands, AU macros and C-language statements. It can be created with the command *edau*. A simple AU program which performs the *efp* command on a series of dataset *expno*'s is:

```
#include <lib/util.h>
int first, max;
char string[80];
first = expno;
GETINT ("Enter first expno to process : ",first)
max = 10;
GETINT ("Enter number of expnos : ",max)
WPAR("tmpmefp","proc")
expno = first;
TIMES(max)
RPAR("tmpmefp","proc")
EFP
IEXPNO
END
DEXPNO
DELPAR("tmpmefp")
QUITMSG("--- multiefp finished ---")
```

Note that TOPSPIN commands like EFP and RPAR and AU macros like IEX-PNO are written in upper case letters whereas C-language statements like are written in lowercase letters. Once created, an AU program can be executed by entering its name on the command line.

For more information on writing AU programs:

 $\mathbb{R}$  Click  $Help \rightarrow Manuals \rightarrow [Programming Manuals] AU programming$ 

## **21.4 Python Programs**

A Python program may contain TOPSPIN commands, User Interface functions and Graphic functions. It is created with *edpy*.

The Python program below reads a region of the real part of a spectrum and the corresponding region of the imaginary part and displays both. The simplest form of DISPLAY\_DATALIST is used.

from TopCmds import \* import math region = [80, 72] # define region in ppm

```
# open testdata, don't display
testdata = ["exam1d_13C", "1", "c:/Bruker/topspin", "guest"]
RE(testdata, "n")
# read real and imaginary points of the region
reals = GETPROCDATA(region[0], region[1])
imags = GETPROCDATA(region[0], region[1], data-
const.PROCDATA_IMAG)
if reals == None or imags == None: EXIT()
# set up list of data to be displayed and respective axis info list
dataList = [reals, imags]
# display the data in the list
DISPLAY_DATALIST(dataList)
```

For more information on writing Python program:

```
Reference Click Help \rightarrow Manuals \rightarrow [Programming Manuals] Python programming
```

## 21.5 Button Panels

A button panel is a window with user-defined buttons for executing TOPSPIN commands, AU programs, Python programs or macros. It appears as an integral part of the active data window and acts on that. Bruker delivers a few standard button panels like *bnmr* and *bnmrse1*. To create your own button panels, you can modify one of these or write them from scratch.

In this description we will create a very simple button panel with some 1D processing commands and print/export buttons (see Fig. 21.2)

1D Processing Panel			
Close	To 2D	<ul> <li>Tips</li> </ul>	
EM	FT	PK	
Print	EXPORT	SEND TO	

Figure 21.2

To write this button panel, take the following steps:

1. Open the Windows Explorer and navigate to the subdirectory

of the users properties directory <sup>1</sup>.

2. Create a text file with the name

cmdpanel\_<name>.prop

where <name> is the name of the button panel.

- **3.** Enter the button definitions including *Panel title*, *Colors*, *Toggle buttons*, *Top buttons*, *Panel layout*, *Panel buttons* and *Tooltips*.
- 4. Save the file under a name cmdpanel\_<xxx>.prop

where <xxx> is the actual name of your command panel.

Make sure the extension of the file is .prop and not .txt, .prop.txt or anything else.

5. Enter *bpan* <*xxx*> on the command line to open the button panel.

Here is an example for a small button panel for 1D processing:

```
# Color definitions used in this file (RGB)
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$ $FT$ $PK$ $
```

1. To locate this, enter *hist* and look for the entry "User properties directory=".

```
TOP COLORS=YELLOW1$ YELLOW1$ YELLOW1
TOP CMDS=em$ ft$ pk
TOP TIPS=Exponential multiplication $\
Fourier transform$
Phase correction
# Panel button definitions
# LAYOUT format: rows columns hgap vgap
PAN_LAYOUT=1$ 3$ 8$ 8
PAN BUTTONS=Print$ $ EXPORT$ $SEND TO$ $
PAN COLORS=BLUE1$ BLUE1$ BLUE1
PAN CMDS=prnt$ exportfile$ smail
PAN TIPS=Print the spectrum<br>>
as it appears on the screen\
Export the dataset<br>
to png, jpg, bmp etc.\$
Send the dataset by email
```

If you type *bpan exam*, a panel with 75 buttons will appear: 5 rows and 15 columns. The corresponding panel file is called cmdpanel\_exam.prop, which resides in the directory:

```
<tshome>/classes/prop/English
```

In the same directory, you can find the files cmdpanel\_bnmr.prop and cmdpanel\_bnmrsel.prop, which are used to display the *bnmr* and *bnmr*. *sel* panels described above.

The texts displayed on the buttons can be graphically adjusted in various ways, because the text may optionally be specified in html format. In the example above, the PAN\_BUTTONS property has no html tags, therefore the texts are displayed in black using the default TOPSPIN *Dialog window font* as specified in the User Preferences (command *set*). If you replace the text Print by the following:

```
<html><font size=10><font
color=\"00BF00\">Print<br>Now</font></html>
```

then the new text "Print Now" is displayed in green (the color to be specified in RGB hex code), with 10 points font size. Also, "Now" is display below "Print" due to the html <br> (= break line) tag.

Note that:
- The *Close* button and *Tips* switch are automatically created. You don't need to specify them.
- The TOGGLE button is typically, but not necessarily, used to call another button panel. In this example it calls the panel *bproc2d*. If TOGGLE\_BUTTON is specified without a value, i.e. the entry is "TOGGLE\_BUTTON=" instead of "TOGGLE\_BUTTON=action text", the corresponding button is not shown in the panel.
- Items must be separated with the "\$" character, button items with "\$
   \$"
- A "\" followed by "end of line" continues an item on the next line.
- Tooltips may use html tags for text formatting.
- Commands may be specified as single commands like "em" or as composite commands like "em\nft\npk". Note that in the latter case, the commands must be separated by "\n".
- When the *bpan <name>* command comes up with an error message, carefully check the syntax of your cmdpanel file. A common mistake is to specify the button items incorrectly. With the keyword PAN\_LAYOUT you define the number of rows and columns, and the number of items will become rows\*cols. All specifications such as PAN\_BUTTONS, PAN\_COLORS, etc. must have this number of members, otherwise you will get some kind of TOPSPIN error. Please insert the "\$" separator to make sure the item count is correct.

# 21.6 Adding User Defined Buttons to the Toolbars

The upper and lower toolbar at the top of the TOPSPIN window can be extended with user defined buttons. They can be assigned to any TOPSPIN command, macro, AU program or Python program.

To create a user defined button, take the following steps:

- 1. Right-click at an empty area of the toolbar.
- 2. In the appearing popup menu, click:

#### Add User-Defined Button

Reactivate All Invisible/Inactive Buttons Add User-Defined Button... Change Icon Size...

Change Toolbar Offset...

Hide Toolbars (type SHIFT ESC to reset)

- 3. In the appearing dialog box (see Fig. 21.3)
  - a) Choose between the options *text label* or *icon* The corresponding parameters are enable/disabled.
  - b) Enter the *command name*, the *tool tip* and the *label text* or *icon file* pathname.
  - c) For a text label: set its *font*, *text color* and *background color*.
  - d) For an icon label: specify the icon image filename
  - e) Set the *separator* flag to *yes* or *no* and select the data *dimension*(s) for which the button must appear.

For an icon label, you must stored the icon image file in one of the following directories:

- <user-home>/.topspin-<hostname>/prop/userdefined (only available for this user)
- <tshome>/classes/prop (available for any user)
- any directory (the full pathname must be specified in the icon label field)

The formats .gif, .jpg, .jpeg and .png, are supported. Standard TOP-SPIN toolbar icons have a size of 16 \* 16 pixels. If your own icons have a different size, they are automatically rescaled and displayed at the standard size.

🍓 Add tool button	$\overline{\mathbf{X}}$
_Options	
Add a button with a text label	
Add a button with an icon	
Required parameters	
Assign this command to button =	ft
Button tool tip =	1D Fourier T∤ansform
Button label text =	FT
Icon image file name (.gif, .jpeg, .png, .jpg) =	
Font of button label text =	Dialog / Plain / 11 Change
Button label text color =	Change
Button background color =	Change
Append separator to button =	yes 💙
Show button only for data of this dimension =	1D 💙
	OK <u>C</u> ancel <u>H</u> elp

# Figure 21.3

In the example above, a button **FT** is created with a separator, which only appears for 1D datasets, and executes the command ft.

# How do I Remove a User Defined Toolbar Button

Right-click the toolbar button and click:

Remove this user-defined button...

in the appearing popup menu (see Fig. 21.4).

# How do I Shift a User Defined Toolbar Button to the left/right

Right-click the toolbar button and click:

Shift left or Shift right in the appearing popup menu (see Fig. 21.4).



Figure 21.4

The button definitions are stored in the file toolbar\_user.prop which resides in the subdirectory userdefined of the user properties directory. To locate this directory enter the TOPSPIN command *hist*. A dialog box will show the contents of the history file. Near the top of this file, you will see an entry "User properties directory=".

For icon image buttons, the formats <code>.jpg</code>, <code>.jpg</code>, <code>.jpg</code> and <code>.png</code>, are supported. Standard TOPSPIN toolbar icons have a size of 16 \* 16 pixels. If your own icons have a different size, they are automatically rescaled and displayed at the standard size.

# 21.7 Adding User Defined Menus to the Menubar

The menubar at the top of the TOPSPIN window can be extended with user defined menus. They can be assigned to any TOPSPIN command, macro, AU program or Python program. They are specific for the dimensionality of the active dataset.

To create a user defined menu, take the following steps:

1. Open a dataset of the desired dimensionality.

- 2. Right-click at an empty area of the menubar.
- 3. In the appearing popup menu, click:

# User\_defined Menus

User-Defined Menus Change Menu Font Define Right-Click Action Hide Menubar (type SHIFT ESC to reset)

- 4. In the appearing dialog box (see Fig. 21.5).
  - a) Click *Add Menu* and specify the **Menu Name** in the appearing dialog.
  - b) Click *Add Menu Item* and specify the **Menu Item** name and the corresponding **Command** in the appearing dialog.
  - c) Click Apply.

🍓 User-Defined Menus	$\mathbf{X}$
Menu Name	Menu Item / Command
Add <u>M</u> enu Add Menu <u>i</u> tem <u>R</u> emove <u>U</u> p <u>D</u> own	
	Apply Apply+Close Cancel

Figure 21.5

The new menu will appear in the menubar.

Furthermore the dialog box in Fig. 21.5 contains the following buttons:

• Remove : Remove menu names and/or menu items

- Apply+Close : Apply any changes and close the dialog box
- Up/Down : Move up/down the menu name list
- *Cancel* : Close the dialog box discarding any changes.

User defined menu definitions are stored in the file umbar\_menubarld.prop, umbar\_menubar2d.prop Or umbar\_menubar3d.prop depending on the data dimensionality. These files resides in the subdirectory userdefined of the user properties directory. To locate this directory enter the TOPSPIN command *hist*.

# 21.8 Adding User Defined Guides

TOPSPIN offers several guides like the Acquisition Guide (command *aqguide*), the Processing Guide (command *prguide*) and the T1/T2 Guide (command *t1guide*). You can set up your own guides, which can be adaptations of Bruker guides or new written ones. In order to do that, you must edit the file toolbar\_user.prop and cmdtab\_user.prop in the directory:

<user properties directory>/userdefined/

To identify this directory, enter the command *hist* in TOPSPIN.

The file toolbar\_user.prop contains the guide definition. If the file does not exist, it must be created. Here is an example of a user-modified T1/T2 guide.

```
MyTlT2Toolbar=\
NM=tlfid_40.gif, NM2=$Extract fid, TIP=$Do rser,
CMD=_t1_fid, END=,\
NM=tlspec_40.gif, NM2=$Transform, TIP=$Do ef+apk,
CMD=_t1_spec, END=,\
NM=tlranges_40.gif, NM2=$Ranges, TIP=$Enter integ. mode,
CMD=_t1_ranges, END=,\
NM=tlscreen_40.gif, NM2=$Relax. Window, TIP=$Enter Relax
mode, CMD=_t1_relax, END=,\
NM=-, END=,\
NM=-, END=,\
NM=myicon.gif, NM2=$Fit Methods, TIP=$Select fit funcs.,
CMD=_t1_func, END=,\
NM=c:/myicon1.gif, NM2=$Start, TIP=$ct1,ct2, simfit,
```

```
CMD=_t1_start, END=,\
NM=c:/myicons/myicon2.gif, NM2=$Show Report, TIP=$report,
CMD=_t1_report, END=,\
NM=tlprint_40.gif, NM2=$Print it, TIP=$print,
CMD=_t1_export, END=
```

Notes to this guide definition:

- The original Bruker guides are defined in the file toolbar.prop in the directory <tshome>/classes/prop. The corresponding commands are defined in cmdtab\_main.prop in the same directory.
- The bold lines in the example above are user-modified lines.
- NM=tlfid\_40.gif: a Bruker defined icon with a size of 40x40 pixels
- NM=myicon.gif: a user-defined icon, which must be located in the user properties directory (Caution: not in its subdirectory userdefined)
- NM=C:/myicons/myicon1.gif: a user-defined icon located C:/myicons. Using the absolute pathname allows you to store icons in an arbitrary directory.
- NM=- : indicates the start of the second icon column
- NM2= : the text to appear underneath of the icon. The \$ sign is mandatory.
- CMD= : the command to be executed when the icon is clicked. This can be a regular TOPSPIN command, a macro or an AU or Python program.
- TIP= : the tooltip to be displayed when the cursor is held over the icon. Note that the \$ sign is mandatory.

Before you can start a user defined guide, you must edit the file cmdtab\_user.prop and define the corresponding command in the file, for example:

```
mytlguide=EM=J, MC=N, CL=tutor.TutStarter, ME=startTuto-
rial,AR=MyT1T2Toolbar;My T1 T2 Tutorial=
```

Here:

• "MyT1T2Toolbar" is the toolbar identifier as it is used in the file toolbar\_user.prop.

• "My T1 T2 Tutorial" is the title as it appears at the top of the guide.

If your guide is a Bruker modified guide, you can also redefine the original Bruker command, i.e. specify tlguide instead of mytlguide. Note that the original Bruker guide is then no longer accessible.

If you want to access a user defined guide from the TOPSPIN toolbar, you have to create a new toolbar button. To do that, right-click in an empty area of the toolbar and define a button in the appearing dialog.

# Index

#### Symbols

\*2 command 35, 42, 118, 159 \*8 command 35, 118, 159 .2d command 34 .3d command 34 .all command 36, 119, 161 .basl command 215 .bmp files 25 .bzip files 27, 76 .cal command 205, 246 .co command 173 .dec command 194, 200, 217, 231 .dopt command 149, 150, 159, 312 .dx files 76 .emf files 25 .f1r command 161 .f2r command 161 .gif files 360, 362 .gr command 172 .hr command 36, 119 .hz command 145, 169 .im command 176 .inc command 194, 200, 217, 231 .int command 195, 233 .jpeg files 25, 360, 362 .jpg files 25, 360, 362 .keep command 36, 120, 161 .ls command 176 .lt command 178 .lv command 174 .md command 24, 207 .ov command 146, 169 .ph command 45, 191, 225 .ph180 command 193 .ph90 command 193 .phr command 193 .png files 25, 114, 360, 362 .pp command 220

.pr command 24, 170 .prop files 256 .ret command 194, 205, 214, 218, 219, 224 .retsab command 219 .s2d command 194 .sd command 37, 120, 162 .sino command 260 .sl command 37, 120, 162 .sl0 command 37, 120 .sr command 37, 120, 162 .sr0 command 37, 120 .sret command 194, 204, 217, 224 .st command 176 .su command 37, 120, 162 .tif files 114 .txt files 153 .vr command 36, 118, 159 .wmf files 25, 114 .y command 146 .zi command 36, 119, 161 .zl command 36, 119, 161 .zo command 36, 119, 161 .zx command 36, 119, 161 /2 command 35, 42, 118, 159 /8 command 36, 118, 159 ? command help 46

#### Numerics

12 23 180 degree phase correction 1D 193 2D 231 3D molecule viewer 259 -90 degree phase correction 1D 193 2D 231 90 degree phase correction 1D 193 2D 231

# Α

abs command 99, 103, 194, 195, 198, 214 absd command 214 absorption mode 192, 193, 229, 230, 231 acqu command 275 acquisition commands 274, 278 mode 300 parameters 93, 94, 287 status bar 276. 289 toolbar 273, 275 Acquisition Reference Manual 21, 97, 282, 283, 300 AcquPars tab 93, 123, 165, 287 activate a data window 251 the next data window 256 add comment to audit file 308 directory to the browser 22 functionalities to Topspin 29 peak in 2D phase correction 227 peak to peak list 222 add increment in 2D levels 174 align intensities in multiple display 212 peak positions in multiple display 212 Alt-F11 key 118, 158 Alt-F4 key 41, 47 Alt-F6 key 47 Analysis menu 25, 26, 33 apk command 99, 103, 191 apks command 191 arrange data windows 252 data windows horizontally 254 data windows vertically 253 rows/columns in 2D phase correction 232 ascii files 86, 153 ased command 96, 123 Aspect 3000 data 75 ATM probehead 279, 280 atma command 280 AU macros 29, 354, 355 AU program reference manual 104

AU programs 20, 29, 103, 300, 354, 359, 362 audit trail check 307 automate data acquisition 30 automatic 1D baseline correction 99 1D calibration 99, 205 1D integration 194 1D peak picking 220 1D phase correction 99, 191 2D calibration 246 compilation of an AU program 303 configuration of a datastation 299 selection of the first expno/procno 69 tuning and matching 280 automatic mode of the Acquisition Guide 272 of the Processing Guide 26, 101 automation 29, 30, 300 autoplot command 103, 110 autostart.mac file 332 Avance spectrometers IV, 299 axis units 35, 145, 169, 206, 247

#### В

background of a data window 338 Backspace key 38 backward peak picking 222 baseline correction 1D 99, 214 mode 35, 214 bcm command 217 bias correction 199 bio-molecular experiments 30 bnmr command 356 bnmrsel command 356 bpan command 357 browser 31, 32, 41, 57, 68 font 343 in multiple display mode 209, 240 Bruker AU programs 30, 302 data format 21, 27, 28, 71, 75, 76, 85 example datasets 22, 64 BSMS control panel 282

BSMS display window 256 bsmsdisp command 282

#### С

calibration 99 1D interactive 205 2D interactive 246 mode 35, 205, 246 cf command 20, 49, 297, 298, 299 chemical shift 212 chemical shift distance 1D 260 2D 247 CHEMSTR parameter 143 C-language 29, 103, 354, 355 clevels file 176 clipboard 25, 41 close active data window 255 lock display window 281, 282 the active data window 41 close command 41 cmdhist command 38 cmdindex command 46 cmdtab user.prop file 47 collapse a data directory 57, 62 color scheme 337 colors of data objects 336 of the lock display 337 on the printer 336 command definition 47 dialog box 89 help 44 index 46 line 37, 38, 345 command line commands 274 focus 37. 41 font 344 history 37, 38 preferences 345 resize 346 usage 37

Command Prompt 19, 298 compile AU program 302, 303 components of a spectrum 24 composite commands 100 configuration commands 20 customized 299 default 299 directory 299 name 299 of a datastation 20 of a spectrometer 20 of the acquisition status bar 276 of the tab bar 335 of the Topspin menu 348 password 297 consistency check 307 contour display 226 of 2D spectra 173 of 3D planes 180 contour levels 158, 174 control keys 40 convdta command 78 convert data to JCAMP-DX 78 data to text 78 data to ZIP 78 copy & paste data 33, 73, 76 copy command 25, 34, 113 copy data 77 C-program 103 create an AU program 29, 104, 302, 354 an empty data window 68 data window color scheme 337 dataset 34 macro 29. 354 new data window 21 new dataset 65, 286 plot layouts 25, 112 Python program 30, 355 set of user preferences 329 user defined command 29

user notebook 353 C-statements 29 Ctrl key 62, 69, 81, 118, 159, 208, 209 Ctrl-c key 38, 41, 133 Ctrl-d key 31, 41 Ctrl-f key 41 Ctrl-F3 key 47 Ctrl-F5 key 47 Ctrl-F6 key 47 Ctrl-n key 34, 41, 65, 286 Ctrl-o kev 34, 41, 70, 75 Ctrl-p key 25, 34, 41, 112, 133 Ctrl-s key 27, 34, 41, 77, 78 Ctrl-v key 38, 41 Ctrl-w key 41 cube display 179 cubic spline baseline correction 218 cursor information 148 customized configuration 299 cut integrals 203

## D

data area 22, 31, 68, 73, 76, 249, 252, 255 compression 28 dimensionality 32, 92, 97, 122, 123 directory 57, 64, 81 field 37, 115, 120, 157 object colors 336 data window 21, 31, 33, 68, 73, 76 2D 157 3D 179 color scheme 337 contents 25, 113 creation 68 handling 33, 249 in 1D peak picking mode 220 in 1D phase correction 192 in 2D calibration mode 246 in 2D multiple display mode 239 in 2D phase mode 226, 233 in baseline correction mode 215 in calibration mode 206 in integration mode 195 in multiple display mode 208

in S/N measurement mode 261 in spline baseline correction mode 218 objects 24 popup menu 146, 162 printing 109 reopen 116 tab bar 1D 121 tab bar 2D 165 toolbar 24 dataset active 251 colors 214 dir 21, 305 directory tree 21, 72 expno 21, 60, 65, 305 files 86, 153 handling 29, 57 last 2D 34 last 3D 34 last used 332 name 21, 60, 65, 73 procno 21, 60, 65, 305 procno directory 73 properties 150 selection in multiple display 209 specification 72, 251 title 65 top level directory 60 user 21, 60, 65, 305 variables 78 datastation configuration 299 dcon command 28, 350 dconpeaks.txt file 28 deconvolution 28 default color scheme 338 command line size 345 configuration 299 find criteria 83 menu font 342 pivot point in 1D phase correction 192 pivot point in 2D phase 229 plane in 3D display 179 printer 111

Tab bar 335 zero order phase correction 193 define cubic spline baseline points 218 integral regions 196 NMR ADMINISTRATOR password 297 NMR SUPERUSER 297 peak ranges 221 peaks 222 de-iconify data window 255 delete AU program 303 data 79 integrals from display 201 noise region S/N 262 peaks from a peak list 223 signal region S/N 262 spline baseline points 219 Delete key 38 depth cueing in 3D 183 deselect data in multiple display 209, 210 integral regions 197 dialog box font 343 difference spectrum in baseline correction 217 in multiple display 210 dimensionality of a dataset 32, 92, 93, 97, 122 dir command 22 disable commands 348 menus 348 toolbar buttons 347 Display button 21, 74, 84 menu item 68, 69, 208 display 1D acquisition status parameters 123 1D data 115 1D FID 145 1D integral list 134 1D peak list 125 1D processed data 121 1D raw data 145

1D spectrum 121 1D spectrum overview 145 2D contours 173 2D data 157 2D FID 169 2D grid 172 2D integral list 167 2D peak list 166 2D projections 170 2D spectrum in contour mode 173 2D spectrum in obligue mode 176 2D spectrum in pseudo color mode 176 3D cube 182 3D data 179 columns in 2D phase correction 226 contours in 2D phase 226 data from the browser 22, 59 data from the portfolio 59 data in multiple windows 116 dataset file list 151 dataset properties 150 expno/procno list 69 found dataset 83 full spectrum in 2D phase correction 227 integrals 23 JCAMP data 28 manipulation 117 manipulations 35 mode of the lock window 281 molecule structure 143 options 35 options 1D 145 peaks 23 planes of 3D data 179, 180 positive/negative 2D levels 178 processing status parameters 1D 122 projections 23 rows in 2D phase correction 226 settings 34 special data formats 75 spectra 21 spectrum overview in 2D 169 status parameters 92, 96 sum/difference spectrum 210 superimposed 1D spectra 207

superimposed 2D spectra 238 y-axis 35, 146 zipped data 27 display properties 23 distance measurement 1D 260 2D 247 mode 35 double-headed arrow 250, 261 Down-Arrow key 38, 41, 42 dpa command 123 dpp command 92, 96, 122 drag & drop data 73, 76

# Ε

eda command 93, 94, 123, 165 edasp command 97, 123 edau command 30, 104, 300, 302, 354 edcpul command 125 edit AU program 303 commands 38 contour levels 174 integral ranges 199 pulse program 125 signal/noise regions 262 title of a dataset 124 Edit menu 33 edlev command 158, 174 edlock command 97 edmac command 29, 354 edp command 26, 89, 90, 122, 165 edprosol command 96 edpul command 125 edpy command 30, 355 edti command 124 ef command 100, 103 efp command 100, 289 em command 26.99 email data 28 empty data window 68 enable disabled commands 350 menus/commands 346 Enter key 42, 59

equidistant sequence of levels 174 Esc key 37 execute AU program 300, 303 macro 29, 354 Python program 30 exit command 41, 48 expand a data directory 42 data directory 21, 22, 57 data directory in the browser 62 individual spectra in multiple display 212 spectrum 28 expand a region 23 experiment time 275 expinstall command 20, 49, 274, 297, 298, 299, 300 expl command 73, 86, 87, 153 Explorer 72, 86, 153 expno 65, 69, 72, 78, 151 exponential baseline correction 216 window multiplication 99, 100 export data 24, 114 expt command 275 extend the Topspin functionality 353 external projection 24 extract a row/column in 2D 244

#### F

F1 dimension 162, 169, 225 F1 key III, 41 F1-F2 plane 180, 183 F2 dimension 162, 169, 225 F2 key 41, 61 F2-F3 plane 181, 183 F3 key 47 F3-F1 plane 179, 181, 183 F5 key 47 F6 key 41, 47, 252 fid command 145, 169 FID display 274, 278, 284, 288 Fid tab 145, 151, 169 File Chooser 21 File menu 21, 33 file size of raw data 275 files of a dataset 73, 78, 86, 151, 153 find command 41, 82 find data 33, 82 first order phase correction 1D 193 2D 229, 231 fitting peaks 28 fmc command 100 focus 37, 41, 61, 62 font of dialog windows 343 of the browser 343 of the command line 344 of the interface 340 of the menu 341 of the status line 344 of the tab bar 342 forward peak picking 222 Fourier transform 99, 100 fp command 100 fromjdx command 28 fromzip command 27 ft command 25, 26, 99 ftf command 26, 348 function keys 40

#### G

Gaussian deconvolution 28 Gaussian window multiplication 100 genfid command 78, 79 genser command 79 geometric sequence of levels 174 geometry of a Topspin window 256, 257 getprosol command 96, 123 gf command 100 gfp command 100 Gnome Mozilla 86 grab rows/columns in 2D 242 gradient enhanced spectroscopy 29 graphic functions 355 graphics files 25, 114 grid display 35, 172, 281 window arrangement 252

gs command 93, 276, 284 GS parameter adjustment window 284

#### Н

halt an acquisition 274, 275 halt command 274, 276, 288 Hardware requirements V helium level 282 Help button 46 menu 33, 45 help in Topspin 44 on commands 46 help command 46 Hertz axis units 145, 169 hist command 47, 50, 357, 362, 364 history file 362 hostname of a remote system 323 HTML page 46

# I

iconify all data windows 256 data window 254 iconnmr command 30 image display of 2D data 176 of 3D planes 180 import data 28 inconsistent dataset 92 initial guess 268 install AU programs 20, 300 pulse programs 20 Topspin 297 installation directory 64, 298, 299 installnmr script 298 int command 149 Integral list 2D 167 integral bias 199 display 23 label 197

list 1D 134 regions 195, 196, 197, 198, 203 scaling factor 203 slope 200 trails 149, 203 values 196 Integrals tab 134, 167, 205 integrals.txt file 205 integration 1D automatic 194, 198 1D interactive 194, 195, 198 mode 35, 195, 204, 205 intensity alignment in multiple display 212 decrease 1D 118, 158 increase 1D 118, 158 manipulation 35 reset 1D 36, 118, 158 scaling 2D 159 interactive 1D baseline correction 214 1D calibration 205 1D data manipulation 189 1D integration 194 1D peak picking 220 1D phase correction 189, 191 1D signal to noise calculation 260 2D calibration 246 2D data manipulation 225 2D phase correction 225 data manipulation 25, 34, 335 modes 34 parameter adjustment 93, 284 processing 99 Processing Guide mode 103 interface fonts 340 internal projection 24 Internet Browser 73 intrng file 199, 202, 204 IP address of a remote system 323 **IUPAC** standard 28

#### J

JCAMP-DX format 28, 75, 76, 78 Jeol spectrometer 75 Jmol molecule structure viewer 143 JNMR data 75

#### Κ

KDE konqueror 86 keyboard commands 33 kill command 53 Konqueror 86, 153

#### L

Left-Arrow key 38, 42, 62 Levenberg-Marguardt algorithm 268 li command 134, 195 Liouville equation 29 lipp command 134 lippf command 134 list 167 1D integrals 134 2D integrals 167 2D peaks 166 AU programs 300 baseline points 218 Bruker AU programs 302 color schemes 338 data files 85, 151 **EXPNOS/PROCNOS 69** found data 83 integrals 112, 204 macros 29 opened datasets 59, 60, 61 parameter sets 65 peaks 112, 222 peaks 1D 125 plot layouts 110 solvents 65 user defined AU programs 302 local Topspin interface 319 lock parameters 97 signal 281 lock command 282 lock display colors 337 mode 281

window 256, 275, 277, 281 lockdisp command 275, 281 lock-in procedure 281 Lorentzian deconvolution 28 lower toolbar 35

#### Μ

macros in AU programs 103, 355 in Topspin 29, 47, 100, 354, 359, 362 magnitude calculation 100 matching the probehead 279 MAXI parameter 222 maximize all data windows 256 data window 255 maximum command line size 346 MC2 parameter 93 menu bar 33 commands 33 configuration table 348, 350 entries 33, 348 font 341, 342 settings 329 MI parameter 222 minimize data window 254 minimum command line size 346 Minus key 42 mixtures 29 molecule structure viewer 143 mouse sensitivity in 1D baseline correction 217 in 1D integration 200 in 1D phase correction 194 in 2D phase correction 231 move data window 250 Mozilla 86, 153 multiple display 1D 35, 207, 238 1D/2D 24, 69, 74

2D 24, 238 in deconvolution 28 multiple display mode 69, 207 multiple window display 116 multiplet 196 multiply with increment in 2D levels 174

#### Ν

nbook command 353 negative 2D levels 178 new command 34, 41, 65, 286 newtop command 48 next channel for wobbling 280 command 41 dataset in Browser 42 parameter field 92, 96 plane in 3D 181 row/column in 2D phase correction 231, 243 window in data area 41, 252, 256 NMR ADMINISTRATION password 297 NMR SUPERUSER 297 nmradminpassword file 297 nmrsim command 29 nmrsuperuser file 297 noise region 260, 261 NOISF1 parameter 260 NOISF2 parameter 260 notebook 353 NS parameter 274

#### 0

O1 parameter 275 O2 parameter 275 O3 parameter 275 objects of a dataset 24, 116, 250, 329, 335, 336, 337 oblique display of 2D spectra 176, 178 of 3D planes 180 online help 45 online manual plot editor 112

Topspin 44 open browser/portfolio 61 data 34, 41, 57, 68, 70 data from the browser 21 data from the command line 73, 76 data from the Explorer 72 data from the menu 21 IconNmr interfaces 30 Linux Shell 19 new data window 252 new procno 74 online help documents 45 special format data 75 Topspin command index 46 open command 34, 41, 70, 75 Options menu 33 overview spectrum 1D 145 2D 169

#### Ρ

paper format 300 paracon command 300 parameter adjustment window 93, 284 change 92, 96, 97 display 23 editor 89, 90, 93, 94 field 91, 92, 95, 96 files 85 handling 89 name 89.93 search 122, 123 value 91, 95 parameter set 65, 78 PARMODE parameter 123 paste command 34, 73, 76 peak alignment 24, 212 display 23 fitting 28 group 28 labels 149, 150, 222 list 223, 224

list 1D 125, 222 list 2D 166 picking mode 220 position 260 position alignment 212 ranges 224 peak picking 1D automatic 220 1D interactive 220 mode 35 mode 1D 220 ranges in 1D 221, 222 peak.txt file 224 peakrng file 224 Peaks tab 112, 125, 166 phase correction 1D automatic 99, 100 1D interactive 191 2D interactive 225 first order 1D 193 mode 34 mode 1D 192 mode 2D 226 pivot point in 1D 192 values 1D 194 zero order 1D 193 PHC0 parameter 91, 193, 230 PHC1 parameter 193, 231 pivot point in 1D phase correction 192 in 2D phase correction 229 pk command 194 plane display in 3D 180 plot data from the menu 109 data from the Plot Editor 112 data from the Processing Guide 111 layouts 25 plot command 110, 112 Plot Editor 25, 110 Plus key 42 polynomial baseline correction 215 position of a Topspin window 257

position of a Topspin window 256 position the baseline of a row/column in 2D 245 positive 2D levels 178 pp command 133, 149, 150 PPARMOD parameter 92, 97, 122 ppl command 222 ppm axis units 145, 169 pps command 220 preferences 33, 329 pre-scan-delay 300 preview the baseline corrected spectrum 216 previous commands 37 dataset in browser 42 parameter field 92, 96 plane in 3D 181 row/column in 2D phase correction 231, 243 print 1D peak list 133 active window 25, 110 colors 337 data from the menu 109 data from the Processing Guide 111 integral list 112 metafiles 113 peak list 112 the current dataset 41 print command 34, 41, 109, 112, 133 printer colors 336 prnt command 110 probehead/solvent dependent parameters 96 proc 1d AU program 103 process data 25, 33 from the command line 99 from the Processing Guide 100 with AU programs 103 with composite commands 100 processing parameters 89, 90 parameters 1D 122 parameters 2D 165 Processing Guide 26, 101, 103 Processing menu 25, 26, 33

Processing Reference Manual 23 procno 69, 74, 78, 86, 152 ProcPars tab 26, 89, 90, 122, 165 projections of a 2D spectrum 23, 170 properties of a dataset 150 of a printer 110 prosol parameters 287 pseudo raw data 78 pulse program 20, 29, 62, 125 display 125 parameters 96, 123, 287 PulsProg tab 125 Python programs 30, 355, 359, 362

#### Q

QUIT AU macro 104 QUITMSG AU macro 104

#### R

re command 22, 73, 207 read color scheme 338 data formats 75 integrals from disk 198 the prosol parameters 287 window layout 256 reb command 21.74 re-enable disabled commands 350 reference peak in 1D calibration 206 in 1D phase correction 192, 193 in 2D calibration 247 in 2D phase correction 229 referencina 99 reg file 204 relaxation curve 263 remote connections 329 remove commands 348 data from multiple display 210 menus 348 toolbar buttons 347 reopen a dataset 116

reopen command 67, 116 rep command 22, 74 repw command 74 rescale 2D projection 171 data in multiple windows 117 reset 1D baseline correction 217 1D phase values 193 3D cube size and orientation 183 F1 zoom factor in 2D 161 F2 and F1 zoom factor 161 intensity 1D 118 intensity in 2D 159 search mask 83 zoom factor 36, 119 resize command line 346 data window 250 graphics 113 resolution of a screen dump 25, 114 restore adjusted acquisition parameters (GS) 286 size and position of a data window 255 toolbar 348 uncorrected baseline 217 retrieve previously entered commands 37, 38 rew command 22, 74 Right-Arrow key 38, 42, 62 rotate 3D cube 178, 182 routing parameters 97

# S

S/N value 262 Sample tab 142 sav command 34, 41 save 1D baseline correction 217 1D integrals 204 1D phase correction 194 acquisition data 78 adjusted acquisition parameters (GS) 285 AU program 30, 302 color scheme 337

cubic spline baseline points 219 current window layout 256 data 27, 34, 41, 77 data in analog filtered format 78 data to a JCAMP-DX file 28 data to a ZIP file 27 data window to a graphics file 25, 114 entire dataset 77, 78 integral regions 203 macro 29 parameters 122, 123 peak list and peak ranges 224 phase correction 2D 229, 232, 238 processed data 78 processed data as pseudo raw data 78 pulse program 142 sum or difference spectrum 210 title of a dataset 124 scale 1D integrals 202 1D spectrum 118 2D spectrum 158 3D cube 183 individual spectra in multiple display 24, 207,212 row/column in 2D phase 230 scaling factor of integrals 203 scan planes of 3D data 181 rows/columns in 2D 242 screen dump 25, 114 scroll bar 92, 96 search criteria 82 data 82 field in the parameter editor 91, 95 result window 83 select AU program 303 color scheme 338 data 57 data in multiple display 208, 209 data window 251 default printer 300

expno/procno combination 69 first expno/procno 69 folders in the browser 62 font 342, 343, 344 integral regions 197, 199 lock signal color 337 multiple datasets 69 multiple folders 62 peaks in 2D phase correction 226 plot layout 110 printer 110 remote system 323 row/column in 2D phase 229 spectra in 2D multiple display 241 spectrum color 336 spectrum print color 337 Topspin window 257 selective excitation 29 semi-automatic peak picking 222 processing 100 sensitivity of the GS slider 284 of the mouse 194, 200, 217, 231 serial command 104 serial processing 104 Server ID 323 set 1D acquisition parameters 123 2D acquisition parameters 165 2D processing parameters 165 colors for multiple display 214 contour levels 174 lock parameters 97 phase pivot point 192 processing parameters 89 processing parameters 1D 122 routing parameters 97 user preferences 330 set command 121, 329 SFO1 parameter 275 Shell 19 shift 1D data down 120 1D data smoothly 120

1D data to the extreme left 120 1D data to the extreme right 120 1D data to the left 120 1D data to the right 120 1D data up 120 1D/2D data 37, 42 2D data down 162 2D data smoothly 162 2D data to the left 162 2D data to the right 162 2D data up 162 data in multiple windows 117 individual spectra in multiple display 24, 207, 212 row/column in 2D phase 230 Shift key 62, 69, 81, 208, 209 Shift-Tab key 92, 96 short description of an AU program 303 shortcuts for processing 100 show command 53 SIGF1 parameter 260 SIGF2 parameter 260 signal region 260, 261 signal to noise calculation 260 Simplex algorithm 268 simulating experiments 29 sine baseline correction 216 single commands 99 slider sensitivity 284 slope correction 199 smail command 28, 34 smooth 1D phase correction 230 1D scaling 36 1D shifting 120 1D zooming 36, 119 1D/2D shifting 37 2D shifting 162 scaling of 1D integrals 202 scanning of planes in 3D 181 shifting of 1D integrals 203 solvent 65 spec command 121

special format data 28 spectrometer frequency 275 spectrometer hardware 20, 21 Spectrometer menu 33, 273 spectrum display 1D 121 objects 329, 330 overview 1D 145 overview 2D 169 Spectrum tab 121, 145, 152 square 2D layout 160 square brackets 33, 45, 116, 121 sref command 99, 103, 205, 246 stacked multiple display 211 Start button 72 startup actions 329 status line font 344 status parameter change 93 display 96, 149 display 1D 122, 123 stdisp command 292 stop an acquisition 274 stop command 274, 276, 288 store 2D contour levels 175 structure file 143 Structure tab 143 sum spectrum in multiple display 210 superimpose 1D spectra 207 cursor information 148 electronic signature 150 integral trails/labels 149 main status parameters 149 peak labels 149 spectra 24 title of a dataset 149 SW parameter 275 swap data windows 257 sweep width 275 swin command 257 switch

to the last 2D data 34 to the last 3D data 34

#### Т

T1 calculation III T1/T2 Relaxation 263 t1quide command 263 T2 calculation III Tab bar 1D 116, 121 2D 158, 165 configuration 121, 335 font 342 usage 121 Tab key 92, 96 tabbed pane 165, 335 TCP/IP port 321 temperature unit window 256 Terminal Window 19 time domain signal 29 title bar 115, 116, 157, 250, 251, 254, 255, 256, 303 title file 124 title of a dataset 23, 62, 65, 124, 149, 286, 337 Title tab 124 toccpn command 78 tojdx command 28, 78 toolbar 1D 189 2D 225 configuration 347 extension 359 for acquisition 273 icons 360, 362 of the data window 24, 145 of the FID display window 288 tips 45 usage 34 tooltips 44, 45 top level directory 21, 22, 57, 64 Topspin color schemes 338 data area 73, 76 fonts 341 help 44

installation 299 installation directory 299 startup V, 19 tailoring 329 window 31 topspin command 19 Topspin icon 19 totxt command 78 tozip command 27, 78 tshome directory 19, 45, 299 tuning the probehead 279

#### U

undo last parameter change 92, 96 last region operation 204 unzip utility 28 Up-Arrow key 38, 41 upper toolbar 1D 34, 189 2D 225 user defined AU programs 300 buttons 359, 362, 364 commands 26, 29 functions keys 47 plot layouts 111 User Interface functions 355 user preferences 329 user properties directory 47

#### V

Varian spectrometer 75 vertical scaling 118, 159 View menu 33, 148 virtual spectrometer 29 VNMR data 75

#### W

walk-up 30 wbst command 280 wbsw command 280 wildcards 81 window layout 256 Window menu 33, 257 WINNMR data 75 wm command 26, 89 wmisc command 78 wobb command 276, 279 wobble display 277 frequency 280 procedure 279 steps 280 sweep width 280 window 279 wpar command 78 wra command 78 wrp command 78 wrpa command 27, 77, 78

## Х

xau command 303 x-axis rotation in 3D 178, 182 xmac command 29

#### Υ

y-axis display 35, 146 y-axis rotation in 3D 178, 182

# Ζ

z-axis rotation in 3D 182 zero order phase correction 1D 193 2D 229, 230 zg command 274, 276, 287 ZIP data format 27, 75 zoom 1D data 36, 119 2D data 161 in 2D phase correction 227 zoom 1D/2D data 42

I-16